

Present Status of RIST in Promotion of High Performance Computing Infrastructure in Japan

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Research Organization for Information Science & Technology

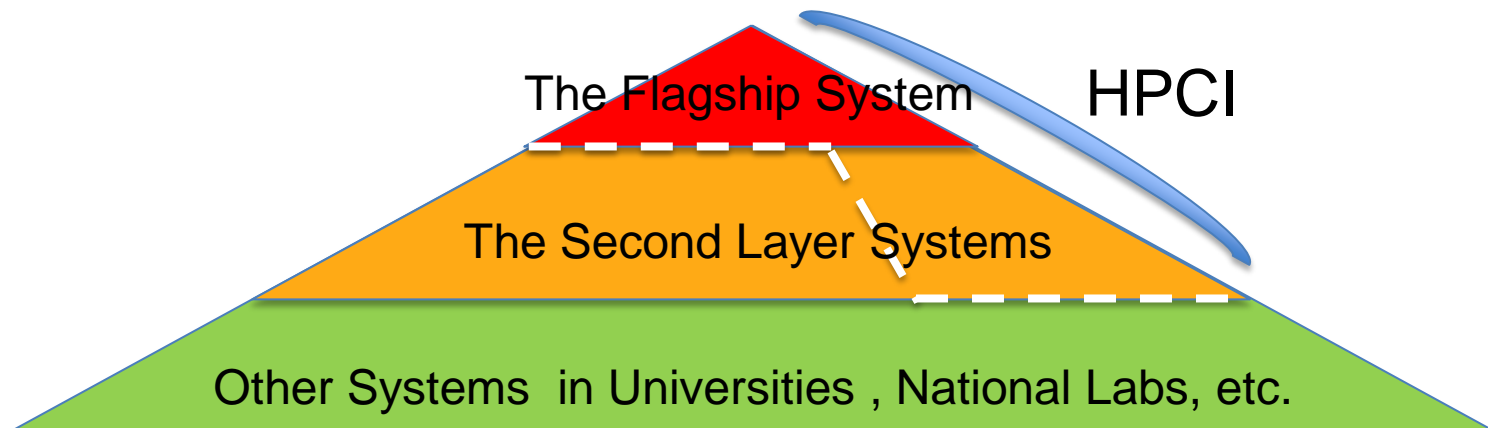
Contents

- High Performance Computing Infrastructure (HPCI)
- Role and Task of RIST in HPCI System
- Shared Use of K computer
- Screening Process of the General Use Category Projects
- Supporting Activities for Shared Use
- Promotion of Industrial Use
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- Recent Research Highlight
- Future Plan
- Conclusion

HPCI

The High Performance Computing Infrastructure in Japan

- HPCI has been established as a platform to realize integrated use of high performance computer resources including K computer.
- HPCI now consists of 12 computers, with K computer as the flagship and others from the second layer systems.
- All the HPCI resources are connected via high speed network and are operated with a policy of single-sign-on.



Constituents of HPCI System

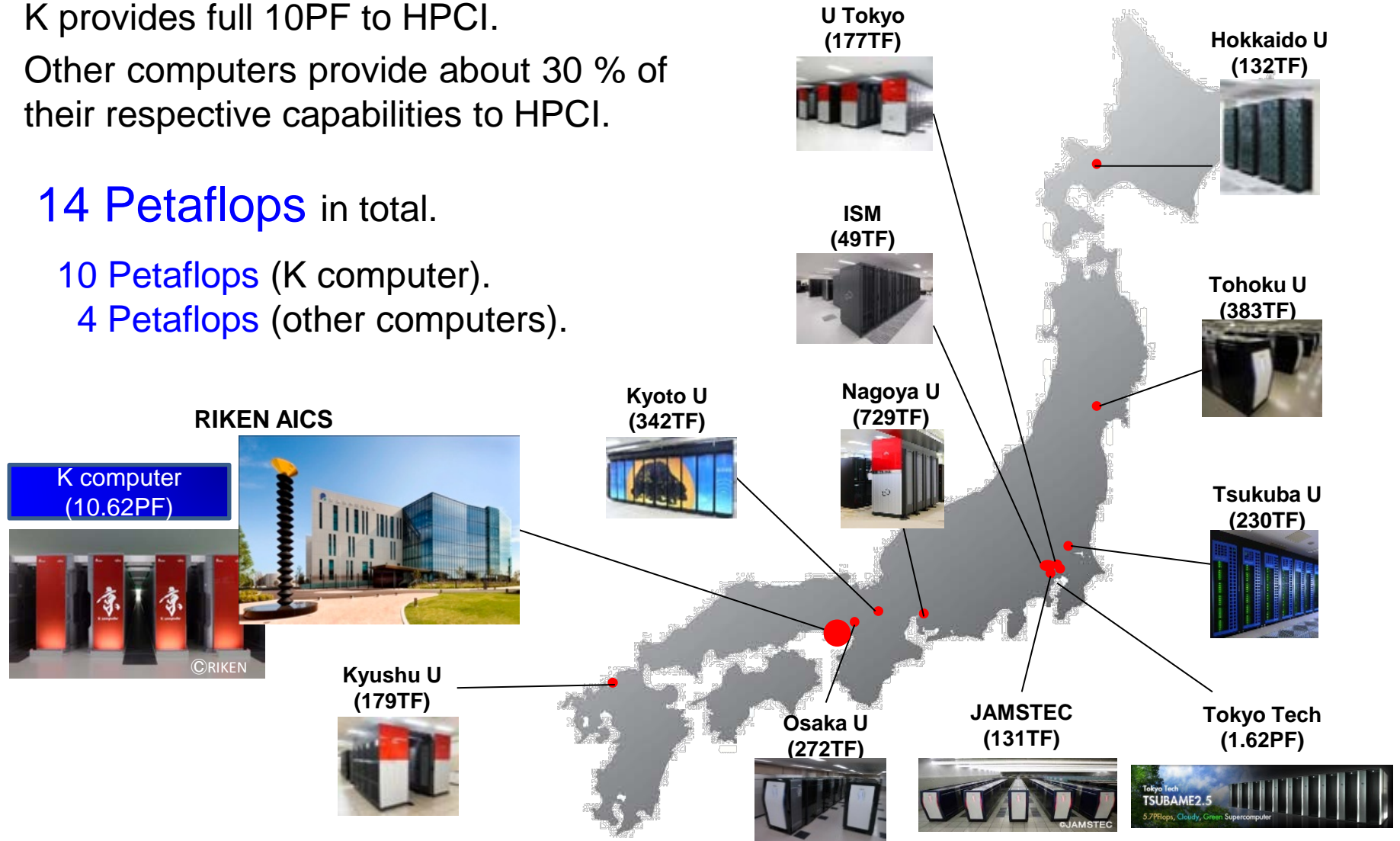
K provides full 10PF to HPCI.

