Advanced Fluid Information Research Center

Institute of Fluid Science, Tohoku University

AFI-NITY

AFI Next-generation Integrated supercomputer for Promoting fluid science and Technology

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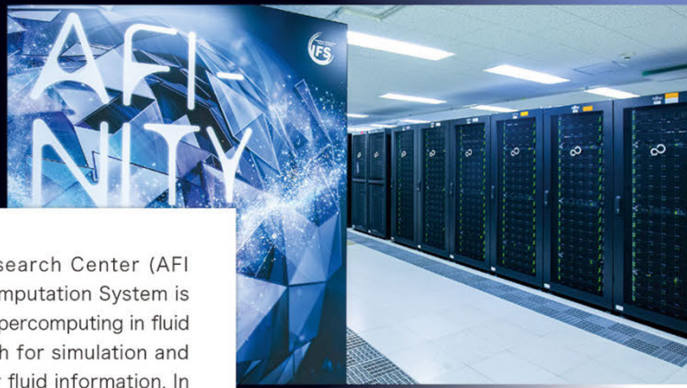
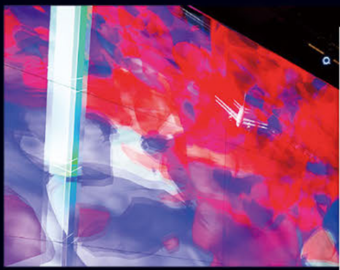
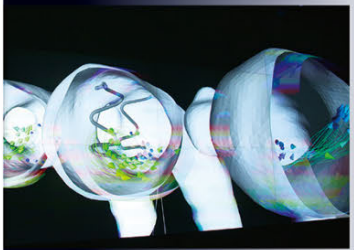




At the Advanced Fluid Information Research Center (AFI Research Center), the Integrated Supercomputation System is employed in diverse applications such as supercomputing in fluid science, measurement-integrated research for simulation and experiment, and advanced visualization for fluid information. In addition, the AFI Research Center conducts international symposiums and shares research results via its database.
The Integrated Supercomputation System plays a pivotal role in research projects which are screened and evaluated for their achievement of high academic and social research goals. The Institute of Fluid Science' s mission is to integrate the fundamental study of fluid science with advanced academic fields and enable applications of fluid science in the field of science and technology, thereby helping to make the AFI Research Center 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 is 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



Kaoru Maruta
Director
Institute of Fluid Science,
Tohoku University

The AFI Research Center, Institute of Fluid Science, established the "Integrated Supercomputation System (AFI-NITY)" with distributed / shared memory parallel computers, FUJITSU PRIMERGY CX2550M4 in August 2018, in order to lead the fluid science and technologies that is the foundation of the sustainable development in human society in harmony with the global environment.
The center is promoting researches on "Advanced Fluid Information" not only for conventional fluids but also for flows of heat, energy, electromagnetic waves and information from macroscopic and microscopic points of view.

The center aims to develop various control and design methods for flow phenomena that lead to the sustainable development of human society and to elucidate unknown complex fluid phenomena by advanced visualization and data mining of massive fluid information obtained from large-scale computations as well as "Integrated Supercomputing Method" that unifies computation and experiment where the system is directly connected to the experimental equipment.

The AFI Research Center, as the international hub for fluid information research, has organized an international symposium on advanced fluid information every year since 2001, and actively promotes collaborative research projects with domestic and overseas universities and enterprises.

Information

■Fluid Science Database

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

Available on the IFS website, this database features many research results on fluid science, including large-scale numerical computations performed on supercomputers, under the goal of sharing and leveraging research results on "flow" as "fluid information."

