Overview of RIKEN AICS and International Collaborations in 2015/2016

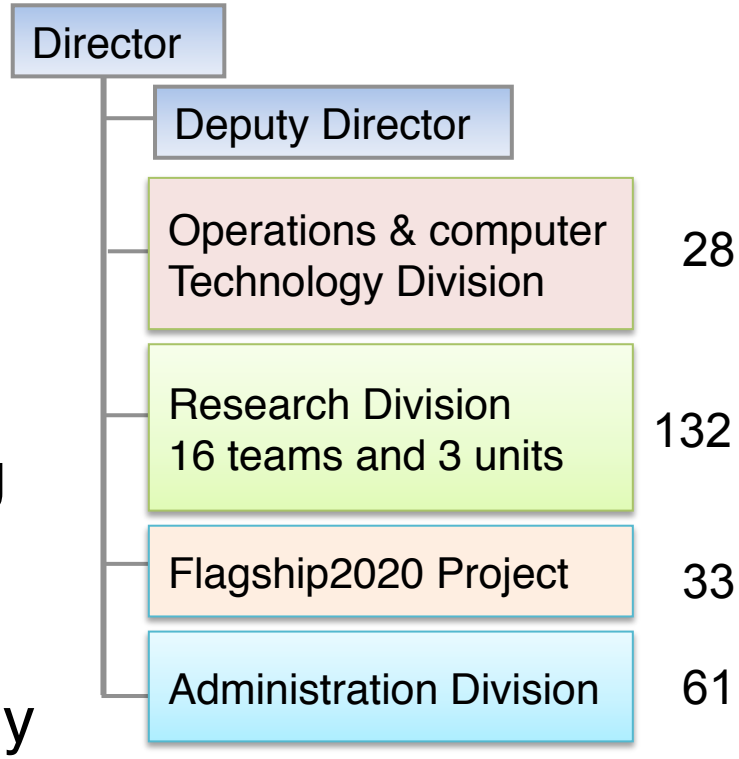
Akira Ukawa
Deputy Director, RIKEN AICS

京
K computer

RIKEN AICS

Foundation and missions

- Foundation : July 2010
- 3 Missions :
  - Operation of K computer for research including industry applications
  - Leading edge research through strong collaborations between computer and computational scientists
  - Development of Japan‘s future strategy for computational science, including development of the post K computer
- #Personnel : 258 (1 Feb. 2016)

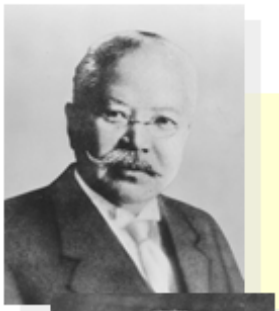


RIKEN　理化学研究所

RIKEN at a glance

- National institute for basic research in Japan covering physical to biological sciences
- Foundation in 1917
- 3,000 researchers, 400 administrators
- 14 centers in 9 sites across Japan including AICS in Kobe
- 10 joint laboratories abroad
- Annual budget: 83 billion JY (690M$)

History of RIKEN



TAKAMINE Jokichi

SHIBUSAWA Eiichi

OKOCHI Masatoshi

SUZUKI Umetaro

1917– RIKEN private foundation

RIKEN Konzern (Industrial Group)
In 1939, 63 companies and 121 plants

NISHINA Yoshio

YUKAWA Hideki

1948– Scientific Research Institute Ltd. (KAKEN)

TOMONAGA Shinichiro

1958– RIKEN public corporation

1967 moved to Wako

NOYORI Ryoji

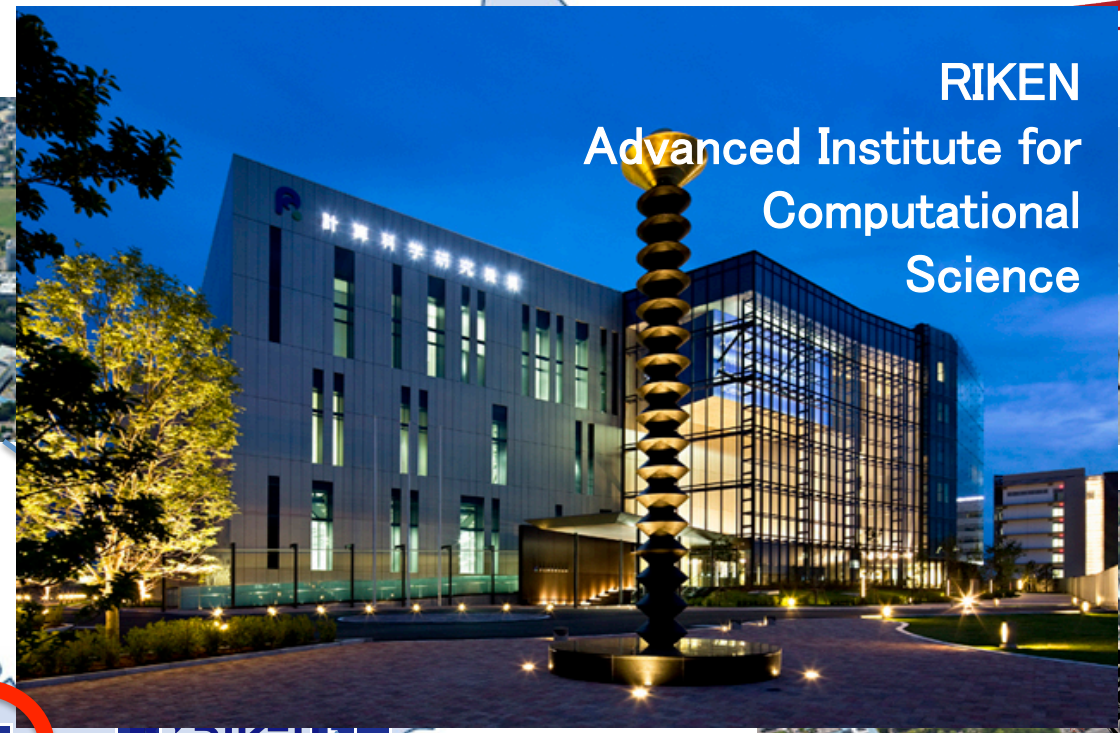
2003– RIKEN Independent Administrative Institution

