

Computer simulations create the future



# An Introduction to AICS Software Center

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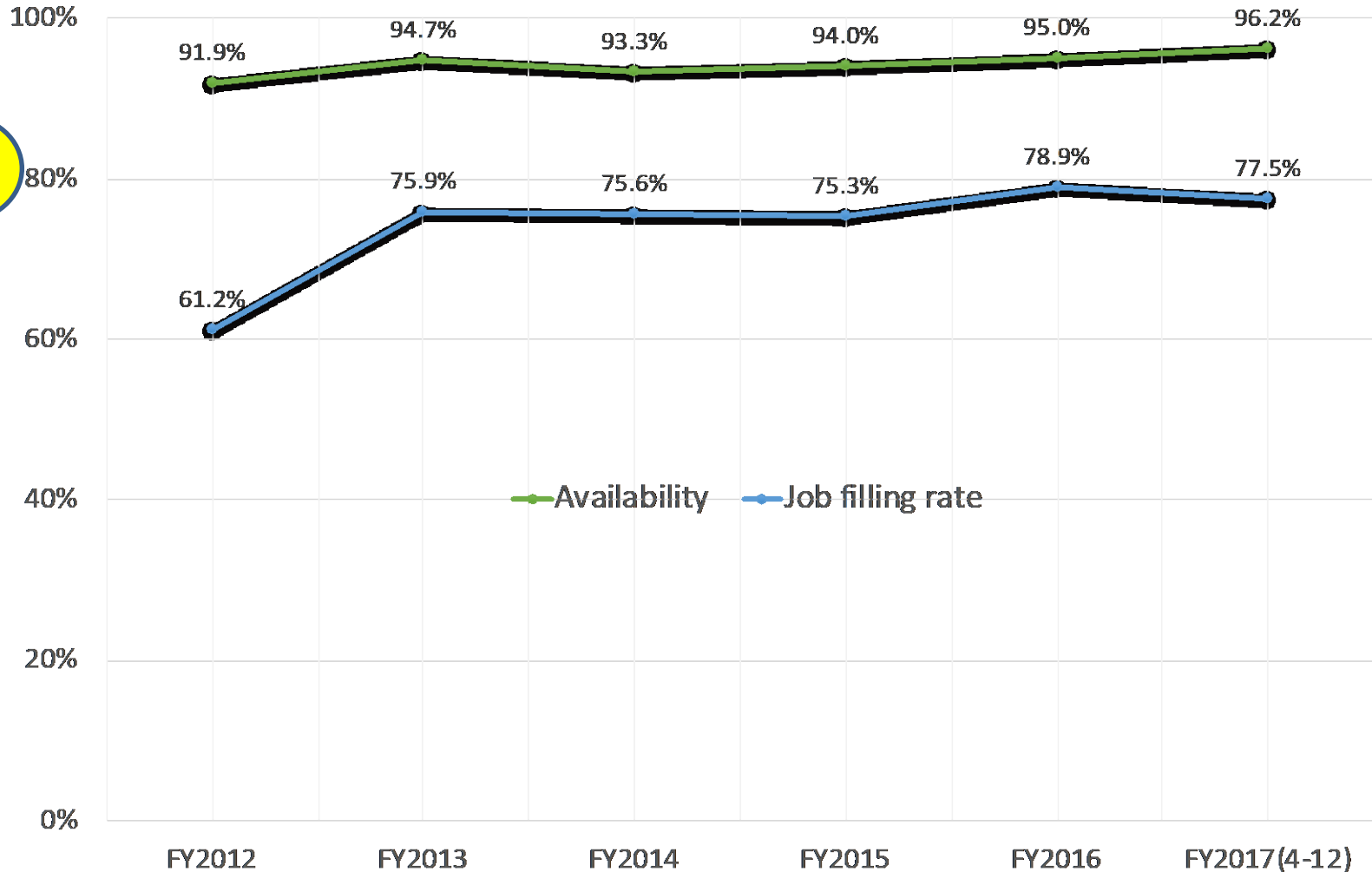
7-8 February, 2018



K computer

# Operation of K computer(1/3)

## Yearly system availability and job filling rate



→ The operation of the K computer is very stable.

