Computer simulations create the future

NEXT Numerical Experiment Tokamak Kyoto Terrsa March 10, 2016

Great Opportunity and Great Challenge in Advanced Computing

KIMIHIKO HIRAO

Advanced Institute for Computational Science (AICS)

RIKEN

K computer

Science in the 21st Century

The Role of Science in the 21st Century

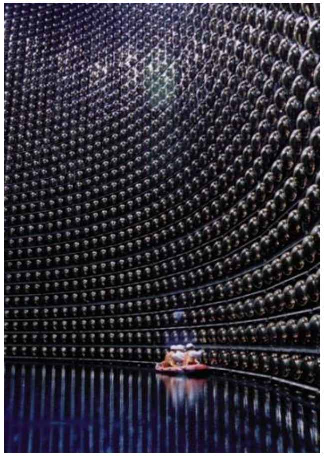
- The role of scientific research in solving the problems we face is more relevant and feasible than ever in the 21st century.

- The world is dramatically being reshaped by scientific and technological innovations, global interdependence, cross-cultural encounters, and changes in the balance of economic and political power.

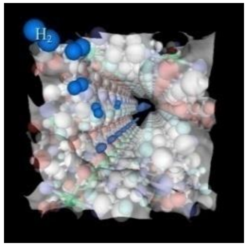
- Humanity's most urgent priority is to bring people out of poverty.

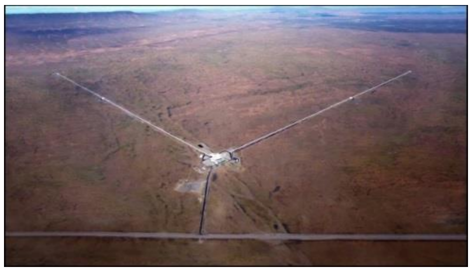
- Science and technology must contribute to protecting the basic right to exist of all peoples.

Technology-driven Science







Recent years have seen remarkable and rapid advances in the technological tools.

Powerful scientific instruments continually advance knowledge and open up new field of science. For example, high-energy particle accelerators, such as the Large Hadron Collider discovered the Higgs boson in 2013, powerful astronomy instruments such as

Supercomputers will undoubtedly accelerate this trend

ecology.

Very recently NSF's LIGO (Lase Interferometer Gravitational-Wave Observatory) has detected gravitational wave 100 years after Einstein's prediction.

Supercomputer is a key technology

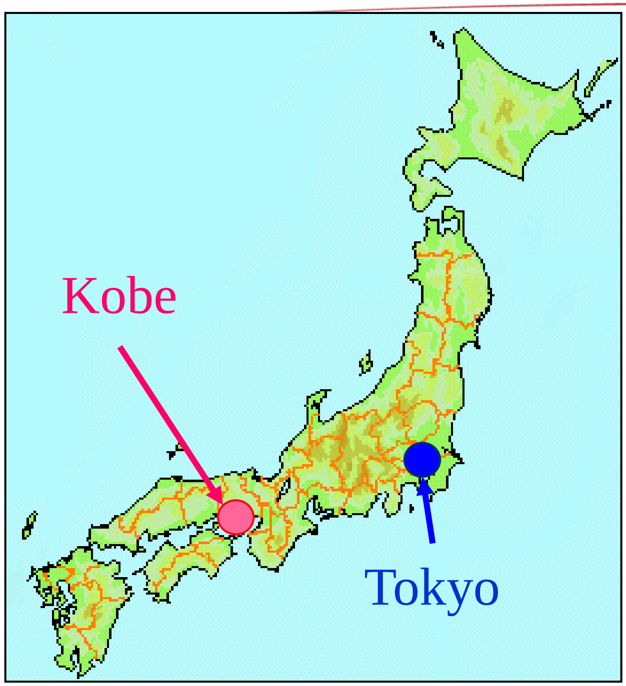
- Supercomputer is applicable to all areas of science and engineering unlike other tools, which are limited to particular scientific domains.

- Supercomputer has been increasingly recognized as a key technology for accelerating major scientific discovery and engineering breakthroughs, fostering economic competitiveness and improving society.

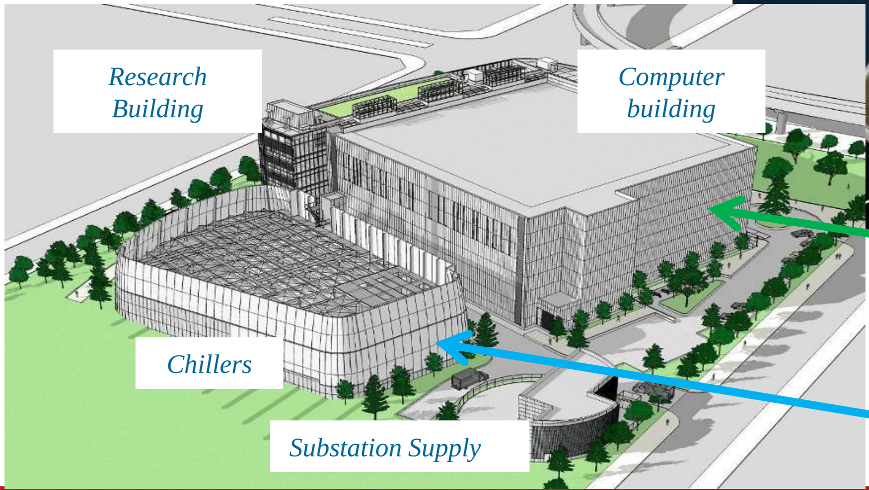
- Simulations performed on the supercomputer will drive progress in science and technology and play an important role in solving difficult problems that we face as a society. There are very **critical issues** that need to be solved
  - *global warming, alternative energy, disaster mitigation, medicine & public health, security, etc.*

Overview of AICS and K Computer

Site of the K Computer & AICS



423 km (263 miles)west of Tokyo



Computer room 50mx60m=3,000m^2
Electric power up to 15MW
Water cooling system

Gas-turbine co-generation 5MW*2

Advanced Institute for Computational Science (AICS)

Established in July 2010. AICS is the Japanese flagship research institution in computational science and computer science

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 the path to exascale computing

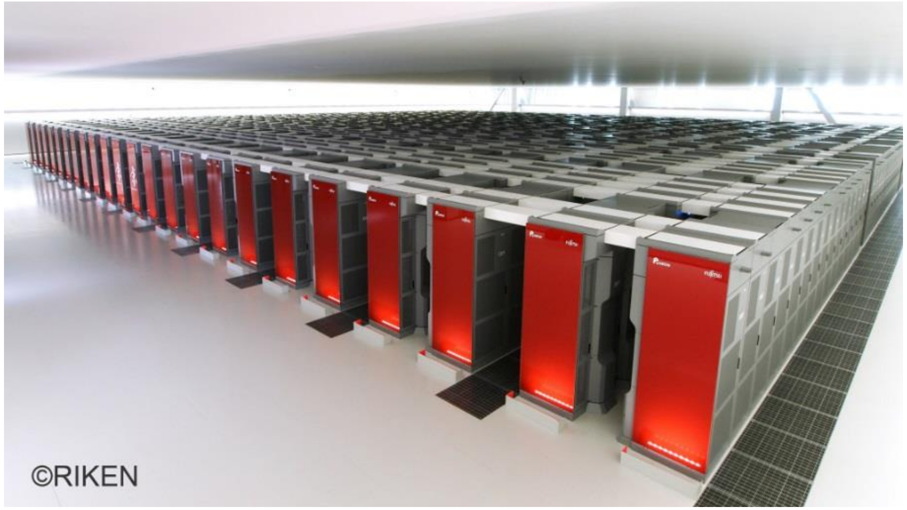
#Personnel: 259 (Feb 2016)

- **Director**
  - **Deputy Director**
  - **Operations & Computer Technologies Division**
  - **Research Division**
    16 teams and 3 units
  - **Exascale Computing Project**
  - **Administrative Division**

K computer

Specifications

- General-purpose supercomputer
- Peak performance is 11.28 Petaflops (PF) with 88,128 nodes (# of cores: 705,204)
- 1.27 PB (16GB/node) memory
- Two-level local(11PB)/global(30PB) files
- 6 dim mesh-torus network
- The architecture balances processing speed, memory, and communication



Top 500 ranking

LINPACK measures the speed and efficiency of linear equation calculations

Real applications require more complex computations.