MATSUMOTO Hiroshi

2015- RIKEN National Research& Developmen Institution

RIKEN sites

- A Sendai
- B Tsukuba
- C Wako
- D Tokyo
- E Yokohama
- F Nagoya
- G Osaka
- H Kobe
- I Harima

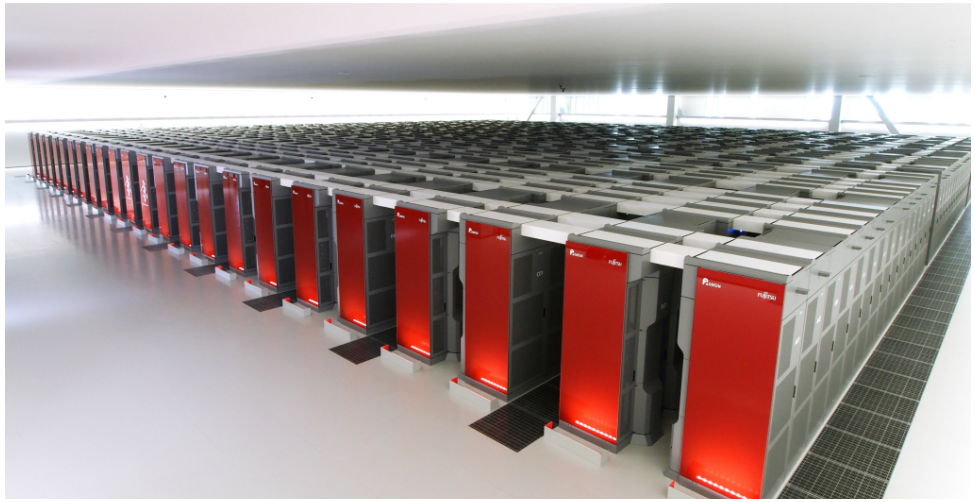


Operating the K computer

K computer

- Specifications
  - 11.28PFlops with 88,128 nodes
  - 1.27PB(16GB/node) memory
  - 6 dim mesh-torus network (5GB/s x 2)
  - 30PB disk
- Top 500 rankings
  - No. 1 in Jun. & Nov. 2011
  - No. 4 in Jun. 2013 - Nov. 2015
- Graph 500 rankings
  - No. 1 in Jun. 2014
  - No. 2 in Nov. 2014
  - No. 1 in Jun. 2015 – Nov. 2015
- HPCG rankings
  - No. 2 in Nov. 2014 – Nov. 2015

