2. Establishment of the Research System for Computational Science

High Performance Computing Development

Management of computational resources

We are working to operate and maintain computing environments required for the efficient use of computational resources offered by the High Performance Computing Infrastructure, with the K computer as a primary resource for a number of researchers (including members of health care and pharmaceutical industries) to realize the potential of researchers in Strategic Field 1.

K computer-use support

Advanced skills and capabilities for parallel programming are required to use the K computer. Thus, we provide highly skilled technical staff, and offer technical workshops including parallel programming and usage of software, to best utilize computational resources.

Education and Outreach

Education

We provide support programs for human resource development in high schools, universities and industries.

SCLS Supercomputer System (Public invitation for research theme proposals)

We offer a K computer-compatible supercomputer system, "SCLS supercomputer system" to encourage researchers in life sciences to make active use of the K computer and the HPCI environment.

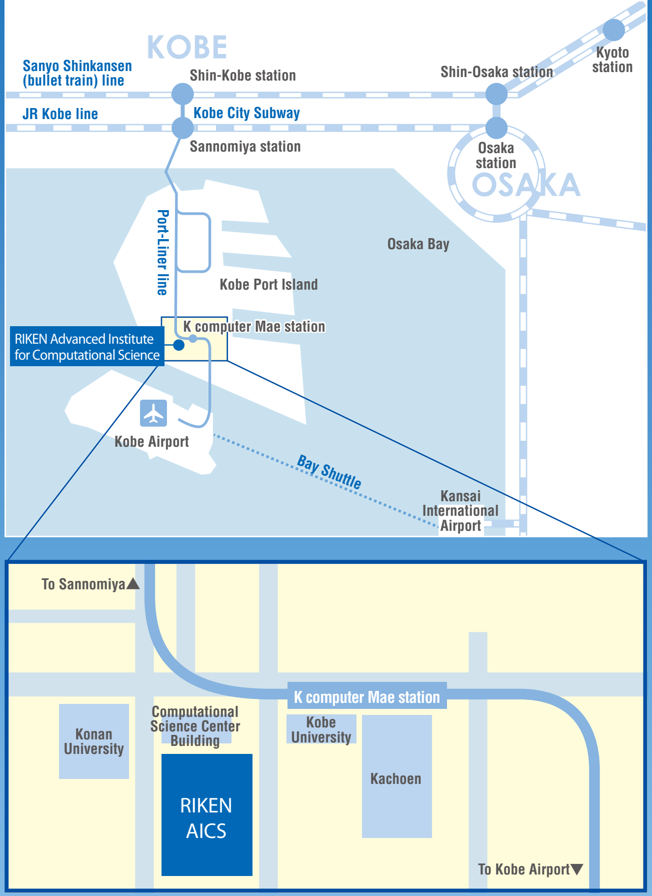
Human Network

We hold symposia and seminars to introduce our activities in the HPCI programs to life science communities. We plan to support researchers in Japan and abroad in the use of the K computer.

Public Relations

We carry out public relations activities aimed at communicating our project to the public and gaining long-term support.

ACCESS MAP



- JR Shinkansen (Bullet) Train (Arriving at Shin-Kobe Station)

JR Shin-Kobe Station	Kobe City Subway 2 minutes	Sannomiya Station	Port-Liner line 15 minutes	K computer Mae station	3 minutes	RIKEN AICS

- Flight

Kansai International Airport	Bay Shuttle Ferry 30 minutes	Kobe Airport	Port-Liner line 5 minutes	K computer Mae station	3 minutes	RIKEN AICS
Kansai International Airport	Limousine Bus 65 minutes	Sannomiya Station	Port-Liner line 15 minutes	K computer Mae station	3 minutes	RIKEN AICS
Osaka International Airport	Limousine Bus 40 minutes	Sannomiya Station	Port-Liner line 15 minutes	K computer Mae station	3 minutes	RIKEN AICS

RIKEN HPCI Program for
Computational Life Sciences
Planning and Coordination Group

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http://www.kobe.riken.jp/stpr1-life/en/