- No.1 in Jun. & Nov. 2011
- No.4 in Jul. 2015

Graph 500 ranking

"Big Data" supercomputer ranking

Measures the ability of data-intensive loads

- No.1 in Jul. & Nov. 2015

New HPCG ranking

measures the speed and efficiency of solving linear equation for large sparse matrix using HPCG

better correlate to actual applications

- No. 2 in Nov. 2015

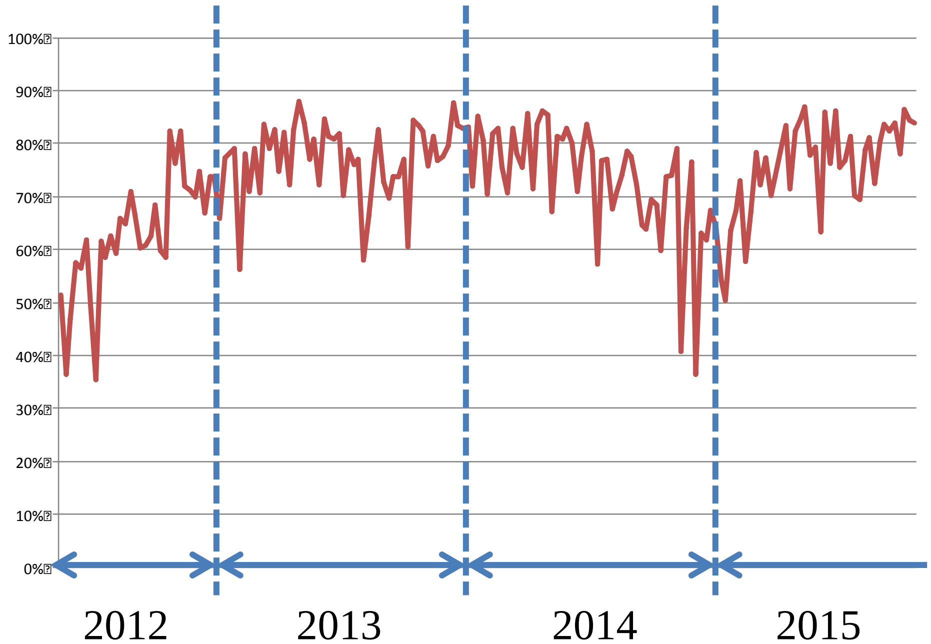
Real application performance on K

Program Name	Area	# of nodes used	Performance
Modylas	Molecular Dynamics	65,536	3.45 PF (41%)
NICAM	Global Climate	81,920	1.05 PF (10%)
Seism3D	Earthquake	82,944	2.02 PF (19%)
GAMERA	Urban Earthquake Simulator	82,944	1.97 PF (19%)
PHASE	Materials	82,944	2.12 PF (20%)
RS-DFT	Physics/Chemistry	82,944	5.84 PF (55%)
NTChem	Chemistry	71,288	2.90 PF (32%)
FrontFlow/Violet	Computer Fluid Dynamics	82,944	1.20 PF (12%)
Lattice QCD	Particle Physics	82,944	1.59 PF (15%)

K is capable of sustained performance of one petaflops on real applications in a wide range of science and engineering.