# Operation of K computer(2/3)

## K computer in major rankings

System (Nation)	TOP500	Graph500	HPCG	Entry/Upgrade
Taihu light (China)	1	2	5	06/2016
Tianhe-2 (China)	2	10	2	06/2013
Piz Daint (Switzerland)	3	N/A	4	06/2017
Gyokou (Japan)	4	N/A	N/A	06/2017
Titan (USA)	5	N/A	9	11/2012
Sequoia (USA)	6	3	8	06/2012
Trinity (USA)	7	N/A	3	11/2015
Cori (USA)	8	N/A	7	11/2016
Oakforest-PACS (Japan)	9	N/A	6	11/2016
K computer (Japan)	10	1	1	11/2011

K computer is still competitive for real applications.

→ The K computer project is almost succeeding.

## Publication database

	Kinds of Projects (Publications due to multiple projects will be counted as the number of each cell) <span style="float: right;">Display Mode</span>										Total	Number of publications
	Research Areas of HPCI Projects											
	Bio-science, Life Science	Matters, Materials, Chemistry	Environment, Disaster Prevention, Mitigation	Manufacturing Technology, Industrial Innovation	Fundamental Physics, Elementary Particles, Space Engineering	Energy	Information Engineering, Computer Science	Computational Science	Other Areas	K for Enhancement		
Refereed Paper	128	285	130	127	115	34	4	15	20	47	905	837
Non-refereed Paper	30	15	41	29	10	5	0	1	4	6	141	133
International Conf., Symp.	217	279	335	221	264	92	1	12	12	174	1607	1493
Domestic Conf., Symp.	348	281	231	321	175	65	2	8	24	93	1548	1452
Research Meeting, etc.	164	119	111	58	107	9	1	4	11	60	644	608
Public Lecture meeting, etc.	144	31	36	27	34	0	0	0	1	18	291	277
Media: Newspaper, TV, etc.	291	50	154	10	55	0	0	1	3	0	564	558
Books	8	2	5	0	0	0	0	0	1	0	16	15
Code, Database published	5	3	0	1	0	0	0	0	0	1	10	10
PAT, applied	3	7	0	0	0	0	0	0	0	0	10	10
PAT, granted	0	3	0	0	0	0	0	0	0	0	3	3
<b>Total</b>	<b>1338</b>	<b>1075</b>	<b>1043</b>	<b>794</b>	<b>760</b>	<b>205</b>	<b>8</b>	<b>41</b>	<b>76</b>	<b>399</b>	<b>5739</b>	<b>5396</b>

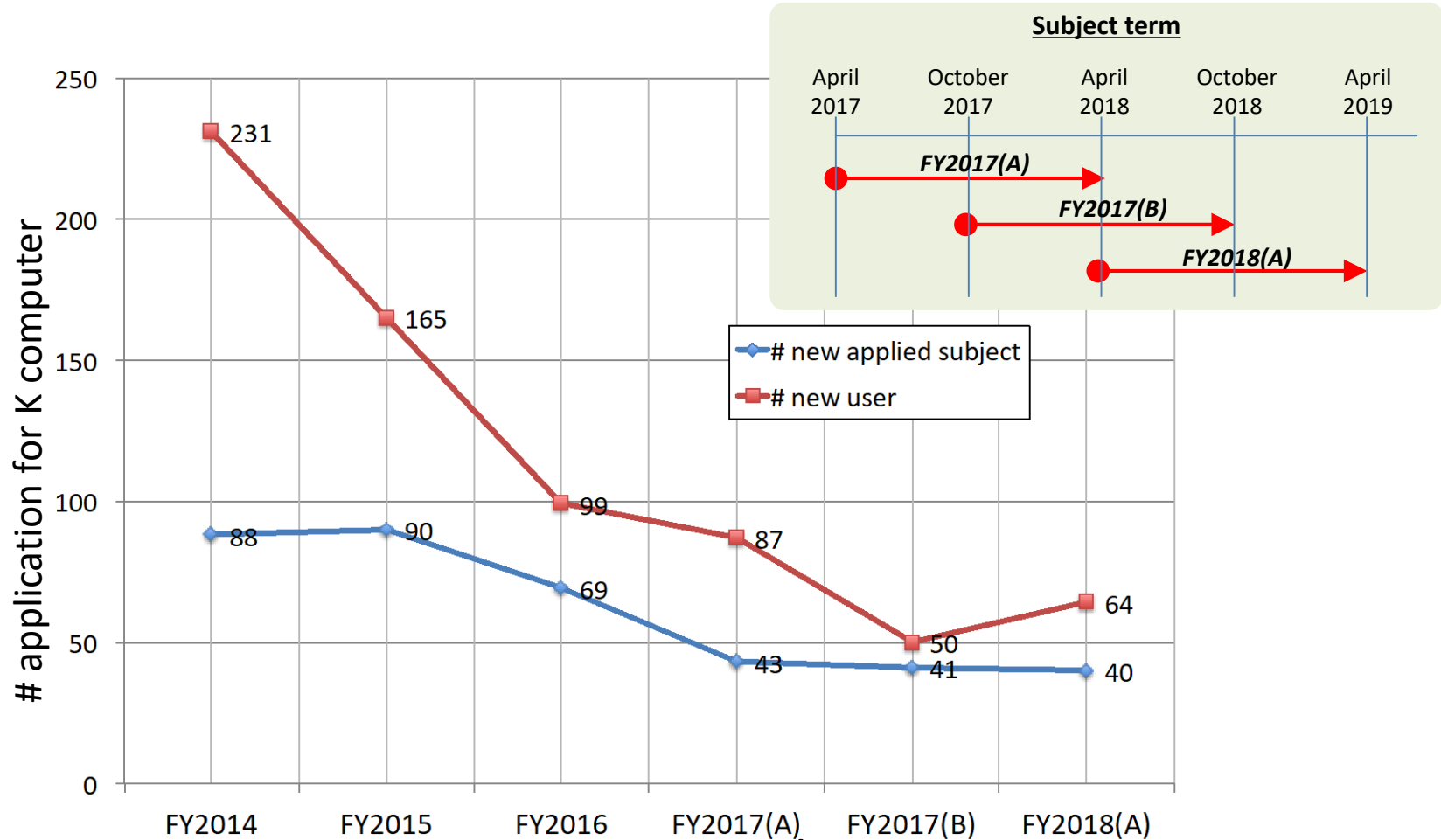
<https://www.hpci-office.jp/hpcidatabase/publications/search.html?lang=en>

