Report of the 2016 RIKEN AICS Advisory Council

Meeting of the Advisory Council of the RIKEN Advanced Institute for Computational Science (AICS), August 29 – August 31, 2016, Kobe, Japan

1. Preliminary Information

Members of the AICS AC

Jack Dongarra	Prof. Dr.	University of Tennessee, USA		Computer Science
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William Kramer	Dr.	Director, Blue Waters, NCSA, USA		Computer Science
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Hiroshi Niino	Prof. Dr.	Atmosphere and Ocean Res. Inst., University of Tokyo, Japan		Atmospheric Science
Satoshi Sekiguchi	Dr.	Director General, Nat. Inst. of Adv. Ind. Science & Tech. , Japan		Computer Science

Information provided to the AICS AC

- Meeting Program of AICS AC 2016
- White Paper of AICS AC 2016 (Basic Information, Overview, Future Plans, Appendix)
- Activity Report of AICS AC 2016 (Operation and Computer Technologies Division)
- RIKEN AICS Brochure (K Computer: System, Facilities, Research, Future, Post K)
- AICS' Research Teams Brochure (Research Highlights of R&D Activities)
- Presentations of RIKEN and AICS Leading Scientist: Yoichiro Matsumoto, RIKEN Executive Director; Kimihiko Hirao, AICS Director; Fumiyoshi Shoji, Director of Operations und Computer Technologies Division; Akira Ukawa, Director of AICS Research Division and Deputy Director of AICS; Yutaka Ishikawa, Project Leader of Flagship2020 Project;
- Presentations of Research Teams
- Interviews with Team Leaders and Researchers

Tasks of the AICS AC

The AICS AC is tasked with reviewing the activities of AICS from 2010 to 2016 following the ToR for review as laid out by the RIKEN President, which is supplemented by the ToR laid down by the AICS Director. Both ToR are included in the White Paper of the 2016 AICS AC.

Information and recommendations from previous reviews

Since the RIKEN AICS was founded on July 2010, no previous review of the AICS by the AC under the RAC framework has taken place. Hence, the present review is the first one.

Glossary

AC	Advisory Council
AICS	Advanced Institute for Computational Science
HPCI	High Performance Computing Infrastructure
JLESC	Joint Laboratory on Extreme Scale Computing
MTBF	Mean Time between Failures
MTTR	Mean Time to Recovery
PUE	Power Usage Effectiveness
RAC	Riken Advisory Council
RIST	Research Organization for Information, Science and Technology
ToR	Terms of Reference

2. Introduction

The meeting of the Advisory Council of the RIKEN Advanced Institute for Computational Science (AICS) took place from August 29 to August 31, 2016, in Kobe, Japan. The period under review, 2010 to 2016, enjoyed the internationally celebrated highlight of the inauguration of the K Computer System of 2011, from this time on for two periods being at position one of the fastest supercomputer systems worldwide on the Top500 list, and being present among the top 5 ever since then. This success is not accidentally; as corroborated by the first position of the K computer in the Graph500 list and the second position in the new HPCG benchmark, it demonstrates Japan's strategic vision as to the K computer together with high operational quality and impactful accompanying research at AICS.

In section 3 of this report, the AC presents the evaluation of AICS. Section 4 conducts a SWOT analysis of strengths, weaknesses, opportunities and threats as distilled in Section 3. In section 5, a summary of specific measures is given, while, Section 6 lists the AC's recommendations.

3. Evaluation and Findings

In the following, the evaluation of AICS by the AC is described in the order of the ToR of the AICS director. The report of the AC is taking into account the ToR of the President of RIKEN in the evaluation comments.

3.1 Operation and Management of the K Computer

The first major objective in the threefold mission of the AICS is "to operate the K computer and to provide its top-level resources to users both in academia and industry". These tasks comprise operation, management and R&D for the enhancement of the system along with the peripheral facilities like networks system, air conditioning, chillers, and power generators. This objective entails in addition the technical coordination of the HPCI system operation along with R&D for its enhancement.