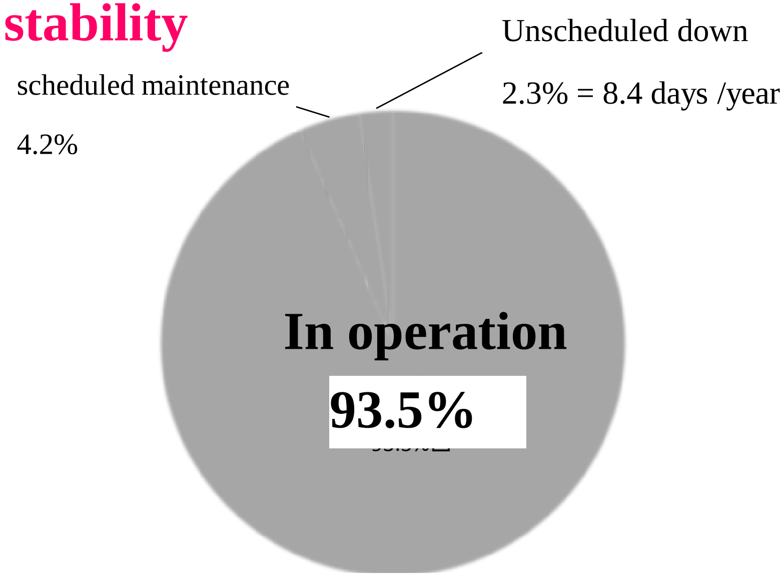
Operation and Use of K computer

weekly node utilization rate

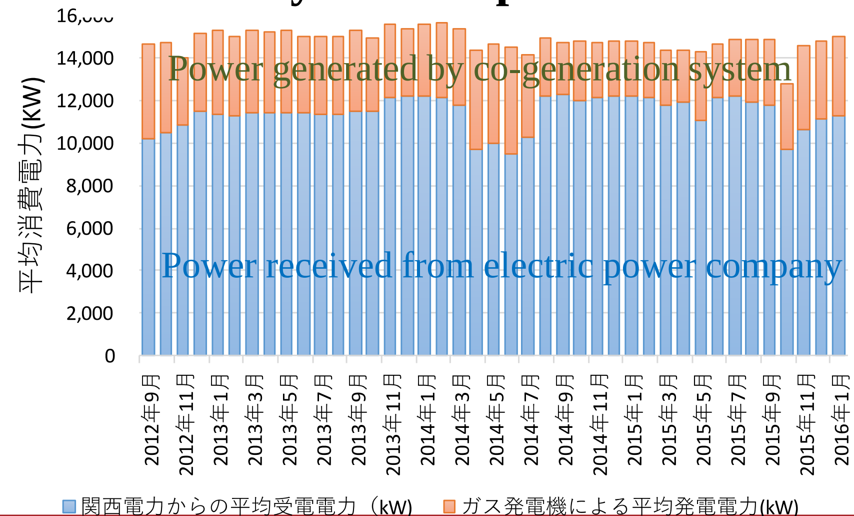


kept around 70-80%

K demonstrates an extraordinary level of stability



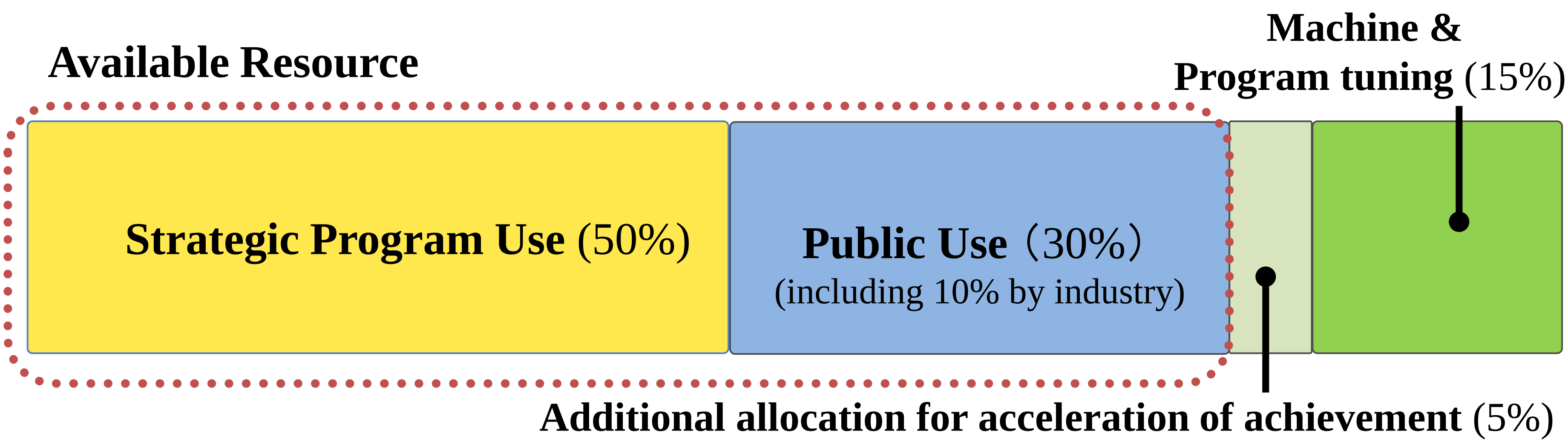
Electricity Consumption for one month



Who Uses the K computer?

- **Strategic Program Use**

  priority use by the five Strategic Application 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



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Strategic Application Areas

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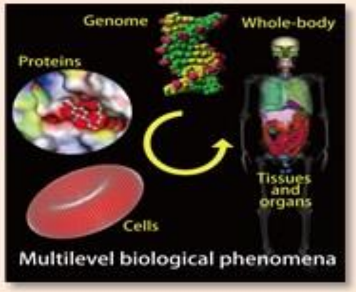
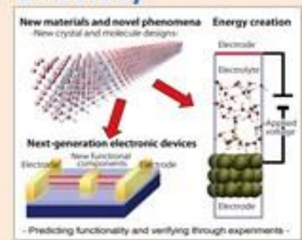
Life Science / Drug Manufacture

RIKEN



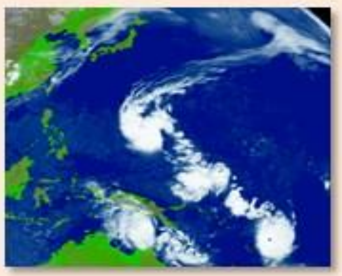
New Materials and Energy Creation

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)

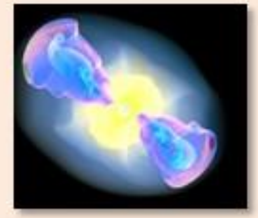


Monozukuri (Industrial Innovation)

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



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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.

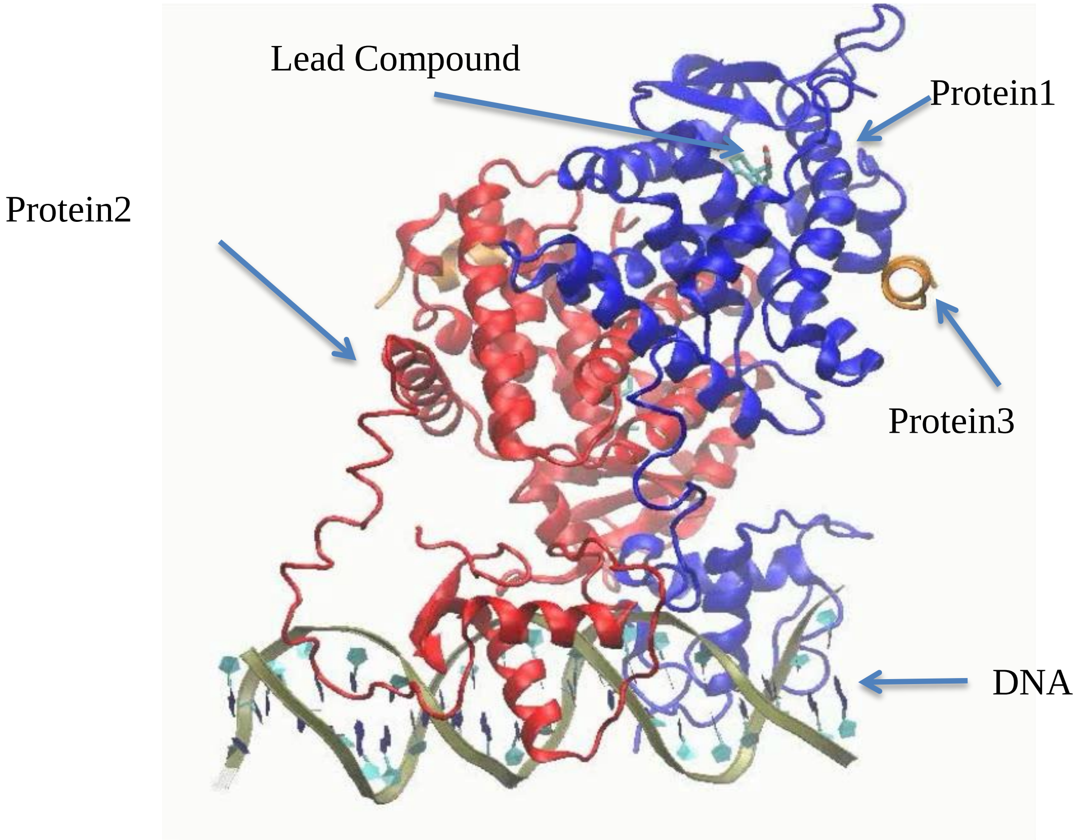
Incentives to promote the industrial usage

- 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

Some Research Highlights on K

Protein Simulation and Drug Design

The rapid advance of computer technology, force-field developments, and simulation methods has made MD simulation more easily and reliably useful in dynamics based drug design.



For the three types of cancer for a target protein more than 10 lead compounds have been identified through MD simulations. Two of them are now under pre-clinical safety evaluation.