More than 5,000 publications derived by K computer have already been released.



# Operation of K computer(3/3)

## # new application for K computer based on user/subject



Applications from new subjects/users are decreasing.

→ **Promotion for new users and fields is needed.**

# New users/fields? How?

- **Improvement about hardware**
  - Cloud type Pre/Post environment of K computer for various use including new fields of science (e.g. Data analysis, AI, etc.)
- **Improvement about software**
  - Increasing ready-to-use software (incl. “**AICS software**”) which is attractive to new users on K computer
- **Improvement about others**
  - Selection method for pioneering and innovative subjects
  - Remote-controllable data (HDD) delivery service
  - Active tuning support based on job execution data analysis

# “AICS Software”

- The software developed and ported by RIKEN AICS
- Current line up consists of about 40 software (listed below)

<http://www.aics.riken.jp/en/k-computer/aics-software>

Name	Description
<b>System Software Research Team</b>	
Carp	Carp is software to parallelize computation for any possible combination of two records in dataset. The software users do not need to write any parallel program, but write just sequential programs. All parallelizing tasks are done by the Carp software.
EARTHONIX	EARTHONIX on K is a derivative version of EARTH (Effective Aggregation Rounds with Throttling) optimization framework towards high performance MPI-IO. EARTHONIX on K is optimized to achieve high performance MPI-IO using a local file system (LFS) of the K computer.
NetCDF	NetCDF is a set of software libraries and self-describing, machine-independent data formats that supports the creation, access, and sharing of array-oriented scientific data. We provide NetCDF library and related libraries (HDF5, Parallel NetCDF and Szip) on the K computer compute hosts and frontends.
PRDMA	The PRDMA library provides a fast implementation of MPI Persistent Communication primitives to reduce the communication latency and to improve the overlap between computation and communication over an RDMA-enabled interconnect.
<b>Programming Environment Research Team</b>	
MUMPS	MUMPS (Multifrontal Massively Parallel sparse direct Solver) is a package for solving sparse linear systems using the direct method. MUMPS supports MPI parallel procedures.
Omnix ScalableMP	Omnix ScalableMP is a compiler for a parallel programming language ScalableMP which is a directive-based language extension for Fortran and C. Using Omnix ScalableMP, you can develop parallel programs effectively.
Scalasca	Scalasca is a software tool that supports the performance optimization of parallel programs by measuring and analyzing their runtime behavior. The analysis identifies potential performance bottlenecks - in particular, those concerning communication and synchronization - and offers guidance in improving their causes.
<b>Large-scale Parallel Numerical Computation Technology Research Team</b>	
EigenXa	EigenXa is a high performance eigenvalue solver, which is developed as a successor of EigenK. It is turned up on the K computer. As EigenK does, EigenXa also solves a standard eigenvalue problem for a dense real symmetric matrix, and it performs very fast even with large-scale parallel computations and small scale problems.
EigenK	EigenK is an eigenvalue solver, which is developed to work on the K computer efficiently. EigenK solves a standard eigenvalue problem for a dense real symmetric matrix. EigenK performs large-scale parallel computation and small scale problem faster than the existing eigenvalue solvers do.
SMATH_RANDOM	A library of random number generator by the Mersenne Twister, a high-quality pseudorandom number generator, for a distributed parallel processing environment. Available for Fortran 90, C, and C++.