Other computers provide about 30 % of their respective capabilities to HPCI.

14 Petaflops in total.

10 Petaflops (K computer).

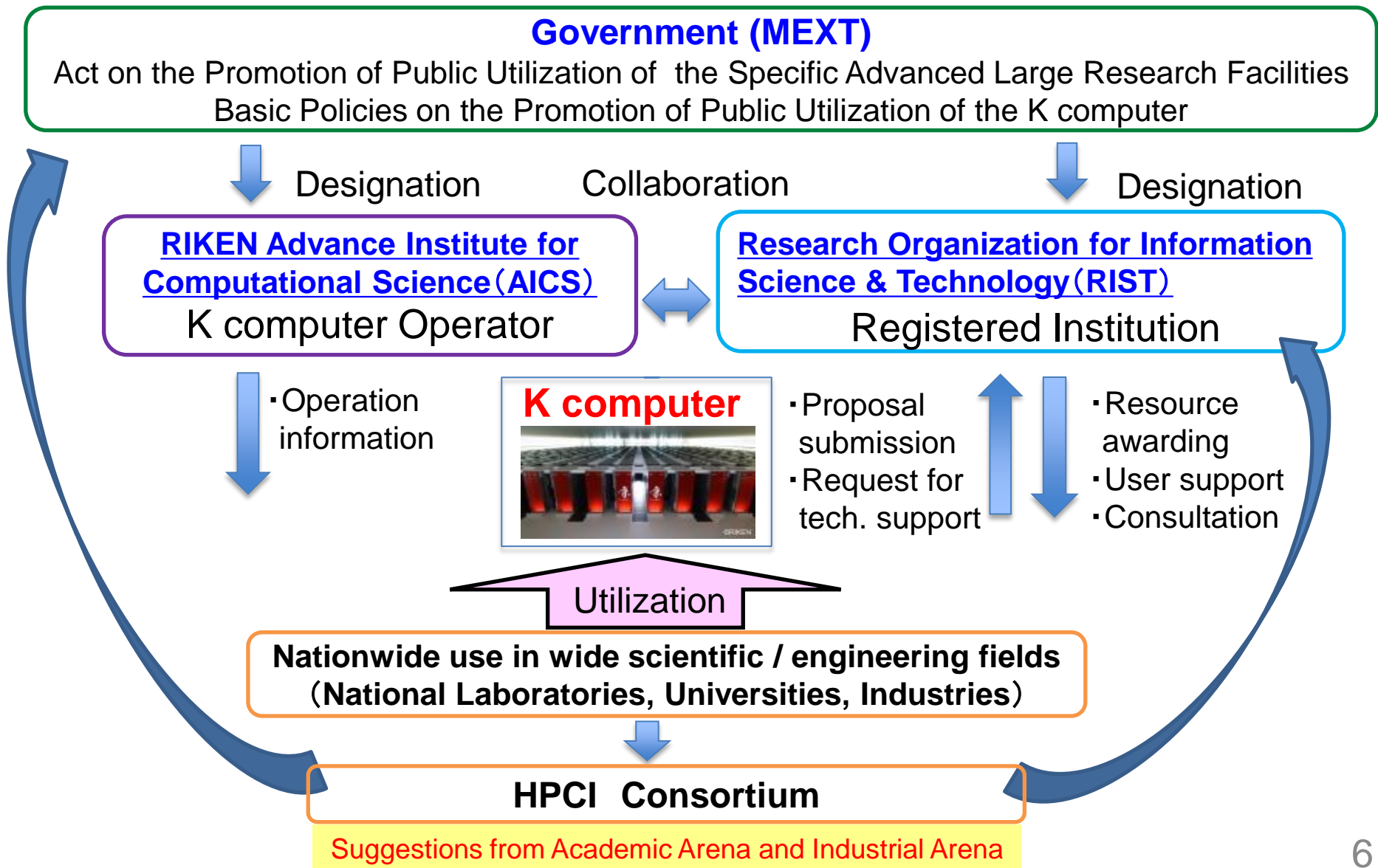
4 Petaflops (other computers).