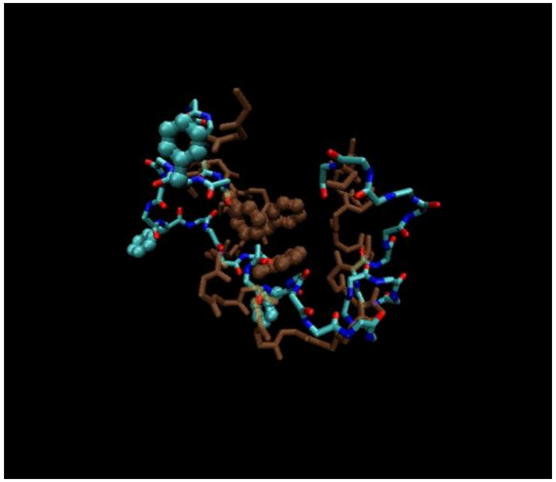
A lead compound in drug discovery is a chemical compound that has pharmacological or biological activity and whose chemical structure is used as a starting point for chemical modifications in order to improve potency, selectivity, or pharmacokinetc parameters.

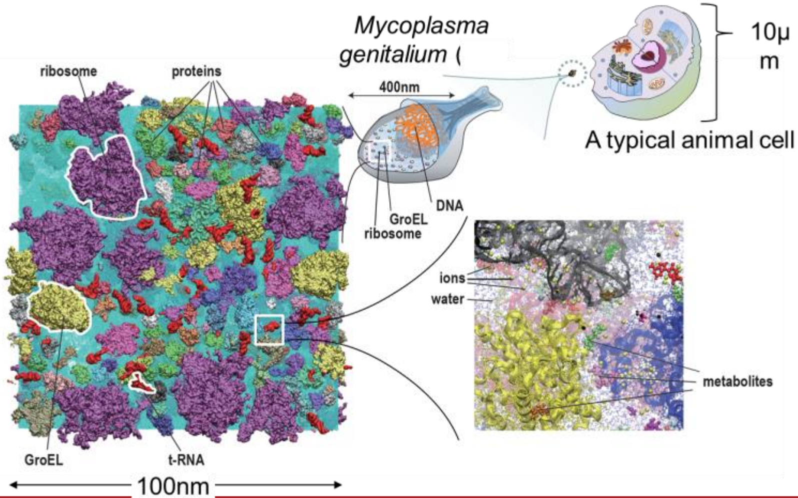
All atom MD simulations of cytoplasm of mycoplasma genitalium with GENESIS

Y Sugita (AICS)

