Conference on Computational Physics (CCP2012)

special event

(October 18, 11:00 - 12:30)

Will computational science be able to provide answers to important problems of human society?

Panel discussion on computational science, with the media and 400 participants

Overview

Shared use of the K supercomputer began on September 28, 2012. To mark this occasion, the Conference on Computational Physics (CCP2012) organized under the auspices of the International Union of Pure and Applied Physics (IUPAP) was held in Japan from October 14 to October 18. More than 400 participants from 44 countries participated. On the last day a panel discussion on the theme, "Will computational science be able to provide answers to important problems of human society?" was held as a special event. The general public was represented by members of the media and the discussion involved the researchers in the field of computational science participating to the conference. Simultaneous interpretation was available. With respect to the K supercomputer, which became widely known as a result of the government's budget screening scheme, debate will also focus on how computational science programs using the supercomputer should fulfill its accountability to the taxpayers. The keynote speech was given by Atsuko Tsuji, an editorialist with the Asahi Shimbun. The title was "Requests and expectations for computational science". This was followed by a free discussion with Ms. Tsuji.
Requests and expectations for computational science

by
Atsuko Tsuji
(Asahi Shimbun)

Atsuko Tsuji, science journalist, is editorial writer for the Asahi Shimbun.

She earned her B.A. from Tokyo University in History of Science and Philosophy of Science in 1976. After joining the Asahi Shimbun in 1979, she has been working as a staff writer in various sections as the science news section and the American General Bureau in Washington DC. She was a Knight Science Journalism Fellow at MIT in 1989 and a Reuters Fellow at Green College of Oxford University in 2004.

*Introduction*

I have been told that this CCP2012 conference is attended by over 400 computational science experts and budding researchers from around the world. As a scientific journalist, normally, I would be the one visiting each of you for interviews, so please excuse me for being very nervous about standing here and addressing you, the experts. My role here is to act as a spokesperson for the general public outside and to convey their requests and expectations for computational science. Communication between expert groups and society has become increasingly important. That's why I mustered up the courage to come today, to help in this cause in some small way. I, therefore, appreciate your kind understanding.

First, the poster for this conference caught my attention. It lists everything from physics, chemistry and engineering through related academic fields and industrial applications. This broad scope of applications is one of the key features of computational science. I hear that Dr. Takabe, the chairperson of this event, made it a point to invite researchers from many different fields. In an age
when interdisciplinary collaboration between various fields has become a big issue, I think that it is significant that researchers of various fields have come together in this way. In particular, while it has always been said that engineering and science should work hand in hand, we have not seen much progress in this area, perhaps hampered by cultural differences and other complex hurdles. Breaking through these barriers is a key issue, not only for computational science, but also for Japan's science and technology communities as a whole.

There are, in fact, other issues that have clearly emerged in computational science that are also commonly found in Japanese science and technology today. Some of these may be unique to Japan; others may be found in other countries too. I hope we can learn about, and get your thoughts on, these wide-ranging issues in the discussion to follow. Please look upon my speech as a prelude to that discussion.

**Computational science and the press**

While computational science plays a major role in society, this may not be widely known among the general public. When I checked the Asahi Shimbun article database on how many times the word "computational science" has appeared in our newspaper, I found that it has only appeared in 62 articles. In most of these instances, it was merely used in organization names; there were very few articles on the subject of computational science itself. It first appeared in 1994. This was in reference to a budget request for 2.9 billion yen lodged to the Science and Technology Agency at the time. This would equate to around 30 million dollars. This resulted in the launch of the Earth Simulator project, which became number one in the world in 2002. I also found an article about the establishment of the Frontier Research Center for Computational Sciences at the Tokyo University of Science in 1997 as Japan's first research center for computational science.

What about the word "simulation"? In the mid-1980s, there were only around 40 articles a year containing this word, but more than 100 articles made mention of it for the first time in 1989. From 2000 onwards, there have been around 400 articles a year. This means that, on average, we see the word "simulation" appearing somewhere in the papers every day. Of course, not all of these relate to computational science. Some are used in reference to professional baseball managers "simulating" the game in their mind and various other situations. Nonetheless, at present it would appear to be rare for the field of computational science to come up in the readers' thoughts. This may partly be because it is a relatively new field. Getting the field recognized by more people is a big issue for the future.
The K computer

I heard that the purpose of this conference is also to celebrate the start of the shared use of the K computer, a state-of-the-art supercomputer earmarked by the Japanese government as a key national technology. Shared use was originally scheduled to start in November, after this conference, but was moved forward and has been in operation since September 28. As a Japanese citizen, I hope that K will produce results that only it could provide.