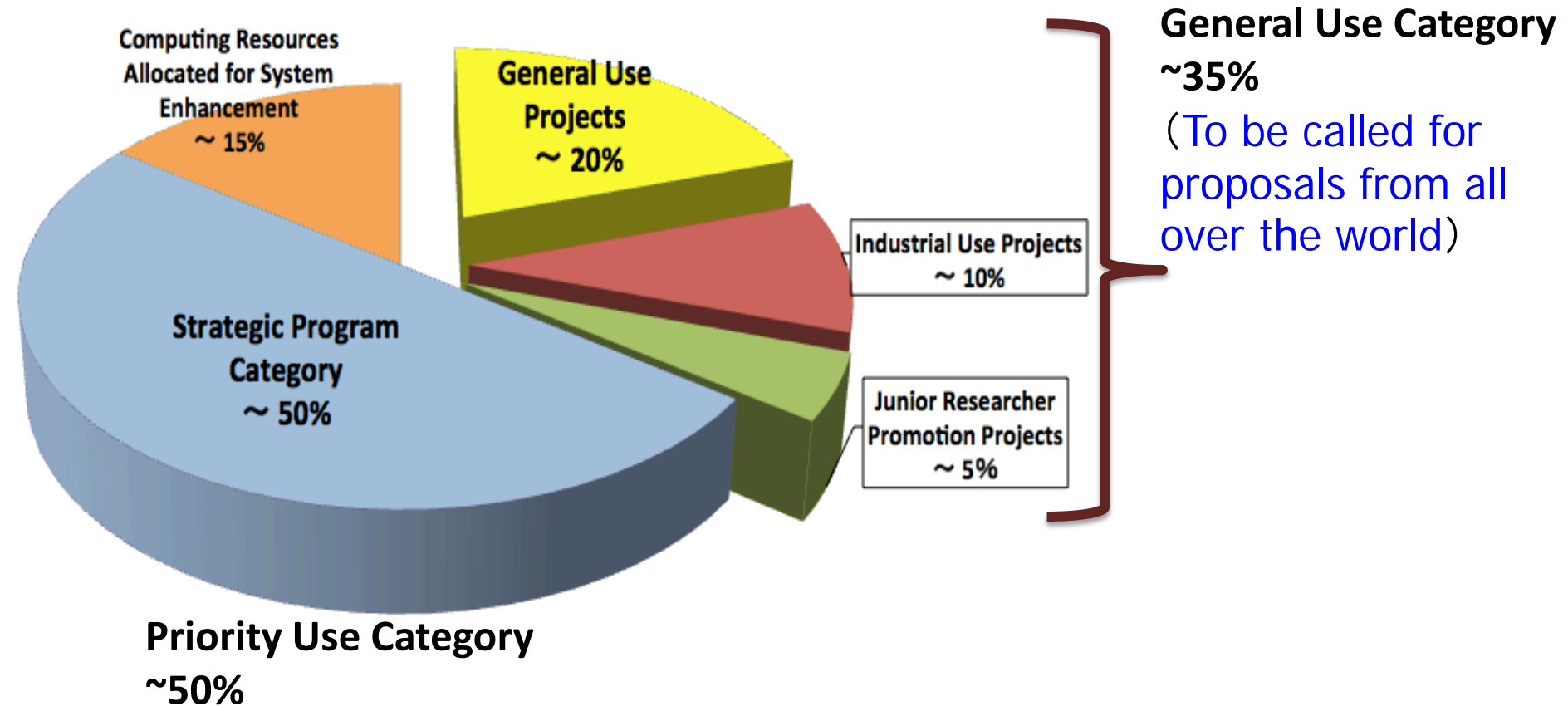
Role and Task of RIST in HPCI System

- RIST has been designated as the Registered Organization for the K computer by the Japanese government (MEXT) since 2011.
- The Task of Registered Organization includes:
 - Call for proposals
 - User selection, awarding K computer resources
 - Support of K computer users
 - Promotion of shared use of K computer
- RIST has been playing practically the same role in other HPCI supercomputers.

Framework for the use of K computer



Resource Distribution for K computer



HPCI Strategic Programs for Innovative Research (SPIRE)

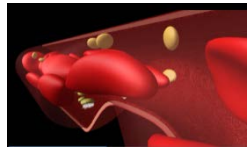
Scope

SPIRE aims at (1) innovative scientific discoveries and technologies, (2) fostering of human resources capable of fully utilizing state-of-the-art computing environments, and (3) establishment of leading-edge research and education hubs by making the most use of HPCI with the K computer as its core.

Project Outline

(Field 1)

Supercomputational
Life Science

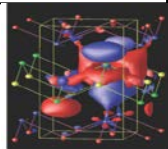


RIKEN

(Field 2)

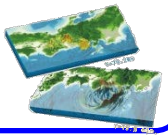
Institute for Solid State Physics,
University of Tokyo
Institute for Molecular Science etc.

Creation of new
materials and energy



(Field 3)

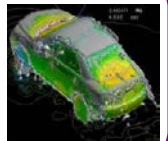
Advanced Prediction Researches
for Natural Disaster Prevention
and Reduction



(Field 4)

Institute of Industrial Science,
University of Tokyo

Industrial
Innovation



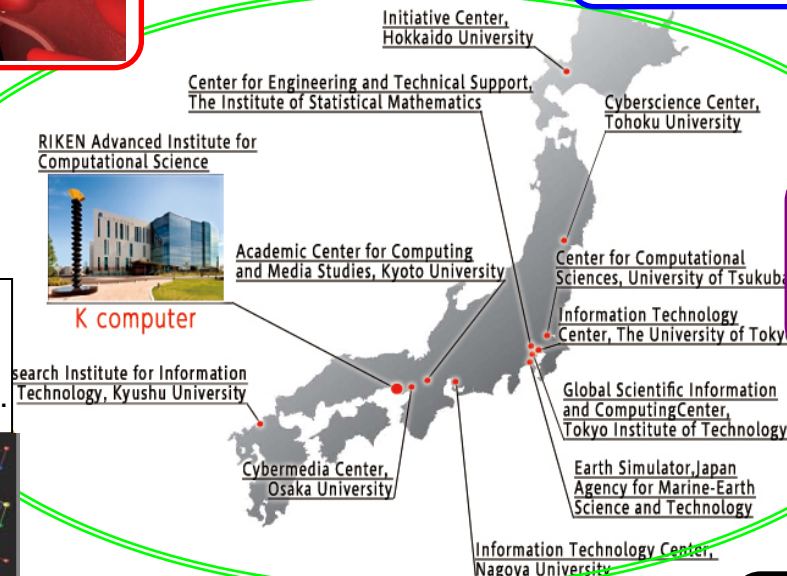
(Field 5)

University of Tsukuba etc.

