Institute of Fluid Science, Tohoku University

Advanced Fluid Information Research Center

AFI-NITY II

AFI Next-generation Integrated supercomputer for promoting fluid science and TechnologY

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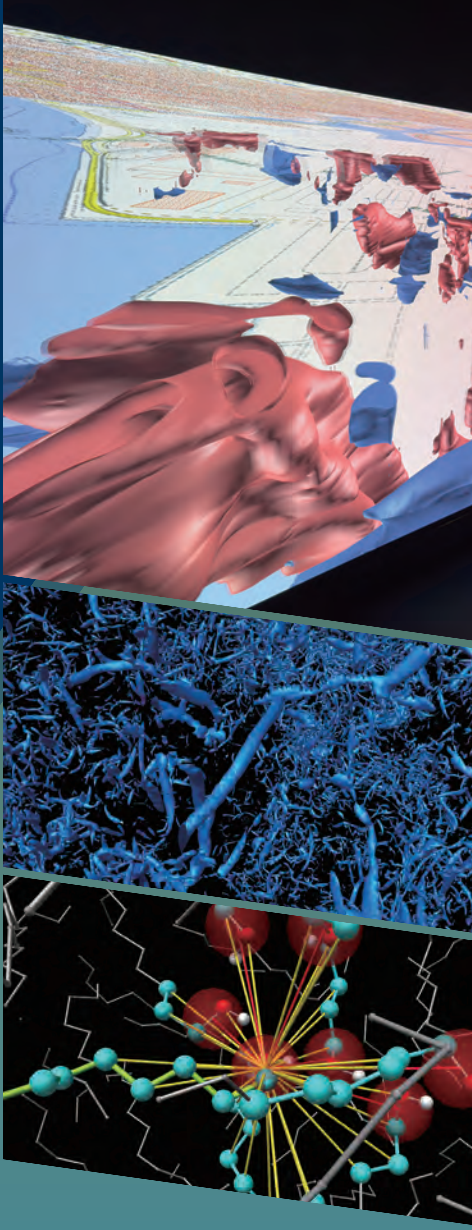


At the Advanced Fluid Information Research Center（AFI Research Center）, the Integrated Supercomputation System is employed in diverse applications such as supercomputing in fluid science, measurement-integrated research for the simulation and experiment, and advanced visualization for fluid information. In addition, international symposiums are conducted by AFI Research Center and the center's database is used to spread the research results. From the academic and social viewpoints, the Integrated Supercomputation System plays a pivotal role in research projects, which are screened and evaluated, for achieving high research goals. The Institute of Fluid Science' s mission is to make contributions, such as integrating the fundamental study of fluid science with advanced academic fields and focusing on the applications of fluid science in the field of science and technology, toward the promotion of AFI Research Center as a world-class research center.

HISTORY

Dec.	1990	Cray Y-MP8/8128 becomes operational
Oct.	1994	Cray C916/161024 becomes operational
Sep.	1999	Advanced Fluid Information Research Center was founded
Nov.	1999	SGI Origin 2000, NEC SX-5/16A become operational
Nov.	2005	SGI Altix 3700, NEC SX-8 become operational
May	2011	SGI Altix UV1000, NEC SX-9 become operational
May	2014	SGI UV2000 is added to the above
Aug.	2018	System based on Fujitsu Server PRIMERGY becomes operational
Aug.	2024	System based on HPE CRAY XD2000 becomes operational

GREETING

Integrated Flow Science pioneered by Next Generation Integrated Research System

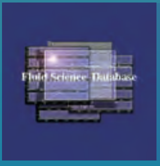
Kaoru Maruta
Director of Institute of Fluid Science, Tohoku University

To lead the continuous development of fluid sciences and technologies, which form the foundation for the sustainable development of human society in harmony with the global environment, the AFI Research Center introduced a new system called the "Next Generation Integrated Research System II（AFI-NITY II）" in August 2024, a distributed memory parallel computing system based on HPE CRAY XD2000. The center conducts research on advanced fluid information from both macroscopic and microscopic perspectives, targeting not only fluid flow, but also the flow of heat, energy, electromagnetic waves and information. By analyzing complex flow fields using next-generation integrated research methods that directly link to experimental equipment, integrate experiments and calculations, and employ large-scale numerical calculations, as well as advanced visualization and data mining of the vast amounts of obtained fluid information, we elucidate previously unknown complex flow phenomena. Furthermore, we develop control mechanisms and design methods for various flow phenomena that contribute to the sustainable development of human society.
As an international hub for advanced fluid information research, the AFI Research Center has been organizing international symposiums on advanced fluid information annually since 2001 and actively promotes collaborative research projects with domestic and overseas universities and enterprises.
Through the particular development of the Integrated Flow Science, the research center also contributes to the training of researchers and engineers, aiming for the international dissemination of research results and their development.
We look forward to your continued support of the AFI Research Center's activities.