<b>HPC Usability Research Team</b>	
CGA/EST	For improving the performance of an application, we have to comprehend the application's source code. In order to facilitate comprehension of source code written in Fortran, this utility analyzes its syntactic/semantic structures and then provides outline views of loop-nests and call trees decorated with source code metrics.
Estree	Estree is the package devoted to generate Paraver trace-files for a post-mortem analysis. MPI applications written in Fortran, C, or C++ can be analyzed in detail using the trace files with Paraver.
Eclipse PTP for K and FX10 computers	This software is necessary for using Eclipse PTP IDE with K and FX10 computers. It consists of 2 packages: (1) Target System Configurations: necessary for submitting jobs to K and FX10 computers. (2) LSL-DIA Driver for PTP: to be installed on K and FX10 user home directory to enable Eclipse PTP monitoring feature.
TAU	TAU Performance System is a portable profiling and tracing toolkit for performance analysis of parallel programs written in Fortran, C, C++, etc. It supports performance instrumentation, measurement, analysis and visualization. Application profiles show the exclusive and inclusive time spent in each function, how many times each function was called, how many profiled functions did each function invoke, and what the mean inclusive time per call was. Application traces show when and where event occurred in terms of the process that executed it and the location in the source code.
Xcrypt	Xcrypt is a scripting language that enables us to easily write a script to manage a number of concurrently running jobs. It provides a unified interface that handles differences in system interfaces of various supercomputers; users do not need to learn each interface. Furthermore, Xcrypt has a mechanism that allows users to add various useful features as modules; some important features are integrated in Xcrypt as standard modules.
<b>Discrete Event Simulation Research Team</b>	
OACIS	OACIS runs as a web server on Mac or Linux to manage simulation executions and their results. After a user sets simulation parameters, OACIS creates shell script files for these parameters and submits them to the specified remote hosts. After these jobs are finished, the results are automatically downloaded and stored in the specified directory.
<b>Computational Molecular Science Research Team</b>	
NTChem	NTChem is a high-performance software package for the molecular electronic structure calculation for general purpose on the K computer. It is a comprehensive new software of ab initio quantum chemistry made in AICS from scratch. NTChem contains not only standard quantum chemistry approaches but also our own original approaches. NTChem is expected to be a useful tool in various computational studies for large and complicated molecular systems. *Web Page: Under construction
<b>Computational Materials Science Research Team</b>	
2D-DMRG	The 2D-DMRG is developed to study quantum lattice systems. The 2D-DMRG is optimized to perform high performance massively parallel computations on the K-computer. Although the DMRG method is used to study one-dimensional systems, the 2D-DMRG can be used for higher dimensional systems. Also, the 2D-DMRG can be employed to investigate an arbitrary shape of systems and many kinds of quantum lattice models. *Website is in Japanese