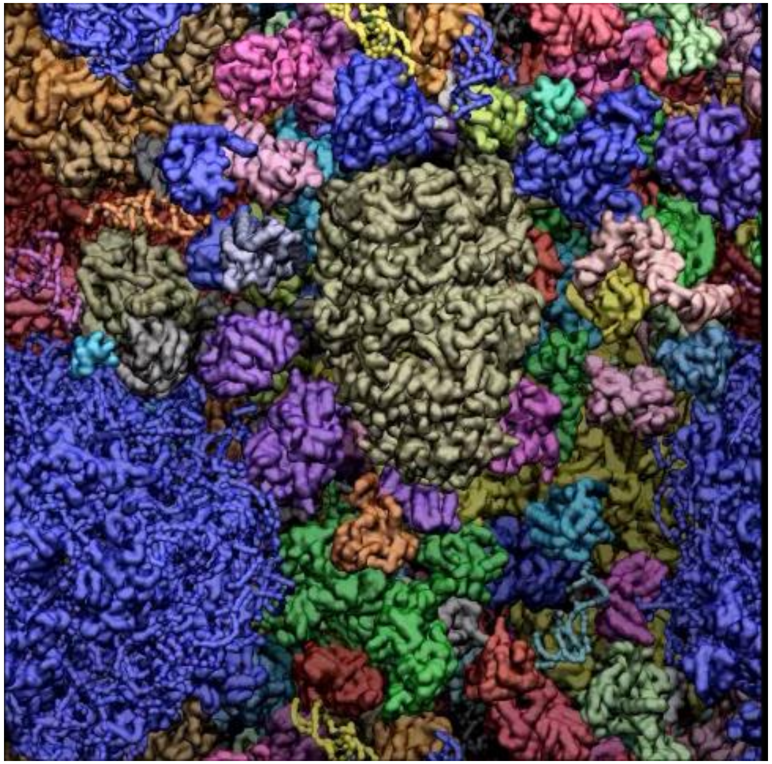
Protein Simulation

Folding of Villin





All atom MD simulations of cytoplasm of mycoplasma

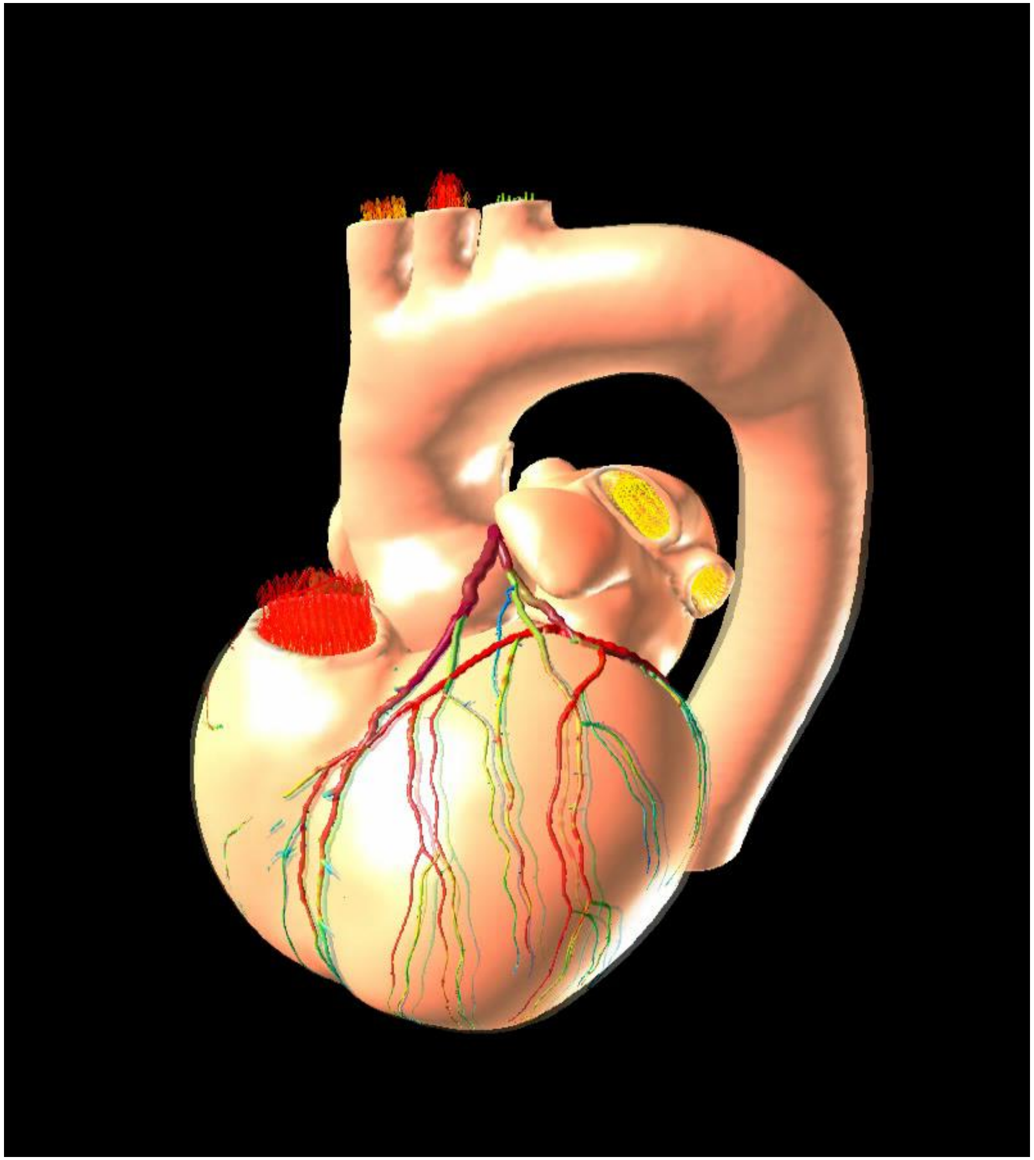


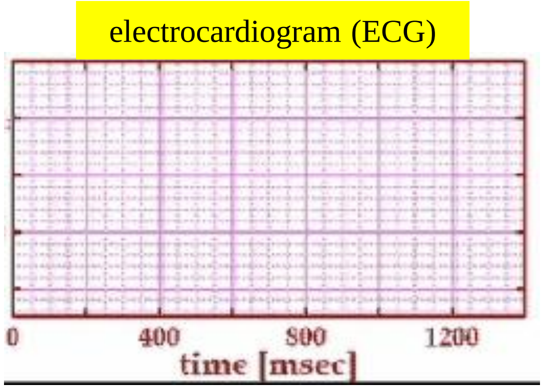
One hundred million atoms

100 ns MD simulation

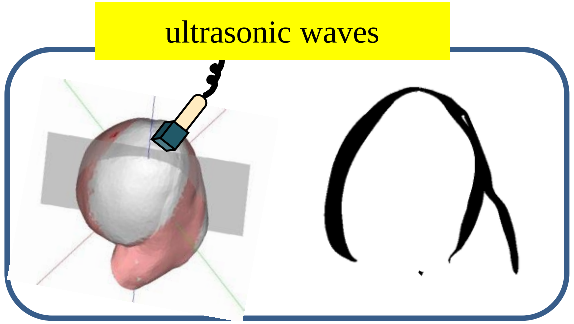
Heart Simulator

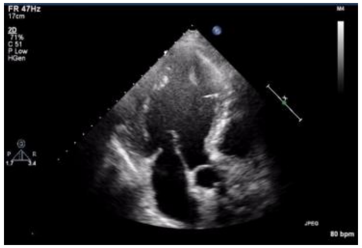
Hisada & Sugiura (UT)





UT Heart is a multi-scale (molecules, cell, tissue, organ) and multi-physics simulator and describes the dynamics of various ion currents and sarcomeric proteins.





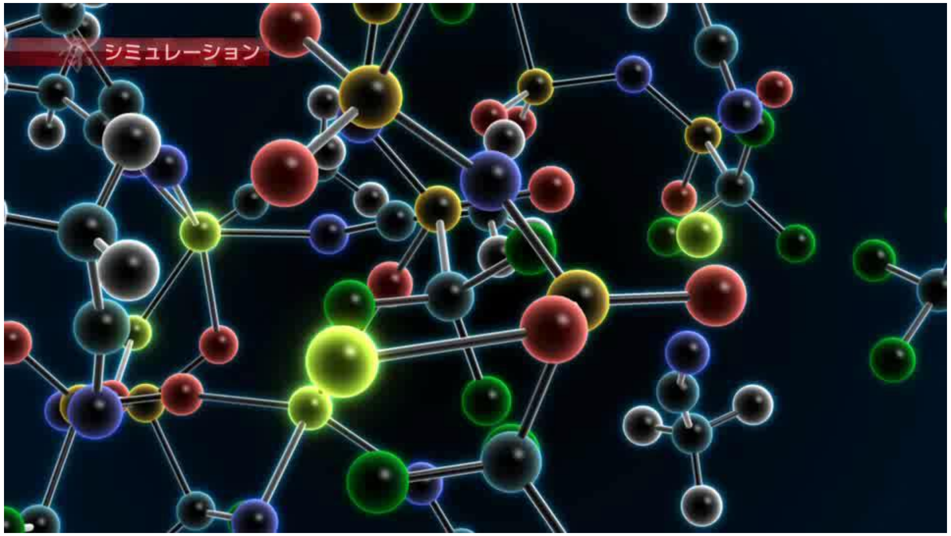
Heartbeat, blood ejection, coronary circulation are simulated consistently, producing the blood pressure, electrocardiogram (ECG) etc, precisely.

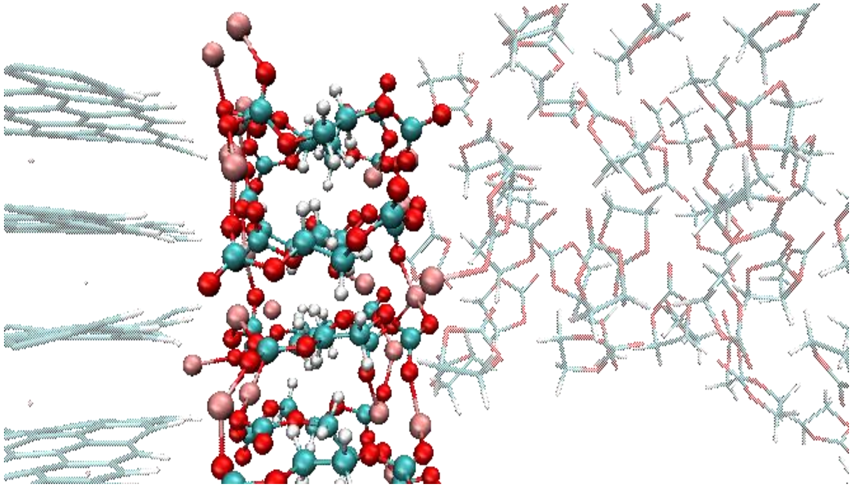
Heart model for each patient can be rebuilt
Applied to congenital heart diseases
Screening for drug-induced irregular heartbeat risk

Super-concentrated electrolyte for Lithium Ion Batteries

- Functional and stable electrolyte is a key for high performance of LIB
- First principle molecular dynamics simulation show that a super-concentrated electrolyte has
  - A fluid polymeric network of anions and Li+ cations, leading to
  - A remarkably fast reaction kinetics (1/3 charging time)
  - A high reductive stability

SEI（Solid Electrolyte Interphase）



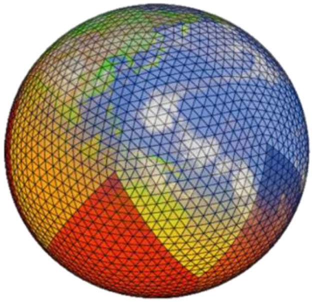


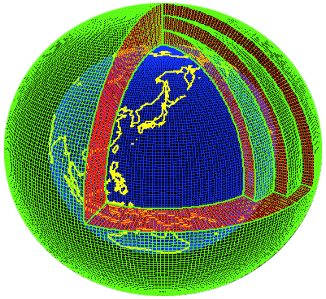
Y. Tateyama (NIMS) et al   J. Amer.Chem.Soc. 2014

Yamada et al (U of Tokyo) J.Amer.Chem.Soc.2014

Global Climate Simulation (Tomita)

Previous NICAM simulations with 3.5 km resolution is quite accurate but not able to resolve individual cumulonimbus clouds. Global cloud resolving model **with 0.87 km-mesh** much closer to the actual process of cumulonimbus development. Month-long forecasts of Madden-Julian oscillations in the tropics is realized.

