Center for Research on Innovative Simulation Software

Institute of Industrial Science, The University of Tokyo

Message

Center Director, Professor Chisachi Kato

Chisachi Kato

The Center for Research on Innovative Simulation Software (CISS) was inaugurated in January 2008 as the official research center of Institute of Industrial Science (IIS) of The University of Tokyo. Since 2008, the CISS has focused on the following objectives: (1) research and development of advanced, world-leading simulation software, (2) dissemination of research products to the community, and (3) reinforcement of our educational capacity to increase the human resources available for the development and use of advanced simulation software.

One of the objectives of the first phase of the CISS (from October 2008 to March 2013) was to power the project "Research and Development of Innovative Simulation Software," which was sponsored by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan. In addition, from 2011 to 2015, the CISS promoted the Strategic Programs for Innovative Research; Field 4: Industrial Innovation, which was also sponsored by MEXT. Within these projects, the CISS established a strong collaboration between industry, academia, and government to develop fundamental simulation software that runs efficiently in high-performance computing environments. The CISS then tested and verified this software by using the K computer. These simulations are sufficiently accurate to replace wind-tunnel and water-tank tests and can even work in real-time.

The CISS is now in the third phase of its program to achieve its three main objectives and extend its activity. In this phase, the CISS not only continues to promote the collaboration between industry, academia, and government to develop advanced simulation software but also encourages its use in real-world applications. The overarching objective of the advanced simulation software developed by the CISS was to use supercomputer Fugaku to contribute to resolving a host of social and scientific issues. This is exemplified by projects such as "Priority Issue 8: Development of Innovative Design and Production Processes that Would Lead the Way for the Manufacturing Industry in the Near Future" (from 2014 to 2019), which was sponsored by MEXT. The software FrontFlow/blue that was developed in this project makes calculations 50 times faster on Fugaku than is possible on supercomputer K. In addition, starting in fiscal-year 2020, the CISS is undertaking the three-year project "Program for promoting researches on the Supercomputer Fugaku: Research and development of an innovative fluid-dynamics simulations for aerodynamical/hydrodynamical performance predictions by using Fugaku," which is sponsored by MEXT. The goal of this project is to verify the large-scale simulation capacity by using the application software developed in Priority Issue 8 on Fugaku. Also, the CISS is developing an original computational science methodology that combines the principles of large-scale data analysis and original algorithms for future computing environments. Thus, through its research and its dissemination of results, the CISS contributes significantly to the industrial competitive advantage of Japan.

We appreciate your continued support for the CISS.

※The results obtained on the evaluation environment in the trial phase do not guarantee the performance, power and other attributes of supercomputer Fugaku at the start of its operation.

Overview

The objectives of the CISS are as follows:
- Research and development of advanced simulation software to change the future manufacturing methods.
- Demonstration of the effects of the developed simulation software and their practical applications.
- Creation of human resources able to use and develop such advanced simulation software.

In the execution of these objectives, the CISS develop original HPC applications, which help to enhance the industrial competitive advantage and cope with the changes in the manufacturing environment, and study their effects.

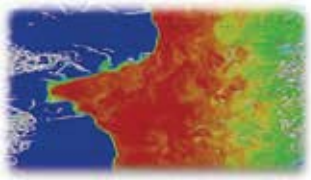
Research and development fields of the third phase of the CISS

The R&D of original design and evaluation technologies by incorporating principles of large-scale data analysis engineering has been organized as follows.

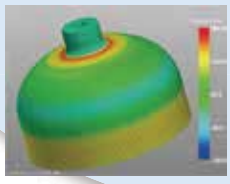
Manufacturing

- Mathematics of turbulence — Prof. Fujihiro Hamba
- Reliability engineering — Prof. Nobuhiro Yoshikawa
- Engineering for propulsion conversion — Prof. Chisachi Kato
- Engineering for optimized design — Associate Prof. Yosuke Hasegawa

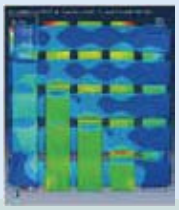
Design of ships, vehicles, and other transportation means (Courtesy of Shipbuilding Research Centre of Japan) [Kato]



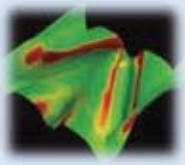
Turbulence modeling and control [Hamba, Kato, Hasegawa]



Optimized design of carbon fiber reinforced plastic (CFRP) tanks [Yoshikawa]



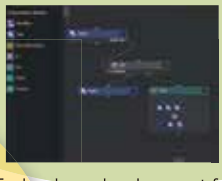
Mesoscale strength analysis [Yoshikawa]



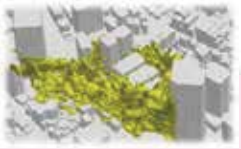
Shape optimization [Hasegawa]

Large-scale data analysis

- Large-scale data analysis engineering — Visiting Prof. Kenji Ono

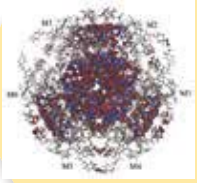


Technology development for upstream design process [Ono]

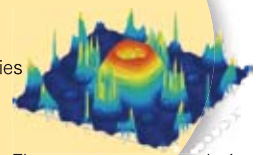


Prediction on urban environment [Ooka]

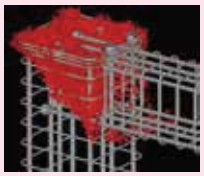
Evaluation of physical properties [Umeno]



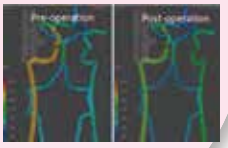
Protein design [Sato]



Electron spectrum analysis [Mizoguchi]



Product monitoring [Nagai]



Medical diagnostics [Oshima]