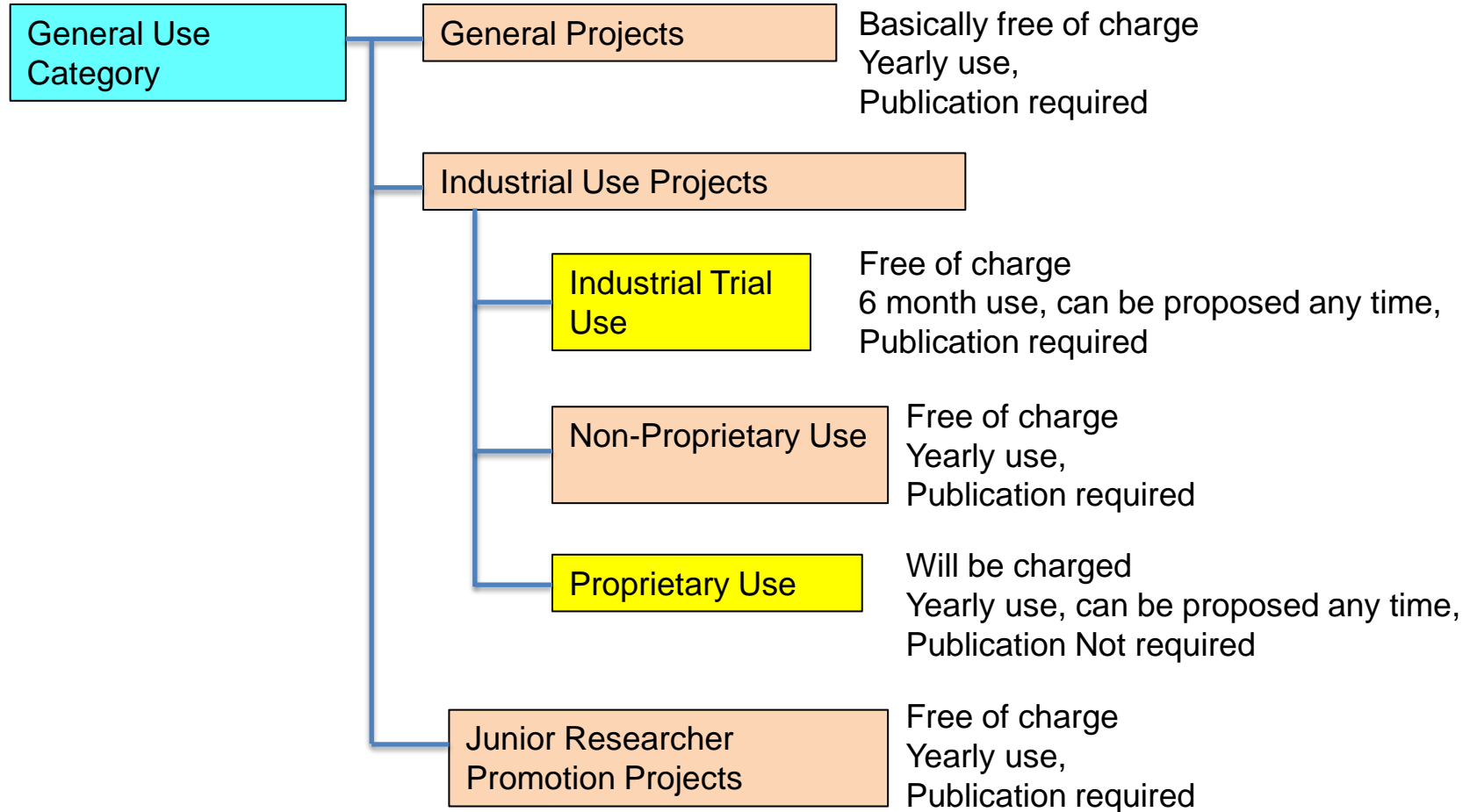
The origin of matter
and the universe



Revolutionary research outcomes through building
strategic computational science infrastructures

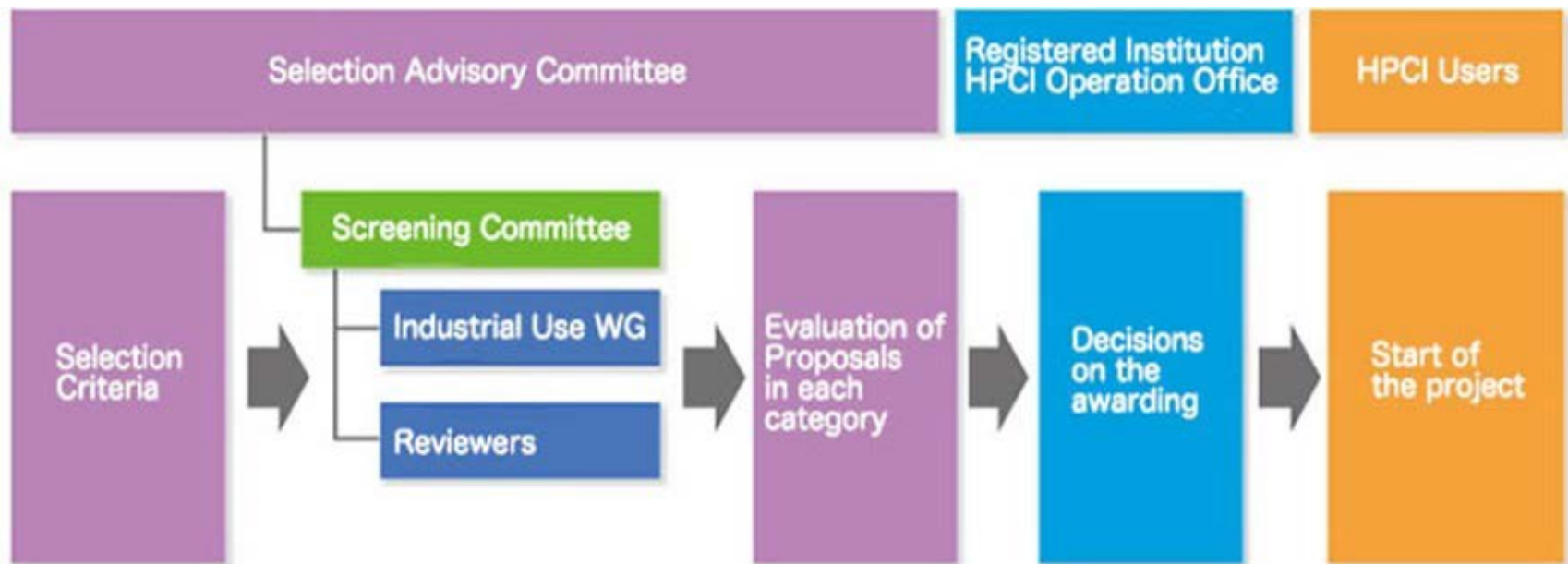


General Use Category



Screening Process for General Use Category

- Call for proposals to access HPCI resources including K computer is basically scheduled once a year
- Proposals for Proprietary Use and Industrial Trial Use projects are acceptable at any time through a year
- Peer review process is used for proposal screening