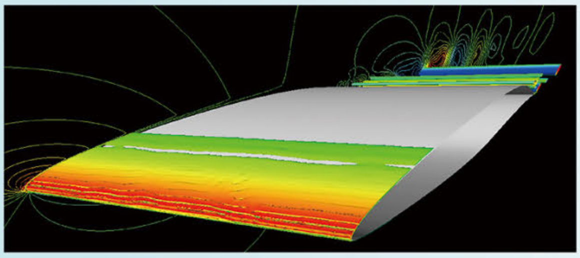
■International Symposium on Advanced Fluid Information (AFI)

We have organized this symposium on advanced fluid information every year since 2001, and share research results on "flow" with the global community. By enabling domestic and overseas researchers to collaborate on fluid information, we seek to further develop "advanced fluid information research."

We also disseminate research results through published reports and presentations at Tohoku University and related international conferences.

Research Topics

Laminar-turbulence transition phenomena near the leading edge of a swept wing



During the flight of a commercial aircraft, about half of the total energy loss stems from friction drag due to the viscosity of the air. Turbulent flow increases friction, but 10% of the total drag can be reduced if the laminar flow can be maintained at 50% of the wing surface. Recent advances in numerical simulation technology and surface processing technology have made it possible to achieve higher performance by the laminarization technique than ever before.

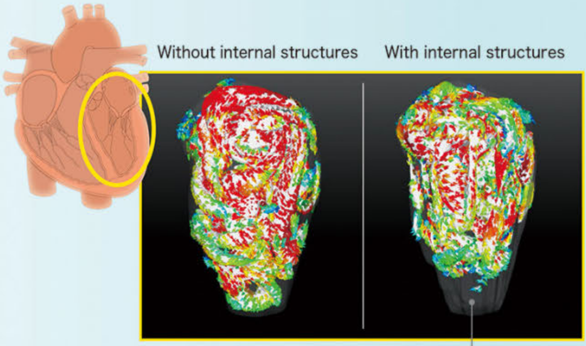
While a sweep angle on the aircraft's main wing reduces the effect of shock waves, this complicates the air flow and causes the unique laminar-turbulence transition. By carrying out direct numerical simulation through large-scale parallelization, we aim to clarify the details of the transition mechanism on the swept wing, improve the accuracy of the transit ion prediction technique, and develop a new laminarization technology.

(Joint research: JAXA, Mitsubishi Heavy Industries)

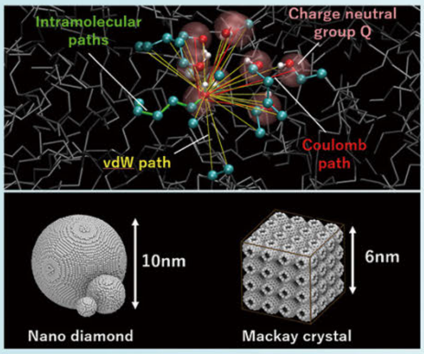
Blood flow analysis in the left ventricle

Thrombus formation was not expected to occur in the left ventricle, a chamber of the heart which pumps blood to the circulatory system, due to its high blood flow velocity. However, recent studies have indicated otherwise.

In this research, we have developed a left ventricular model that includes the chamber's typical internal structures, and are investigating left ventricular blood flow with the Institute of Fluid Science's supercomputer. The images on the right visualize the vortex structure in the left ventricle model without (left) and with (right) the internal structures. The white areas indicate the shape of the vortex. This analysis confirmed that the internal structure prevents the vortex from reaching the apex of the left ventricle. In addition to visualizing the vortex, studying various other parameters has shown that the internal structure has a significant impact on causing a tendency for blood flow to stagnate. Moreover, this analysis technique is also being used to study the effect of valvular heart disease.



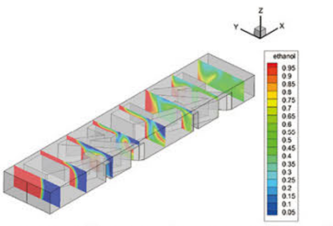
Elucidation and control of the molecular mechanism that determines the thermal conductivity of a heat medium



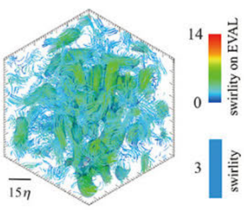
Modern electronic devices and other industrial products require advanced thermal management to control heat generation and dissipation. Consequently, this has increased demand for technology that enables us to design a heat medium with desired characteristics at the molecular level. Knowledge about the mechanism of macroscopic heat conduction at the molecular level is essential to the 'molecular design' of a heat medium. However, studies of such mechanisms in liquids and soft materials, where the molecular configuration and dynamics are irregular, are insufficient compared with those of gas and crystalline solids.