Design of molecular and nanoscale materials and devices

- Biomaterial engineering — Prof. Fumitoshi Sato
- Material science and creation — Prof. Teruyasu Mizoguchi
- Applied material engineering — Associate Prof. Yoshitaka Umeno

Medical engineering / Urban safety

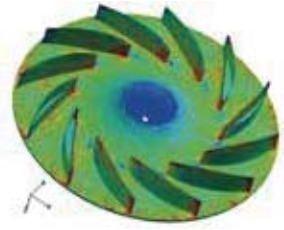
- Medical engineering — Prof. Marie Oshima
- Urban energy engineering — Prof. Ryozo Ooka
- Social infrastructure engineering — Associate Prof. Kohei Nagai

Research members & Research contents

Chisachi Kato — Center Director, Professor

Field: Fluid Fow and Thermal Energy Systems Control

My research interests are as follows: 1) development of simulation methods to predict flow and flow-induced noise in turbomachinery, automobiles, and ships and R&D advancement in the related applications, 2) clarification of the issues involved in large-scale parallel computation with tens of billions of grids for the next generation computing environments, and 3) use of the simulation software developed within the collaboration among industry, academia, and government to improve the performance and reliability and lower the noise of the various flow-related products. Regarding the energy field, I focus on the research and development of new types of windmills generating power with little noise even in relatively low-wind locations, advanced noise and cavitation models, and ultra-micro gas turbines (UMGTs).

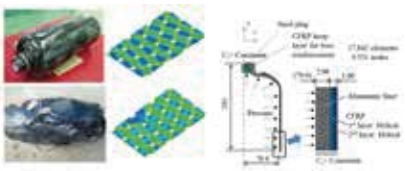


Absolute vorticity in a centrifugal blower

Nobuhiro Yoshikawa　Center Vice Director, Professor

Field: Multi-scale Solid Mechanics

We have investigated a methodology to develop carbon fiber reinforced plastic (CFRP) components based on strength and design simulations in the framework of high-performance computing. Mesoscale simulations to distinguish between carbon fibers and resins seem promising for overcoming the conventional trial-and-error design method. This methodology is currently applied to the design of CFRP hydrogen tanks in terms of mesoscale parameters such as winding path, resin strength, and manufacturing error. In addition, from the viewpoint of formability, carbon fiber reinforced thermalplastic composites are promising. We have been developing a simulation system to predict the mesoscale structure of carbon fibers after forming.

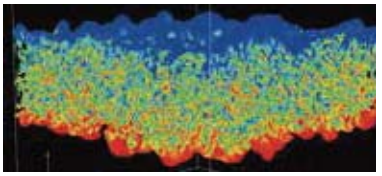


Burst pressure prediction of a hydrogen tank for fuel cell vehicle by means of zooming mesoscale simulation

Fujihiro Hamba　Professor　* Cooperating Member

Field: Fluid Physics

We are developing modeling and computational methods for turbulence as a basis for fluid simulation software. In spite of the recently advanced computers allowing large-scale simulation of complex fluid phenomena, the improvement of basic physical models and computational methods remains essential. We are trying to develop computational methods for fluids applicable to large-scale and high-speed flows by improving turbulence models based on their elucidated statistical and physical properties. To understand these properties, we rely on the theoretical analysis based on fundamental flow equations and large-scale numerical simulations of basic flow fields. In addition, we are studying the turbulence of electrically conducting fluids such as liquid metals and plasma fluids as examples of fluid motions exhibiting complex physical phenomena.

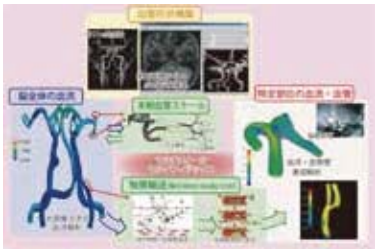


Contours of turbulent kinetic energy in a rotating system. Red and blue denote the right- and left-handed helical motions, respectively.

Marie Oshima　Professor　* Cooperating Member

Field: Bio-microfluidics

Vascular diseases such as myocardial and cerebral infarctions are blood vessel disorders triggered by the mechanical stress induced by blood flow obstruction and subsequent degeneration of vascular tissue. The aim of our research is to develop an integrated simulation system based on image-based modeling and multiscale calculations. In particular, we aim at modeling both the dynamic influences on the blood vessel walls and the physiological influences of, e.g., changes in cell functions by studying conditions such as atherosclerosis and cerebral aneurysms while considering the blood vessel hierarchical structure, which presents various spatial scales. We aim at developing a simulation system for the diagnosis and treatment of individual cases based on medical imaging and measurement data to elucidate the disorder mechanisms in terms of clinical applications.

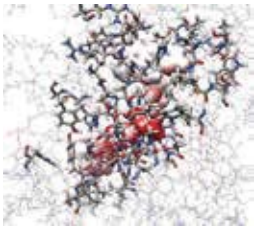


Schematic of the integrated simulation system M-SPhyR Circulation(multiscale and physics simulator for circulation)

Fumitoshi Sato　Professor

Field: Computational Biomolecular Science, Quantum Molecular Biology

Proteins are intricate molecules working efficiently with a minimal amount of energy. The remarkable functions of proteins are inseparable from their large-scale and complex structures. The straightforward approach for explaining and predicting the essence of the protein functions is the analysis of the reaction mechanisms using quantum chemistry based on the entire molecular structure. Our group is investigating and developing simulation systems using ProteinDF/QCLO, an all-electron calculation program for proteins based on the density functional theory (DFT) that succeeded in developing the 3rd generation algorithm for supercomputers. We aim at designing new enzymes and nanomaterials for industrial and societal use by combining various simulation methods and original software.