versatile performance for a wide spectrum of computing needs



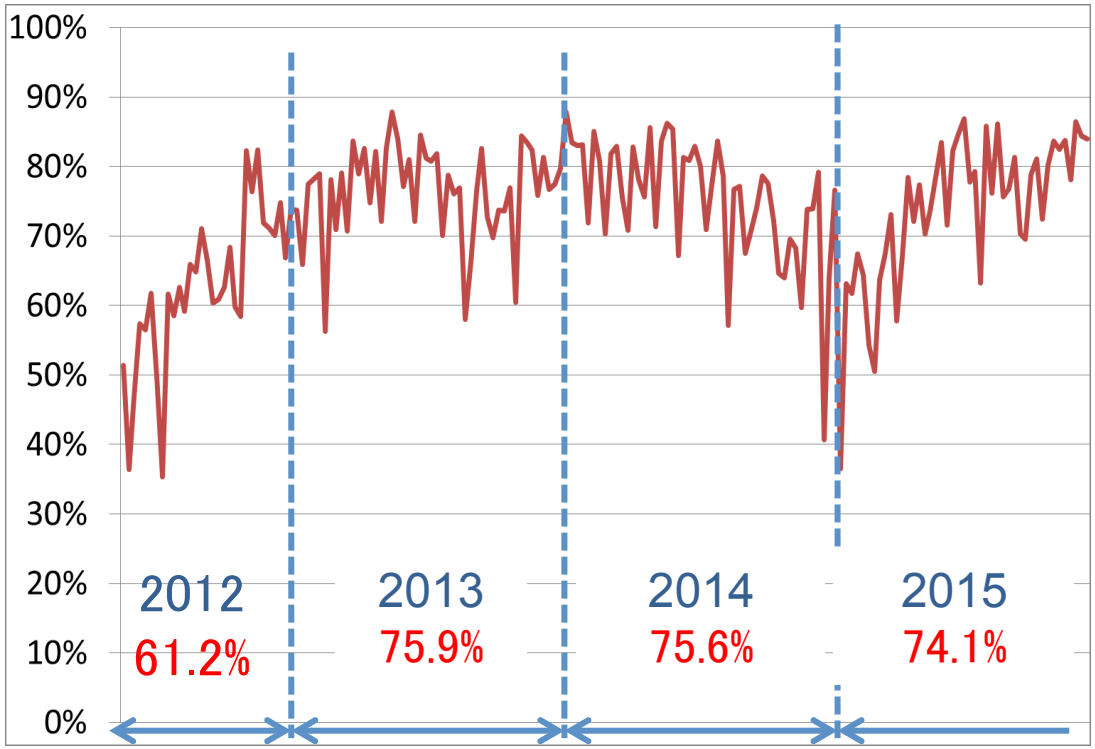
Real application performance on K

Name	Area	# of nodes	Performance
NICAM	Global climate	81,920	1.05PF (10%)
Seism3D	Earthquake	82,944	2.02PF (19%)
PHASE	Material	82,944	2.12PF (20%)
RSDFT	Material	82,944	5.84PF (55%)
FrontFlow/Blue	Flow analysis	82,944	0.64PF (6%)
LatticeQCD	Particle physics	82,944	1.59PF (15%)

Operation of K computer

Weekly node utilization rate

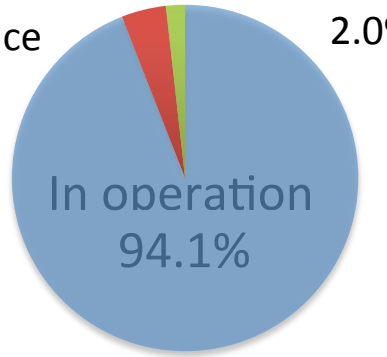
kept around 70-80%



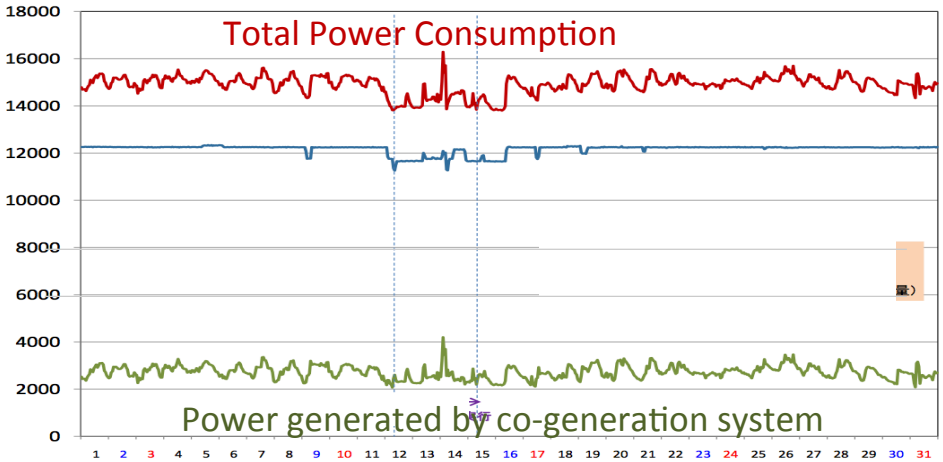
Extraordinary level of stability

scheduled maintenance 3.9%

Unscheduled down 2.0%=7.3 days/year



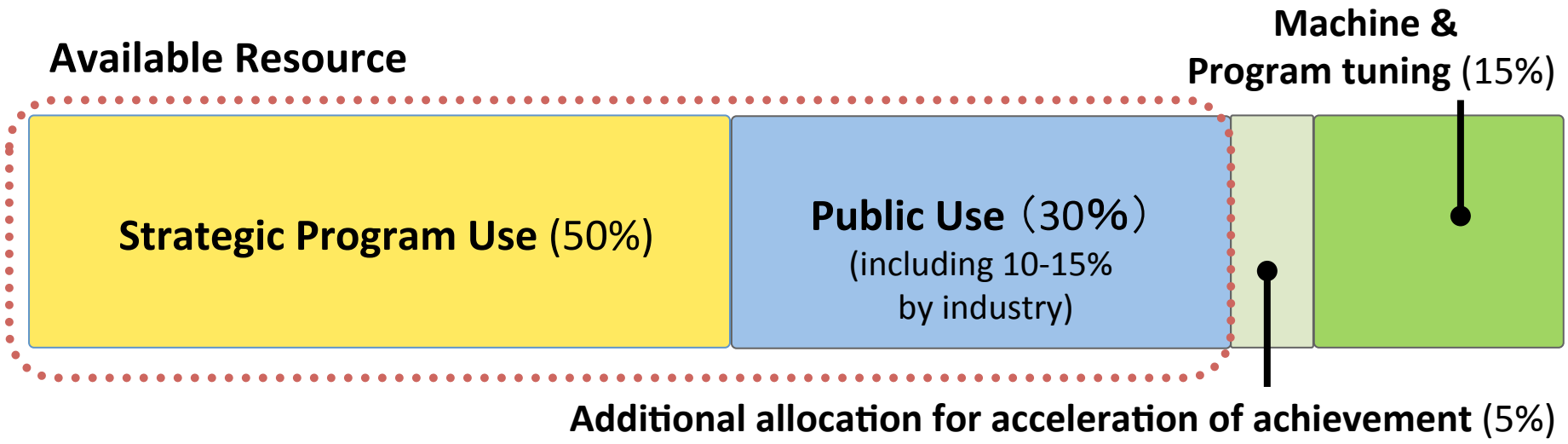
Electricity Consumption for one month



Who has been using the K computer?