INFORMATION

Fluid Science Database

In the Fluid Science Database, many research results on fluid science, such as obtaining large-scale numerical computations using supercomputers, have been released on the website of IFS（http://afidb.ifs.tohoku.ac.jp）. The aims of this database are sharing and leveraging the results of research on "flow" as "fluid information."



http://afidb.ifs.tohoku.ac.jp

International Symposium on Advanced Fluid Information（AFI）

We have organized this symposium on advanced fluid information every year since 2001, and dispatch the research results on "flow" to the world. While sharing, linking, and using fluid information with domestic and overseas researchers, we aim to further develop "advanced fluid information research."
Furthermore, we disseminate the research results by publishing a report on results and actively making presentations at open events at Tohoku University and related international conferences.

Integrated Supercomputation System

AFI-NITY II

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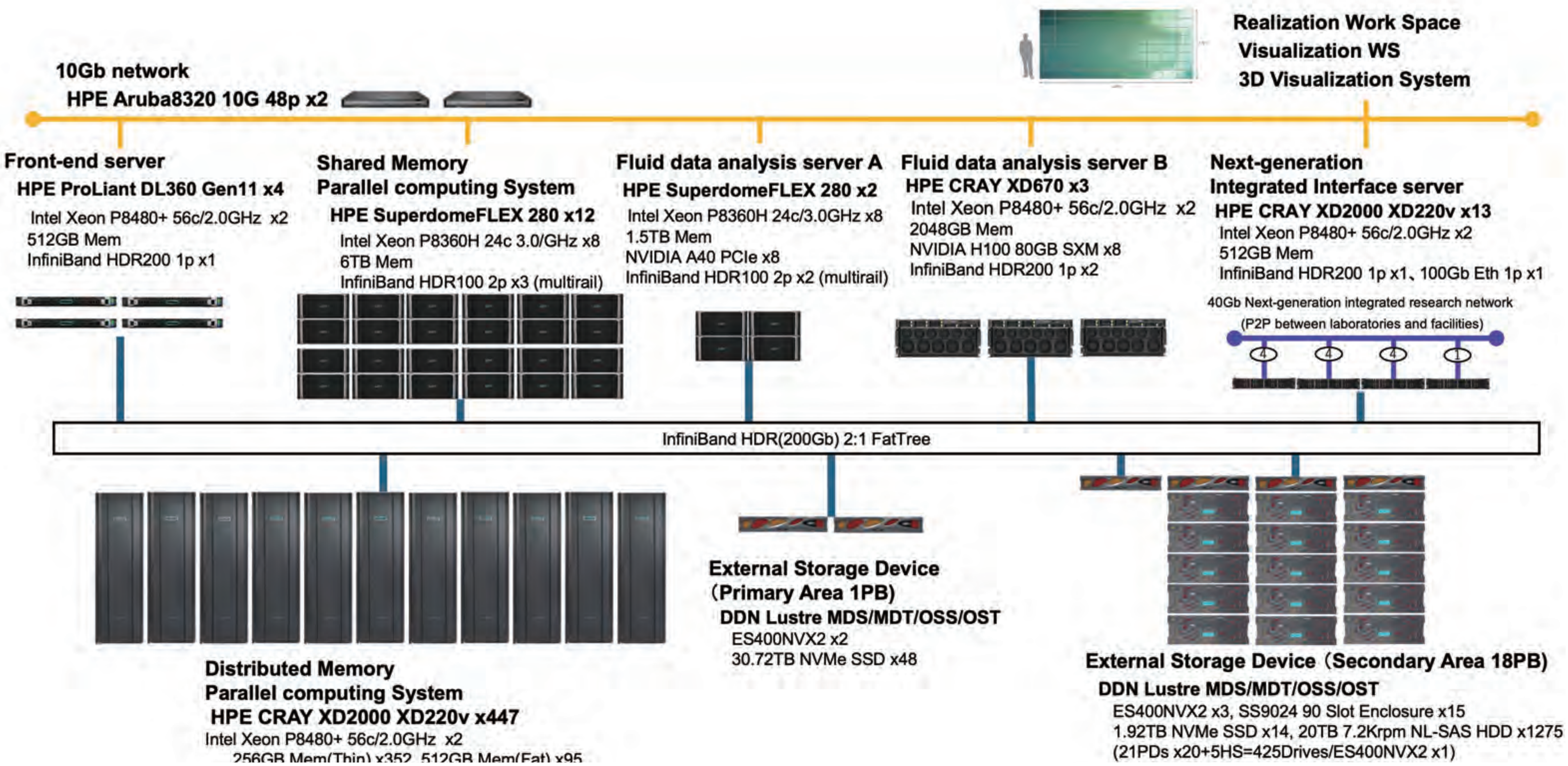
A New Era of Research Pioneered by "AFI-NITY II"

