Computer simulations create the future

Progress and Future of Computational Sciences
The 25th Anniversary Memorial Symposium of Center for Computational Science
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From K to post K

Great Opportunity and Great Challenge

in Advanced Computing

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RIKEN

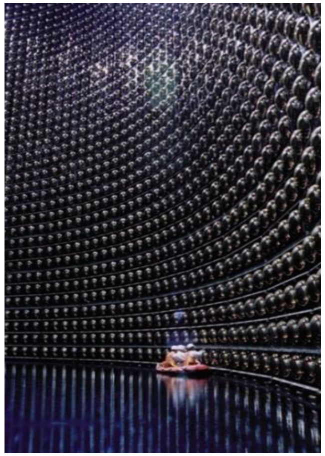
Contents

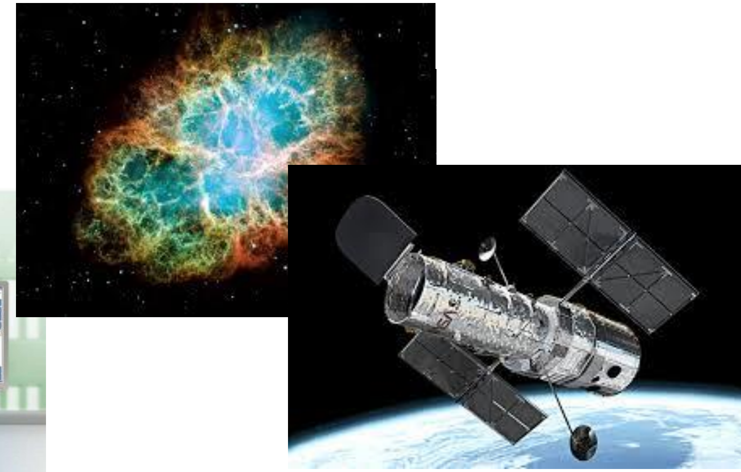
- Science in the 21st Century
- HPC in Japan and K Computer
- Some Research Highlights on K
- Flagship 2020 Project

The Role of Science in the 21st Century

- The role of scientific research in solving the problems is more relevant and feasible than ever in the 21st century.
- The world is 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 contribute to protecting the basic right to exist of all peoples.

Most Exciting Era of Science and Technology





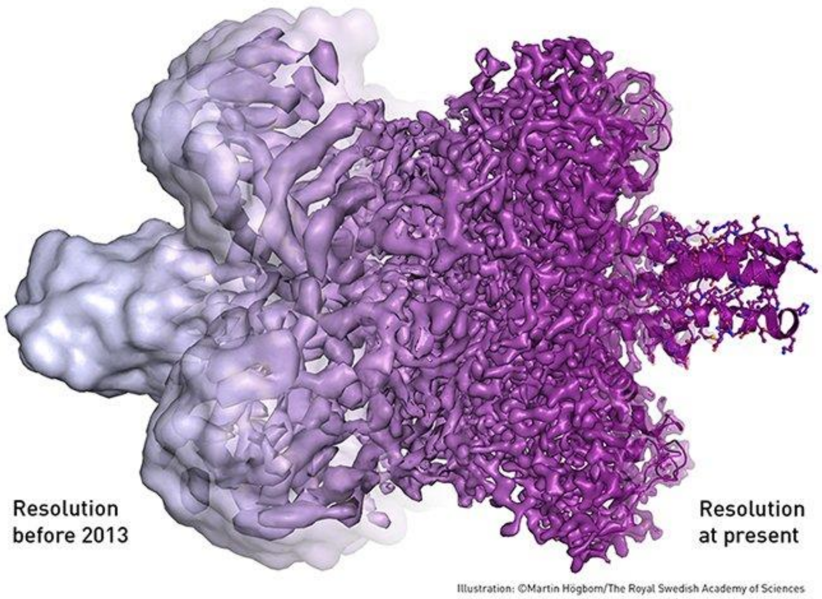
Recent years have seen remarkable and rapid advances in the technological tools. The 21st century is the age of **technology-driven science**.

For example, high-energy particle accelerators, such as the **Large Hadron Collider** confirmed the Higgs boson in 2013, powerful astronomy instruments such as the **Hubble Space Telescope** yielded insights into the universe's expansion, **high-throughput DNA sequencers** has revolutionized medicine and biomedical research, etc.

2017 Nobel Prizes in Physics and Chemistry

The Nobel prize in physics 2017 was awarded to three physicists for decisive contributions to the **LIGO** detector and the observation of gravitational waves.

The Nobel Prize in Chemistry 2017 was awarded to three biophysicists for developing **cryo-electron microscopy** for the high-resolution structure determination of biomolecules in solution.



The age of technology-driven science

- Powerful scientific instruments continually advance knowledge and open up new field of science.
- **Supercomputer** undoubtedly accelerates this trend.
- Unlike other tools which are limited to particular scientific domains, the supercomputer is **applicable to all areas** of science and engineering.
- Supercomputer is also a fundamental technology for data science, deep learning, IoT etc.
- Supercomputer will **drive progress** in science and technology and play an important role in **solving difficult problems**.

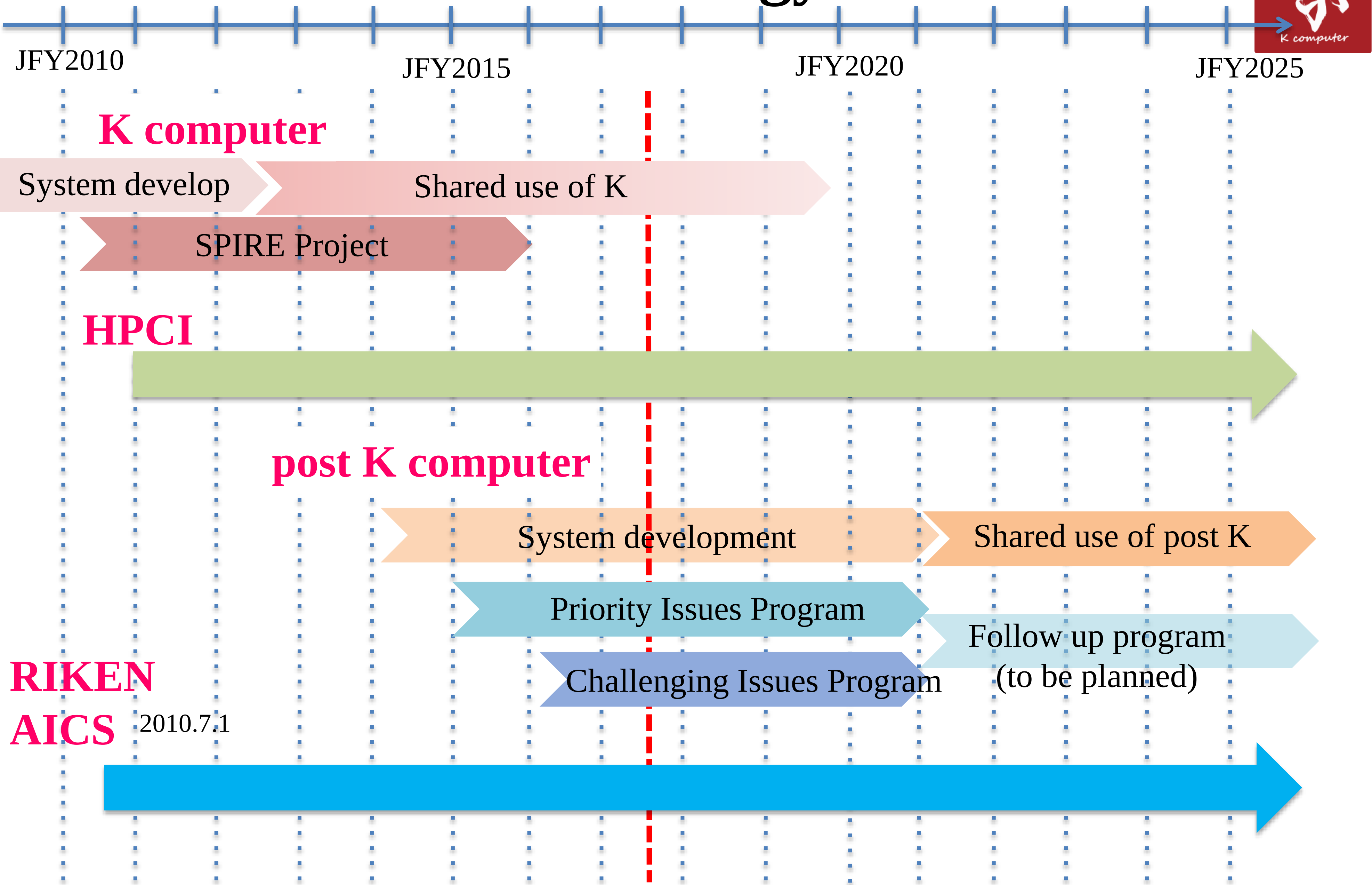
HPC in Japan and K Computer

HPCI (High Performance Computing Infrastructure)

- **Multi-component Project by MEXT**
  - Development of the K computer (2006 – 2011)
  - Foundation of AICS (2010)
  - Buildup of HPCI (2012 –)
    - National infrastructure for HPC in Japan
    - Tier-0 /Tier-1 supercomputers and storages connected via SINET network
  - SPIRE (Strategic Program for Innovative Research) (2011 – 2015)
    - 5-year national program for promoting computational science
    - Strategic usage of the K computer for computational science

- **Continuing on to the next stage**
  - Development of post K computer (2014 –)
  - Priority Issues and Challenging Issues Programs (2016 –)

Chronology



JFY2010
JFY2015
JFY2020
JFY2025
K computer
System develop
Shared use of K
SPIRE Project
HPCI
post K computer
System development
Shared use of post K
Priority Issues Program
Follow up program
(to be planned)
Challenging Issues Program
RIKEN
AICS
2010.7.1

HPCI Project (1)

- **Established massively parallel computation in Japan**
  - Recovered from the "Lost Decade" of the 2000's; caught up and even surpassed the world frontier in HPC
  - Massively parallel application codes successfully developed and widely spread among researchers
- **Produced many great results at the forefront of research**
  - Significantly enhanced the resolution both in precision and spatial and temporal sizes through massively parallel computation
  - Capacity computing (Ensemble computing) addresses uncertainty of highly complex phenomena and optimization in multi-dimensional spaces
- **Pulled up the level of computational science in Japan**
  - The execution of the national strategic program, SPIRE, has quickly and powerfully pulled up the level of computational science in Japan in a short time

HPCI Project (2)

- **Great progress in industrial utilization of supercomputers**
  - Supercomputers provide essential infrastructure for enhancing the international competitiveness of industry
  - Illustrated the powerful merits for time/cost reduction, improvement of product performance, search for best design solution, replacing experiment etc.