- **Strategic Program Use (JFY2012～JFY2015)**
  priority use by the five SPIRE areas

- **Public Use**
  - Annual call for proposals
  - Joint application for K and other resource of HPCI
  - Selection by peer review
  - Special allocation for junior researchers and industrial use

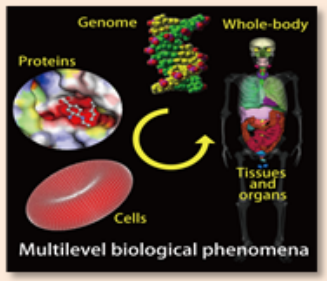


Strategic Program for Innovative Research (SPIRE JFY2011～2015)

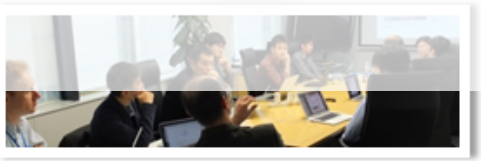
- 5-year national program for promoting computational science

Life Science / Drug Manufacture

RIKEN

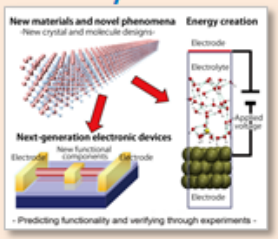


RIKEN AICS



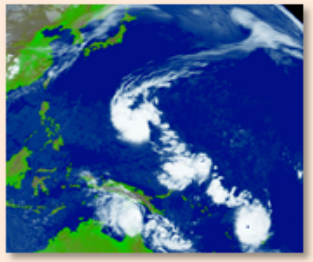
New Materials and Energy Creation

University of Tokyo
National Institute of Natural Sciences,
Tohoku University



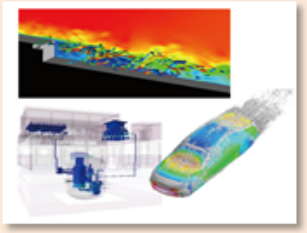
Global Change Prediction for Disaster Prevention/Reduction

Japan Agency for Marine-Earth Science and Technology (JAMSTEC)



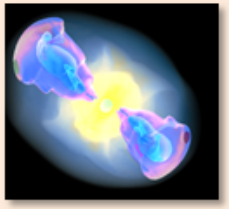
Monozukuri (Industrial Innovation)

The University of Tokyo,
Japan Atomic Energy Agency (JAEA),
Japan Aerospace Exploration Agency (JAXA)



The Origin of Matter and the Universe

University of Tsukuba, High Energy Accelerator Research Organization
National Astronomical Observatory of Japan

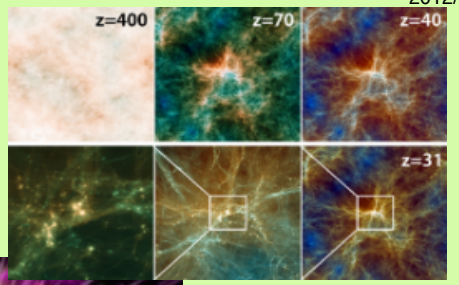


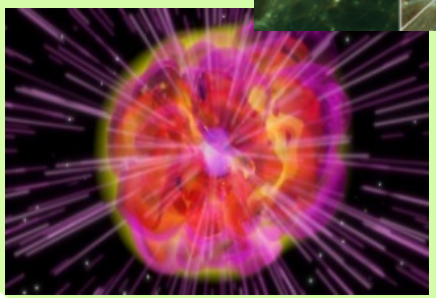
Some recent results from the K computer

Fundamental science

2012/11/17

Dark matter with $2x10^{12}$ particles Gordon Bell 2012

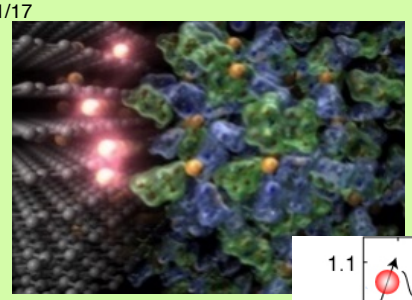




Supernova explosion through neutrino heating

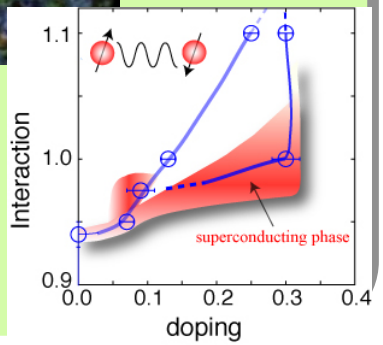
Materials& Energy

2014/03/30
2014/03/27



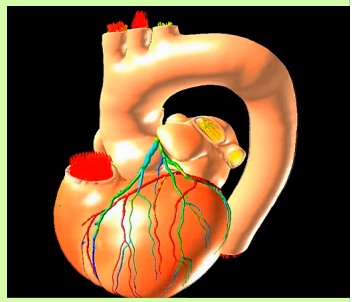
Fast Charging mechanism of Lithium Ion battery