Awarding results for the fiscal year, 2015

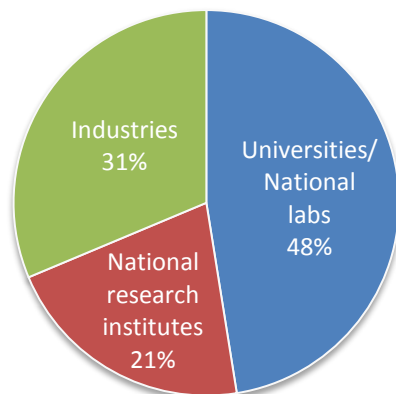
Number of Proposals submitted and awarded

			submitted	awarded	ratio
The K computer	annual	General Use	78	24	31%
		Junior Researcher Promotion	23	12	52%
		Industrial (non-proprietary)	37	31	84%
		Total	138	67	49%
	all times	Industrial (Industrial Trial Use)	3	3	100%
		Industrial (proprietary)	5	5	100%
HPCI System Computers other than the K computer			127	67	53%

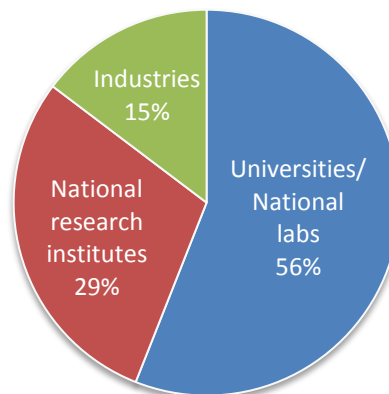
**Number of K users:
1,095
including
Industrial and
Strategic Program
users:**

(as of April 1, 2015)

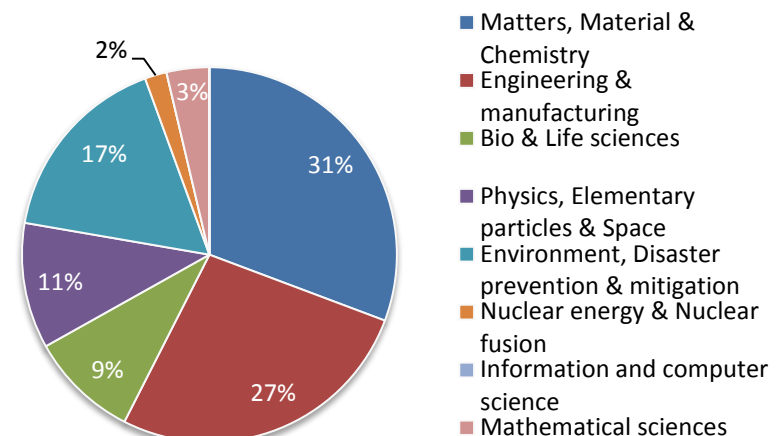
Number of awarded proposals for the K computer (classified by affiliation type)



Awarded resources for the K computer proposals (classified by affiliation type)



Awarded resources of the K computer (classified by research areas)



User Support

- Help Desk is operating with One-Stop Service philosophy so that User can solve every problems when using K computer:
 - User consultation
 - Consulting about Porting, Compile, Library, Tools, etc.
 - Technical support
 - Program Tuning for K computer
 - Research support
 - Research consultation provided by collaboration with many research organizations
 - Promotion for Industrial Use
 - Consultation and assistance before submitting proposal
- Collaboration with other organizations
 - RIKEN AICS
 - 11 HPCI organizations providing High Performance Computing Infrastructure
 - Strategic Programs for Innovative Research

User Support page of the HPCI Portal Site:
http://www.hpci-office.jp/folders/e_user

Support Framework

RIST

All Users

One
Stop
Service

Help Desk

User
consultation

Technical
Support

Research
Support

Industrial Use
Promotion

**Collaboration
with**

AICS

HPCI System
Providers

SPIRE^{*1}

^{*1}Strategic Programs for Innovative Research (Field1, ..., Field5)

Technical Support

- Tuning Support made by 30 Research Consultants

- Supporting period is about 3 months a project.
- Free of charge
- Number of Projects supported
 - FY2013.....37 projects
 - FY2014.....29 projects



- Support for using OSS

- Scalability of commercial software is not enough for large scale simulation.
- Necessity of OSS becomes higher and higher.
- Confirmation of OSS performance and provision of OSS information for Users
 - Ex) CFD: OpenFOAM, MD: LAMMPS

Training for Users' skill-up (Free of charge)

- Achievements

- Effective usage of K computer
- Contribution to effective research implementation

- Seminars

- 22 times at Tokyo and Kobe etc. in FY2014
- 751 participants: 130 Industrial participants

- Workshops

- Information exchange for advanced tuning on K computer
- Case study for using OSS on K computer
- 111 participants: 80 Industrial participants



Industrial Use Promotion

- Objectives of Industrial Use

- To demonstrate effectiveness and values of large scale HPC (Not production run) in Non-proprietary use
- To carry out confidential projects at its own expense in Proprietary use

- Staff for Industrial Promotion

- 7 consultants at Kobe Center
- 6 consultants at Tokyo branch office
 - Tokyo Access Point



(Support center for industrial users : 2 secured rooms with technical staff)
230 HPCI users used Tokyo AP in FY2014.