Electrostatic potential on the flavin adenine dinucleotide

Teruyasu Mizoguchi　Professor　* Cooperating Member

Field: Nano-materials Design

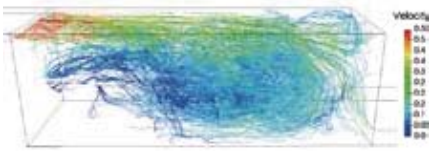
Further technological developments now require materials with significantly higher performance and reliability. For electroceramic materials, such as multilayer ceramic capacitors and varistors, the grain size diminishing down to approximately 1 mm or less improves the properties of each grain and grain boundary further. To achieve this, it is crucial to clarify the atomic and electronic structures and develop a method to improve their properties. In our group, we investigate such atomic and electronic structures and their relationship with the material properties by combining electron energy loss spectroscopy (EELS), transmission electron microscopy (TEM), and first-principles calculations.

Wave function at the bottom of the conduction band of MgO in the ground state (top), the Mg2p orbital core-hole state (middle), and the Mg1s orbital in the core-hole state (bottom)

Ryozo Ooka Professor * Cooperating Member

Field: Urban Energy Engineering

We study urban environment and energy in the Ooka laboratory. Computational fluid dynamics (CFD) models are used to analyze the flow field in and around buildings, wind environment, urban atmospheric environment, and urban heat island. The results are used for urban design to improve the urban environment and for the development of fundamental science. Recently, the future weather data for building design under climate changes have been predicted. Furthermore, for the resolution of the urban energy problem, a net energy building zeroing method and an optimized operation for urban energy systems using metaheuristics and machine learning have been developed. We aim at suggesting the way of the future city.



Analysis of a flow field in and around a building using the lattice Boltzmann method (LBM)

Kenji Ono Visiting Professor

Field: Large-scale Computer Engineering

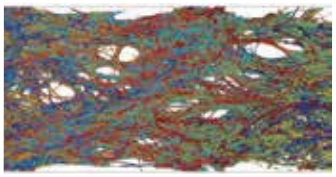
The capacity computing approach, computing many cases employing a huge computational resource and derives useful information from the results, has changed the paradigms of industrial product design via robust design, optimization, and uncertainty quantification. This approach requires the integration of high-throughput simulation, workflow, post-processing, and data science technologies for large-scale datasets. Our laboratory aims at constructing an advanced simulation system combining the latest achievements in computer engineering and computational science and to apply it to high-end product design.

Web-based workflow system WHEEL

Yoshitaka Umeno Associate Professor

Field: Nanostructured Materials Strength and Science

To reveal the physical and mechanical properties of nanostructured materials, our group performs simulations based on atomistic and electronic modeling, such as classical molecular dynamics and ab initio (first-principles) density functional method calculations. In addition, we work on multiscale mechanical simulations based on the knowledge of nano and microscale phenomena. Our research topics include the ideal strength of crystals, structural instability analysis of atomic systems, deformation and fracture of power semiconductors, deformation and multiphysics of low-dimensional nanostructures, chemical reaction of electrode materials in solid oxide fuel cells (SOFC), multiscale analysis of deformation and fracture of polymer materials, and optimized structure design of environmental barrier coatings for ceramics.

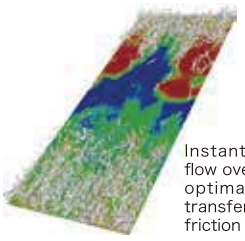


Deformation of polycarbonate simulated with a coarse-grained particle model

Yosuke Hasegawa Associate Professor

Field: Interfacial Transport Engineering

To improve environmental predictions and energy use efficiency, we investigate the turbulent flows and the associated transport phenomena. In particular, to identify the scalar sources in turbulent flows, we are developing novel strategies integrating finite sensing data into numerical simulations to obtain three-dimensional (3D) flow structures and the associated thermal and concentration fields. In addition, by applying the optimal control theory, we aim at deterministically optimizing various energy devices without relying on the subjective insight of the investigators. We have recently conducted flow simulations inside 3D complex geometries, such as vascular networks in biological systems and heat exchangers, and developed algorithms to optimize such complex geometries for better performance.

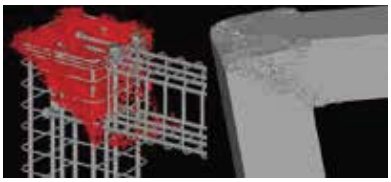


Instantaneous turbulent flow over a flat plate under optimal control for heat transfer enhancement and friction drag suppression

Kohei Nagai Associate Professor * Cooperating Member

Field: Infrastructure Management for Developed Society

We developed a 3D rigid body spring model (RBSM) to simulate a failure of a reinforced concrete (RC) structure at the mesoscale, with the shape of the steel bars directly modeled. In reality, not only are RC structures subjected to mechanical loading, but they are subject also to environmental conditions. Hence, to broaden the applicability of 3D RBSM, a truss network is being developed to model the substance movement because of the environmental exposure. A combination of both of the simulations could be a powerful tool for assessing the deteriorated RC structures on site and predicting their life span.



Failure of an RC beam–column joint simulated by 3D RBSM

Projects for developing advanced simulation software

The Center for Research on Innovative Simulation Software (CISS) is promoting national projects and is leading the research and development of advanced, applied simulation software.

Projects promoted by the CISS

Ministry of Education, Culture, Sports, Science and Technology (MEXT) (2020～2022)

Program for Promoting Researches on the Supercomputer Fugaku

Research and development of innovative fluid-dynamics simulations for aerodynamical/hydrodynamical performance predictions by using Fugaku

Issue Representative
Chisachi Kato

Because turbomachines and vehicles are at the core of the energy and transportation industries, respectively, we develop application software that is optimized for high-performance computing infrastructure, including Fugaku, to help streamline manufacturing processes.