The “Integrated Supercomputation System,” which currently consists of the distributed memory type parallel computing system, the shared memory parallel computing system, fluid-data analysis server, and the Measurement Integration Interface Server to link the supercomputer and experimental measurement system, started operation in November 2005 and was updated in May 2011, May 2014, August 2018, and August 2024. The data storage system (magnetic disk), which has petabyte class capacity, is connected to the servers using a storage area network (SAN) . The Realization Workspace and peripherals with stereo visualization devices are also involved in the system. For the supercomputing servers, 447 nodes of HPE CRAY XD2000 are used as the distributed memory type parallel computing system, while the shared memory parallel computing system consists of HPE SuperdomeFLEX 280, providing a total peak performance of 4.4 PFLOPS together with fluid-data analysis server, maximum shared memory of 6 TB, and total storage capacity of 223 TB. The network which connects the servers and users has a 40 Gbit Ethernet as the backbone, and facilitates clients’ work, including high-speed data transfer and image processing at each laboratory in the Institute of Fluid Science (IFS).



Hardware

The performance of the supercomputer servers (the distributed memory type parallel computing system, the shared memory type parallel computing system, and fluid-data analysis server) is listed in the Table.

	Peak Performance [PFLOPS]	Total Memory [TB]
Distributed memory type parallel computing system	3.2	135.5
Shared memory type parallel computing system	0.2	221.2
Fluid data analysis server	0.8	6.0

Software

Various applications are installed to support research on the Integrated Supercomputation System. Some of them are listed below:

●Computational Fluid Dynamics
ANSYS, FaSTAR, CONVERGE

●Structural Analysis
Abaqus, LS-DYNA, ANSYS

●Molecular Dynamics and Quantum Mechanics
Materials Studio, Gaussian, Amber, Amsterdam Modeling Suite, Cantera

●Others
Comwave, COMSOL Multiphysics, JMAG

●Optimization
modeFRONTIER

●Compilers
Intel oneAPI (C/C++, Fortran), GCC, NVIDIA HPC SDK

●Libraries
Intel MPI, IMSL Fortran, OpenMPI, OpenMP

●Visualization
[Visualization of CFD results]
FIELDVIEW, Tecplot, AVS/Express
[Visualization of Structural Analysis]
Abaqus/CAE
[Visualization of Molecular Dynamics and Quantum Mechanics]
Materials Studio Visualizer, GaussView

●Modeling
[Modeling in CFD]
ANSYS, CATIA
[Modeling in Structural Analysis]
Abaqus/CAE, CATIA
[Modeling in Molecular Dynamics and Quantum Mechanics]
Materials Studio Visualizer, GaussView
[Others]
Materialise Magics

●Mesh Generation
[For CFD]
ANSYS, Pointwise, ICEM CFD
[For Structural Analysis]
Abaqus/CAE

User Support

The office of the R & D Division of AFI Research Center, supervised by the Director of the center, operates the Integrated Supercomputation System and supports the users of the system. The organization and the duties of the AFI Research Center are listed below:

●Steering Committee
Determines the policy of the AFI Research Center

● Selection and Examination Committee
Screens and evaluates the research projects of the AFI Research Center

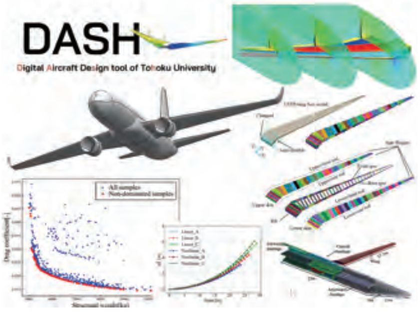
●Office of R & D Division
Operates the Integrated Supercomputation System and the network of IFS; supports the users of the system; does clerical work, planning and advertisement of the AFI Research Center