In this research, we used molecular dynamics simulation to develop a method to express macroscopic heat conduction as an accumulation of microscopic energy transfer due to single interaction (i.e., the atomistic heat path, see upper illustration on the left) between atoms and molecules. Using this method, we have clarified the connection between molecular features, like backbone structure and functional groups, and thermal conductivity for typical liquids including alkanes and alcohols. Moreover, nano-composite materials, where carbon nanomaterials (see lower illustration on the left) in the forms of nano-particles are dispersed in a matrix, are attracting much attention as promising heat media, and analysis with such materials is ongoing.

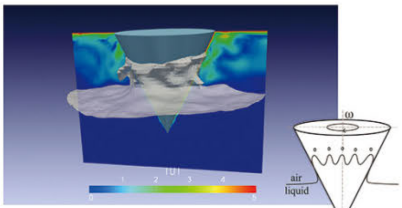
(Joint research, Toyota Motor Corporation)



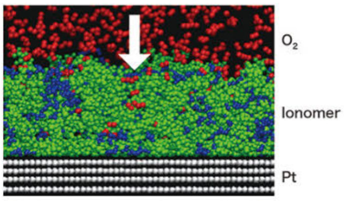
Phase contours in several cross-sections of the optimized micromixer



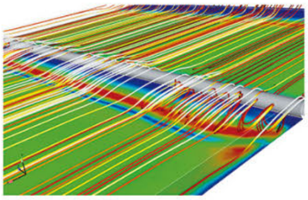
Vortical region represented by swirlity and traced eigen-vortical-axis lines (EVAL) in a decomposed scale in isotropic homogeneous turbulence



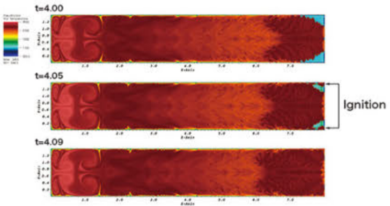
Disturbance wave at the water surface induced by Rayleigh-Taylor instability



Molecular dynamics study of oxygen permeation through ionomer thin film on Pt surface