Many of you have probably seen it already. I also had the chance to see the K computer at the ceremony held prior to the start of shared use. It was quite a sight seeing 864 units lined side by side, each unit just a little taller than an ordinary person measuring 2 meters in height. It reminded me of the Terracotta Warriors and Horses in China’s ancient capital, Xian. Needless to say, the terracotta figures were an army of soldiers made of clay that were placed there to protect the body of Shi Huangdi, the first Qin Emperor, in the netherworld. Shi Huangdi commanded a powerful army and overwhelmed surrounding states in numbers during China’s Warring States period, unified the country and became its first emperor in 221 BC. Even today, more than 2000 years later, the wordless statues speak volumes of Shi Huangdi’s immense power. In contrast, the K computer will not endure for so long. The game is about how much it can achieve in a much shorter period of time. The person giving the commands holds the key to this. For the terracotta army, this was Shi Huangdi, for K, it's you. It is up to you
whether you can take advantage of K's capabilities. Of course, the strength of an army is not determined merely by its size. We find many examples of this worldwide, a typical example being the Battle of Red Cliffs in the *Chronicle of the Three Kingdoms*, which gained public attention through the movie *Red Cliff*. Your strategies for controlling your soldiers and your ability to read ahead like Zhuge Kongming (the chancellor of the state and military strategist of Shu Han) will determine whether you can use K wisely or let it go to waste. As researchers, you bear a grave responsibility. Whether we will see revolutionary results will depend on the ingenuity and foresight of the researchers using the computer. In that sense, I think it is particularly important to foster personnel with a wide vision.

The K computer faced many challenges before it was completed. Many of you living outside Japan may not be aware of this, but after the Democratic Party of Japan took over the government, in November 2009, it embarked on "budget screening" to filter out wasteful expenses in government projects and cut down on their budget. This was carried out in the open and attracted much public attention as a new initiative. The K computer, which was under construction at the time, was also subjected to examination. In regards to its development aim of becoming the world's fastest computer, lawmaker Renho asked the representative from the Ministry of Education, Culture, Sports, Science and Technology, "Why No. 1? What's wrong with being No. 2 in the world?" The developers were unable to provide her with a satisfactory answer and a harsh verdict was reached that the budget should be slashed. This footage was aired over and over again, and became a famous symbol of the budget screening initiative. The science community reacted strongly and Nobel laureates joined in issuing a statement in protest. They expressed their fierce objection saying, "If you don't aim to become No. 1, you cannot even become No. 2 or No. 3." In some ways, however, the lawmaker's question was very legitimate; it was something that had to be asked. In the end, the project received virtually the same budget as originally allocated and actually received an extra budget to speed up development. Last year, the K computer was ranked number one in

![Image](image.png)

*Figure 3. Lawmaker Renho at a budget screening on the K computer project. Her comment on K "Why No. 1? What's wrong with being No. 2 in the world?" became very famous.*
the world's top 500 rankings, twice. It was ousted from this top position in June this year by the supercomputer, Sequoia, developed by the Livermore Laboratory in the United States, so it was no longer the fastest when shared use began.

Questions arise, first of all, regarding the method for determining these projects. It is not hard to imagine that those involved in K's development wanted to show off to the rest of the world the advanced level of Japan's supercomputer technology, which came to be known thanks to Fujitsu's Numerical Wind Tunnel and NEC's Earth Simulator. Becoming No. 1 in the world was not one of the Earth Simulator's objectives, but it took the world by surprise when it rose to that position in 2002 and remained there until 2004. As a result, the K computer project got underway with the clear-cut goal of retaking the top position, which was consistent with political and administrative intentions. It is only natural that Ms. Renho asked, "Would you spend 100 billion yen to be No. 1? Is there any point to that?".

As an aside, the term “No. 1 in the world" reminds me of a story I heard from Mr. Sakurai, a former manager of the Honda team which was a constant winner in Formula 1 racing. He was asked by a company executive if it was possible to cut down on the expenses a little, even if the team were to drop to second place, because it was costing the company the not inconsiderable sum of several billion yen a year. To this he answered, "The moment we say it's okay to be second, you'll find we won't even be able to be No. 2". He meant that it is only when you strive desperately to become No. 1 that you have any chance of achieving this, if all goes well. Even then, you could still end up becoming No. 2 by the slightest margin. If you're going to do something, you have to aim for the top.