●Supporting WG
Supports the users of the system

Aircraft Design Based on Fluid-Structure Interaction Analysis and Multi-Objective Optimization

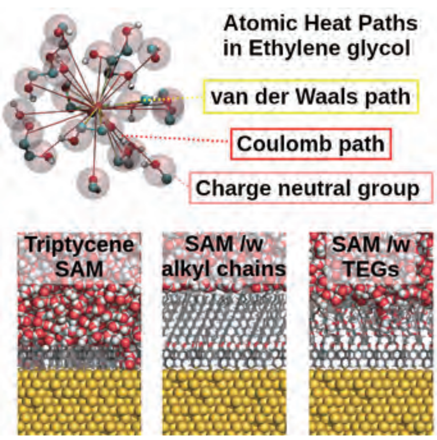
In the aircraft design, it is essential to consider the interaction between aerodynamic forces and structural deformation through fluid-structure interaction analysis, and to conduct multi-objective optimization, such as minimizing aerodynamic drag and structural weight. In this study, we developed an aircraft design tool for carbon fiber reinforced plastic (CFRP) materials, which is named as the Digital Aircraft deSign tool of ToHoku University: DASH [1]. This tool enables material property prediction through multiscale analysis, aeroelastic analysis of CFRP wings under various flight conditions, structural optimization with aeroelasticity, and multi-objective optimization of wing geometries using Bayesian optimization. In particular, we have successfully quantified the changes in wing performance due to differences in carbon fibers, and clarified the effects of reduction on structural weight and wing deformation when using the next-generation carbon fiber, TORAYCA®T1100G [2]. Currently, we are also developing design tools for aircraft with complete configuration, while also conducting fundamental research on coupled analysis methods to apply more advanced and high-fidelity simulations.

[1] https://www.ifs.tohoku.ac.jp/mulphd/softwares/DASH/docs/_build/html/index.html
[2] Aerospace Science and Technology, Vol. 124, 2022, 107565 https://doi.org/10.1016/j.ast.2022.107565



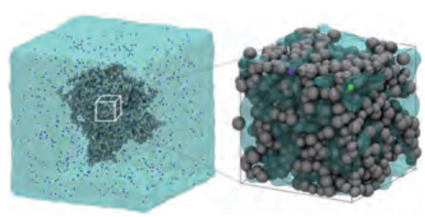
Elucidation and Control of the Molecular Mechanism that Determines Thermal Transport via Molecular Dynamics Simulation

Advanced thermal management is urgently needed to further improve the performance of semiconductor electrical components. Therefore, there is a need for technology to design heat medium and thermal interface materials with desired properties at the molecular level. In order to enable such " molecular design," it is necessary to understand the molecular scale mechanism of macroscopic heat conduction. However, compared to solid crystals and gases, the molecular arrangement and motion of liquids, soft matter, and their interfaces are irregular, making it difficult to research.
In the present research, we have developed an analytical method via molecular dynamics simulations to express macroscopic heat conduction as an accumulation of microscopic energy transfer due to interactions between individual atoms and molecules (i.e. atomic heat path, see upper subfigure) . By doing so, we have clarified the connection between the molecular structure, functional group characteristics, and heat transport in self-assembled monolayers (SAMs) at the solid-liquid interface (lower subfigure).



Theoretical Design and Control of Liquid-Liquid Phase Separation Using Artificial Proteins

It is known that proteins and RNA can self-assemble to undergo liquid-liquid phase separation, forming droplets or gel-like structures within cells. In the crowded and chaotic intracellular environment, these droplets create order by concentrating specific molecules while excluding others, thereby regulating various biological processes such as transcription, translation, and signal transduction. However, it is challenging to experimentally observe the internal structure of such dynamic and reversible droplets at atomic resolution, and current methods rely on trial and error when exploring the types and combinations of constituent molecules. In this study, we aim to theoretically design artificial proteins that undergo phase separation using molecular simulations, in order to elucidate the mechanisms of droplet formation and control their fluidity. In collaboration with experimental groups, we also synthesize and evaluate these proteins experimentally, working towards a bottom-up understanding of intracellular phase separation. Additionally, we seek to develop methods for controlling the function of specific proteins within cells by selectively trapping them inside droplets.



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