First of all, the AC acknowledges that the AICS Operation and Computer Division is delivering outstanding work in operating, managing and improving the K computer, having reached a world-class level. Given the sheer size and complexity of the machine as well as of its technical and support periphery, the AC considers the well-balanced division structure with 24 technicians and researchers for this task – supported by about 30 technicians of Fujitsu – as fully adequate, absolutely necessary and as the major strength of the division. The users enjoy high system availability with an MTBF of more than 18 days, excelling most leadership-class systems in China, Europe and the USA. At the same time, its MTTR is only about 10 hours. In addition, a careful tuning and optimization of power generation, consumption and heat re-use has been successfully achieved, leading to a remarkably low PUE. The development of a smart energy management system is a major opportunity that the AC encourages the team to pursue.

The division has managed by various means, e.g. resolving the early time file system problems and introducing asynchronous file staging, to boost the job-filling rate from 60% to 75%, a fully adequate value, given the more effective block-wise node allocation chosen. Still, the AC considers it as an important opportunity to continue the efforts in improving the job-filling rate without compromising the capability of the system. This might be realized by a combination of improved back-filling methods with a closer involvement of the users in the monitoring of the system, by offering a 3D-realistic web-based system allocation panel.

The AC is concerned about the apparent separation of AICS with respect to the end users of the K computer. The AC sees this separation as a structural weakness that concerns both the AICS Operation and Computer Division and the AICS Research Division. The AC has the feeling that only an indirect communication channel to the users via the RIST 2nd-level support team is established at this time. Both, 1st-level support as provided by the AICS Operation and Computer Divi-

sion, as well 3rd –level support as provided by the AICS Research Division through community oriented methodological research would strongly profit from more transparent and direct ways of user feedback. A unified trouble ticket system might be a first step in this direction. The positive effects on the co-design activities of the Flagship2020 Division through direct user feedback with the AICS teams seem evident.

While one might consider the number of publications per person of this division as a weakness of the division, the AC recognizes that technical work very often must be prioritized against research publications. The AC welcomes further that the division is prepared to increase their publication rate according to their self-assessment, which is certainly in the genuine interest of the majority of team members with fixed time contracts.

Indeed, the AC is concerned about limited permanence of positions, which poses some threat of loosing or not being able to attract good people in the future, especially in the operational sector. This was discussed in the interviews of researchers.

3.2 Research in Computer Science and Computational Science

The second major objective of the mission of the AICS is "to carry out leading-edge research toward breakthroughs in science and technology through the close cooperation of computational science and computer science". This comprises "research of basic technologies for advancing the usage of the K computer" and "advanced research in computer and computational sciences". As detailed below in the summary of the team leader presentations, this young division is able to present a huge mass of very impressive results in research and development for many use cases.
On the one hand, the algorithms, tools, models and methods developed to advance the usage of the K computer, funded through MEXT's grant-in-aid, enjoy a steadily increasing utilization by the user community (including more than 140 companies). In fact, the AC is absolutely con-vinced that the performance improvements reported pay off by factors through a much more effective exploitation of the system by the users of these software instruments, compared to the expenditure required to fund about 110 researchers in the 16 teams of the division.
On the other hand, all these developments created are, at the same time, investments into the future, as they also help defining scientific requirements on the post K architecture, see section 5.3, and will be available for the post K system right from its start. 18 computer scientist and 14 computational scientists from the Research Division are also involved in the activities of the Flagship2020.
What is more, the advanced research of the division in computer and computational sciences, co-funded through bottom-up external funding by the Hyogo Prefecture and the City of Kobe, competitive funding through JST, JSPS, MEXT, and a small management expenses grant by MEXT, has considerably increased AICS' excellence in science.
The unifying paradigm and unique feature of the division's research strategy is the living interaction between computer science and computational science, which is – to the satisfaction of the AC – realized in a multitude of activities between the fields. Many scientific highlights, 32 codes at full scale on the K computer and an impressive number of papers and citations prove the strength of the division.
The group has created important cooperations with the leading supercomputing centers worldwide showing its international standing; one example is the JLESC consortium. Quite a few international scientific symposia have taken place in the reporting period.
Finally, the AC would like to comment on weaknesses, opportunities and threats for the division: Smaller weaknesses appear in the educational activities: the training would certainly have high-er impact if it was held in English and transmitted via web broadcast. A systematic visitor's pro-gram would be desirable as well.