<b>Computational Bioinformatics Research Team</b>	
GENESIS	GENESIS is a high performance molecular dynamics and modeling software. It consists of two simulators, ATDYN and SPOYN. SPOYN shows high speed and good scalability on massively parallel computers. ATDYN is capable of multi-scale simulations using coarse grained models and all atom models. Generalized ensemble simulations including replica-exchange molecular dynamics and replica-exchange umbrella sampling methods are available.
<b>Particle Simulator Research Team</b>	
FDPS	FDPS is an application-development platform. It helps researchers to develop software for particle simulations which run efficiently on massively parallel computers such as K computer. By using FDPS, researchers without much experience in tuning or parallelization can develop applications which run efficiently on tens of thousands of nodes.
<b>Computational Climate Science Research Team</b>	
SCALE	A library for weather and climate simulations, and an atmospheric large-eddy simulation model using the library. These are developed with co-design by researchers of computational and computer sciences to achieve high performance in massive parallel computer systems.
<b>HPC Programming Framework Research Team</b>	
Apache Spark	Spark is a big data processing framework developed by Apache Software Foundation. It has been built to use on K computer as well as R language on K computer. The installation also includes scripts to use Spark as a job on K.
KMR	KMR (K Map-Reduce) is a high-performance map-reduce library designed to ease programming on data processing on the K computer. It is based on the popular framework in the cloud computing, but its execution is much efficient by exploiting the power of supercomputers.
Fortran90c6	Patched LLVM compiler for using Fujitsu extensions of SPARC64.
<b>Advanced Visualization Research Team</b>	
CDIO	This CDIO library provides following functions for the Cartesian structured data. - Management of distributed files - Restart from previous calculated data (standard) - Restart from previous calculated data of the number of different process - Restart from previous coarse data with interpolation - Raging helper - File converter utility
CPMD	CPMD is a C++ class library to efficiently assist the development of unsteady physical simulations. This library provides functions such as the management of partitioned subdomains by domain decomposition method and wrapper functions for neighbor and global communications.
GridB	This C++ Information library provides functions to calculate intersection between polygon face and background grid, and to manage generated information. Both Cartesian and Octree grid data structure can be utilized for the background grid. <i>Previous version</i> is available as public software.
FFV-C	FFV-C is a 3D unsteady thermal flow simulator developed to execute high-performance simulation of fluid flow around complex geometries by using Cartesian grid. One of the major features of this simulator is the automation of the grid generation process, widely recognized as a difficult task in fluid flow analysis, which makes it possible to reduce considerably the large-scale simulation time. Another noteworthy feature is the fine-tuning implementation which contributes for a weak scaling performance of over 90%, using the full computational nodes of the K computer. The FFV-C has continuously been developed to aggregate functionalities for assisting real-world design tasks in the engineering fields.