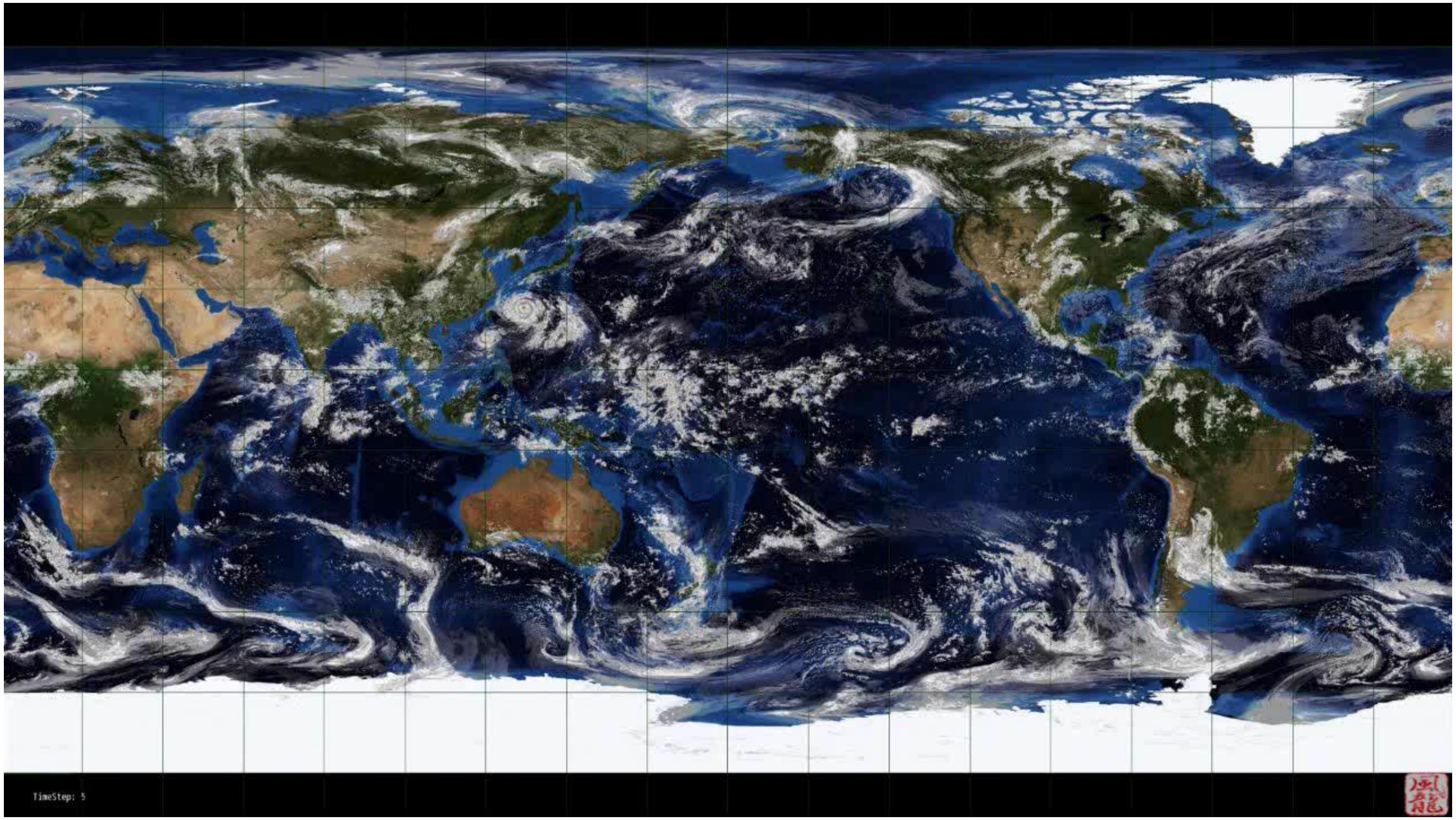




Global cloud resolving model

Weather forecasting and climate prediction are performed using climate models. To run a model, we divide the planet into a 3-dimensional grid, apply the basic equations, and evaluate the results.

Global Cloud Resolving Model with 0.87 km-mesh on K computer



Miyamoto et al (2013) , Geophys. Res. Lett., 40, 4922–4926, doi:10.1002/grl.50944.

3.11 East Japan Earthquake and Tsunami

by Furumura and Maeda (U of Tokyo)

Reproduction of 3.11 East Japan Earthquake

Coupled calculations of earthquake, crustal deformation, and tsunami

Direct comparison with observed records
Planning countermeasures against complex disasters involving multiple elements

#nodes: 2,304
Time: 3 hours

Simulation of Nankai Trough Earthquake and Tsunami

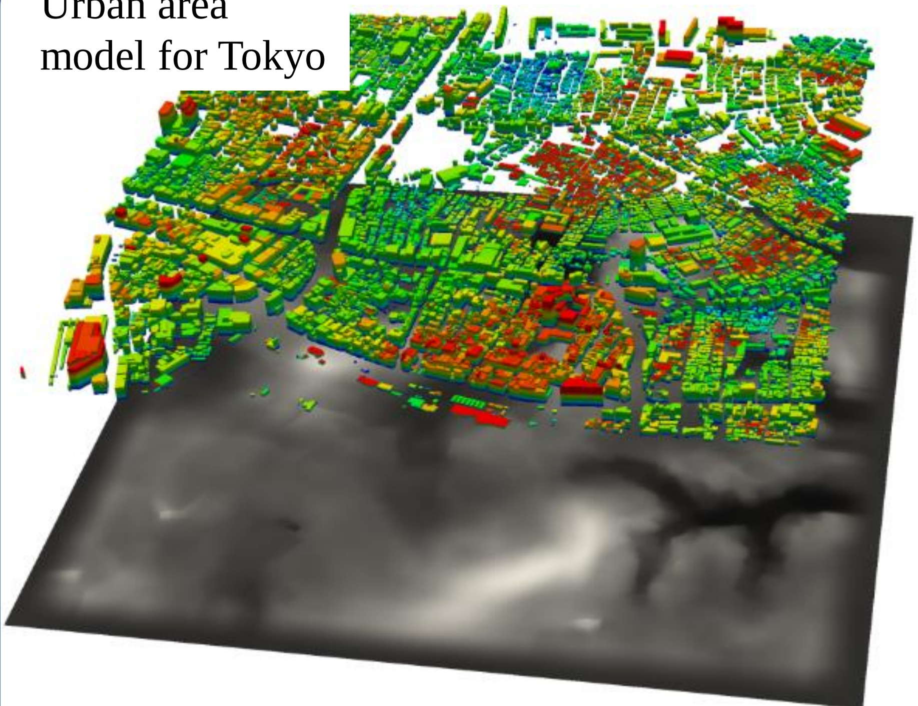
Coupled calculations of earthquake, crustal deformation, and tsunami