Themes of experimental studies:

Theme 1: Realization of a numerical towing tank and improvement of propulsion efficiency by using energy-saving devices (FrontFlow/blue)

Theme 2: Wall-resolved LES of internal flow in hydro-dynamical and leakage-flow passages of multistage centrifugal pump (FrontFlow/blue)

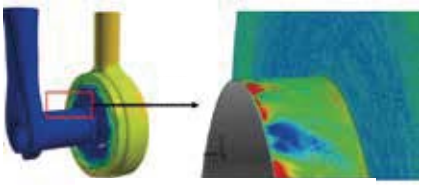
Theme 3: Direct analysis of compressor surge (software of DES (Detached Eddy Simulation) analysis of compressible flow for turbomachines)

Theme 4: Prediction of real aerodynamic performance of automobile in road conditions (CUBE)

Theme 5: Prediction of automobile aeroacoustics in road conditions (CUBE, FFX)

※ The application software used is given in parentheses.

Examples of analysis using a modest scale model

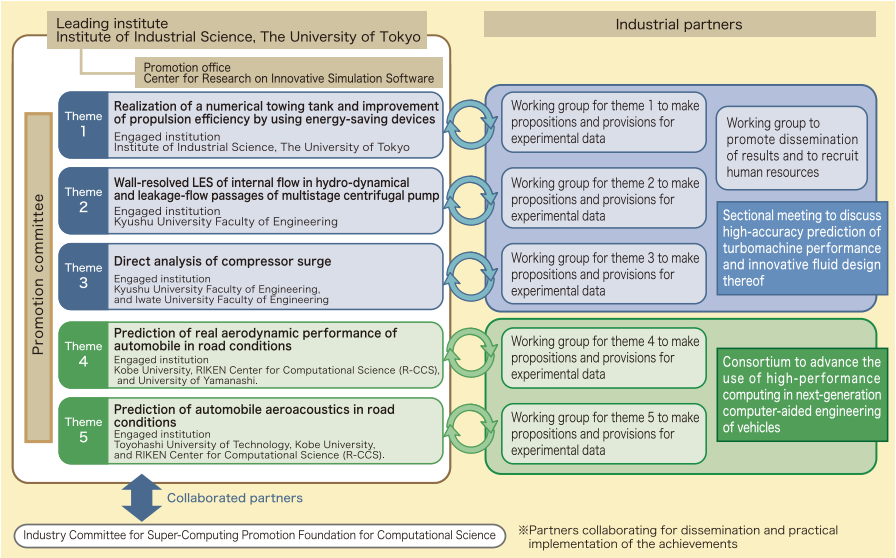


Wall-Resolved large-eddy simulation of internal flow around the stenopeic structure of single-stage centrifugal pump

Provided by SUZUKI

Turnaround time (TAT) for a real vehicle aerodynamic analysis reduced to ≤ 24 h

Organization



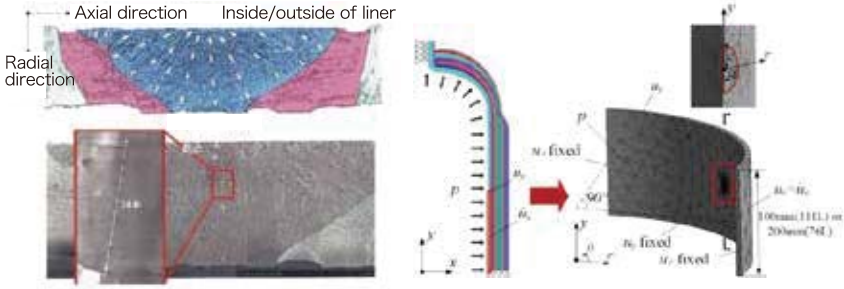
The CISS is conducting research and development in close collaboration with Kobe University, Kyushu University, Iwate University, Toyohashi University of Technology, University of Yamanashi, and RIKEN Center for Computational Science (R-CCS).

New Energy and Industrial Technology Development Organization (NEDO) (2019～2021)

Development of Technologies for Hydrogen Refueling Stations
Development of Technologies for Cost Reduction of Hydrogen Refueling Stations
Establishment of evaluation method for composite pressure vessel・ Technology development for technical standard improvement

Associate Participant
Nobuhiro Yoshikawa

A method of lifetime evaluation as well as extension is developed to reduce cost of composite high-pressure accumulator equipped in hydrogen refueling stations. In concrete terms, evaluation method for pressure -cycle fatigue strength analysis is established through bottom-up analysis using a test piece of pressure vessel material; furthermore, the vessel is fatigue designed by fatigue life design curve, and cumulative damage rule is applied. Consequently, reduction of cost and test time for pressure-cycle fatigue test using actual accumulator and extension of lifetime of accumulator are achieved.



Micro-scale zooming-up simulation for lifetime prediction of fatigue crack growth of composite accumulator

The CISS is promoting this project in close collaboration with Japan Petroleum Energy Center (JPEC) and the High Pressure Gas Safety Institute of Japan (KHK).

Past projects promoted by CISS and its achievements

Ministry of Education, Culture, Sports, Science and Technology (MEXT)

Social and Scientific Priority Issues to be Tackled by Using Post-K Computer

Priority Issue ⑧: Development of Innovative Design and Production Processes that Would Lead the Way for the Manufacturing Industry in the Near Future

Leading Institute

(2014～2019)

We aimed at realizing high value-added manufacturing industries through the development and application of innovative and efficient simulation software maximizing the capabilities and performance of the Post-K computer. We had been using these applications to research and develop innovative design techniques. Hence, engineers will be able to quantitatively evaluate and optimize the product concepts at an initial stage, minimizing the cost and maximizing the precision of the manufacturing processes. We had been developing applications for two main categories, design process innovation and manufacturing process innovation. These applications were in line with the needs of typical industrial fields such as automotive, turbomachinery, and aircraft.

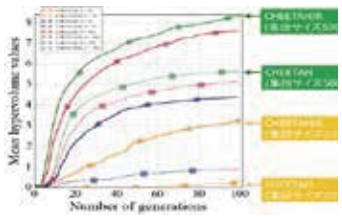
The CISS had been conducting research and development in close collaboration with the Graduate School of Frontier Sciences, The University of Tokyo, Kyushu University, Kobe University, Tohoku University, University of Yamanashi, Tokyo University of Science, Japan Aerospace Exploration Agency (JAXA), and RIKEN Center for Computational Science (R-CCS).