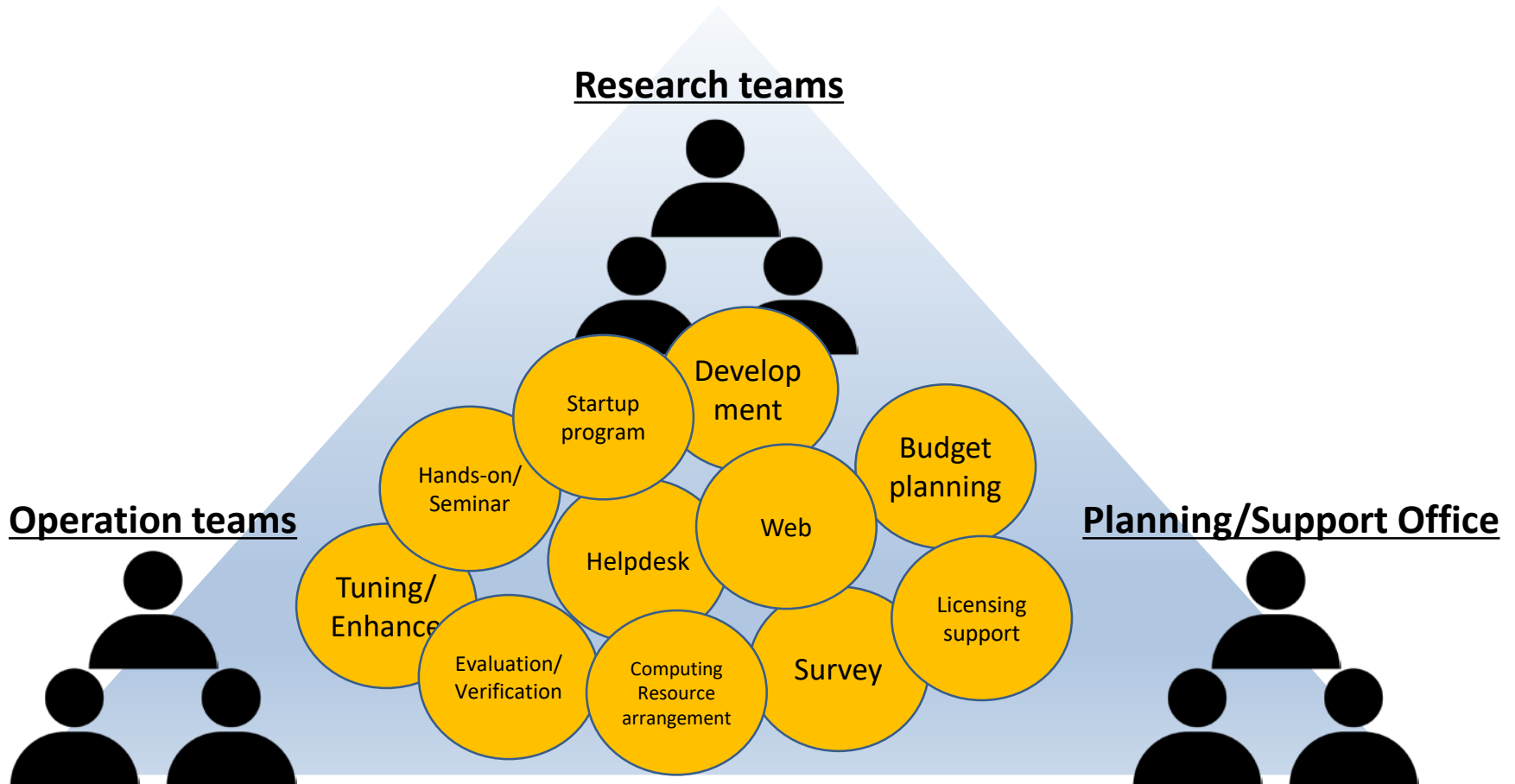
HIVE	HIVE is a visualization framework designed to be user-friendly, functional and convenient in a highly parallel environment. It can perform parallel rendering with multiple nodes on the K computer. It is being developed to be portable to many different computing platforms, be capable of executing in both local and remote mode, be highly scalable, be flexible for aggregating new functionalities, and be easily portable and maintainable. It is currently available as a beta version for Mac and Linux in the binary package format.
Knowledge	A collection of original general-purpose C++ APIs, developed at AICS. Included APIs are: (1) Automatic memory management with flat time-complexity performance, and enhanced stability and debugging features; (2) Object serialization/deserialization API that turns embedded objects to and from XML, BSON, etc.; (3) Broad range of I/O streams including network I/O; (4) Multi-level multi-channel logger; (5) Exceptions with printable/serializable stack trace; (6) Range Arithmetic for facilitation of distributed stencil computation, (7) Thread, Mutex, Condition and Java-like System classes.
KnobRBA	C++ library for creating KnobRA agents. The Knowledge Request-Broker Architecture or KnobRA technology is the world's first distributed programming environment that uses "agents" in place of "objects" as general-purpose programming component models. Its purpose is to offer a higher level of abstraction, and with it higher autonomy, portability, flexibility, extensibility, and stability. Agents created using this library can be executed using KnobRA Agent Runtime Environment (ARE) on a cluster or any distributed system.
PMIO	This Performance Monitor library records arithmetic performance of a user code during its execution and reports the summary. The PMIO is able to use for both serial and parallel environments including hybrid (OpenMP & MPI) code.
PolysB	PolysB is a C++ class library to keep and to manage polygon data, and has following functions: - Load and save polygon data. The file format is STL. - Management of polygon data on distributed parallel environment. - Search and retrieve polygon data - Grouping by input parameter file (text parser format) - Data movement and migration between subdomains <i>Previous version</i> is available as public software.
TextParser	Text Parser library enables us to handle YAML like simple parameter structure instead of a heavy XML parsing library.
<b>Software Development Team</b>	
K-scope	K-scope is a source code analysis tool with graphical user interface for Fortran 90 and FORTRAN 77, which visualizes program structures such as loop, branch and procedure call as bottom-up. By the K-scope, application performance engineer can understand overview of source codes for starters. (This software is Java application for Commodity-PC, not the K-computer.)
Performance Analysis tool by once, "IPAWat"	This software is the tool on the K computer to display the results of the basic performance analysis and time breakdown analysis that are output as profile results by Precision PA analysis function.
<b>System Operations and Development Team</b>	
Waiting for the K	This tool calculates a waiting time of a job on the K computer.

- Information quality of web page strongly depends on developer's effort.
- Promotion activities of AICS software are independent by software.