WSS analysis on endothelial cells around a medical device



Two-dimensional simulations on knocking of n-heptane/air mixture

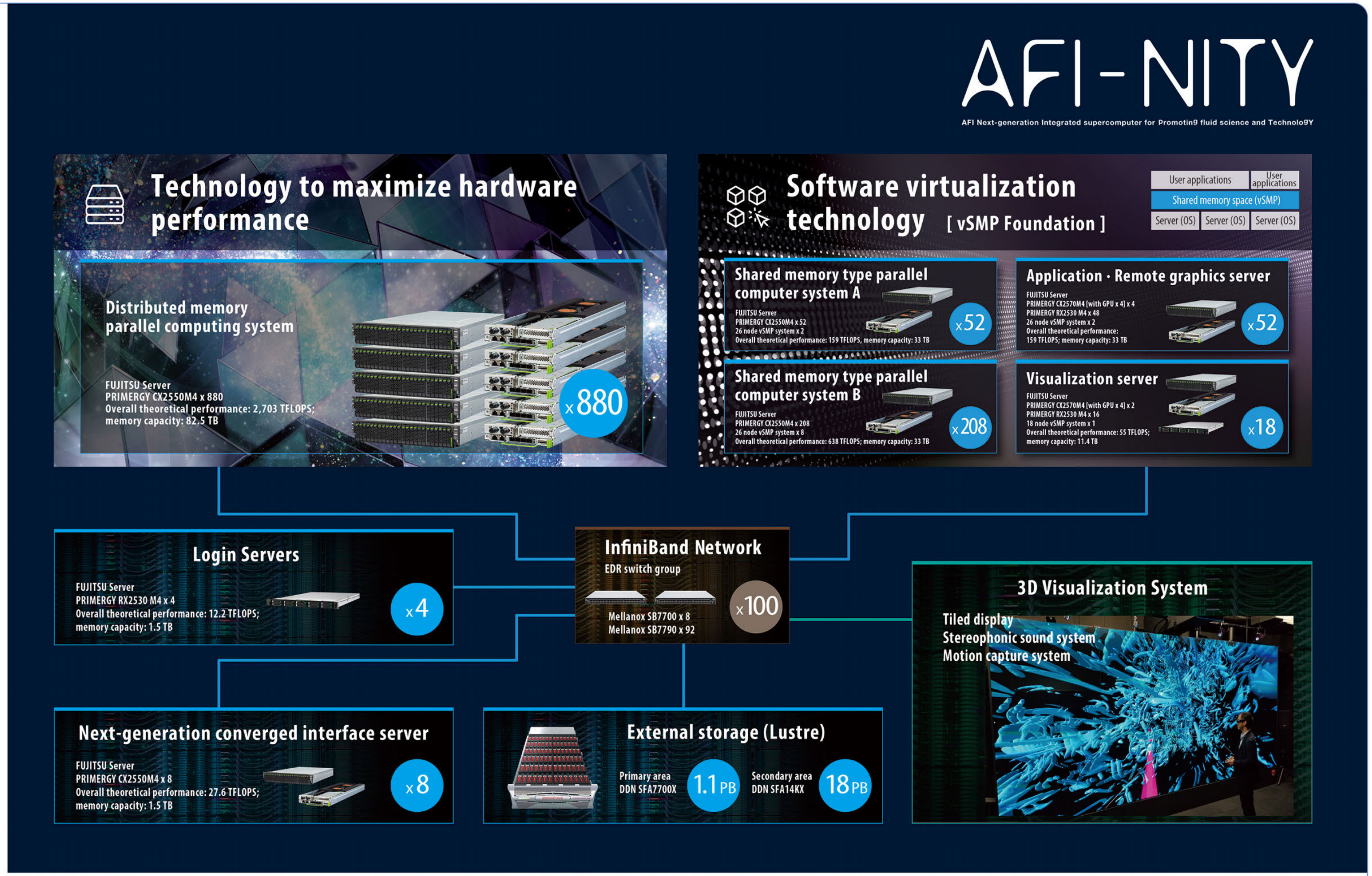
Integrated Supercomputation System

AFI-NITY

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

Leading next-generation fluid science research through the integration of large-scale computing and experimental measurement

The "Integrated Supercomputation System," which currently consists of the distributed memory type parallel computing system, the shared memory vSMP parallel computing system, the Three-dimensional Visualization System for visualization of computation results, 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, and August 2018. 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, Fujitsu servers based on Primergy are used as the distributed memory type parallel computing system and the shared memory vSMP parallel computing system, providing a total peak performance of 3.7 PFLOPS and total memory of 192 TB (maximum shared memory 16 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 and the shared memory vSMP parallel computing system) is listed in the table below.

	Peak Performance [PFLOPS]	Total Memory [TB]
Distributed memory type parallel computing system	2.7	82.5
Shared memory vSMP parallel computing system*	1.0	109.5