Achievements

Sub-issue A

Research and development of multiobjective design exploration and high-performance computing technologies for design innovation

We developed the multi-objective design-optimization algorithm, Cheetah/R, which significantly reduces the optimization time.



Performance of Cheetah and Cheetah/R evaluated by applying to blade-shape optimization problem for a wind turbine.

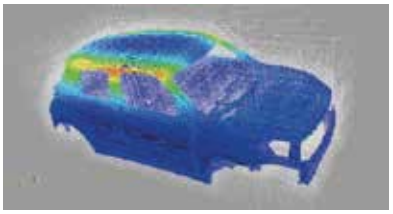
【Engaged institutions】
JAXA, Kyushu Univ., Tohoku Univ., Tokyo Univ. of Science and RIKEN.

【Developed software and/or algorithm】
CHEETAH/R, a low B/F novel iterative method, parallel-in-time method, and Workflow system, called "WHEEL"

Sub-issue B

Research and development of the real-time real-world integrated design system for road vehicles

The aerodynamics of a real vehicle with a complex configuration can be analyzed about ten times faster than before.



Unified coupled analysis of thin-plate automotive structure and fluid flow.
(Provided by SUZUKI)

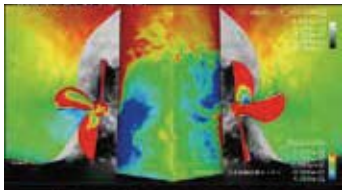
【Engaged institutions】
Kobe Univ., Univ. of Yamanashi and RIKEN.

【Developed software】
CUBE

Sub-issue C

Research and development of a design and evaluation system based on quasi-direct fluid-flow computations for turbomachinery

We have achieved a speed up of the FrontFlow/blue in Fugaku by 50 times.



Benchmark calculation using the KVLCC2 vessel aimed at replacing self-propulsion tests.
(Courtesy of Shipbuilding Research Centre of Japan)

※The results obtained on the evaluation environment in the trial phase do not guarantee the performance, power and other attributes of supercomputer Fugaku at the start of its operation.

【Engaged institutions】
The Univ. of Tokyo, and Kyushu Univ.

【Developed software】
FrontFlow/blue, and FFX (the application code using Lattice Boltzmann Method)

Sub-issue D

Research and development of core technologies to innovate aircraft design and operation

Hierarchical orthogonal grids with equal spacing has been produced for a real aircraft with complicated surface, and a preliminary computation has been conducted.

・JAXA High-Lift Model
・3.1 billion fluid cells and a total of 4.5 billion cells with no layer grids and no wall model

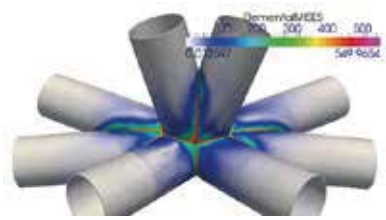
【Engaged institutions】
JAXA, Tohoku Univ., and Tokyo Univ. of Science

【Developed software】
FFVHC-ACE

Sub-issue E

Research and development of advanced press forming and welding simulators for new materials

We have developed an advanced press forming and welding simulator and applied it to the evaluation of deformation of the entire structures and stress distribution of the base material.



Results of simulation of arc welding of large-scale telescope mount (stress distribution).

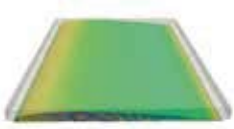
【Engaged institution】
The Univ. of Tokyo (Graduate School of Frontier Sciences)

【Developed software】
FrontISTR

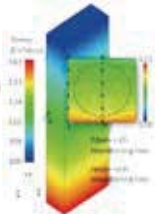
Sub-issue F

Research and development of multiscale modeling simulators for thermoplastic CFRP

Press-forming simulation of structural guide vane done using macro-scale simulator.



Stress distribution



Temperature distribution

【Engaged institution】
The Univ. of Tokyo

【Developed software】
FrontComp

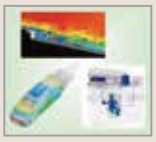
Past projects promoted by CISS

Strategic Programs for Innovative Research (SPIRE), Field 4: Industrial Innovation

Leading Institute
(2009～2015)

◆ Overview: Contribute to the rapid advancement in the next-generation Monozukuri field through innovative and high-performance computing infrastructure

◆ Leading institutions: IIS, The Univ. of Tokyo; JAEA; JAXA



Research and Development of Innovative Simulation Software

Core Institute
(2008～2012)

◆ Overview: R&D and manpower training on advanced practical software for monozukuri including life sciences and nanotechnology, with the goal of contributing to the advancement of Japan's industrial innovation

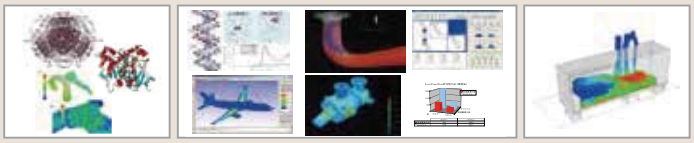
◆ Participating institutions: IIS, The Univ. of Tokyo; Graduate School of Engineering, The Univ. of Tokyo; Graduate School of Frontier Sciences, The Univ. of Tokyo; NIMS; NIHS; Rikkyo Univ.; software vendors; etc.

Revolutionary Simulation Software Project

Core Institute
(2005～2007)

◆ Overview: R&D, promotion, and manpower training on state-of-the-art practical software that is key to the rapid advancement of science and technology in the 21st century

◆ Participating institutions: IIS, The Univ. of Tokyo; Graduate School of Engineering, The Univ. of Tokyo; RACE, The Univ. of Tokyo; NIMS; NIHS; Hokkaido Univ.; Tohoku Univ.; Keio Univ.; Kyushu Univ.; UEC; Rikkyo Univ.; RIST; AdvanceSoft Corp.; etc.