Charge-fluctuation origin of iron-based superconductors



Life sciences

Artificial heart and blood flow



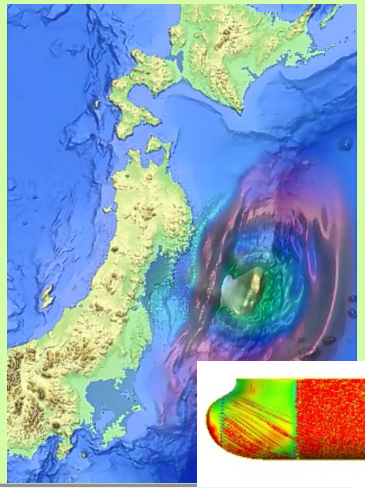
High thruput docking simulation for drug design

Neuronal simulation with 10^13 neurons

Disaster prevention

2013/10/18

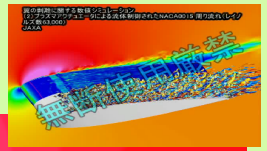
Cloud resolving NICAM runwith less than 1km mesh

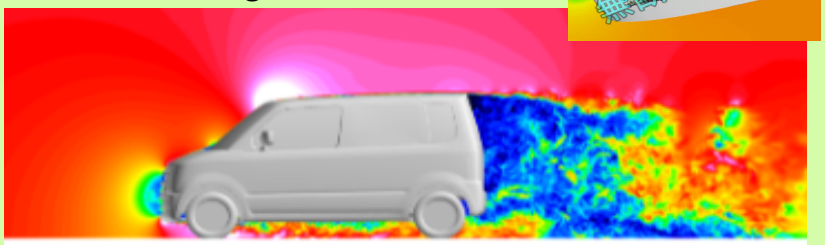


Coupled earth quake-plate dynamics-tsunami simulation

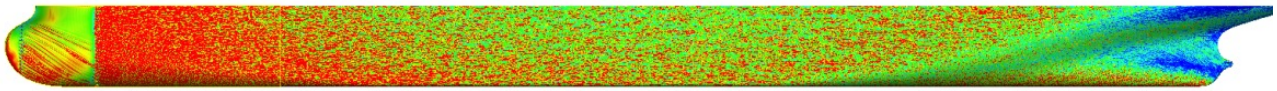
Engineering

Large-scale aerodynamics simulation for accelerated vehicle design





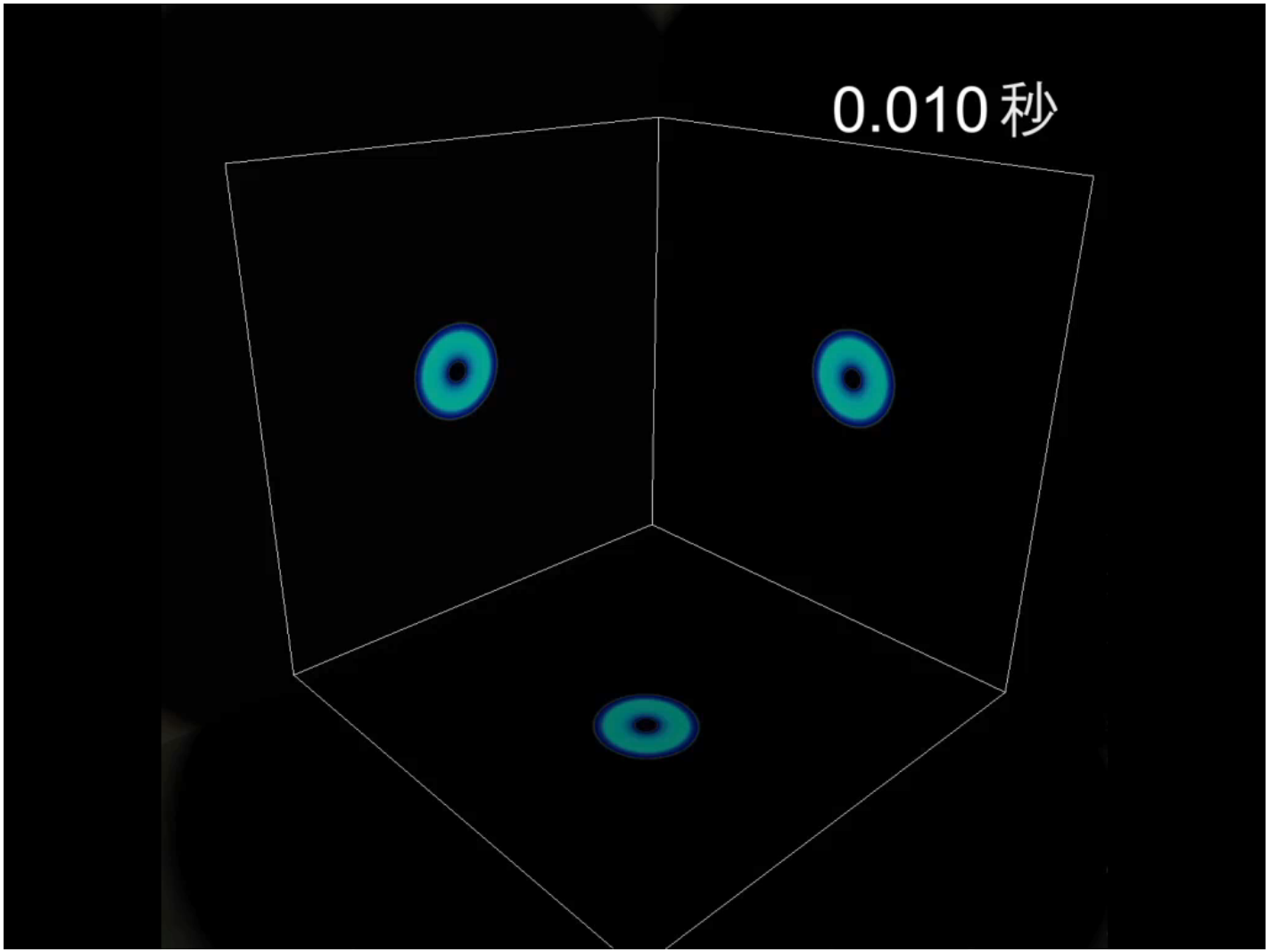
Fluid flow simulation accelerates design of transport vehicles