- **Development of HPCI (High Performance Computing Infrastructure)**
  - Seamless access to K and other supercomputers in 11 major academic computers in Japan
  - Scientists in wide areas of computational science can now access supercomputers with ease
  - Contributed in the overall level-up of computational science and technology in Japan

RIKEN AICS has played a key role in all of these aspects!

Advanced Institute for Computational Science (AICS)

Established in July 2010.

Three Missions

- Operation of world top-class **supercomputer K** for wide community of users in academia and industry
- Leading edge research through strong collaborations between **computer and computational scientists**
- Development of **post K supercomputer**

Director
- Deputy Director
- Operations & Computer Technologies Division
- Research Division
- Flagship 2020 Project
- Administrative Division

#Personnel: 202 (as of 1 Sep 2017)

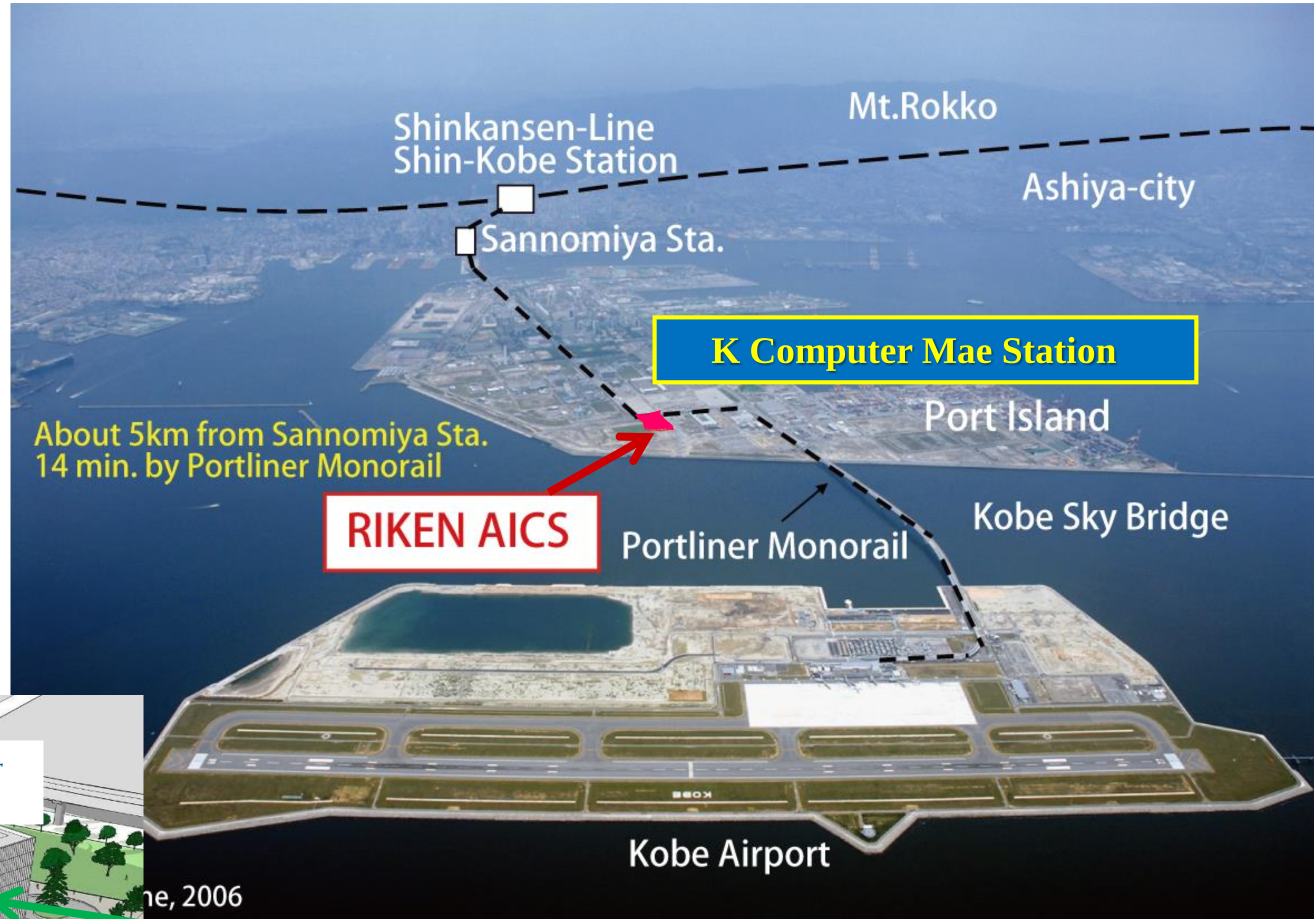
→ Full-time Researchers : 93

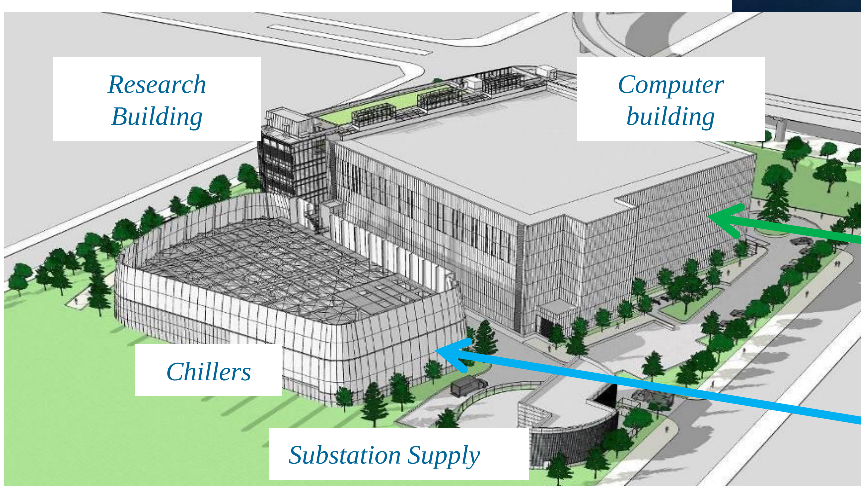
Non-Japanese Researchers : 17 (18%)

Female Researchers : 6 (6%)

Site of the K Computer & AICS

423km (263miles)west of Tokyo





Computer room 50mx60m=3,000m^2

Electric power up to 15MW

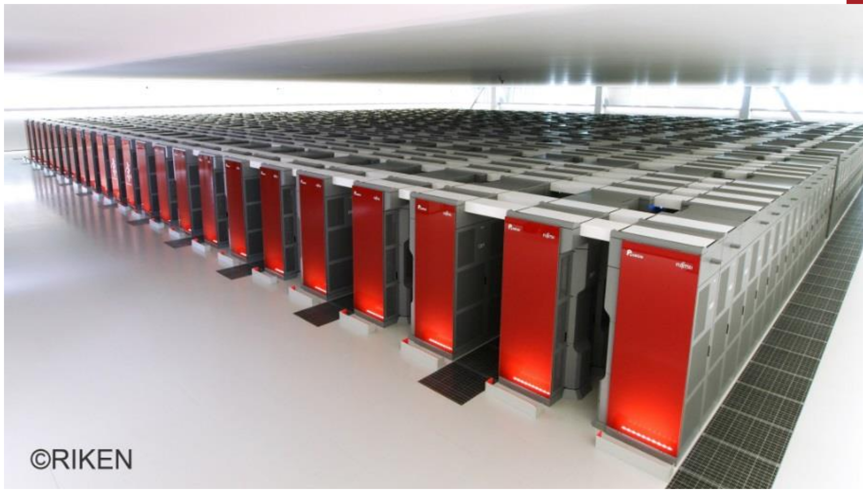
Water cooling system

Gas-turbine co-generation 5MW*2

K computer

Specifications

- Massively parallel, general purpose supercomputer
- No. of nodes : 88,128
- Peak speed: 11.28 Petaflops
- Memory: 1.27 PB
- Network: 6-dim mesh-torus (Tofu)



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.8 in Jun. 2017

Graph 500 ranking

"Big Data" supercomputer ranking
Measures the ability of data-intensive loads

- No.1 in Jun. 2017

HPCG ranking

Measures the speed and efficiency of solving linear equation using HPCG
Better correlate to actual applications