- Service fee

- Free of charge for specific services



Software Development	Software Parallelization	<ul style="list-style-type: none">▪ Performance Analysis▪ Advice for tuning	Software Modification
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Activities for Industrial Use Promotion

- Consultation and Assistance before submitting proposal
 - Consultation and assistance for 49 projects in FY2014
 - Evaluation of program portability and performance with FX10 (K compatible)
- Program Tuning Support
 - 14 companies, 17 projects in FY2014
- Pre and Post processing (Visualization) Support
 - 5 companies, 5 projects in FY2014
- Provision of Application (ISV/OSS) information
 - Preparing makefile, job script and correcting code for OSS (LAMMPS, OCTA/COGNAC83, OCTA/SUSHI9.1, FrontISTR, FrontFlow/blue, REVOCAP_Coupler, etc) for K computer and FX10
 - Performance test for ISV (Poynting, VASP, CzeekS, VSOP, etc.) on FX10 and K computer
 - Collaborative research with AdvanceSoft Corporation for porting 4 applications
- Promotion to increase industrial users
 - 6 Lectures and 4 exhibitions at Industrial seminars in FY2014
 - Workshop on “Let’s use OpenFOAM on K computer”
 - Cooperation with economic organizations and industrial associations

Publication Management

- The research achievements obtained from the use of the HPCI system should be widely disseminated as public intellectual property in society, according to [the Basic Policy on the Promotion of Public Utilization of the Specific High-speed Computer Facilities](#) (i.e., K computer).
- Submission of User Reports.(within 60 days after completion of the projects)
- Publication of research achievements. (within 3 years after completion of the projects)



Search screen for the User Reports
~ List of research areas ~

HPCI Publication Database

- It is encouraged to register research achievements in the HPCI Publications Database as soon as they are published during or after implementation of the projects.

The latest number of registered products : 2755

- The number of peer-reviewed papers has significantly increased since FY 2013.

(as of May 20, 2015)

Q

SEARCH

RESET

Any Publication Date • The Main Resource • Any Language • HPCI Projects Only •

Search fields

Publication Category

Author/Speaker

Title

Journal

Venue

Reference URL

Project Number

Project Title

Project Category

Results publication number that matches the criteria of the current

Date Range: Any Publication Date

Resources that were used: [The main resource for each category](#)

Language: Any Language

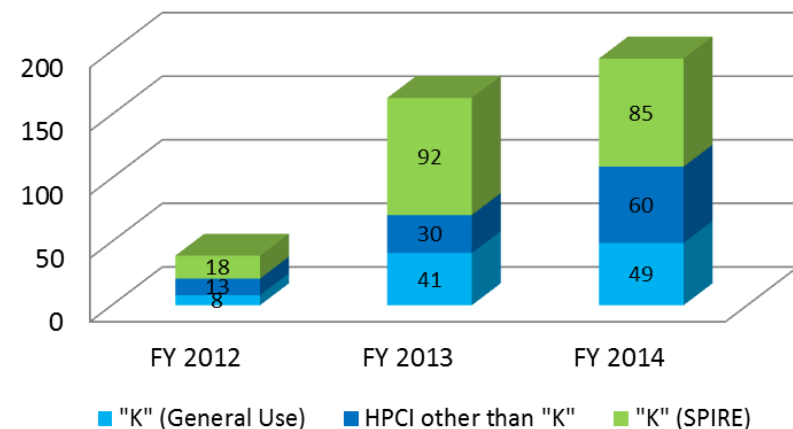
*List will appear when you click on an active cell.

	Project category (Publications due to multiple projects will be counted as the number of each project category.)										Total	Number of publications
	"K"(General use)			HPCI other than "K"		"K"(HPCI Strategic Programs)						
	General use	Fostering young	Industrial use	General use	Industrial use	Field 1...	Field 2...	Field 3...	Field 4...	Field 5...		
Paper(peer-reviewed)	75	20	9	104	3	19	84	38	35	33	420	376
Paper(without peer review)	7	2	6	7	0	15	4	21	12	3	77	75
International Conf., Symp.	158	20	8	140	0	79	152	82	139	87	865	802
Domestic Conf., Symp.	134	24	43	99	3	100	121	88	187	62	861	789
Research Meeting, etc.	77	6	38	42	0	52	53	58	32	57	415	395
Public Lecture meeting, etc.	13	2	15	8	0	26	12	6	10	10	102	99
Media: Newspaper, TV, etc.	14	5	45	20	1	16	32	38	4	32	207	196
Books	2	0	2	5	0	3	1	2	0	0	15	15
Code, Database published	2	1	0	0	0	2	1	0	0	0	6	5
PAT. applied/granted	0	0	0	1	0	2	0	0	0	0	3	3
Total	482	80	166	426	7	314	460	333	419	284	2971	2755
	728			433		1810						

May 20,2015: Last updated database

Publication Trend of HPCI

Peer-reviewed paper



The 1st Project Report Meeting of the HPCI System Including K computer (31 October, 2014, Tokyo)

- Objectives: Promotion of information exchanges and communications between researchers through presentations of research products of the HPCI System
- Highlights:
 - Special talk by Dr. S. Girona, PRACE
 - Ten oral presentations of remarkable results selected from General Use categories
 - Presentations of the five fields of SPIRE
 - 124 poster presentations from General Use categories
 - Prize-giving; HPCI Excellent Result Award to the ten speakers of General Use categories



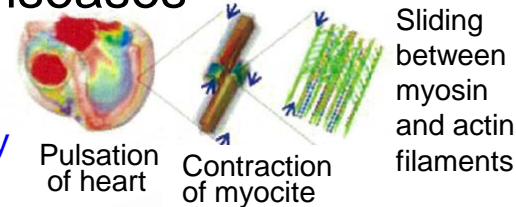
- Participants: 313 persons including 185 from universities and research organizations and 96 from industries

Recent Research Highlight (1)

HPCI Strategic Program for Innovative Research (SPIRE)

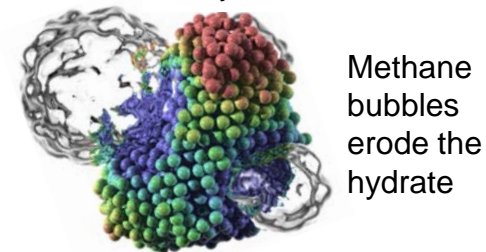
(Field 1) Multiscale and Multiphysics Simulation of Heart Diseases

The performance of the K computer has realized precise heart simulation based on the hierarchical structure ranging from molecules to the whole organ. The developed simulator, "UT-Heart", has made a significant contribution to the study of underlying mechanism of hypertrophic cardiomyopathy.