Simulation of supernova

Tomoya Takiwaki
RIKEN Nishina Center

Fully 3d calculation leads to a successful explosion with energy supplied by neutrino transport



Multiscale modelling of chromatin and nucleosomes

Released 12 Feburary 2016

SPIRE Field 1: Computational Life Science
Hidetoshi Kono （JAEA）
Mitsunori Ikeguchi （Yokohama City Univ.）
Shoji Takada （Kyoto Univ.）

Generated with SCUBA and CafeMol

http://www.scls.riken.jp/en/research/01_dynamics/

Industrial Usage

Significant increase due to the appearance of K

- Supercomputers provide essential infrastructure for enhancing the international competitiveness of industry.
- **Trial use** (50k node*hours/application accepted all year round) and **system for non-disclosed achievements** (fee-based) have been introduced to promote the industrial usage in addition to he public use.
- Even outside the industrial use framework, there are many corporate users. If these are included, ca. 30% of all users are from industry. The number of participating companies exceeds 100.

Incentives to promote the industrial usage

- Expansion of framework for industrial use (5% → 8% → 10%)
- Introduction of an “anytime” application system for industrial use only
- Introduction of a system for priority use → enables use with no waiting time

Research at RIKEN AICS

AICS Research Teams

Computational Science Research Teams

Provide a shared infrastructure to support a wide range of fields in making sophisticated use of the K computer, by developing methodologies required by computational science.

- Particle Physics (Y. Kuramashi)
- Astrophysics (J. Makino)
- Solid State Physics (S. Yunoki)
- Quantum Chemistry (T. Nakajima)
- Computational Chemistry (K. Hirao)
- Biophysics (Y. Sugita)
- Drug Design (F. Tama)
- Earth Science (M. Hori)
- Climate Science (H. Tomita)
- Engineering (M. Tsubokura)
- Discrete Event Simulation (N. Ito)