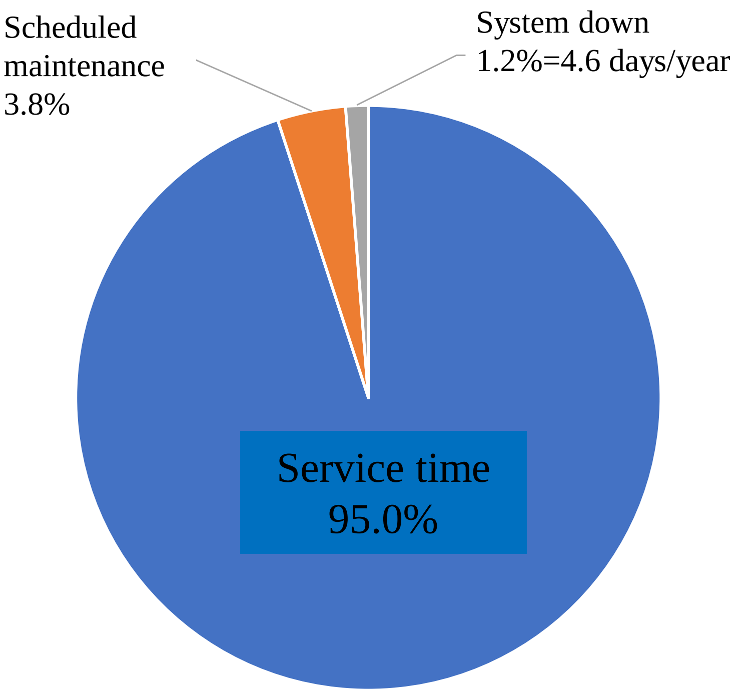
- No. 1 in Jun. 2017

A well balanced architecture with a good floating point rate and a good memory

Operation of K computer

System availability rate

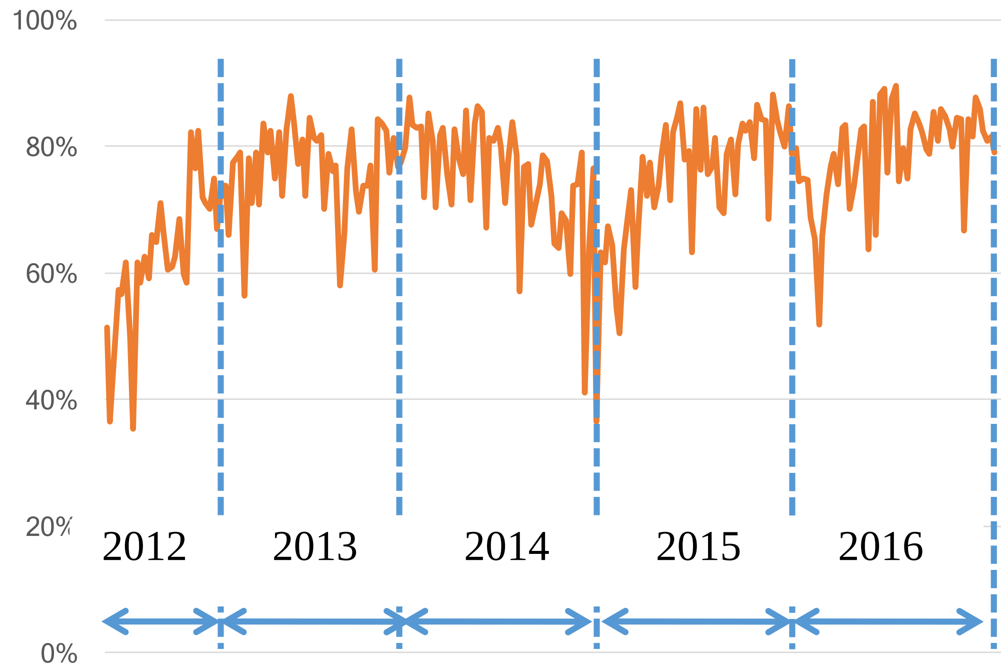
annual percentage of time in operation



JFY2016 statistics

Job filling rate

time which is actually used by user jobs over the available time of the K computer



Maintained high filling rate of over 75%

K demonstrates an extraordinary level of stability

AICS Research Teams and Team Leaders

Computational Science

- Particle Physics (Y. Kuramashi)
- Condensed Matter Physics (S. Yunoki)
- Astrophysics (J. Makino)
- Molecular Science (T. Nakajima)
- Biophysics (Y. Sugita)
- Structural Biology (F. Tama)
- Climate Science (H. Tomita)
- Data Assimilation (T. Miyoshi)
- Disaster Mitigation (S. Ohishi)
- Engineering (M. Tsubokura)
- Discrete Event Simulation (N. Ito)

Computer Science

- System Software (Y. Ishikawa)
- Programming Environment (M. Sato)
- Processor (K. Sano)
- Large-scale Parallel Numerical Computing Technology (T. Imamura)
- HPC Usability (H. Matsuba)
- HPC Programming Framework (N. Maruyama)
- Advanced Visualization (K. Ono)

Promoting strong collaborations between computer scientists and computational scientists

Open Software developed by AICS

Application software, Middleware, Language, and Libraries

Software		
IHK/McKernal	Light-weight OS kernel targeting high end HPC	OS
XcalableMP	Parallel programming language. Awarded HPC Challenge (Class 2) in SC13 and SC14	Language
KMR	MapReduce data processing tool implemented on K computer	Tools
Xcrypt	Parallel job control script language Xcrypt implemented on the K computer	Libraries
EigenExa	Parallel eigenvalue solver. A million dim dense matrix can be solved in 1 hour on K.	Libraries
HIVE	Visualization system of large data directly on K	Science software
FDPS	Application development platform for particle simulations	Particle simulator

Open Software developed by AICS

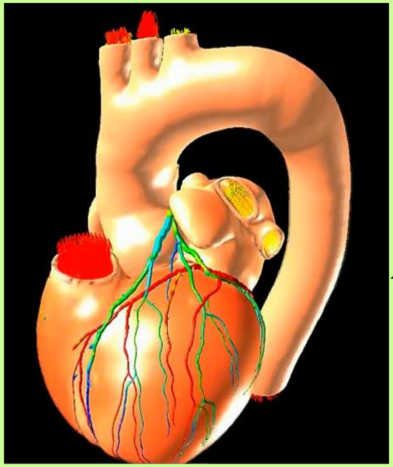
Software		
GENESIS	Parallelized MD library for large biomolecules scaling up to full K nodes for 10^8 atoms	Molecular dynamics
NTChem	Parallel molecular science software	Quantum chemistry
SCQS	Library for strongly correlated systems with quantum Monte Carlo and DMRG methods	MC and DMRG
CUBE	Unified library for complex fluids including heat, sound, structure, and particles etc.	CFD
SCALE	Basic library for next generation climate simulation jointly developed by computational and computer scientists	Weather dynamics
OASIS	Software for discrete events	Social simulation
GAMERA	Software for urban earthquake simulation Gordon Bell Finalist for SC14 and SC15	Earth quake

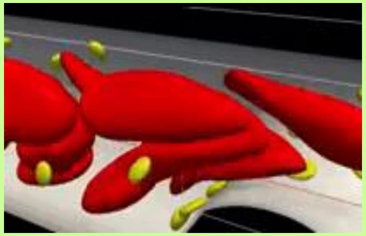
Some Research Highlights on K

Some Recent Results from the K computer

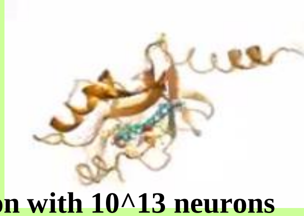
Many projects that use K would be difficult or impossible to do elsewhere

Life sciences





Artificial heart and blood flow

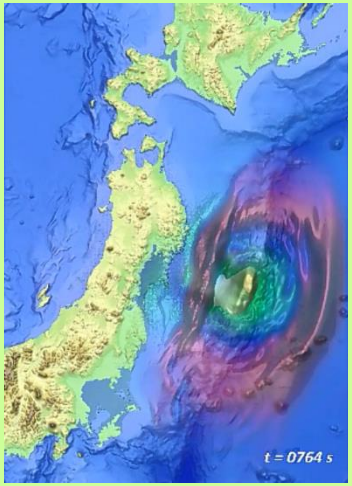


Neuronal simulation with 10^13 neurons

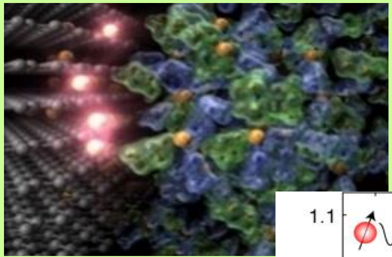
Disaster prevention

Cloud resolving NICAM run with less than 1km mesh

Coupled earth quake-plate dynamics-tsunami simulation

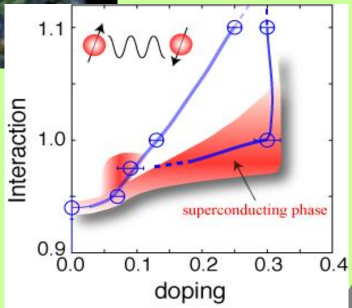


Materials & Energy



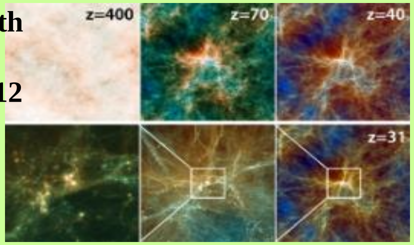
Fast Charging mechanism of Lithium Ion battery

Charge-fluctuation origin of iron-based superconductors



Fundamental science

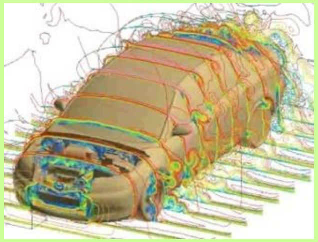
Dark matter with $2x10^{12}$ particles Gordon Bell 2012