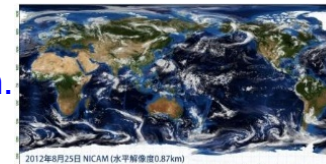
(Field 2) Decomposition of Methane Hydrate

Methane hydrate is the future energy resource abundant at the ocean floors. We perform the large-scale molecular dynamics simulation of its decomposition and propose the way to control the decomposition rate by enhancing / restricting the emergence of methane bubbles.



(Field 3) Weather simulation by Nonhydrostatic ICosahedral Atmospheric Model

An example of three-dimensional distribution of clouds (mixing ratio of hydrometeors) simulated by NICAM of 870m horizontal resolution.

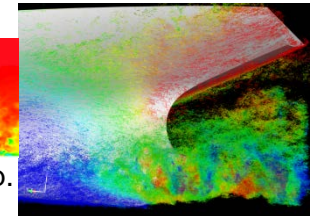


Global distribution of clouds

JAMSTEC and AORI / U. of Tokyo (HPCI SPIRE3) with RIKEN AICS.

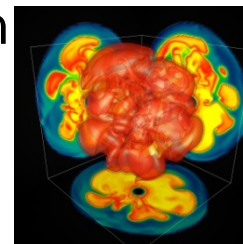
(Field 4) Turbulent Vortex Simulation for Fluidic Device

Turbulence simulations which directly compute dynamics of small eddies with up to 30 billion computational grids were performed by industry & academia cooperation in the field of automobile, turbomachinery, ship and so on.



(Field 5) Simulation of Supernova Explosion

This is a pioneering 3D hydrodynamic simulation that self-consistently solves the radiation equation for neutrinos. The numerical grids employed in the simulation achieve the finest resolution in the world.



Snapshot of the supernova simulation. Yellow and red: convective bubble. Blue: expanding shock wave.

Recent Research Highlight (2)

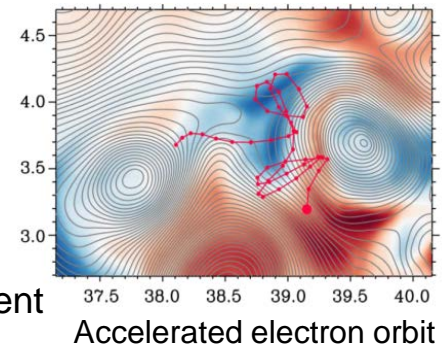
“K” General Use, HPCI General Use other than “K”

“K” General Use category

- Toward understanding cosmic-ray electron accelerations at astrophysical shock waves (hp120222)

Stochastic electron acceleration in a turbulent shock structure was revealed for the first time by ab initio particle simulations.

Y. Matsumoto et. al., “Stochastic electron acceleration during spontaneous turbulent reconnection in a strong shock wave”, Science, 27 February 2015 (Online).

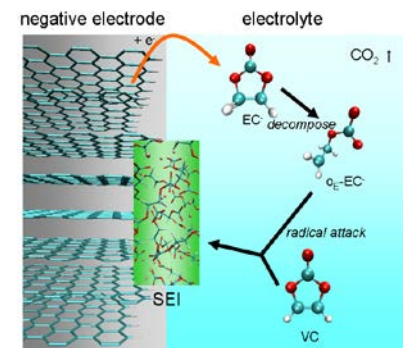


“K” Industrial Use category

- Additive effect on Solid Electrolyte Interphase Formation (SEI) in Lithium-ion Battery (hp120181)

By using density-functional based molecular dynamics method, we can first completely reproduces gaseous products in lithium ion battery and elucidate the effect of additive on SEI formation.

K. Ushirogata et al., “Additive effect on reductive decomposition and binding of carbonate-based solvent toward solid electrolyte interphase formation in lithium-ion battery”, J. Am. Chem. Soc., 135, 11967-11974 (2013)



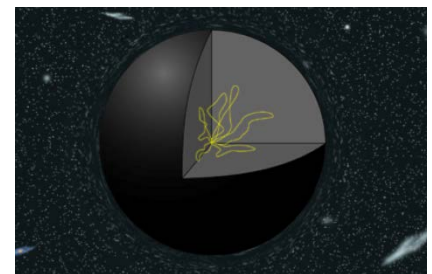
VC additive and EC electrolyte reaction in lithium ion battery

HPCI other than “K” General Use category

- Supercomputer study of superstring theory (hp120162)

For many decades, physicists dreamed of unifying quantum mechanics and general relativity. Superstring theory, with the help from supercomputer simulation, provides us with a promising solution.

M. Hanada et al., “Holographic Description of a Quantum Black Hole on a Computer”, Science, 17 April 2014 (Online)

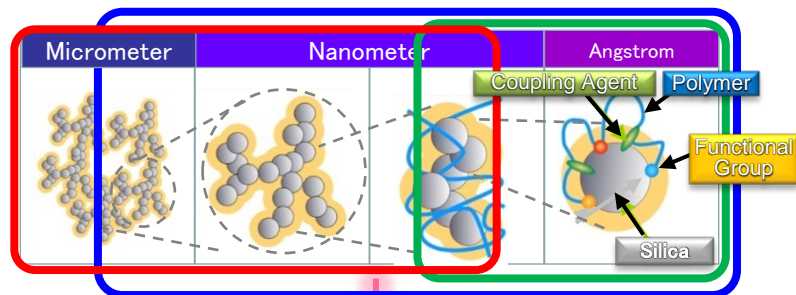


Black hole can be understood as a condensation of strings.