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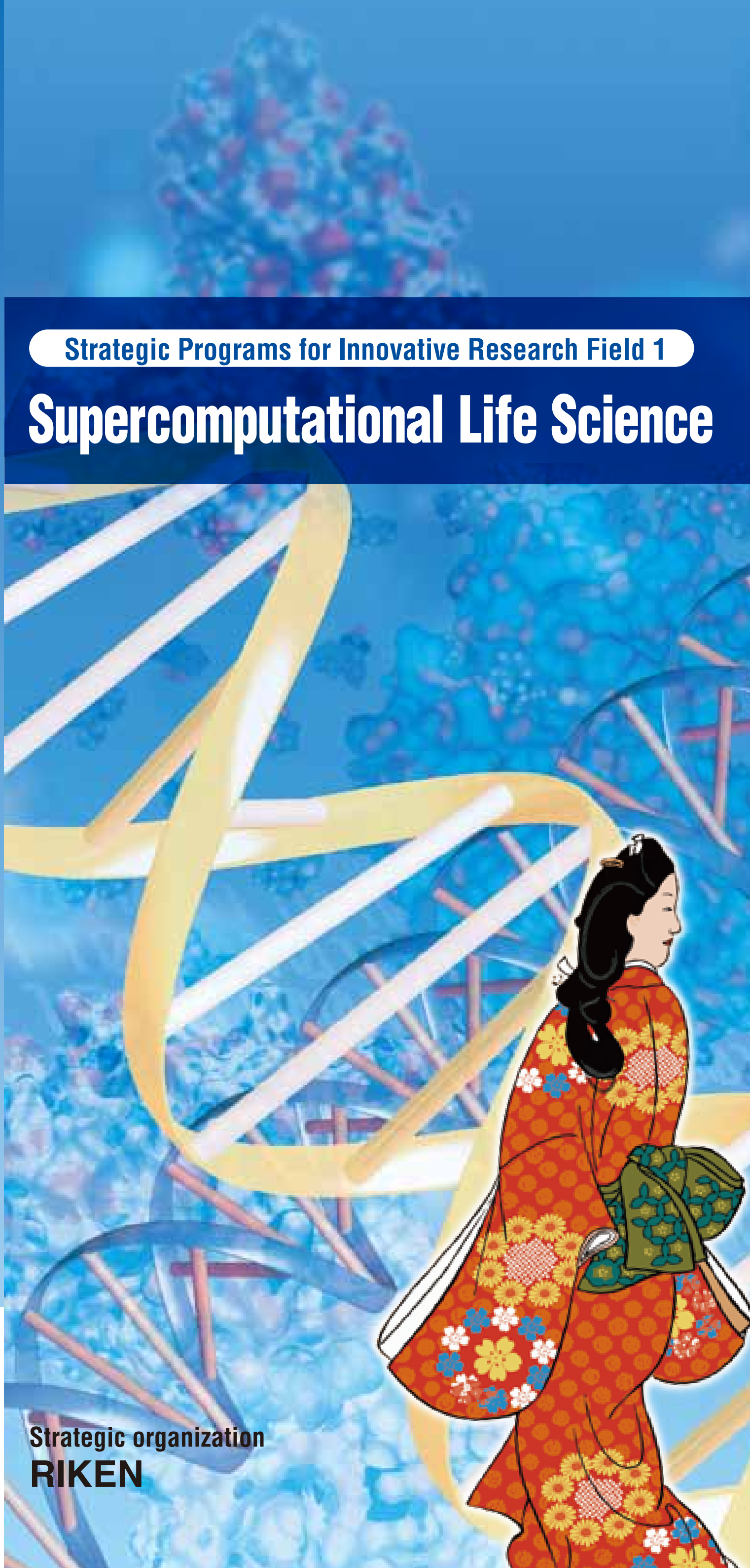
RIKEN 2013-034



Strategic Programs for Innovative Research Field 1

Supercomputational Life Science

Strategic organization
RIKEN

Computational Life Sciences

Biological phenomena are understood as the result of large and complex systems consisting of a variety of elements (these systems form various levels of biological hierarchy such as genomes, biomolecules, cells, and organs). Our approach involves the simulation of biological phenomena by constructing suitable models based on experimental information on the biological systems, and then inputting these models into the computer. The applicability of a given simulation is usually limited by the performance of the computer employed, making it necessary to divide the system into subsystems, to coarse-grain the model, and/or to deal with only short-term phenomena. The K computer makes it possible to simulate a whole system without such limitations. The simulation results obtained by the K computer will reveal the principles of biological phenomena that are hidden behind experimental information and, as a result, will enable greater prediction and control of biological phenomena. In particular, focusing on disease as the target problem, we have set our sights on the ultimate goal of contributing to medical care and drug design using the simulations.