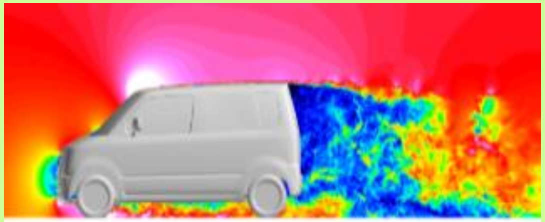


Supernova explosion through neutrino heating

Engineering

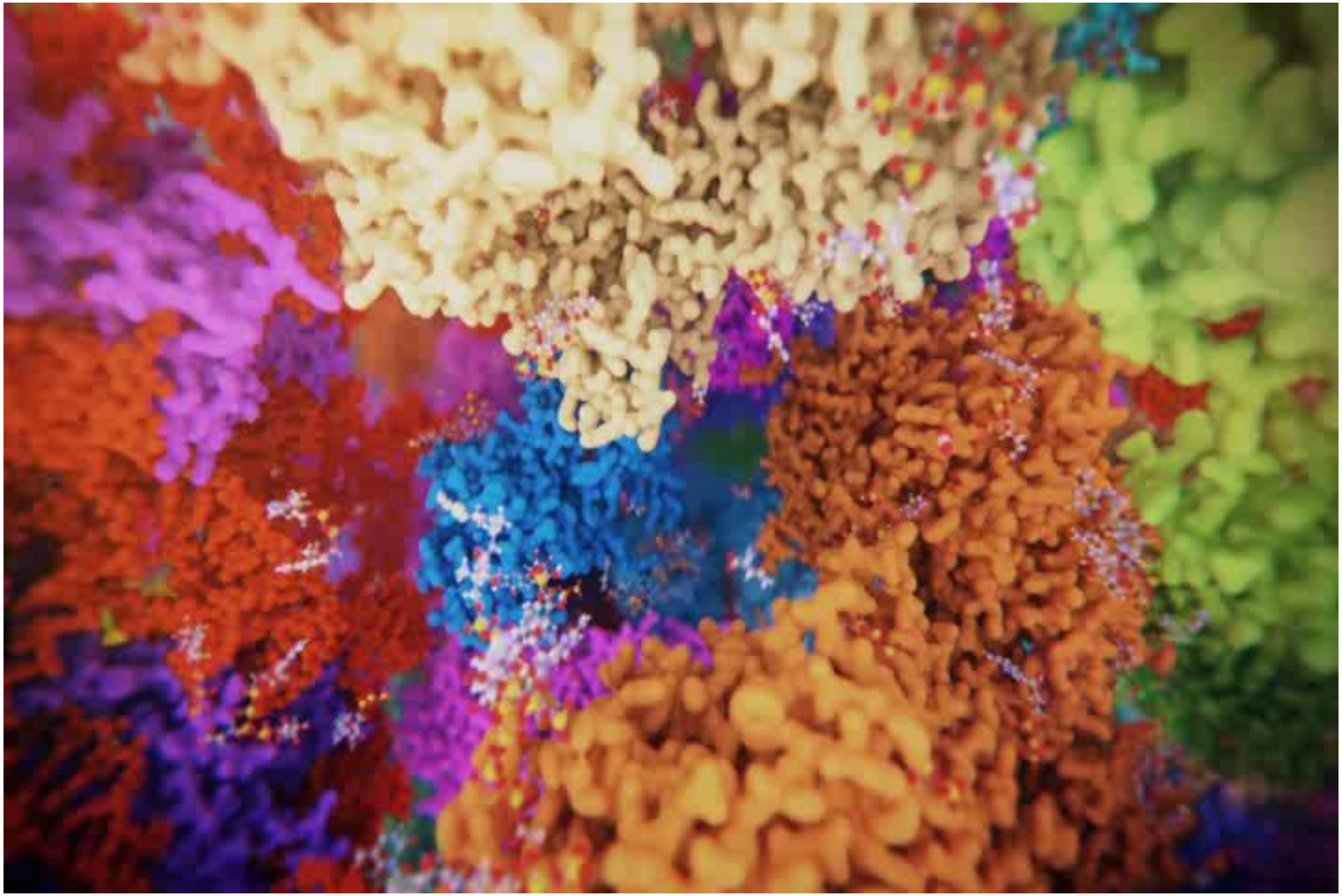
Fluid flow simulation accelerates design of transport vehicles





Computer simulations create the future

All atom MD simulations of crowded cellular environment of mycoplasma genitalium with GENESIS

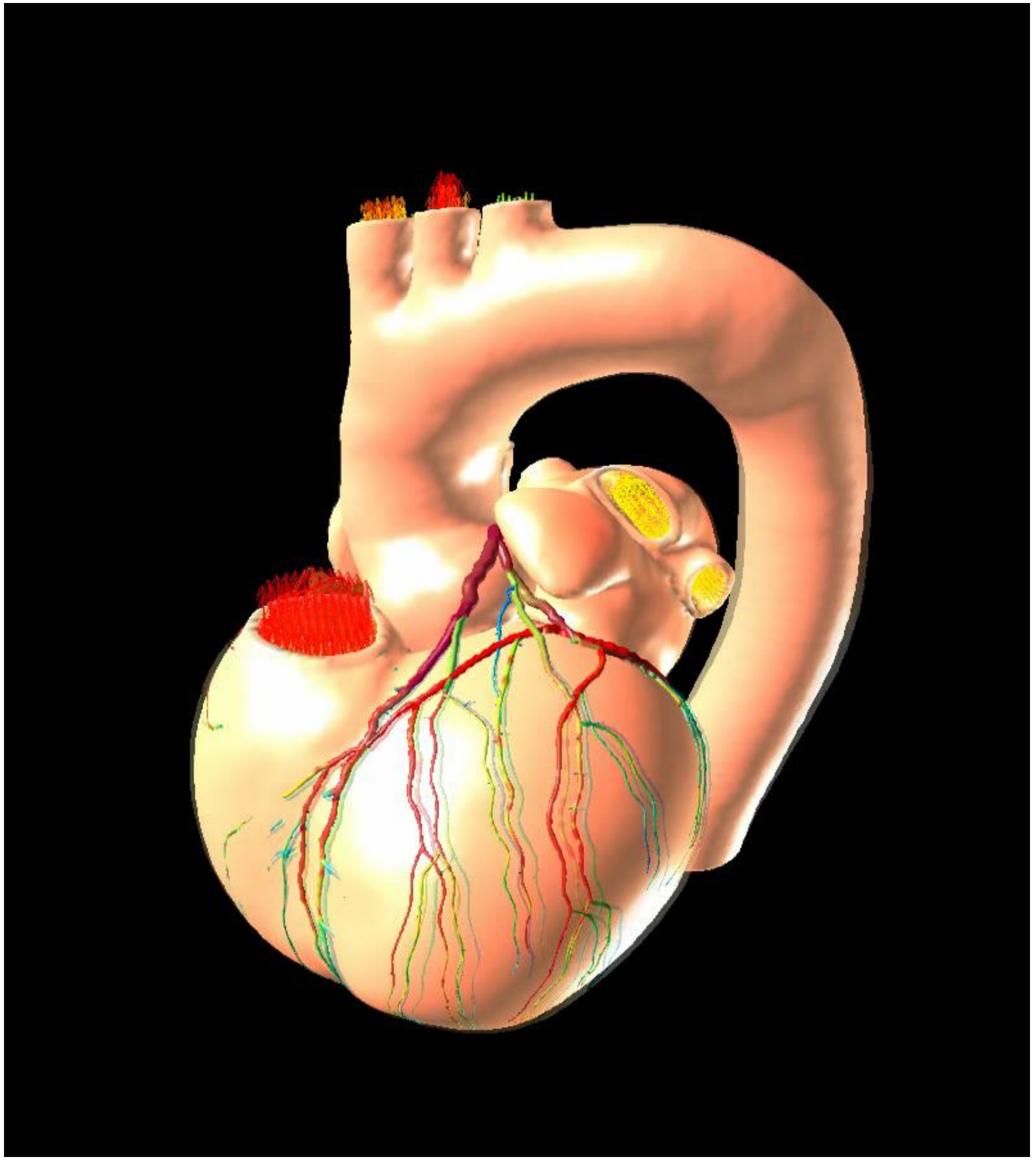


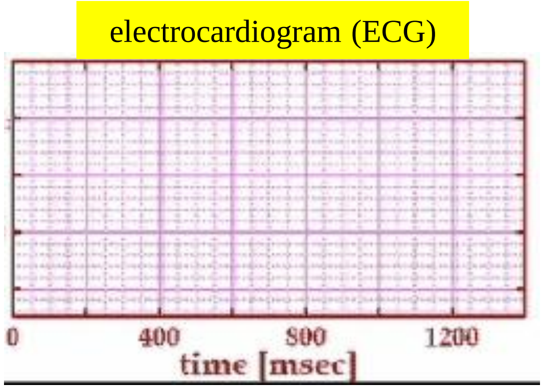
Y. Sugita, J. Jung (AICS), M. Feig (Michigan State Univ.)

103 million atoms in a 100nm cubic box
MD simulations were carried out for 100 ns

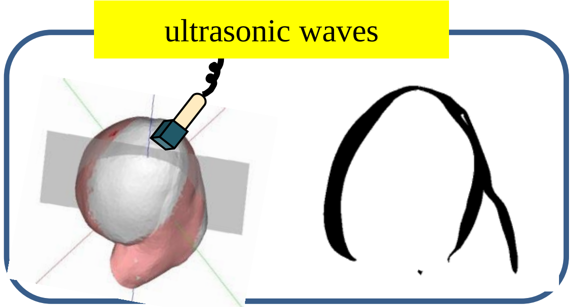
Heart Simulator

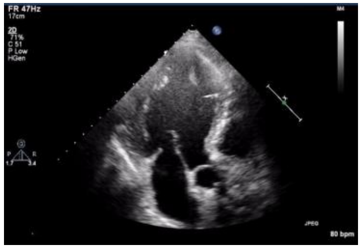
Hisada & Sugiura (UT)





Multi-scale simulator of heart starting from molecules and building up cells, tissues, and heart





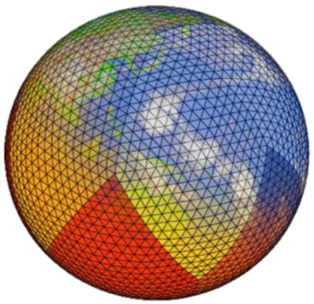
Heartbeat, blood ejection, coronary circulation are simulated consistently.
Heart model for each patient can be rebuilt

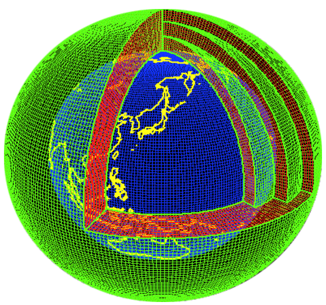
Applications explored

- Applied to congenital heart diseases
- Screening for drug-induced irregular heartbeat risk

Global Climate Simulation (Tomita)