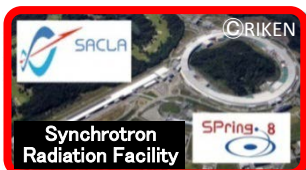
Recent Research Highlight (3)

Complementary use of HPCI with large experimental facilities

SPring-8 / J-PARC / “K” computer



Structural Analysis
+
(Dynamics)

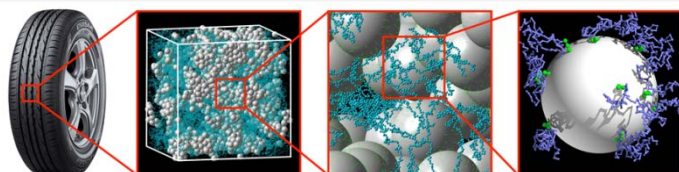


Dynamics



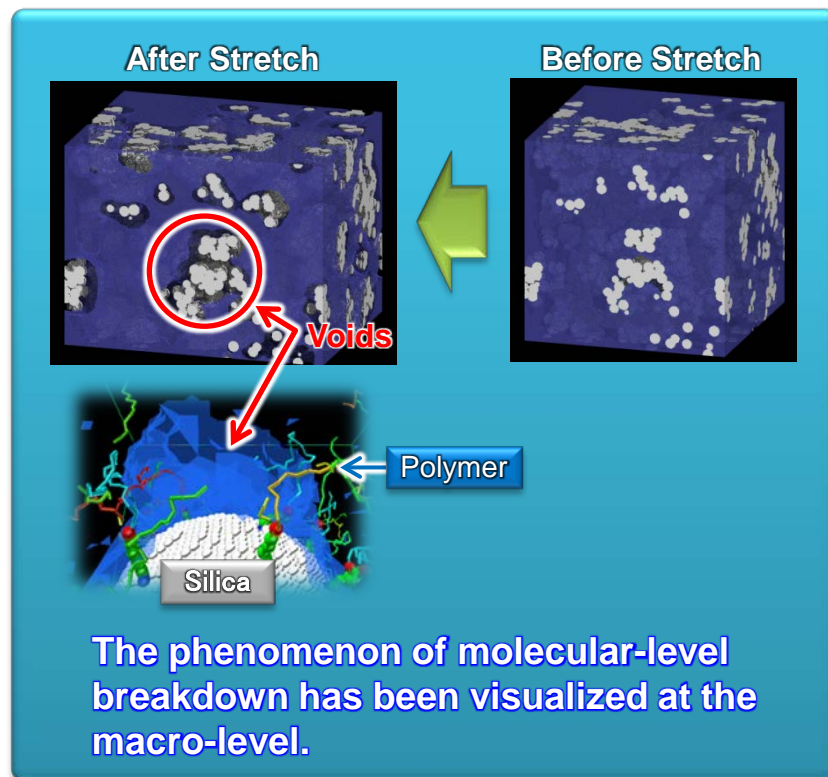
- Prediction
- Material design

Understanding the nano-scale behavior of **real compounds** will lead to **the development of new polymers** and **further innovation in the field of rubber chemistry**.



“K” Industrial Use category

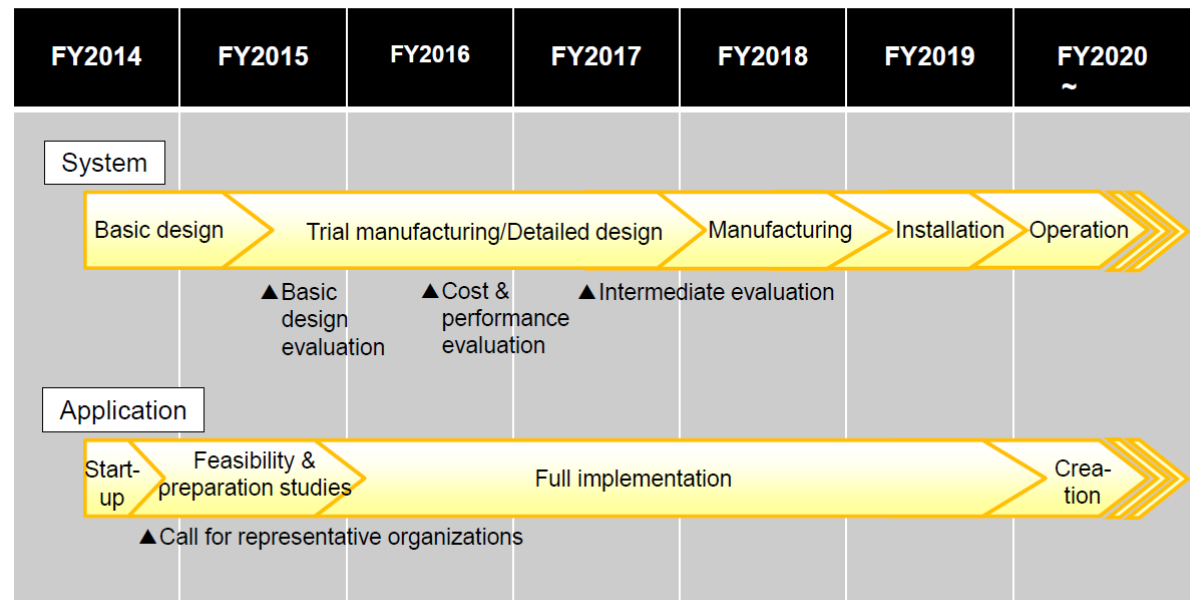
- Development of Tire Material using Large-scale Coarse-grained MD on the K computer (hp120032)



Future Plan

- Flagship 2020 Project (development of post “K computer”) is being proceeded by MEXT, aiming at realization of an exa-scale supercomputer by FY 2020.
- Nine major subjects, which are socially and scientifically important and to be focused in the Flagship 2020 Project, have been identified and each representative organization has been selected by MEXT in 2014.
- Feasibility and preparation studies on the major subjects have started. Some amount of computational resource of “K” will be allocated to them from the latter half of FY2015.

Development Schedule of Flagship 2020 Project



Conclusion

- User selection
- User support
- Industrial use support
- Publication management
- Research highlights
- Future plan



Thank you very much for your attention!

<http://www.hpci-office.jp/folders/english>

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