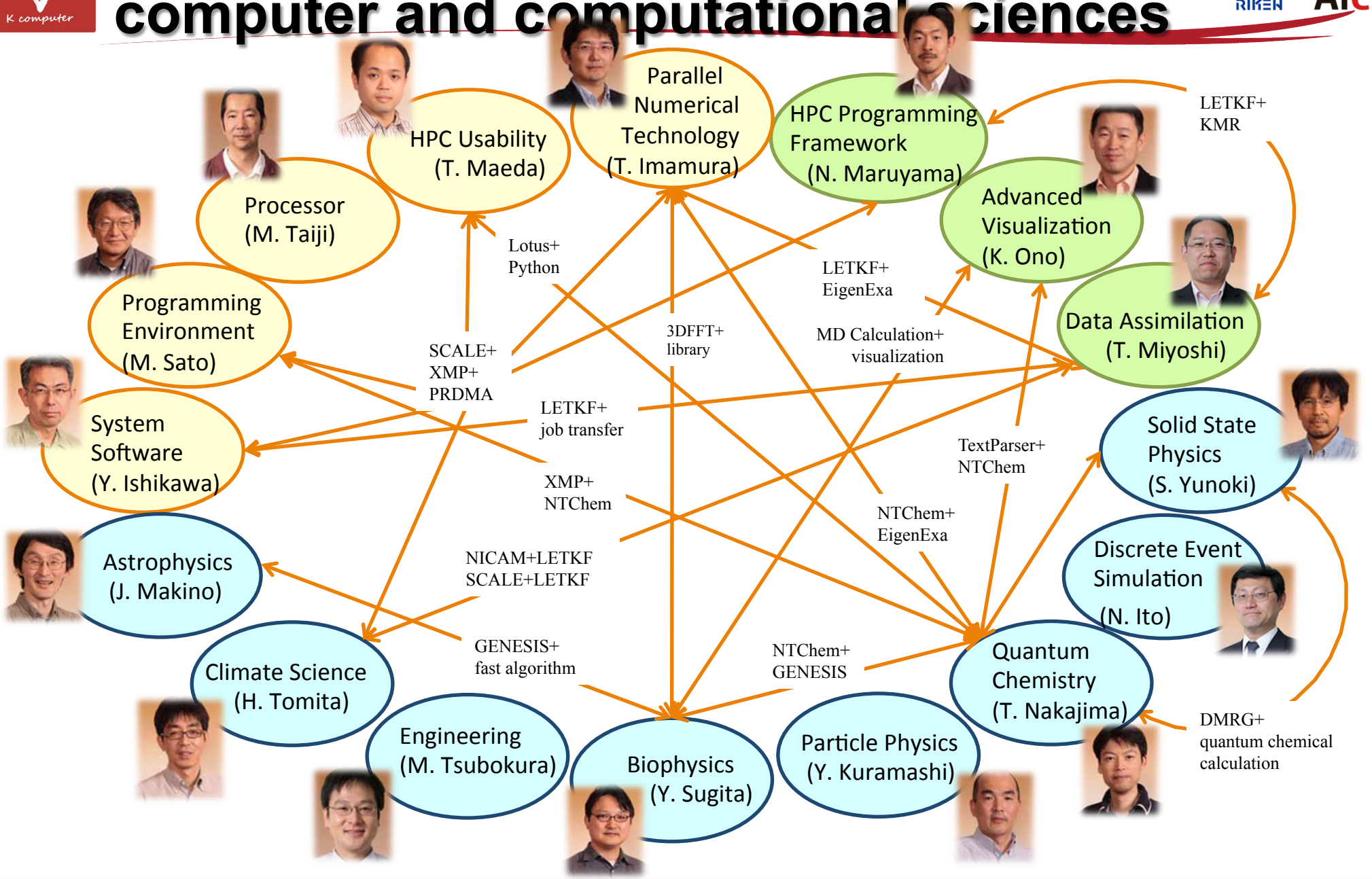
Computer Science Research Teams

Solve issues surrounding the K computer through research in major elemental computer technologies

- Processor (M. Taiji)
- System Software (Y. Ishikawa)
- Programming Environment (M. Sato)
- Large-scale Parallel Numerical Computing Technology (T. Imamura)
- HPC Usability (T. Maeda)
- HPC Programming Framework (N. Maruyama)
- Advanced Visualization (K. Ono)
- Data Assimilation (T. Miyoshi)

Promoting strong collaborations between computer scientists and computational scientists

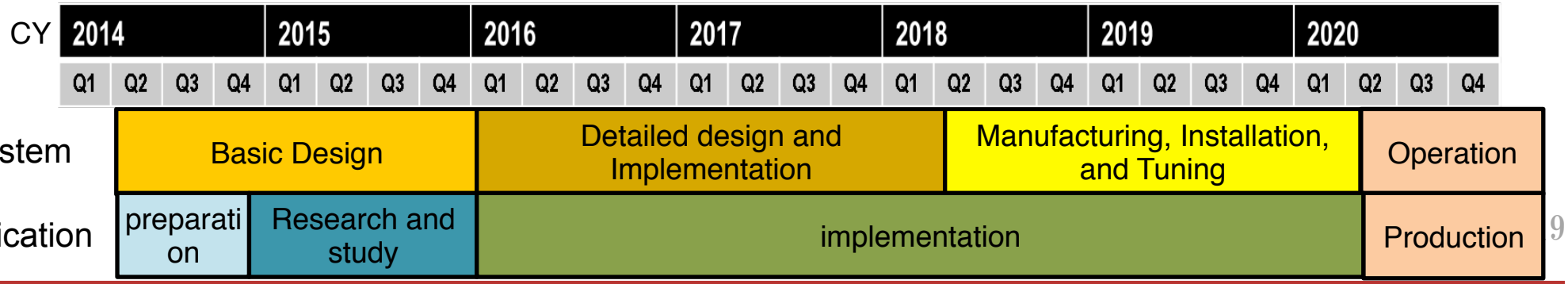
Working across computer and computational sciences



Flagship2020 Project

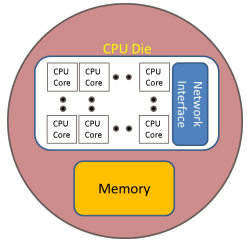
Flagship 2020 Project

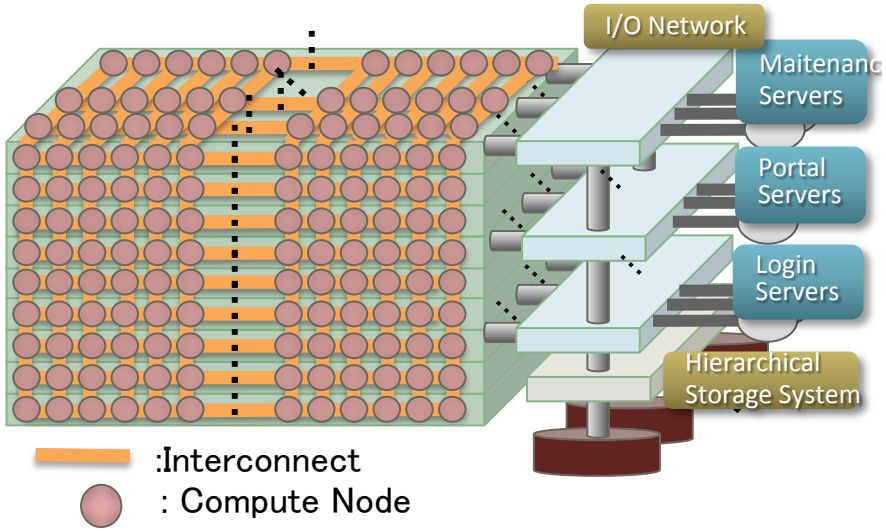
- Dual mission
  - Develop the next Japanese flagship computer, tentatively called *post K*
  - Simultaneously develop a range of application codes, to run on post K, to help solve major societal and science issues
- Budget
  - 110 billion JPY (about 0.91 billion US$ if 1$=120JY)
  - includes:
    - research and development, and acquisition of the post K system
    - Development of applications