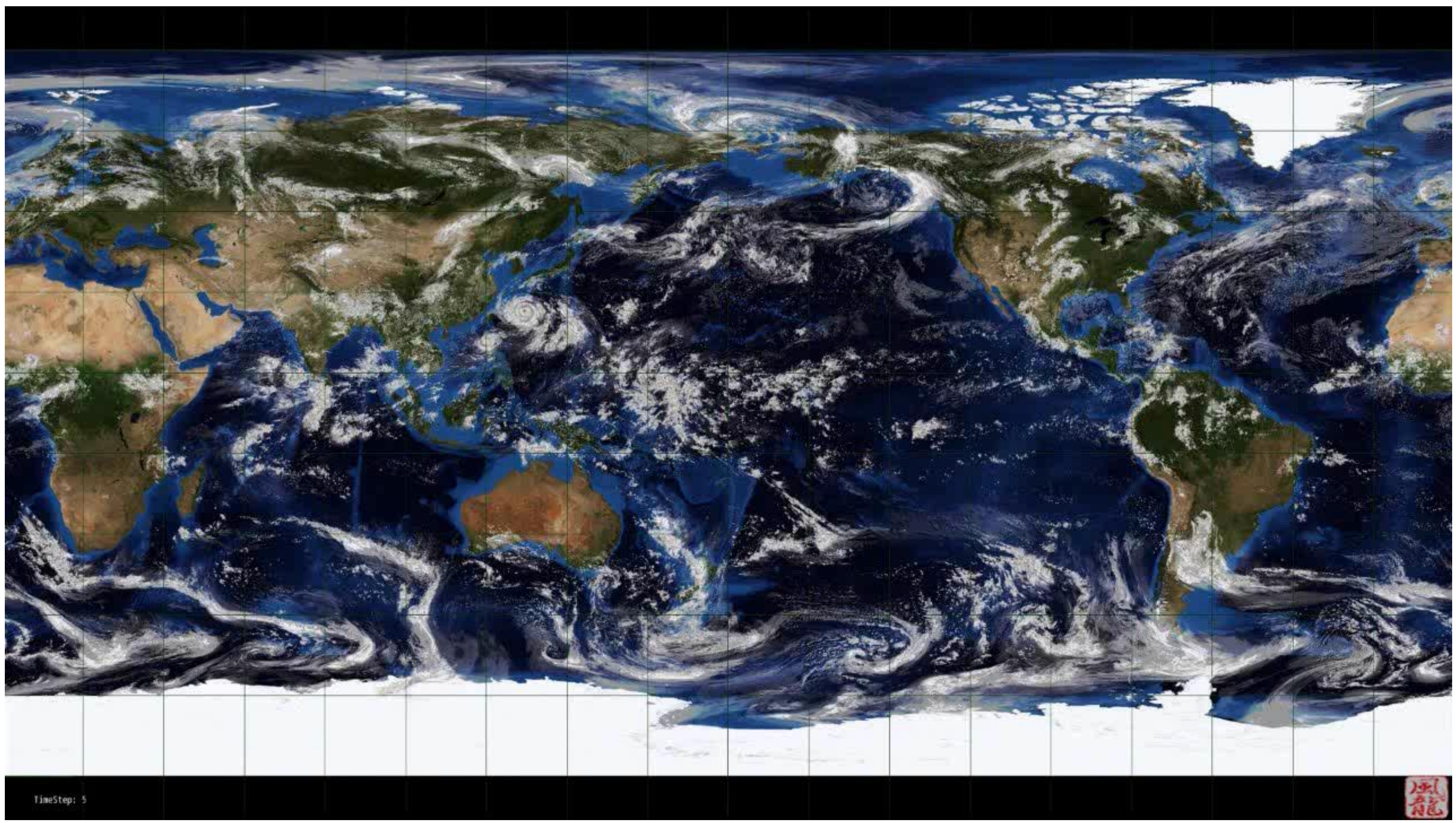
- Previous NICAM simulations with 3.5 km resolution is quite accurate but not able to resolve individual cumulonimbus clouds. Global cloud resolving model **with 0.87 km-mesh** much closer to the actual process of cumulonimbus development.
- Month-long forecasts of Madden-Julian oscillations in the tropics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



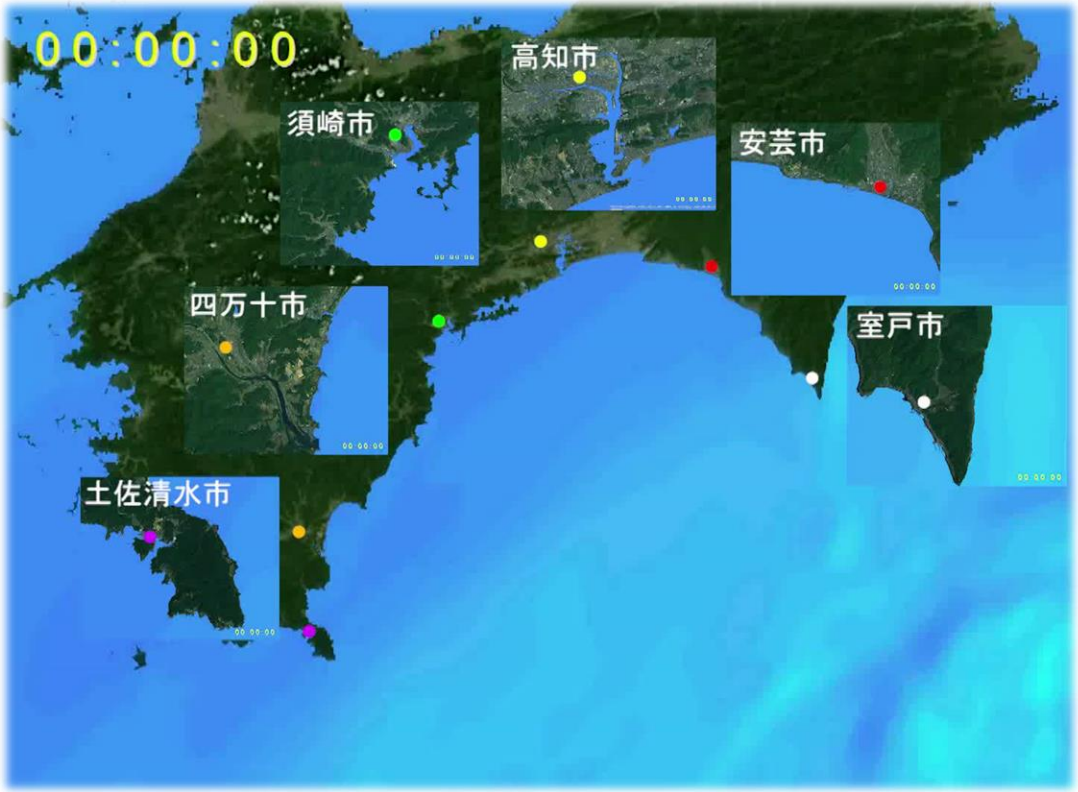
Miyamoto et al (2013) , Geophys. Res. Lett., 40, 4922–4926, doi:10.1002/grl.50944.

3.11 East Japan Earthquake and Tsunami

Coupled calculations of earthquake, crustal deformation, and tsunami

Direct comparison with observed records

Furumura and Maeda (UT)



Nankai Trough Quake Baba (JAMSEC)

Resolution 5m, 6.8 hundred million meshes

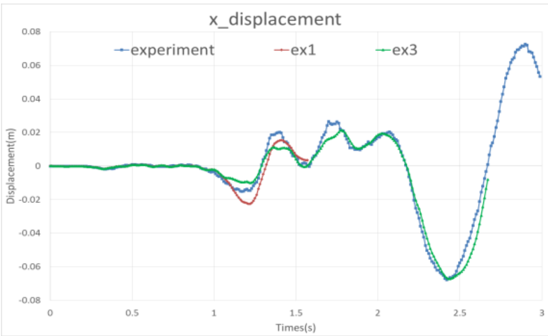
Planning countermeasures against complex disasters involving multiple elements

Disaster Mitigation and Reduction

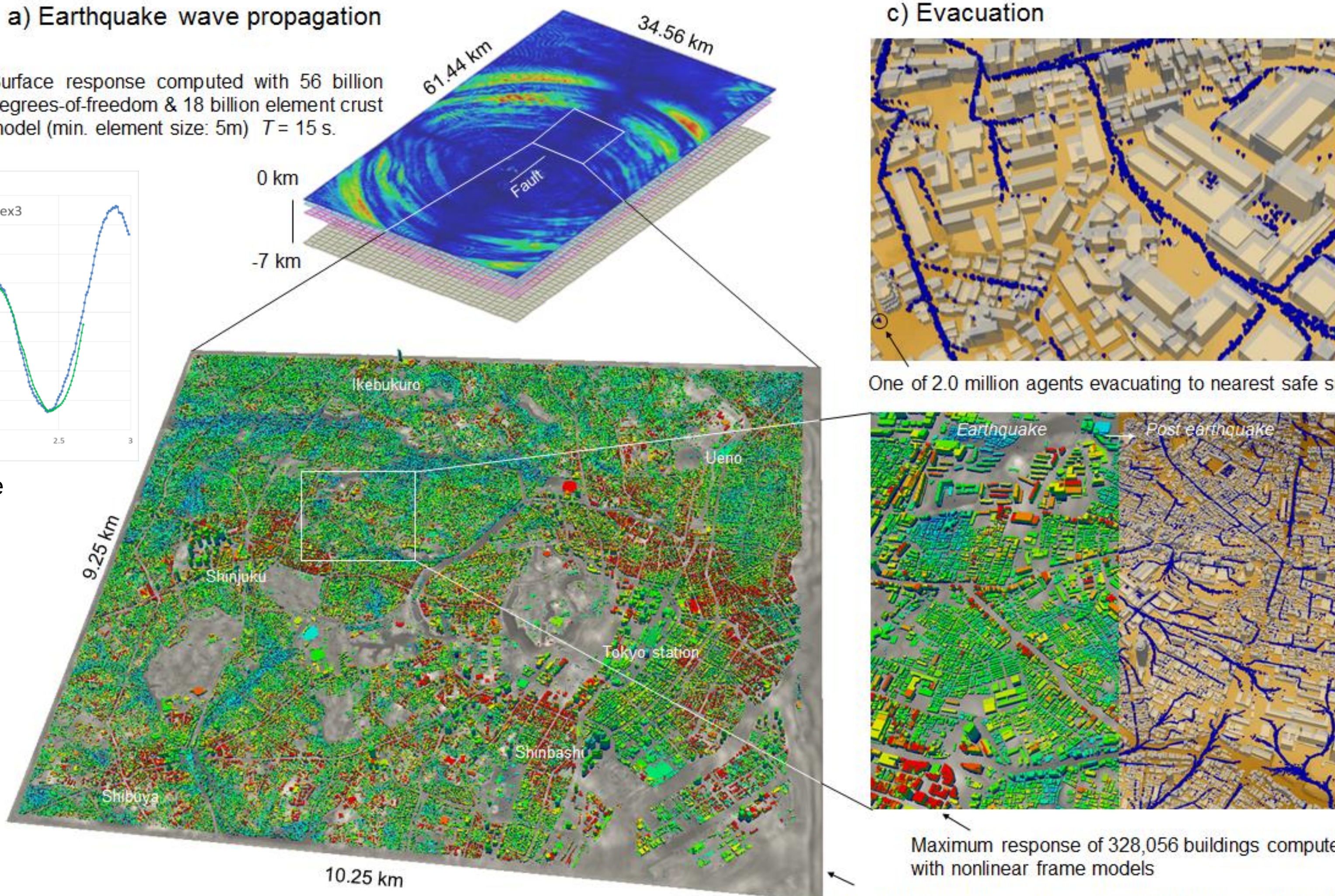
Earthquake that directly hits Tokyo area