While there are discussions on building a Software Center, at this time there is no tangible long-term software maintenance plan, which is considered as a weakness of the AICS.
Data science is ever deeper dominating the entire field of science. The AC considers this an important opportunity for the AICS. Given the huge activities in the direction of data sciences in Japan and worldwide, the absence of an environment and support structure that enables data science focused projects on the K computer, including machine learning, is considered as a threat for the AICS. In fact, the SWOT analysis in Section 6 shows that the AICS can easily com-pensate threats by its strength and is able to turn weakness into pursuing opportunities.

3.3 Development of the Post K Computer

The third major objective of the mission of the AICS is "to lead the development of Japan's future strategy for computational science, including the development of the follow-up to the K computer", i.e., the so-called Flagship2020 project. The ACs judgment is mainly based on information not being under non-disclosure, as given in the division leader's presentation. From this infor-mation, the AC is impressed by the progress in the design efforts achieved. The AC is convinced that expertise and experience in AICS is a huge strength and will enable it to successfully carry out its Flagship2020 responsibilities to develop the post K supercomputer together with the right combination of communities, skills, and collaborations. The selection of ARM as the core technology is an innovative chance for AICS and potentially will have great impact in the entire HPC ecosystem. The post K system based on ARM gives AICS the opportunity for much larger community impact and therefore should be highly visible. It is however important, to start ac-quiring competence with ARM processor technology for a broad range of tools and applications codes very soon.
It is foreseen that other systems in HPCI will help to fill the provision gap when the machines are replaced. A delay in the provision of post K certainly poses a risk to Japan's science infrastructure. The AC thinks, that longer delays could be compensated by provisioning an intermediate system with similar capability as the present K at much smaller footprint and modest expense.
Furthermore, the Flagship2020 project encompasses the development of a wide range of application codes to run on post K, in order to solve major social and science issues. Nine co-design fields have been selected, ranging from protein sciences via weather prediction to fundamental physics.
The AC acknowledges the progress achieved and welcomes the co-design as a most effective means to pursue an application oriented development of post K.

3.4 Feedback from Staff Interviews

The AC has asked for having a direct unbiased discussion with staff. The AC considers the situation, the concerns, the constructive proposals and suggestions of younger team leaders and researchers as very important for inclusion into this evaluation, to sharpen the recommendations.
The conclusion from the interviews is provided to the AICS AC management in form of a sepa-rate document.

4. SWOT Analysis

SWOT	Helpful	Harmful
Internal	**Strengths** 1. Strong and well balanced operation and technology teams 2. Excellence in computer and computational science 3. Convincing R&D structure and organization for post K	**Weaknesses** 1. Only indirect interaction with end users via RIST 2. Competences for data curation and discovery are underdeveloped 3. ARM needs considerable adaption of existing codes
External	**Opportunities** 1. User transparent monitoring can improve K's effectiveness 2. Supporting data science will expand the impact of K systems 3. ARM processor opens door to wider community	**Threats** 1. Decreased interest of young technicians w/o permanent positions 2. Only few users in societally relevant data sciences (medicine etc.) 3. In case of delay of post K, there is a detrimental gap in capability

The AC focuses its SWOT analysis on a few relevant topics in order to derive strategic advice. The discussion follows the numbering in the table for each of the five items:

1. Operation and Management

The AC considers the outstanding operation and technology teams an important strength of AICS. The interviews made evident, that the members of staff want to be able to plan their carrier at AICS, as it is harder to find new job opportunities for technicians than for researchers. Some more permanent position would mitigate this risk.

The AC considers the purely indirect interaction with users as a weak point. Measures like more transparent web-based monitoring or a uniform User Service Request Ticket System accessible byall AICS staff are perfect opportunities to improve on the user interaction and improve effective-ness like the job fill-rate 8

2. Research

AICS excellence in computational and computer science is a good starting point to engage in attracting more users in emerging data sciences, such as medical imaging or other fields relevant for society.
The AC considers data science an important opportunity to enhance the impact of the K systems. An important step can be accomplished by developing proper data curation competences.