*includes Application-Remote graphics server and Visualization server

Software

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

- **Computational Fluid Dynamics**
  ANSYS CFX, ANSYS Fluent, ANSYS Chemkin-Pro, ANSYS Forte, FaSTAR
- **Structural Analysis**
  Abaqus, LS-DYNA, ANSYS Mechanical, ANSYS AUTODYN
- **Molecular Dynamics and Quantum Mechanics**
  Materials Studio (Dmol3, ONETEP, Forcite), Gaussian, Amber
- **Others**
  Comwave, COMSOL Multiphysics, JMAG
- **Optimization**
  modeFRONTIER
- **Visualization**
  Visualization of CFD results : CFD-Post, Ensight, FIELDVIEW, Tecplot, AVS/Express
  Visualization of Structural Analysis : Abaqus/CAE, Patran, Ensight
  Visualization of Molecular Dynamics and Quantum Mechanics : Materials Studio Visualizer, GaussView
- **Modeling**
  Modeling in CFD : ANSYS DesignModeler, CATIA
  Modeling in Structural Analysis : Abaqus/CAE, Patran, CATIA
  Modeling in Molecular Dynamics and Quantum Mechanics : Materials Studio Visualizer, GaussView, xleap
  Others : Materialise Magics
- **Mesh Generation**
  For CFD : ANSYS Meshing, Pointwise, ICEM CFD
  For Structural Analysis : Abaqus/CAE, Patran
- **Compilers**
  Intel Parallel Studio XE(C/C++, Fortran), GCC
- **Libraries**
  Intel MPI, IMSL Fortran, OpenMPI, OpenMP

User Support

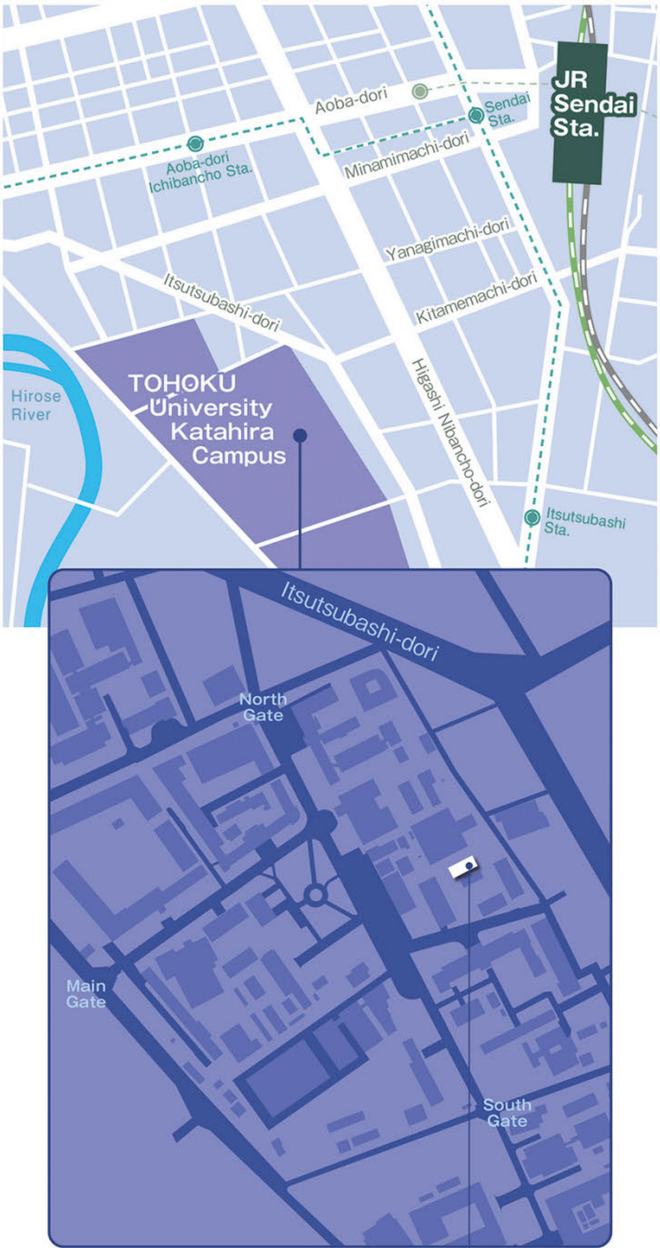
The AFI Research Center's R&D Division office, supervised by the Director of the center, operates the Integrated Supercomputation System and supports the users of system.

Steering Committee
determines the AFI Research Center's policy

Selection and Examination Committee
screens and evaluates the AFI Research Center's research projects

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

Supporting WG
supports users of the system



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