Planning countermeasures against complex disasters involving multiple elements

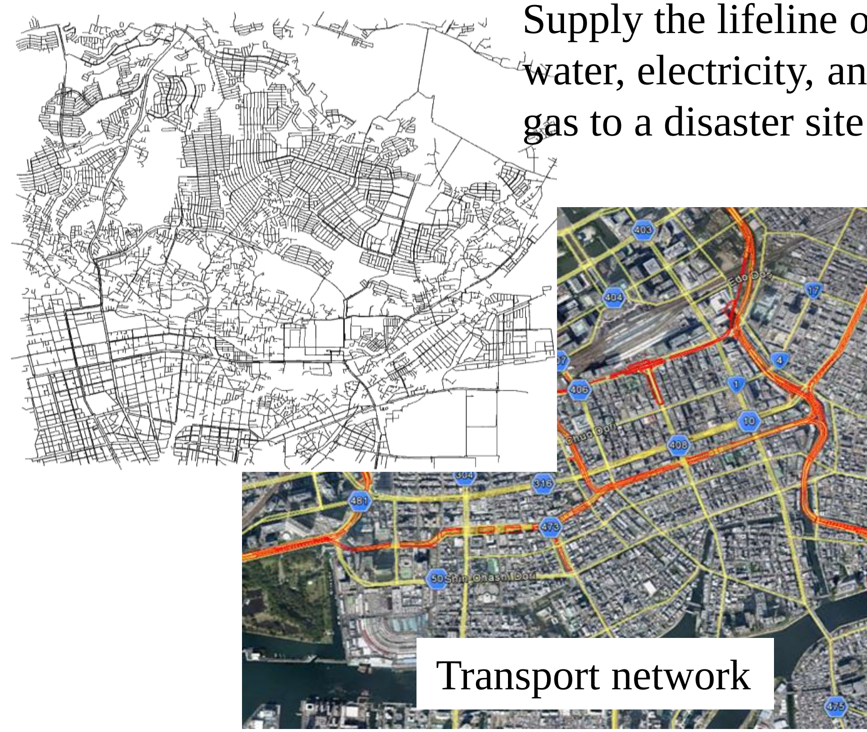
Disaster Mitigation and Reduction

Earthquake that directly hits Tokyo area

- 首都直下地震のさまざまなシナリオを基にした，災害・被害・復旧シミュレーション
- 信頼度に限界がある現行の評価を凌駕する，合理的かつ超精緻な震災評価を提示



Estimating Disaster Damage



Restoration Simulation

「京」の成果を発展させた，ライフライン・交通ネットワークの被害シミュレーション

ポスト「京」で取り組む社会科学シミュレーションを使った復旧シミュレーション

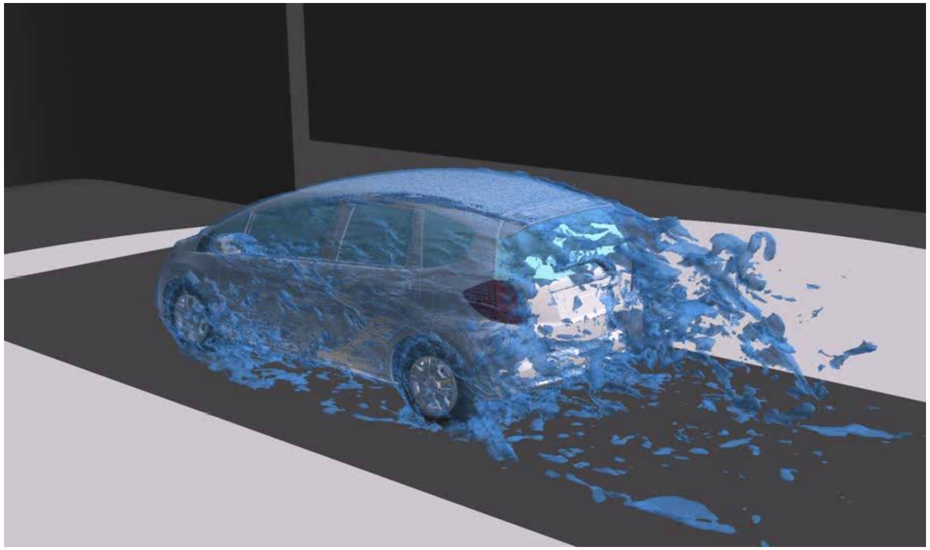
首都直下地震に対し，首都機能を維持する防災減災計画立案に寄与

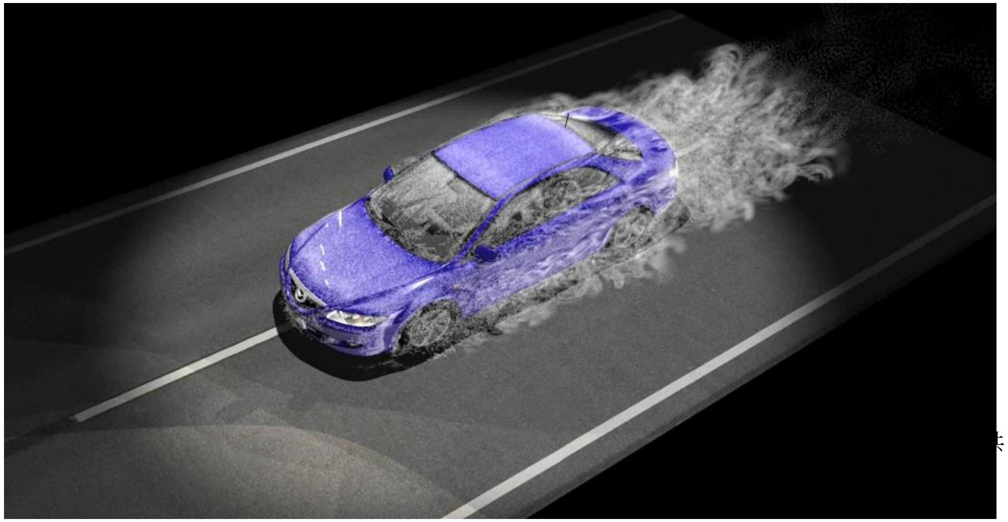
Process Innovation by HPC

Kato (Univ. of Tokyo), Tsubokura (AICS)

So far, CFD has been used as a supplementary tool to wind-tunnel experiment, and has contributed to making the process cheaper and faster. The K can change the process by applying HPC-CFD to the analysis which conventional wind-tunnel measurements cannot treat.

Examples of the next generation aerodynamic simulation





Estimation of high-speed stability during dynamic maneuvering

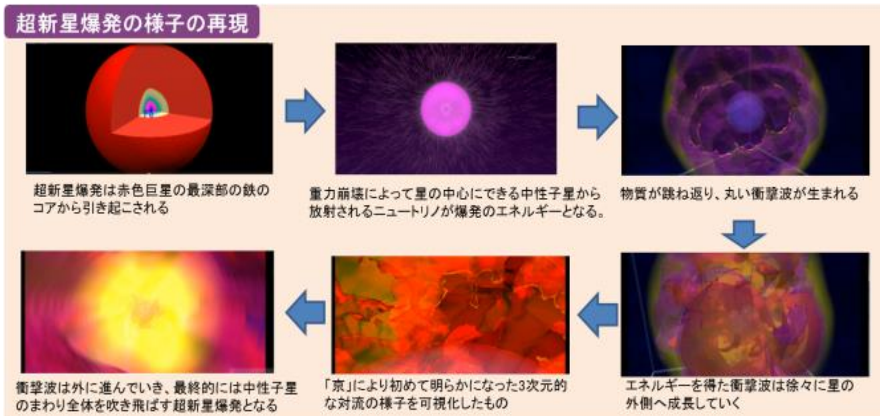
Estimation of safety in crosswind by dynamic coupling of vehicle motion and aerodynamics

Supernova Explosion

Tomoya Takiwaki, Kei Kotake and Yudai Suwa

Core collapse supernovae are stellar explosion of massive stars whose mass is bigger than 8 solar masses. The mechanism of supernovae is not clarified. K first enabled us to perform the simulation with fine numerical grid and the central engine of supernova was reproduced.