3. Post K

A delay in the provision of post K is considered less probable, given the strength of the consorti-um. Still it is a threat of high impact. While HPCI is foreseen to fill the unavoidable provision gap when the machines are replaced, longer delays could be compensated by provisioning an interme-diate system with similar capability as the present K, at much smaller footprint. While the transition to ARM requires substantial adaption of existing codes, this weakness will turn into an opportunity, as the new processor technology will attract a much broader scientific ecosystem.

For all three fields discussed in the SWOT-analysis, weakness can be turned into opportunity and strength can immunize the AICS against risks.

5. Mid to Long-Term Policy (5 to 10 Years)

The AC strongly encourages the AICS to continue to strive being a world-class supercomputing center as a hub for science and technology innovation by doing leading-edge research of basic technologies for advancing the usage of the K systems as well as advanced research in computer and computational sciences to increase excellence. The AC recognizes that the AICS is following the five strategic topics of the initiative on scientific excellence of the RIKEN president and recommends continuing in this direction in a ten years perspective.

5.1 Comments on the Future Plan of AICS

The AC fully endorses the future plan of AICS, presented by Director Hirao. The plan is based on the three mission statements of AICS as presented in sections 5.1, 5.2 and 5.3 of this document. The AC is convinced that, following the plan, AICS will develop a worldwide leading large-scale supercomputer system in Japan, i.e. the post K supercomputer, AICS is will become a world hub for computer and computational science, and AICS will foster breakthroughs in simulation, en-semble computations, data analytics, and data assimilation. The AC is looking forward to see how this vision will materialize..

5.2 Policy on Software Sustainability

The impact of the work at the AICS on novel algorithms for the next generation Exascale com-puters can be greatly increased if key computational kernels developed at AICS can be made available as open source software to be used by the community at large. Development of such software can provide great visibility and reputation to the AICS and help cement the reputation of RIKEN as a "destination". However, this is best done by professionals specialized in the de-velopment of high quality software rather than graduate students or post docs, whose focus, rightly, is on advancing research. Even though hiring professional software engineers can be quite expensive, the AC highly recommends allocating resources to address this need.

5.3 Policy on Data Science

While the AICS has focused on simulation and key mathematical tools such as linear systems solvers, there is an excellent opportunity to expand the focus substantially into the general area of data analytics. This is important for a number of reasons as outlined below.

Progress in science and engineering is increasingly dependent upon our ability to analyze very large data sets that are becoming available due to advances in sensors and instruments as well as computational simulations. This is often referred to as the fourth paradigm of scientific discovery, with theory and experimentation being the first two paradigms and computational simulation as the third paradigm.

Even the massive amounts of computational simulation output create opportunities for novel data analytics. In particular, novel algorithms are needed to extract patterns from space-time data sets that can identify features and regions of interest (e.g., vortices in a CFD simulation) and even help steer the computational simulations.

AICS's expertise in the development of algorithms that are power efficient and minimize data motion (as opposed to arithmetic operations) can be very valuable in improving a host of traditional data analytics algorithms including those that are not based on linear algebra (e.g., association pattern mining, k-means clustering, and deep learning kernels).

In addition, the AICS should carry out further efforts to bridge the integration of simulation and experimental science by data assimilation, in order to accelerate discovery across many areas of science using the K systems.

6. Response w.r.t. ToR of the RIKEN President

The ACs has received evaluation criteria by the RIKEN President: 1. Does the Center possess R&D achievements and personnel meeting international standards, produce world-class results and benefits for society, what is the standing in the field along with strengths/weaknesses and a policy for 5 to 10 years? (Criterion 2. not applicable); 3. Alignment of the activities with five strategic goals, prospects to fulfill them and new policies: (1) pioneer a research management model – (2) lead the world in R&D – (3) become a hub for S&T – (4) be focal point for global brain circulation – (5) foster world class leaders in research; 4. How effective and appropriate does AICS maximize RIKEN's achievements as a whole, including collaboration between the RIKEN centers.