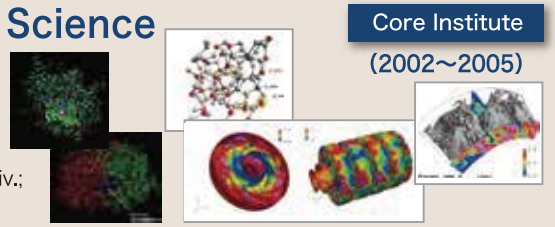


Frontier Simulation Software for Industrial Science

Core Institute
(2002～2005)

◆ Overview: Development and promotion of world-class practical simulation software in computational science

◆ Participating institutions: IIS, The Univ. of Tokyo; Graduate School of Engineering, The Univ. of Tokyo; RACE, The Univ. of Tokyo; NIMS; NIHS; Keio Univ.; Kyushu Univ.; UEC; Rikkyo Univ.; RIST; AdvanceSoft Corp.; etc.



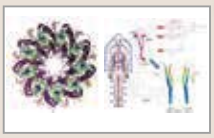
The "Grand Challenge" software applications

Next-Generation Integrated Simulation of Living Matter

Participations
(2006～2010)

◆ Overview: Development of molecular-scale and organ/body-scale analysis systems using ultra-high-speed computer

◆ Affiliated institutions: RIKEN; Osaka Univ.; Kyoto Univ.; Yokohama City Univ.; Keio Univ.; Tohoku Univ.; The Univ. of Tokyo; etc.



Science and Technology for a Safe and Secure Society

Research on Diffusion and Damage Prediction of Dangerous Toxic Material and Disaster Reduction Measures

Participations
(2007～2009)

◆ Overview: Prediction of indoor/outdoor diffusion of dangerous toxic material and development of evacuation-guidance support systems

◆ Affiliated institutions: Mitsubishi Heavy Industries; AdvanceSoft Corp.; AIST

New Energy and Industrial Technology Development Organization (NEDO)

Development of technologies for hydrogen utilization

Participations
(2015～2017)

Development of low-cost equipment and systems for fuel cell vehicles and hydrogen infrastructures

Development of innovative design for composite hydrogen tanks by a multi-filament winding method

◆ Overview: To reduce the overall cost of these systems, diffuse the FCV, and ensure international competitiveness, research and development for low-cost equipment and components for fuel cell vehicles (FCV) and hydrogen infrastructures are performed.

◆ Affiliated institutions : Murata Machinery Limited, Teijin limited

Multi-filament winding machine

Application software developed by the promoted projects

Thermal fluid analysis

Thermal Fluid-Aeroacoustics System

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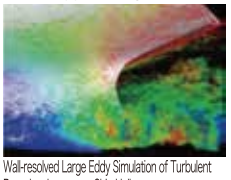
FrontFlow/blue
FrontFlow/blue-ACOUSTICS

Turbulent flow can be accurately predicted by this software. It supports large-scale flow computation with up to 100 trillion grids. Coupled simulations (fluid, structure, and acoustics) with up to 1 billion grids on various types of machine architectures, including a PC cluster and a supercomputer are also possible with FrontFlow/blue. It can be applied to various engineering problems, such as aeroacoustics noise, internal flow of turbo machinery, and predictions of promote resistance for ships.

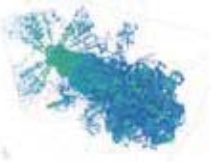


Wall-resolved Large Eddy Simulation of Turbulent Boundary Layer on a Ship Hull
Courtesy of Shipbuilding Research Centre of Japan

High-Performance Parallel Thermal Fluid Simulator on the Cartesian and Hierarchical Cartesian Grids for Practical Complex-fluid Analysis.

FrontFlow/violet
Cartesian(FFV-C)
Hierarchical Cartesian (FFV-HC)

FrontFlow violet (FFV) is an incompressible thermal fluid-flow simulator that covers situations from industrial design to natural structures in the field of biological research. The simulation is enhanced for massively parallel computation environments. The FFV family comprises an FFV Cartesian (FFV-C) and FFV Hierarchical Cartesian (FFV-HC) data structure. These applications employ a unique approach for the grid generation process, thereby enabling the formation of over 30 billion grids and reduction in the time cost of the entire simulation process.



Fine vortex structure of contra-rotating jet visualized by Q criterion

Material structure analysis

Nonlinear Structural Analysis System

Representative/Contact
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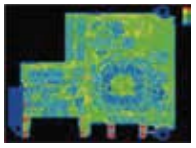
office@frontistr.com
https://www.frontistr.com/

FrontISTR

FrontISTR is an open-source structural analysis system that runs on PCs and parallel supercomputers such as the K computer. A dedicated Pre/Post processor is included in the system. It supports fruitful nonlinear analysis functions comparable to those of commercial codes and exhibits an innovative aspect that addresses large-scale application, parallelism, and programmability. A 7.5-billion DOF problem can be solved in 13.7 h using 65,536 cores of the K computer.



Thermal bending analysis of printed-circuit board (Mises stress distribution) (DOF: 7.5 billion , Minimum mesh size : 7.5 micrometer, Number of cores ("K computer") : 65,536)

Simulation System to Evaluate Strength Reliability of Carbon Fiber Reinforced Plastic (CFRP)

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[Carbon-Fiber-Reinforced Plastic Tanks]

FrontCOMP_FW, FrontCOMP_FW_multi
FrontCOMP_FW_shell, FrontCOMP_tank
FrontCOMP_tank_multi
FrontCOMP_wind_multi

[Forming Carbon-Fiber-Reinforced Plastic Material]

FrontCOMP_cure, FrontCOMP_TP

FrontCOMP is a simulation system that uses mesoscale modeling to evaluate strength reliability of CFRP in term of the fiber bundle and resin system. It strongly supports reasonable optimum design of CFRP pressure vessels for high-pressure hydrogen fuel-cell vehicles. Mesoscale design parameters such as cross-sectional dimensions of fiber bundle, winding path, nonlinear material properties of resin and residual stress after cure processing are explicitly handled to improve the reliability of the system.