Post K computer development

- Fujitsu Ltd. selected as vendor partner through procurement
- Just finished the basic design
  - Many-core CPU
  - Tofu interconnect (6d mesh/torus)
  - Layered storage and I/O
- “co-design” to maximize performance for applications important for solving major social and scientific problems





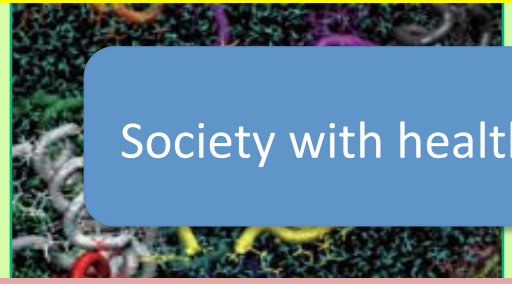
Priority Issues Program

- MEXT selected *9 Priority Issues and 4 Exploratory Issues* based on discussions at a committee of academia and industry members.
- MEXT also selected, through an open call, the research groups/institutions responsible for tackling each issue
- They receive
  - Funding for research, including program development
  - Priority allocation of post K computing time
- Program duration
  - Development phase: 2014～2019
  - Production phase: 2020～

9 Priority Issues

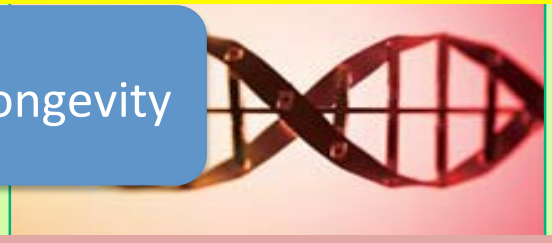
Society with health and longevity

①Innovative Drug Discovery



RIKEN Quant. Biology Center

②Personalized and Preventive Medicine



Inst. Medical Science, U. Tokyo

Disaster prevention and global climate

③Hazard and Disaster induced by Earthquake and Tsunami

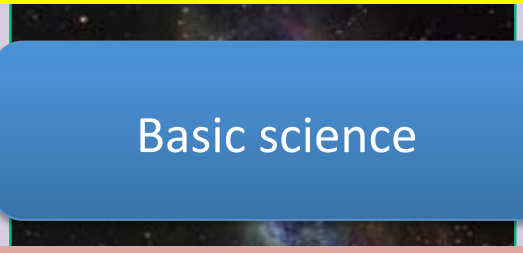
Industrial competitiveness

⑧ Innovative Design and Production Processes for the Manufacturing Industry in the Near Future

C

Basic science

⑨Fundamental Laws and Evolution of the Universe



Cent. for Comp. Science, U. Tsukuba

④Environmental Predictions with Observational Big Data

Center for Earth Info., JAMSTEC

Energy issues

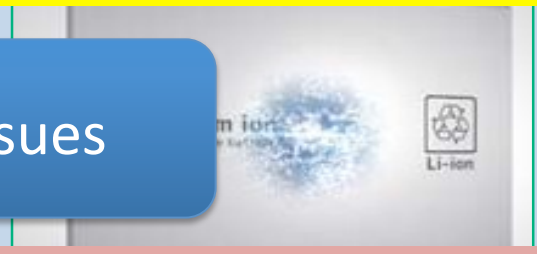
⑦New Functional Devices and High-Performance

Inst. For Solid State Phys., U. Tokyo

⑥Innovative Clean Energy Systems

Grad. Sch. Engineering, U. Tokyo

⑤High-Efficiency Energy Creation, Conversion/Storage and Use



Inst. Molecular Science, NINS

Exploratory Issues

Interactive Models of Socio-Economic Phenomena and their Applications

Frontiers of Basic Science - challenge to extremes -

Formation of exo-planets (second Earth) and Environmental Changes of Solar Planets

Mechanisms of Neural Circuits for Human Thoughts and Artificial Intelligence

Call for proposals expected soon

International Collaborations

"essential to work beyond borders and barriers"

International partnership

AICS serves as a core center for international brain circulation promoting international cooperation

Ongoing partnership

The Joint-Laboratory for Extreme-Scale Computing (JLESC)	USA Europe
Argonne Leadership Computing Facility	USA
National Center for Supercomputing Applications(NCSA)	
University of Maryland	
Jurich Supercomputing Center	Germany
National Computational Infrastructure	Australia
Maison de la Simulation (MDLS), Centra National de la Recherche Scientifique (CNRS)	France
The Scuola Internationale Superiore Di Studi Avanzati (SISSA)	Italia

MOU was signed between Argonne and AICS in SC13, Denver, US

Japan MEXT and US DOE have signed MOU in 2014 in support of computer science and software related to current and future HPC for open scientific research. AICS leads the Japanese teams as the facilitator.

3 themes at this Symposium

- Toward next generation systems development
  - Japan-US DOE-MEXT Collaboration for HPC System Software
- Working through network of leading HPC centers
  - Collaboration between AICS and Francs
  - Collaboration in JLESC
  - Collaboration between AICS and Julich
  - Collaboration in Operation and Management of large systems
- Toward global collaboration in computational science