a) Earthquake wave propagation

Surface response computed with 56 billion degrees-of-freedom & 18 billion element crust model (min. element size: 5m) T = 15 s.



Comparison with E-defence experiment



c) Evacuation

One of 2.0 million agents evacuating to nearest safe site

Maximum response of 328,056 buildings computed with nonlinear frame models

Maximum surface response computed with 133,609,306,335 degrees-of-freedom & 33,212,898,352 element soil model (min. element size: 1m)

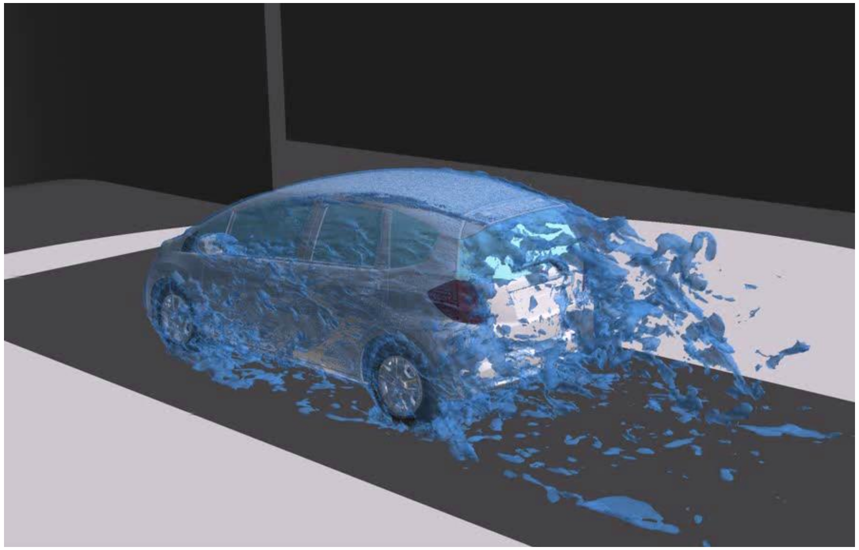
b) Soil amplification & seismic structural response

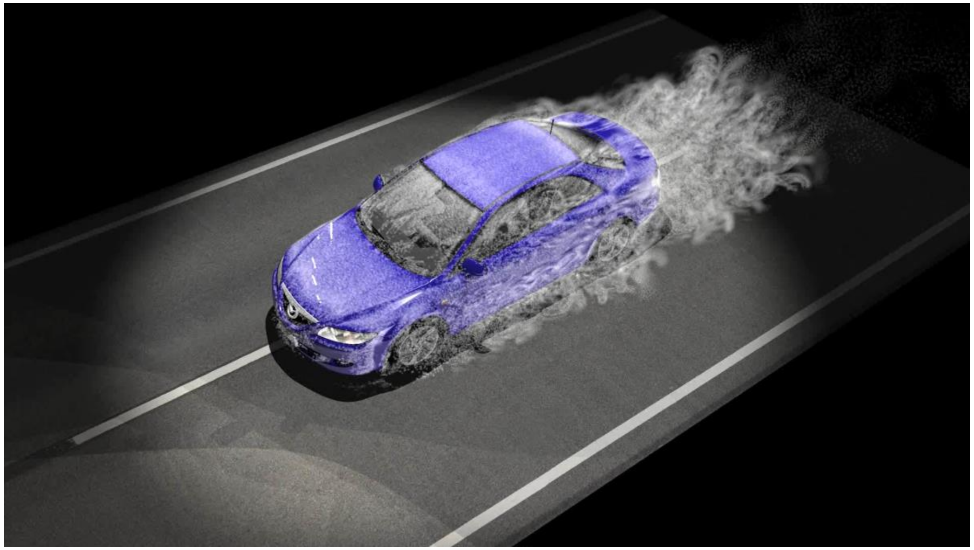
Manufacturing Innovation by HPC

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

- K computer is changing the manufacturing process with the analysis *which cannot be made with wind-tunnel measurements.*

Examples of the next generation aerodynamic simulation





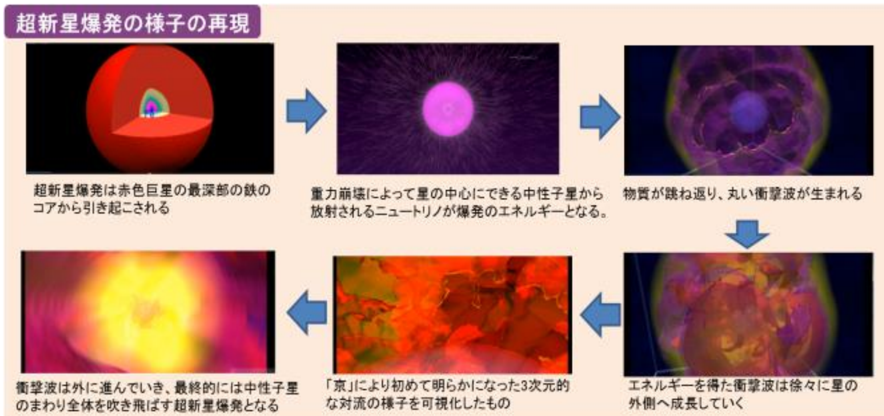
- Estimation of high-speed stability during dynamic maneuvering
- Estimation of safety in cross-wind by dynamic coupling of vehicle motion and aerodynamics

Supernova Explosion

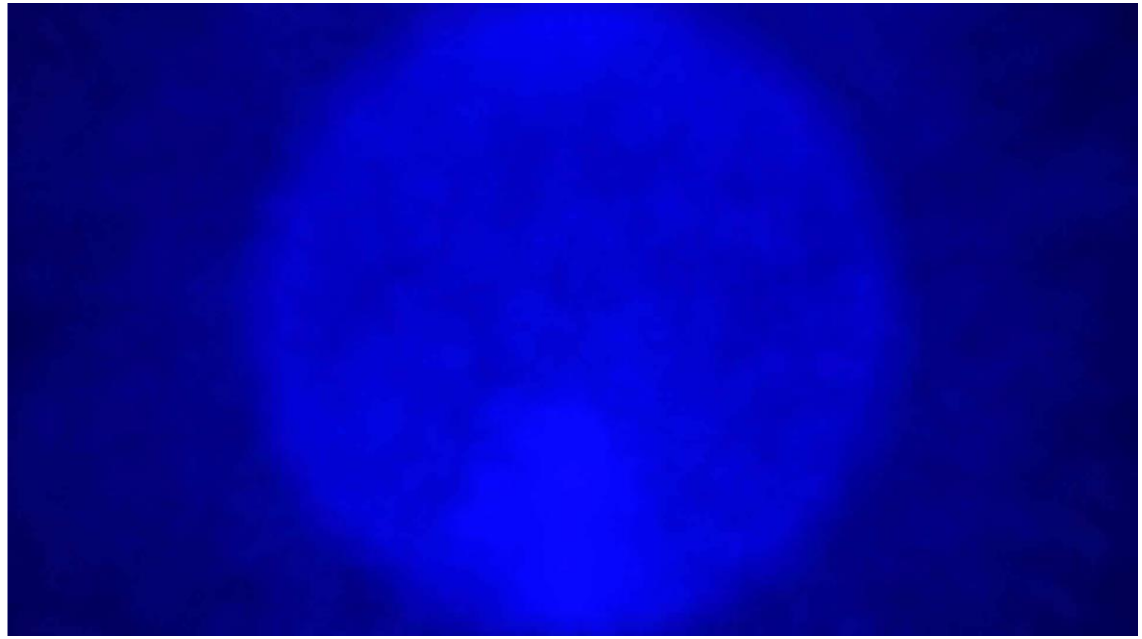
Tomoya Takiwaki, Kei Kotake and Yudai Suwa

A supernova explosion is an astronomical event that occurs during the last stellar evolutionary stages of a massive star's life. The mechanism is not clarified.

K first reproduced the supernova explosion
Support the explosion is driven by the neutrino-heating mechanism



- 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.