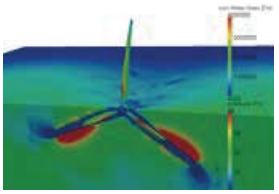
Impact damage of high-pressure hydrogen tank

Coupled analysis

Large-scale Assembly, Structural Correspondence, Multidynamics Simulator

REVOCAP_Coupler
REVOCAP_PrePost
REVOCAP_Refiner

The REVOCAP system enables large-scale coupled analyses of parallel computers by collaborating with FrontISTR and FrontFlow/blue. As an application, the flow-induced vibration analysis of turbine blades has been solved. The system can be also applied to solve magnetostructure interaction analysis and fluid-structure acoustic interaction analysis.



Fluid Pressure Contours, Deformation of blade (x 100)and Mises stress contours on blade surface calculated by fluid-structure interaction analysis

Nanoscale and Biomolecular material analysis

First-Principles Electronic Structure Calculation Software

Representative/Contact
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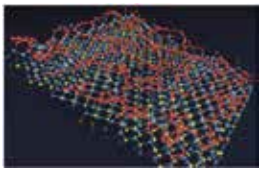
https://azuma.nims.go.jp/

PHASE/0
PHASE-Viewer
ASCOT

The first-principles electronic-structure calculation software PHASE/0 is based on a pseudopotential method within the density functional theory. It uses plane-wave basis sets. This software enables not only fundamental electronic structure analyses, but also advanced analyses of the dynamics, reactions, and spectra of the materials. It runs on various computer platforms, ranging from PCs to PC clusters and supercomputers. ASCOT is used to analyse quantum transport in nanojunction systems.



Large-scale FP simulation for graphene growth on SiC

All-Electron Canonical Molecular Orbitals Calculation of Protein by the 3rd generation DFT method

Representative/Contact
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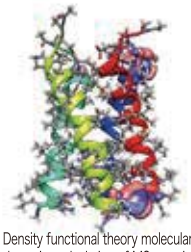
satofumi@iis.u-tokyo.ac.jp
http://proteindf.github.io/

ProteinDF
QCLO

ProteinDF/QCLO is all-electron canonical molecular orbitals calculation software for proteins. It uses a density functional method based on the standard Gaussian function of quantum chemistry. It can be used for state-of-the-art electronic-structure modeling of biomolecules. It runs on all types of PCs, including supercomputers.



Density functional theory molecular dynamics calculation of M2 protein in influenza A virus. The proton transfer process is investigated.

Biomolecular Interaction Simulator

Representative/Contact
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ABINIT-MP
BioStation Viewer

The ABINIT-MP/BioStation Viewer performs systematic interaction analyses of protein-ligand complexes available for rational drug as well as molecular design on the basis of highly parallelized fragment molecular orbital (FMO) calculations. Additionally, this system can be widely used in material designs and nano-bio researches.

Complex structure formed between the main protease (Mpro) of COVID-19 and ligand N3. The crucial residues were identified by applying an interaction analyses based on fragment molecular orbital (FMO) with ABINIT-MP.

See the website of Computer Science Navigator (**http://www.cenav.org/**) for different examples of calculations usingadvanced simulation software.

Dissemination of the developed simulation software and development of human resources

To fulfill the expected, we support the high-performance computing (HPC) manufacturing users.
The Center for Research on Innovative Simulation Software (CISS) disseminates the advanced and practical applications developed, which are incorporated into national policies and can be broadly applied to manufacturing, and trains human resources for the use and development of the simulation software.
As an example, the most recent advances achieved have been effectively communicated via a dissemination framework developed under the Strategic Programs for Innovative Research (SPIRE) "Field 4: Industrial Innovation."

Website "Computer Science Navigator"

Different outreach activities conducted by the CISS are available on the website "Computer Science Navigator" (http://www.cenav.org).

Newsletter

A newsletter presenting the latest R&D outcomes and the examples of their applications in the private sector is being published in an easy-to-understand language and is available on the website.

Software running on supercomputer K, FX10 supercomputers, and PC clusters

Analysis simulators for various fields, including thermo-hydrodynamics, structure, nanotechnology, and life science, and peripheral software can be downloaded from the Software Library section of the website.

HPC application by case analysis database

Analysis of examples collected by various applications are available to the public. The collection, which includes standard analyses in various fields, introduces significant application functions and performance issues, such as examples of massively parallel analysis conducted using supercomputer K. Reproducible datasets are attached to some of the example cases so that the users can gain hands-on experience.

Information shared through FAQs and forums

A collection of frequently asked questions and related answers is available for the users. There are also users' forums, such as GitHub, on problems for all the applications.

Website "Computer Science Navigation"

Software library

Analysis examples posted in database

Manufacturing support for HPC users

We plan to link the HPC to the Foundation for Computational Science (FOCUS) and the Industrial Committee for Supercomputing Promotion (ICSCP) to support the users and to increase their base for applications.

Support for HPC users

For applications in the thermal fluid, material structure, and nano-quantum fields, we support experience-based seminars teaching how to use these applications in a corporate environment, from pre-processing to calculation and post-processing.

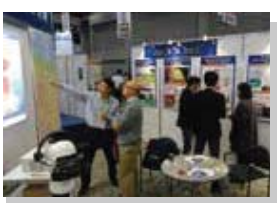
Links to the industry

To demonstrate the applicability of the software developed, we conduct benchmark tests based on actual themes in the industry.