However, you must be able to explain why. A supercomputer is a tool. Developers should aim to become No. 1 with the results of using this tool and should begin by asking what this would require. This was not the case with K and that's where the problem lay.

Moreover, there was much criticism that K became more costly and inferior in performance to Sequoia because of the insistence on the use of Japanese parts. The aim was to provide support to the Japanese semiconductor industry but the manufacturers ended up stopping their chip production nonetheless.
Deliberation on development plans for the next supercomputer to succeed K is currently underway. I think it is vital to formulate a plan with reasonable objectives, following a series of scientific studies into what type of computer should be built and for what purpose. It is precisely because this was lacking that the developers were unable to answer the lawmaker's question properly.

Behind this issue is the lack of mechanism in Japan for delivering scientific assessments to the policy making process. In dealing with the Fukushima nuclear accidents too, scientific findings could not be combined and utilized, resulting in much confusion. Learning from this experience, discussions are presently in progress on creating a framework for incorporating scientific advice into policy making.

**Raison d’être of supercomputers**

What is the purpose of building expensive supercomputers in the first place? As Dr. Takabe mentioned earlier, I think that it is true to say that national defense is the primary objective of building the world's fastest supercomputer in the U.S. The main purpose of the world's fastest Sequoia is said to be to maintain and manage the performance of nuclear weapons. What then is the position of computational science and the reason for having expensive supercomputers in a country like Japan, which does not have nuclear weapons? I guess this would be for fundamental science and industrial applications. But how does that justify the enormous costs? I think computational scientists have a responsibility to answer to the taxpayers.

Needless to say, expensive supercomputers, such as K, are not necessarily essential to computational science. Today, many people have more than one personal computer, and their capacities far exceed that of Cray-1, which appeared in 1976 and is said to have marked the start of the age of supercomputers. The infrastructure for computational science is now available to anyone. The only difference between a personal computer and K is the speed and memory size. It is a known fact that an increase in numbers leads, at some stage, to a leap in quality. But will this vast growth in the number of computers result in scientific discoveries of a different nature from the past? This kind of question also emerges.

**Is computational science necessary?**

Computational science simulation is currently called the third mode of science after theory and experimentation. Would their results, then, merit awards such as the Nobel Prize? In his will, Alfred Nobel skillfully captured the essence of each
field of science by setting out that his awards were for discovery or invention within the field of physics, chemical discovery or improvement, and discovery within the domain of physiology or medicine. How can the expensive computers in existence around the world today contribute to such inventions, discoveries and improvements? There is no denying that technical advances have supported the progress of science, and the Nobel Prize rates development of innovative devices highly. What about the role of the computer?

Looking back on the history of the computer, it goes without saying that it has its roots in the ENIAC developed for military purposes in the United States during World War II. It was developed to calculate the trajectory of ammunition fired from warships and decrypt coded messages, and also used to compute the fluid flow of the type of atomic bomb used at Nagasaki. The computer made it possible to solve non-linear fluid equations that even math geniuses of the likes of Von Neumann could not solve. In the early days, Enrico Fermi and his fellow researchers made a remarkable discovery using a computer in which interacting non-linear systems, which were expected to end up in a disorderly state, went through what is called a recurrence phenomenon and returned to their initial state. Consequently, some expected at the time that the computer would enable an ongoing succession of Nobel Prize-level discoveries. More than half a century has passed since then and computers have undergone astronomical progress in their capabilities. But it seems that computational science discoveries have not thus far produced any Nobel Prize winners. That said, we should not forget that computational science simulations on global warming contributed greatly to the awarding of a Nobel Peace Prize to the Intergovernmental Panel on Climate Change (IPCC) in 2007.