Participants ; RIKEN, Nagoya Univ., The Univ. of Tokyo, JAEA, OIST,
Tokyo Tech., AIST, Osaka Univ., NIG, Yokohama City Univ.,
Kyoto Univ., ISM (abbreviated, in no particular order)

The "Strategic Programs for Innovative Research" is a five-year program of the Ministry of Education, Culture, Sports, Science and Technology (MEXT), aimed at yielding significant social and academic breakthroughs in five 'strategic fields': 1. Supercomputational Life Science, 2. New Materials and Energy Creation, 3. Projection of global change toward the mitigation of natural disasters, 4. Industrial Innovations, 5. The Origin of Matter and the Universe (utilizing the K computer system as a primary resource).

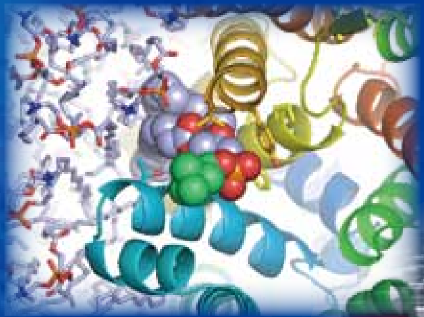
The program was launched in April 2011. RIKEN is a representative organization of Strategic Field 1, and has been developing applied computational life sciences, collaborating with other universities and research institutes in Japan.

In addition, we plan to offer a number of technical workshops and seminars to the social and academic communities, and to contribute to the formation of human networks in computational life sciences.

1.Research and Development

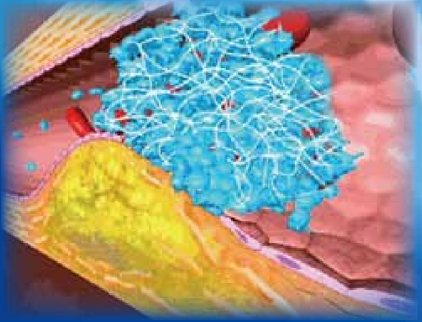
1 Simulations of biomolecules under cellular environments

By using multi-scale molecular dynamics simulations and single-particle simulations as research tools, we aim to investigate biomolecular structures and functions under cellular environments. Molecular transport across biological membranes, protein/DNA interaction, and signal transduction are representative targets in the project. We expect that these simulation studies will contribute to drug design and understanding of cellular functions.



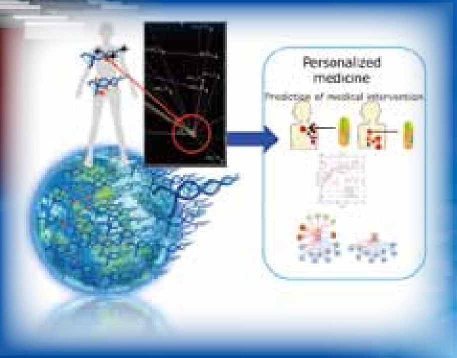
2 Simulation applicable to drug design

We plan to construct a methodology for designing new compounds, and to establish a method for identifying protein-compound binding sites; and then to design and verify drug candidates against several target proteins. In addition, we will develop a method for predicting ligand binding to proteins with flexible binding sites. A highly efficient method of drug design is expected to be established through this research.



3 Hierarchical integrated simulation for predictive medicine

We plan to combine the whole-body musculoskeletal-nervous system simulator, thrombus simulator, heart simulator, and whole-body vascular network simulator, and construct an integrated simulator that can help us understand complex biological phenomena more thoroughly, and can be applied to a wide range of diseases. We expect that these studies will contribute to the development of effective medical treatments (including those for cardiac diseases such as angina pectoris and myocardial infarction, and neurological diseases), as well as to the evaluation of drug efficacy, and prognostic prediction.



4 Large-scale analysis of life data

We will develop a methodology for large-scale analysis of data obtained by cutting-edge technologies such as the next-generation sequencer, to understand diseases and biodiversity, investigate characteristics of cells and cancer, and understand the network of biomolecules. We expect that this research will contribute to personalized medicine and industrial use of genomic information.