View of the seminar

Exhibition activities at international

We set up display booths at the International Conference for High Performance Computing, Networking, Storage and Analysis and the International Industrial Fair Kobe.

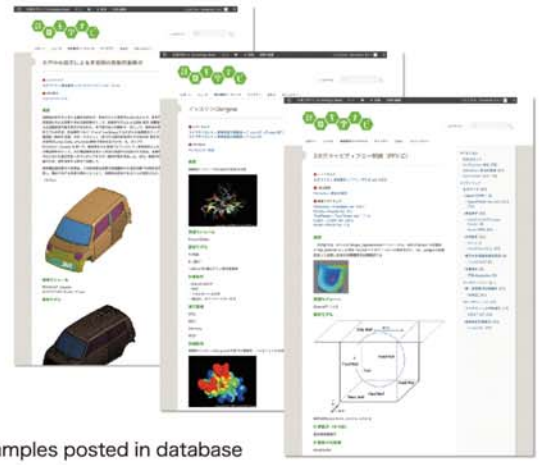


Display booth at the International Conference for High Performance Computing, Networking, Storage and Analysis

Display booth at the International Industrial Fair Kobe

Preparation of the knowledge database

To help to handle the simulation software developed by the promoted projects, a database of knowledge and examples of calculations using it is built and is available on the website (http://www.cenav.org/).



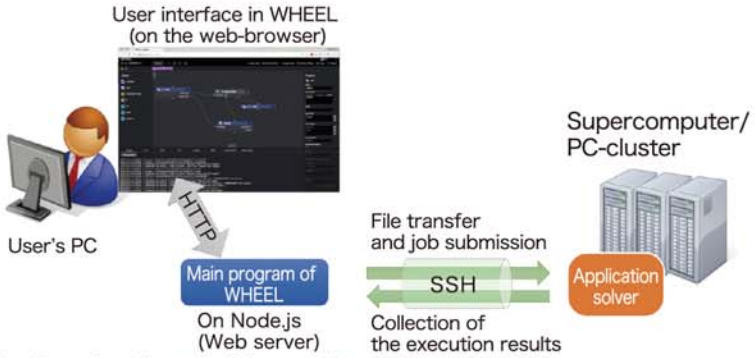
Analysis examples posted in database

Field	Application	Number of the examples
Manufacturing (structural, fluid and acoustic engineering)	FrontFlow/blue	29
	FrontFlow/violet	16
	FrontCOMP	10
	FrontISTR	31
	ADVENTURE	4
	OpenFOAM	16
Design of molecular and nanoscale materials and devices	PHASE	65
	ABINIT-MP	16
	ProtainDF	20
	Total	207

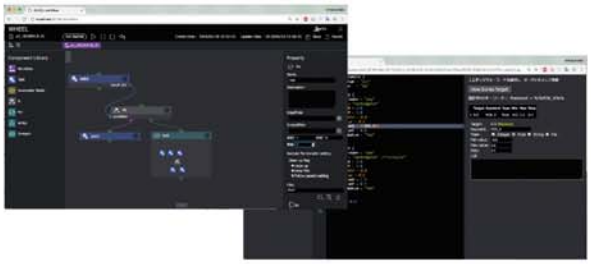
Number of analysis examples posted in database

Development of the workflow system

A workflow system helping to use the advanced and massively parallelized applications for research and design has been developed and is being continuously improved.



Configuration diagram of the workflow system



Example of user interface (on the web browser)

Education of software developers – Hands-on training for the development of advanced simulation software –

In FY 2009, we contributed to the education of developers of simulation software at the School of Engineering of the University of Tokyo.

- Software development in a group with progress and quality management
- Practical training in both software engineering and HPC (with an emphasis of the former one)
- Hands-on lectures held by university and corporate researchers
- Creation of hybrid-parallelized simulation programs for computational fluid dynamics (CFD) and molecular dynamics (MD)
- Development and job submission of the newest supercomputers

ISBN-13:
978-4130624541

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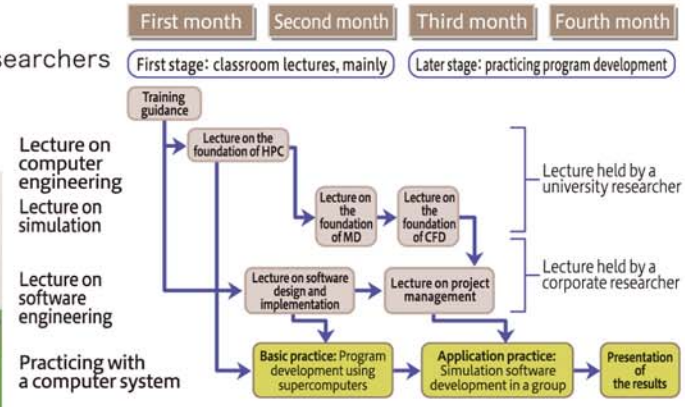

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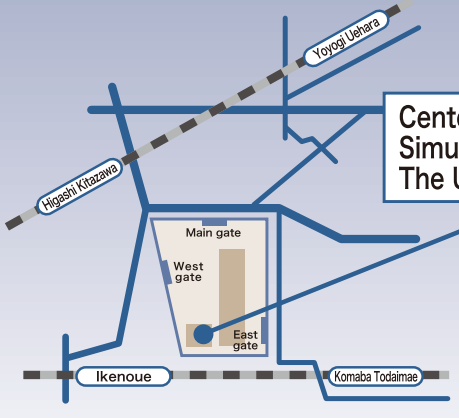

Center for Research on Innovative Simulation Software, IIS, The Univ. of Tokyo, An-604

Odakyu Line / Tokyo Metro-Chiyoda Line
7 min, walk from Higashi Kitazawa Station
12 min, walk from Yoyogi Uehara Station

Keio Inokashira Line
10 min, walk from Komaba Todaimae Station
10 min, walk from Ikenoue Station

Oct 2020