Tomoya Takiwaki, Kei Kotake and Yudai Suwa, *The Astrophysical Journal*, Vol. 786(2): 83, 2014
"A COMPARISON OF TWO- AND THREE-DIMENSIONAL NEUTRINO-HYDRODYNAMICS SIMULATIONS OF CORE-COLLAPSE SUPERNOVAE"

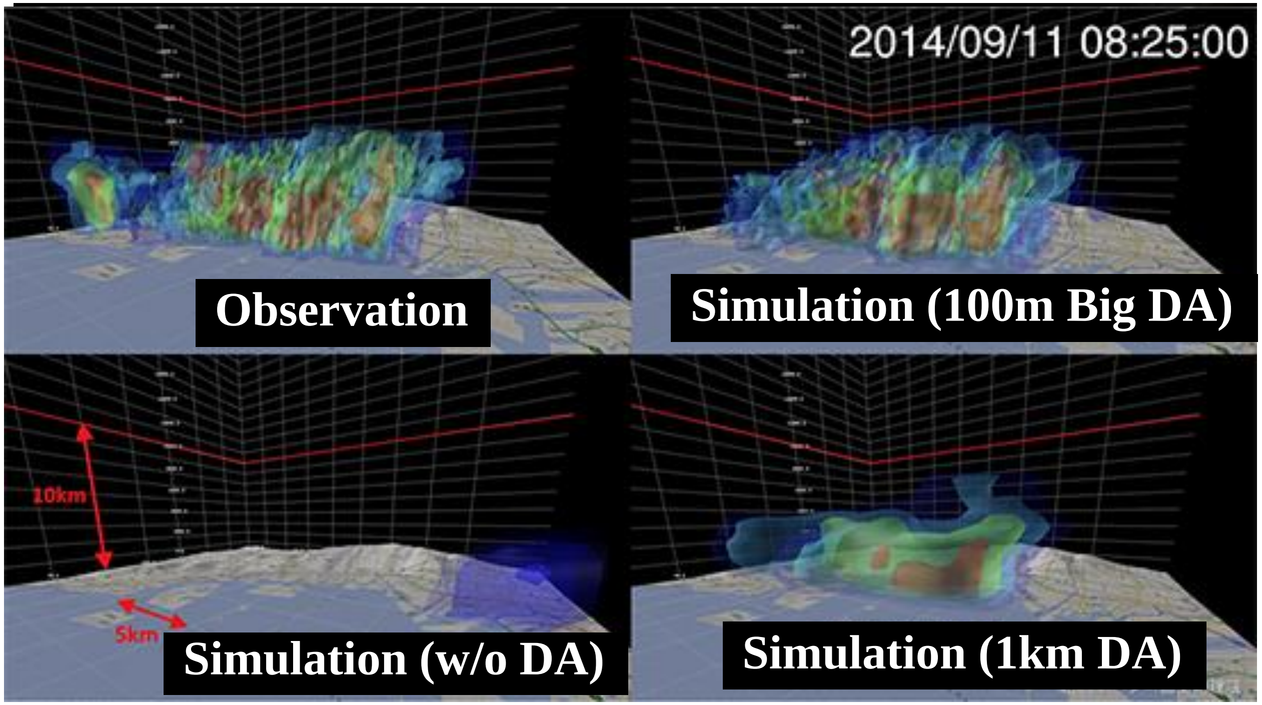
Data Assimilation (DA)

- DA bridges simulations and observations, revolutionizing weather prediction.
- Growing interest in applying DA to other forecasting problems (Climate/Weather, Brain Science, Protein Science, Engineering, etc).

Bridges Simulations and Observations

Climate/Weather Forecasting Research (Miyoshi)

BIG DATA ASSIMILATION bridges simulations and observations



Rainfall distributions

The prototype system (100m grid /100 ensemble simulations and rainfall distributions observed every 30 sec by phased array radar) can predict **sudden torrential rains!**

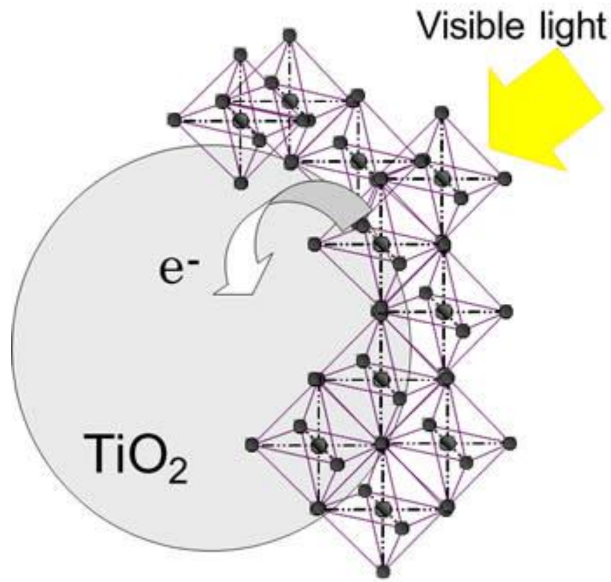
BIG SIMULATION + BIG DATA × Highly sophisticated assimilation = Weather Forecasting Revolution

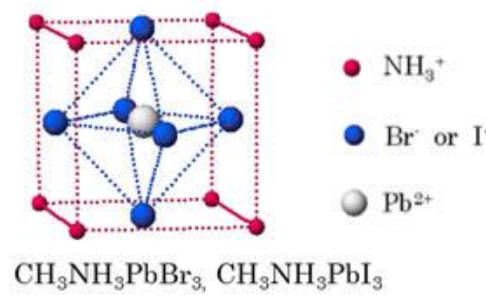
Capacity Computing

Capacity computing addresses uncertainty of highly complex phenomena and search for optimal solutions in multi-dimensional space.

Design of Perovskite Solar Cell

Rapid emergence of a solar cell based on mixed organic–inorganic halide perovskites. Solar cell efficiencies of devices have increased from 3.8% in 2009 to 22.1% in 2016.





Organo metal perovskite as photoconductive material

Capacity Computing for a Perovskite Solar Cell

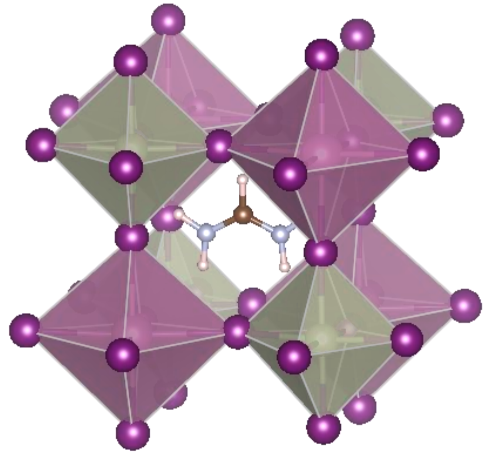
T. Nakajima (AICS)

$A_2BB'X_6$, ABX_3

A: CH3NH3, HC(NH2)2, Cs,

B/B’: Metal atoms, 49 elements ,

X: I, Br, Cl



# of possible combination: 11,025

Periodic Table

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	1 H																	2 He	1
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	2
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	3
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	4
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	5
6	55 Cs	56 Ba	57～71 Lanthanoid	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	6
7	87 Fr	88 Ra	89～103 Actinoid	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og	7
			57～71 Lanthanoid	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
			89～103 Actinoid	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

A Perovskite Solar Cell

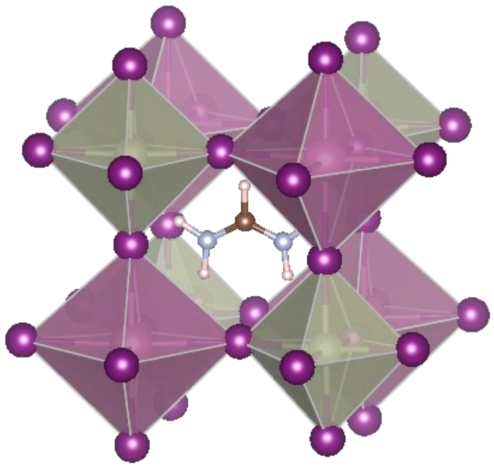
T. Nakajima (AICS) 51 candidates

All candidate perovskites and their lowest band gaps (in eV)							
group-14–group-14		group-13–group-15		group-11–group-11		group-11–group-13	
$CsSnI_3$	0.95	MA_2InBiI_6	0.88	$MA_2AgAuBr_6$	1.27	MA_2CuInI_6	1.29
$FASnI_3$	1.00	MA_2InSbI_6	1.01	$MA_2CuAuBr_6$	1.29	FA_2AuGaI_6	1.44
Cs_2GeSnI_6	1.04	FA_2GaBiI_6	1.10	MA_2CuAuI_6	1.30	MA_2AuInI_6	1.47
$CsSnBr_3$	1.07	MA_2GaBiI_6	1.16	$MAAuI_3$	1.34	MA_2AuGaI_6	1.50
MA_2SiSnI_6	1.22	$MA_2InBiBr_6$	1.18	FA_2AgAuI_6	1.35		
FA_2GeSnI_6	1.24	FA_2InBiI_6	1.19	$FAAuI_3$	1.38	group-11–group-15	
$CsGeI_3$	1.28	MA_2GaSbI_6	1.21	$MAAuBr_3$	1.39	MA_2AgBiI_6	2.09
$Cs_2GeSnBr_6$	1.29	Cs_2GaBiI_6	1.21			MA_2CuBiI_6	2.11
$MASnI_3$	1.43	$Cs_2GaBiBr_6$	1.29	group-9–group-13			
$MASiI_3$	1.44	$MA_2InSbBr_6$	1.29	Cs_2RhInI_6	1.42		
$CsGeBr_3$	1.56	$Cs_2GaBiCl_6$	1.39	FA_2RhInI_6	1.63		**Band gaps**
MA_2GeSnI_6	1.56	$Cs_2GaSbCl_6$	1.43	MA_2RhGaI_6	1.67		(0.8-2.2 eV)
FA_2SiGeI_6	1.66	$Cs_2InBiBr_6$	1.45	Cs_2RhGaI_6	1.68		**Toxic metals** Pb, Hg, Cd, As, Tl
MA_2SiGeI_6	1.82	MA_2GaPBr_6	1.64	$Cs_2RhInBr_6$	1.76		excluded
$MAGeI_3$	1.83	$MA_2GaBiBr_6$	1.72	$MA_2RhInBr_6$	1.83		
$MASnBr_3$	1.89	$MA_2GaSbBr_6$	1.77				

A Perovskite Solar Cell

$A_{1-x}A'_xB_{1-y}B'_yX_{1-x}X'_xY_{2(1-y)}Y'_{2y}$

(x=0, 0.25, 0.5, y=0, 0.25, 0.5)



# of possible combination: Several millions to ten millions

Screened using Post K computer

Flagship 2020 Project

Development of Post-K Computer

- Started in 2014
- AICS appointed as the main organization for the development of the world's top-level general-purpose supercomputer.
- The post K will be used to work on innovative solutions to current scientific and social issues.