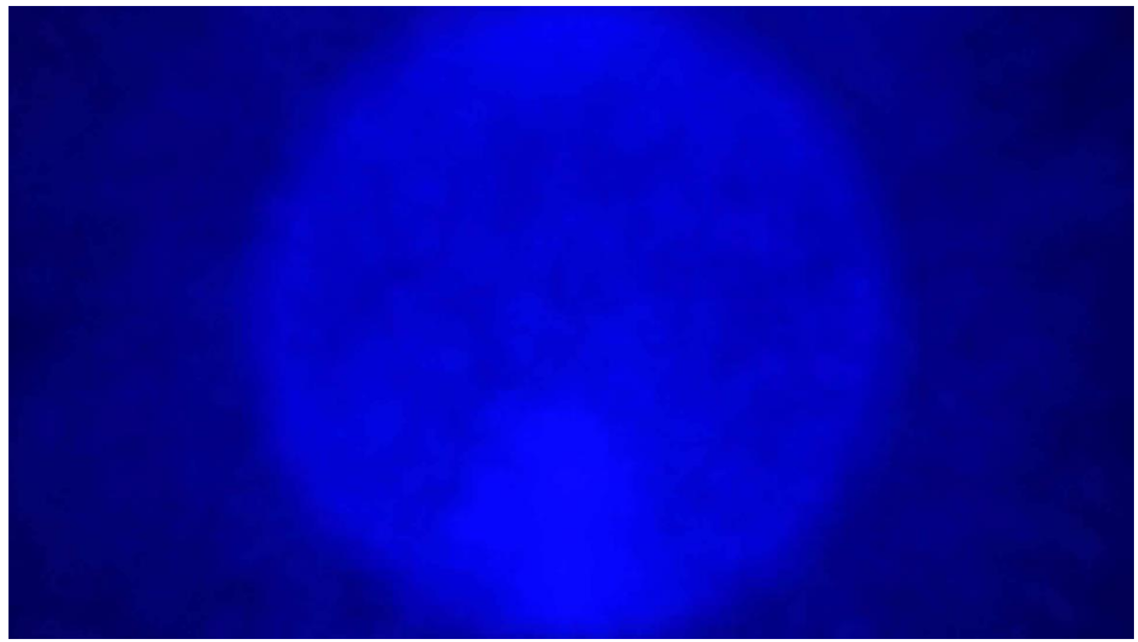
Supernova explosion was first discovered by this 3D simulations with K computer.



The supernova starts at the innermost iron core.

The iron core shrinks by the strong gravitational force. The gravitational collapse does not stop until the core bounce resulted from the birth of proto-neutron star. The shock waves generated.

After the gravitational collapse of iron core, the shock wave generated by the core bounce goes outer ward. That is supernova explosion

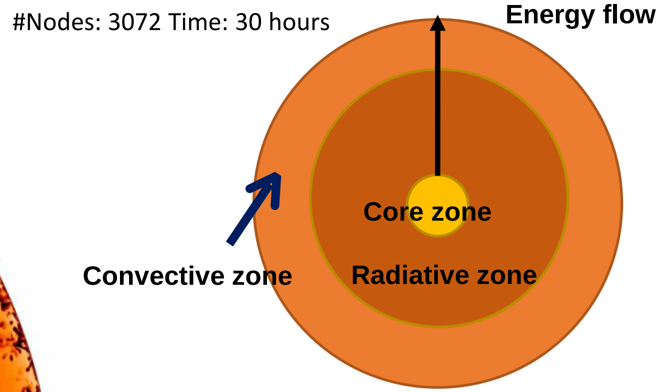


Turbulent flow in the solar global convection

「京」を用いて世界最高の解像度で太陽の対流層を計算

H. Hotta, T. Yokoyama (U. Tokyo), M. Rempel (HAO, USA), Astrophysical Journal, 2014

- Crucial for understanding the formation of magnetic field and sun spots
- High resolution (5x108 → 30x108 mesh) calculation on K with a new algorithm (Reduced Speed of Sound Technique)
- Successfully resolved the structure of the turbulent flow; 1st step toward understanding the solar global convection and sun spots (11 year cycle)



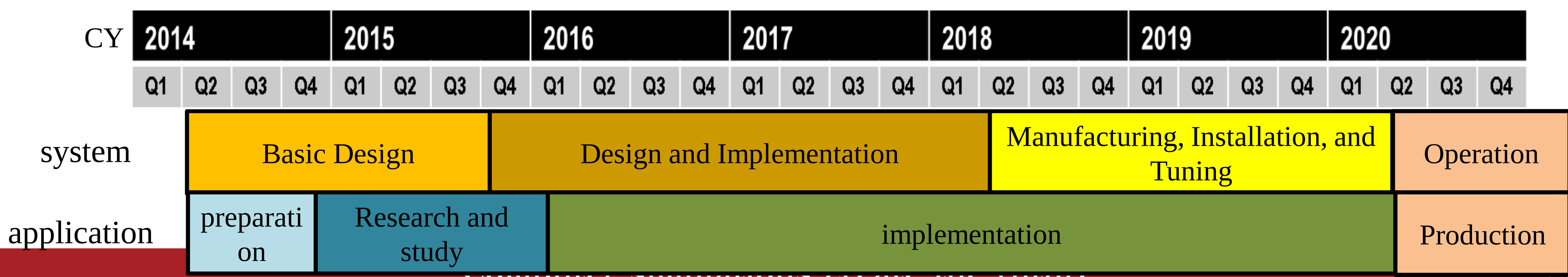
太陽の中心部では核融合でエネルギーが発生する。
放射層では光でエネルギーが運ばれ、対流層では
熱対流という現象でエネルギーが運ばれる。

Movie is courtesy of Dr Hideyuki Hotta: http://www-space.eps.s.u-tokyo.ac.jp/~hotta/movie/conv_spe.html

Development of Post-K Computer

Flagship 2020 Project

- Dual mission
  - Develop the next Japanese flagship computer, *post K*, by 2020
  - 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



Exascale Considerations

- Why push to the exascale? What science (applications) do we want to simulate at the exascale, and why?
- What will systems a hundred times faster than K look like architecturally?
- What should we do about it to prepare algorithmically?
- The system should be "co-designed" of architecture and application.

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) : The University of Illinois at Urbana-Champaign, INRIA the French national computer science institute, Argonne National Laboratory, Barcelona Supercomputing Center, Jülich Supercomputing Centre and the Riken AICS	**USA Europe**
Argonne Leadership Computing Facility	**USA**
Jülich Supercomputing Center	**Germany**
National Center for Supercomputing Applications (NCSA)	**USA**
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.

Computing is a Tool, not the End

- Computer simulation will dramatically increase our ability to understand the world around us
- Big computing and big data will revolutionize science
- AICS is a young institute growing into a world hub for computational science
- Pursuit of further interdisciplinary study encompassing wider spectrum of sciences
- Effort under way toward exascale computational science
- With exascale computing, we are reaching a tipping point in “Predictive Science”