# RIKEN AICS Software Center

- To accelerate the AICS Software activity, RIKEN AICS Software Center was founded in 2017.
- The missions of AICS Software Center are:
  - to develop and deploy high quality applications, libraries, programming tools, etc. (called "AICS Software") for many HPC platforms including the K computer and the successor.
  - to support and collaborate with AICS Software users from various fields of science and engineering to improve and enhance the AICS software.
- Organize
  - AICS Software Committee (Chair: Director)
    - Webpage WG, Tuning/Enhance WG, User support/Promotion WG

# Members & tasks



All tasks & issues are shared and solved by all of members.



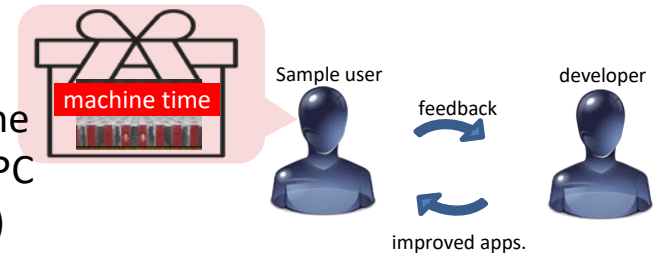


# Actions in FY2017(2/2)

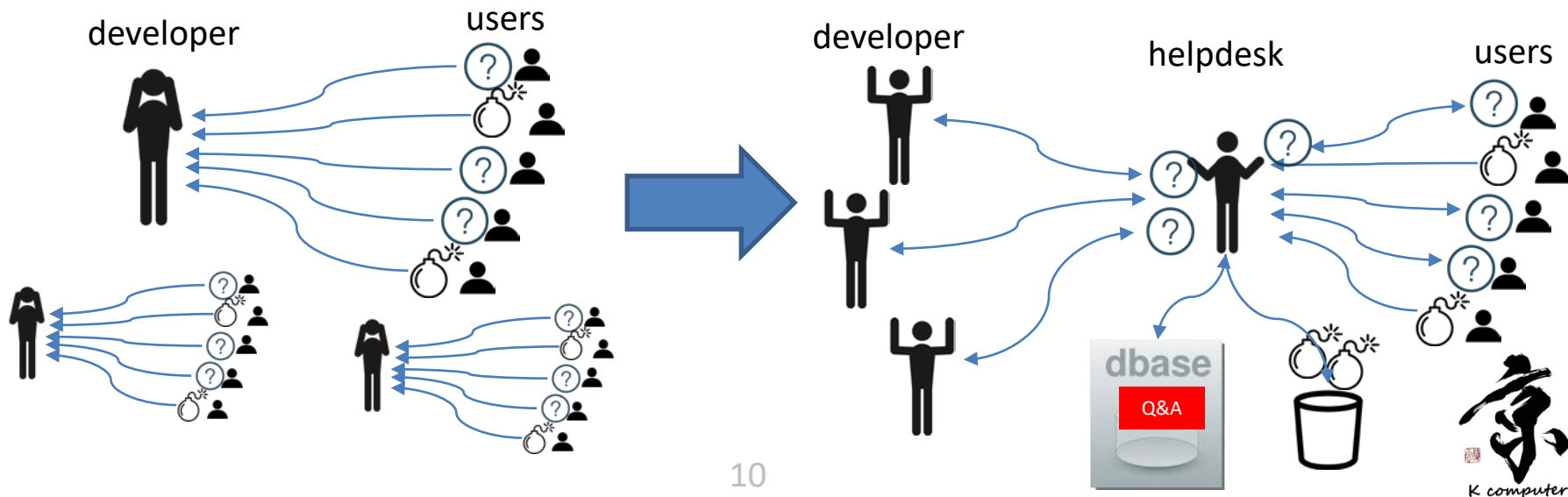
## • “Sample User Program” (in preparation)

A startup program for new HPC users

1. Someone who is interested in AICS Software can apply to join this program as a sample user of AICS software.
2. We provide sufficient machine time of the K computer and special user support for 1 year.
3. Sample user gives us feedback for improvement and enhancement of the software.
4. Developer improve and enhance the software based on the feedback and the sample user experience a world-class HPC environment/Apps.(and grow up to big HPC users/expert.)



## • Reconstruction of helpdesk system (in preparation)



# Plans in FY2018

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- Fix name & logo (AICS → R-CCS)
- Expand the software lineup and web contents
- Ignite the “sample user program”
- Hands-on/seminar support
- Port to the other HPC platforms

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Thank you for your attention