Flagship 2020 Project

- Develop the next Japanese flagship computer, *post K*, which is planned to go on line in 2021/2022
- Simultaneously develop a range of application codes, to run on *post K*, to help solve major societal and science issues

- Co-design of architecture and application is crucial
- Budget:110 billion JPY
- Power consumption: 30～40MW（12.7MW in the case of K computer）

Our aim is to balance various factors, such as

i) power consumption,

ii) computational performance,

iii) user convenience,

iv) ability to produce ground-breaking results

characterized by its all-around capabilities compared to any other system in the world in the 2020's.

Priority Issues Program

Drug manufacture

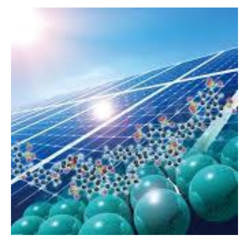
Innovative computing infrastructure for drug discovery using AI

Climate and environment

Meteorological global environmental predictions using big data

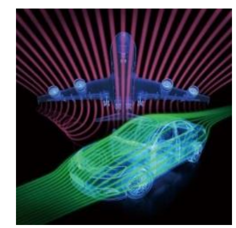
Energy issues

New technologies for energy creation, conversion/storage, and use



Industrial innovation

Development of innovative design and production processes

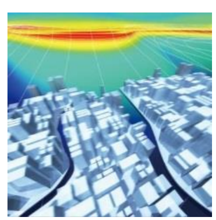


Health and longevity

Personalized and preventive medicine using big data

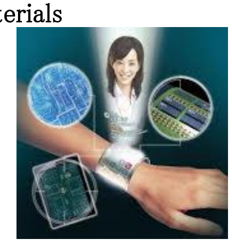
Disaster prevention

Integrated simulation systems induced by earthquake and tsunami



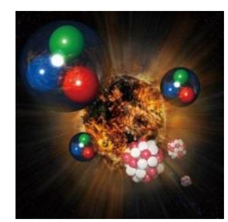
Functional materials

Creation of new functional devices and high-performance materials

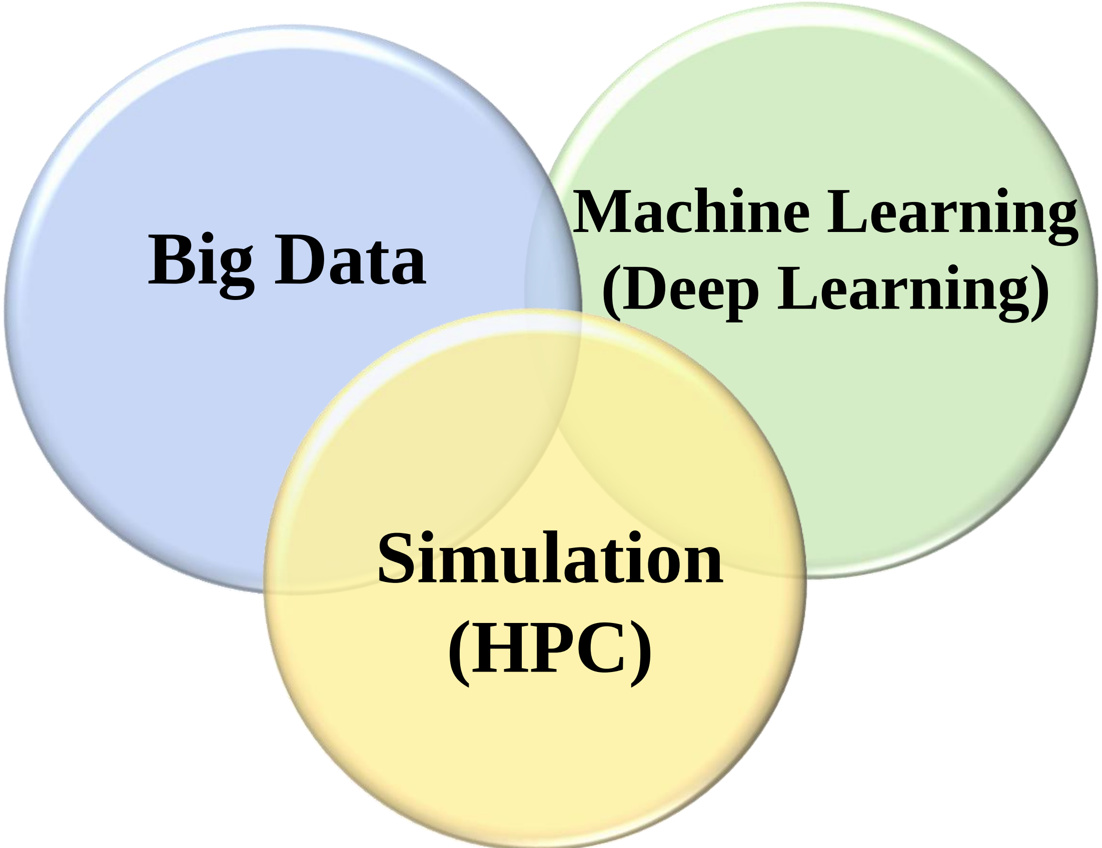


Basic science

Elucidation of fundamental laws and evolution of the universe



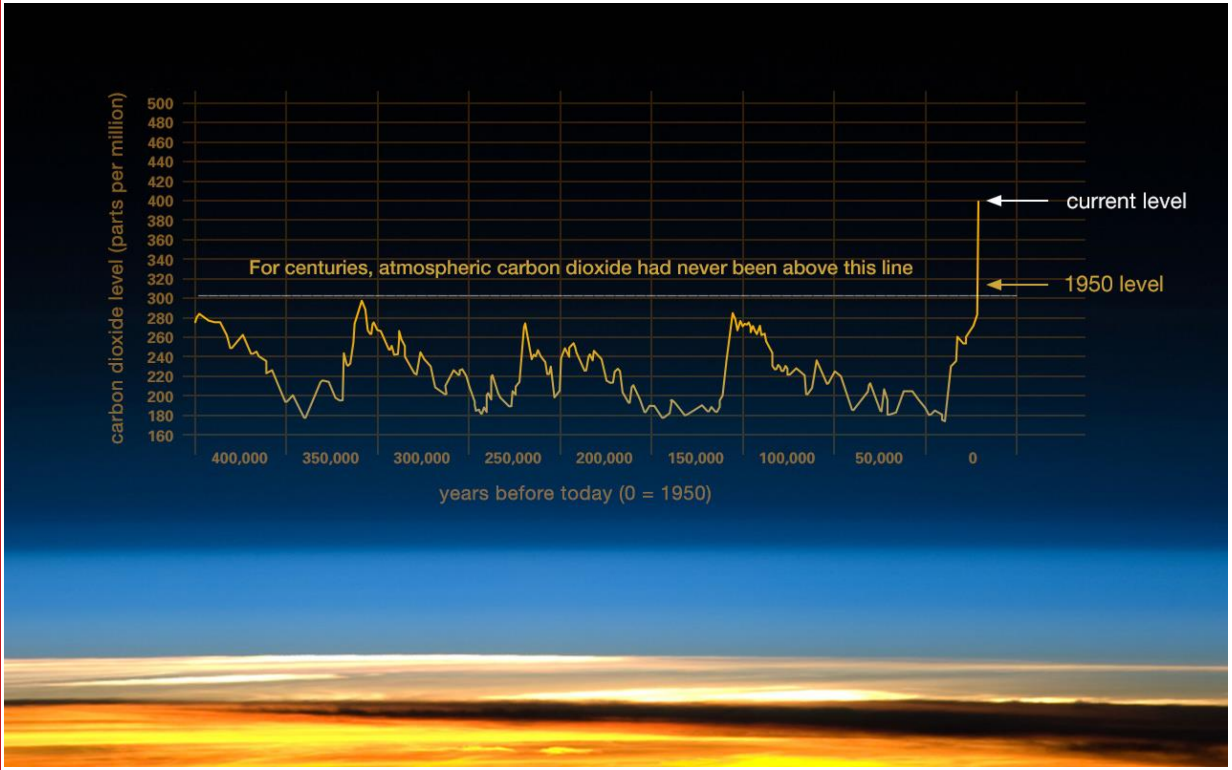
Advanced Computing



- Big data and big simulation are both essential elements of an integrated computing research and development.
- Scientific discovery via computational science and data analytics is truly the “endless frontier”.

Global Warming

CO2 Concentration



Scientific evidence for warming of the climate system

- Global temperature rise
- Warming oceans
- Shrinking ice sheets
- Glacial retreat
- Decreased snow cover
- Sea level rise
- Declining Arctic sea ice
- Extreme events
- Ocean acidification
- ・・・

Warning from Royal Society & US National Academy of Sciences

Even if greenhouse gas emissions were to suddenly stop, it would take thousands of years for atmospheric CO_2 *to return to its levels before the industrial era.*

Save the Planet

When I started my scientific career in the early 70s, **the world was bright**. There was a strong belief that science and technology was able to solve all problems that might occur in the future.

Today **it is different**. We are now living in an endangered world. The climate threat is becoming more and more obvious.

Save the planet. But maybe it is too late. Maybe it is too difficult if not impossible to change the attitudes of people.

“We have met the enemy and he is us” (PoGo).

From Science to Society

- Supercomputer has become a fundamental technology which supports the society today, and pioneers the society of tomorrow.

- Continued development of world top-class supercomputer is vital for the world leadership in science and technology.

- AICS is developing a world's top-class supercomputer, "post K" launching in around 2020 to spearhead the quest for knowledge of human kind.

Thank you for your attention!

K computer