1. The AC is impressed by all AICS divisions delivering world-class results with respect to international standards: (i) AICS' *Operation and Computer Division* is an international role model as to operating, managing and improving the K computer; (ii) AICS' *Research in Computer and Computational Science Division* is pushing the effectiveness of the K computer through algorithms, software and libraries, is highly ranked in the international TOP500 and Graph500 lists, and shows impressive numbers of papers, many in societally relevant fields; (iii) AICS' *Flagship2020 Project Division* brings together strong expertise in AICS and the right combination of communities and collaborations as a sound basis for co-design. As to the knowledge of the AC, there is no comparable co-design project worldwide. Besides strengths, the AC could find only few weaknesses and risks for AICS. By means of a SWOT-analysis, the AC became convinced that any weakness can be turned into an opportunity and that its strengths immunize the AICS against risks.

2. Not applicable.

3. The AC acknowledges that AICS is closely following the five strategic topics of the initiative on scientific excellence of the RIKEN President and recommends continuing on this path: (1) The tri-partition of the AICS and the paradigm of interaction between computer and computational science enables most effective R&D management at AICS. The AC gives recommendations 1 and 2 for closer interaction with the user communities as a new policy; (2) The AC recognizes high flexibility at AICS in pioneering new research, *e.g.* data assimilation. In addition, the AC gives recommendations 3 and 4 to establish a Software Center and to pursue methodologies for Data Science including Machine Learning; (3) The AC sees RIKEN AICS as existing hub of technology and innovation, *e.g.* proven through co-design with industry for the K/post K systems. The AC proposes recommendation 5 to sustain sufficient attraction of excellent developers; (4) In recommendation 5, the AC advices to introduce international recruiting programs; (5) International cooperation with world-class centers exist, including an exchange program (JLESC), demonstrating AICS' pursuit of international brain circulation. In recommendation 7, the AC proposes to internationalize training at AICS by using English as the language and broadcasting via the web.

4. The AICS substantially contributes to RIKEN's achievements and visibility from both a national and an international perspective. The exponentially growing field of data science is a unique opportunity for RIKEN to utilize AICS's resources and competences for RIKEN as a whole.

The AC congratulates RIKEN for having established AICS as a marvel of the Japanese research infrastructure, with a focal role in the HPCI ecosystem and highest worldwide reputation.

7. Recommendations

1. The AICS has the responsibility for the quality of usage of the K computer. The AC believes, that this entails to have direct interaction with the end users. A uniform User Service Request Ticket System for all aspects of the K computer service, comprising users, AICS and RIST personnel, would be an effective first step to improve the integration of support activities.

2. Additionally, the AC encourages AICS to set up a yearly workshop of K computer users, AICS experts and RIST support experts for open discussion on important operational topics.

3. AICS has established system and application software development activities for a variety of software capabilities proven relevant for the HPC user community. In order to create long-term impact, the AC endorses to establish support structures for maintenance and improve-ment of these software products like the planned Software Center. In this manner, AICS will gain international recognition as a home for important community-based software capabilities.

4. The AICS should start to substantially extend data science activities during the remainder of the K computer operation in order to actively push the convergence of simulation and data an-alytics – expected by many international experts – for the post K phase, thus transcending ex-isting research fields. In particular this concerns provisioning novel data analytics and ma-chine learning services, and the suitable design of post K software and workflow environ-ments to support data science workloads.

5. AICS faces work force recruitment and retention challenges within the fields of computational science that are relevant to the mission of AICS. The AC recommends establishing three high profile programs: (i) a highly prestigious postdoctoral fellowship program in the areas of computer science and computational science; (ii) programs to engage more graduate students within the structure of AICS; (iii) a robust visitor program.

6. As a general recommendation, valid for any similar institution, AICS should implement suc-cession planning and leadership development activities at all levels of staff.

7. The AICS should carry out training courses in English language as a means for internationali-zation and in addition should broadcast the courses on the web.

Acknowledgments

The AC members would like to thank the AICS scientists and administration for a very effective organization of the review and the friendly, consructive and pleasant atmosphere during the review. Furthermore, they would like to thank the RIKEN for having established AICS as a marvel of the Japanese research infrastructure, with a focal role in the HPCI ecosystem and highest worldwide reputation.

Jülich, October 15th , 2016

Prof. Dr. Dr. Thomas Lippert

on behalf of the AICS Advisory Council, Prof. Dr. Jack Dongarra, Prof. Dr. Kozo Fujii, Dr. William T. Kramer, Prof. Dr. Haruki Nakamura, Prof. Dr. Hiroshi Niino, Dr. Satoshi Sekiguchi