According to Dr. Takabe, computational science is the optimal research method for fundamental science on the evolution of the universe, particularly because there is no way of carrying out experiments in astrophysics. However, we must verify whether computational simulations are reproducing actual physical phenomena by checking the correctness of the mathematical models used, through simulation experiments or by other means. In light of the rapid advancement in observation technologies, to truly impress astrophysics observation and theory experts with simulations, their programming must be verified. In the materials field too, many researchers are having a go at numerical material design. How close are computer simulations to the prediction of new materials? Computational science has always had to deal with the prejudice that it is just a follow-up study to experiments and theories. To live up to its name as the third mode of science, I feel that computational science is now required to acquire predictive abilities.
Comparison with earthquake science

The day before yesterday, there was a special symposium on earthquake prediction at the Fall Meeting of the Seismological Society of Japan and it made references to computational science. Let me briefly introduce some of the interesting discussions that went on. As you know, on March 11 last year, a huge earthquake of magnitude 9.0 occurred off the coast of the Tohoku region in the northern part of Japan, and the giant tsunami that followed took many lives. It caught people completely unawares. Presently in Japan, only the area off the coast of Shizuoka Prefecture has an extensive system of observation in place for the anticipated Tokai Earthquake and offers any chance of prediction. But the Tokai Earthquake is yet to occur. Instead, we have had frequent earthquakes in other areas such as the Great Hanshin Earthquake and the massive earthquake of last year. Seismologists have lost their confidence and earthquake prediction itself has come under scrutiny. The symposium discussed the history of seismology over the past 50 years, during which observation systems have been reinforced, as well as its outlook for the future. With respect to technical progress, advancement in computational science has enabled simulations using realistic models and there are moves to predict earthquakes through simulations. But the symposium also pointed out certain limitations.

The comment by Dr. Hiroo Kanamori of the California Institute of Technology was especially noteworthy. He said that since we do not have a full understanding of physical phenomena of earthquakes, it is difficult to utilize study results as they are in real-life disaster prevention. He then went on to list three areas in which seismology can meet the demands of society. The first was to reinforce education and research activities and train human resources who have the ability to think creatively and flexibly. This is a common issue in any field, but the fact he mentioned this first reflects his shrewd discernment. This also has to do with the fact that, because new tools such as K have been developed, creativity is required in making the best use of them. Next, he explained that outstanding research results should be utilized effectively in disaster prevention, bearing in mind the uncertainty factor they still possessed, and lastly, that real-time seismology methods should be developed to prevent damage. He emphasized the importance of collaboration with engineers in this regard. Applying this to simulations, this means that models should be verified using observed data, and be utilized in society while remaining aware of their limitations. I think this is an important point.

Future applications of computer science

How then, should we make use of computational science in the years ahead? There is no doubt that it will be used increasingly in various aspects of natural
Besides climate change research, it can be used for disaster prediction as well as studies on energy, genetic information, functions of the brain and heart, and design of new materials. The possibilities would appear to be unlimited. And it is not just in natural science. In the future, there will likely be demand for wide application in the fields of social and cultural sciences too. For example, researchers engaged in social science could input large amounts of data (big data) relating to economic crises or yen appreciation into a supercomputer and perform simulations using mathematical models. Of course, there will still be problems that would be difficult to address in real life. However, I believe that deeper research is required to facilitate evidence-based policy making. It is also important to train computational science experts who will undertake research in various fields.

Take policy making, for instance. In today's world with its vastly improved means of globalization, communication and transport, policy making is an extremely complex task. But with computational scientists working together to create mathematical models of national activities, large amounts of data (big data) held by government offices could be processed so that we can prepare efficient budgets and growth strategies without resorting to budget screening, hurriedly implemented over a short period of time. As a member of the public, I have great hopes in these developments. What do you think?

After last year's nuclear accident in Fukushima, the government asked the public to what extent they thought Japan should rely on nuclear energy for its energy requirements: 0% 15% or 30%? With this too, I thought the government could have prepared simulations in advance on various scenarios for their energy policies until 2030, and then logically explained under what conditions each of those assumptions would be realized, in a similar way to global warming simulations. It is unfortunate that they did not do this because, had they done so, their ideas would have been more widely accepted and the debate would have become much more scientific.

In terms of methodology, it is somewhat similar to statistics. Statisticians are called upon to show interest in various fields, and to try and find solutions to problems in cooperation with experts in the respective fields. Unfortunately, statisticians in Japan tend not to be so enthusiastic in getting involved in outside fields, though this seems to be changing gradually more recently. I hope that computational science experts will be different, and that they will boldly take on challenges in a variety of areas to provide clues for steering society in a more positive direction.

Here are some themes that we can possibly examine in the following discussion:
1. Computational science to address humankind's problems
2. Ideal style of supercomputer development
3. How to inform society
4. How to foster human resources
Will computational science be able to provide answers to important problems of human society?

Part (2)

Record of discussions at the IUPAP Conference on Computational Physics 2012

(This is the record of the comments made by the audience following the keynote address by journalist Atsuko Tsuji on the above theme at the IUPAP Conference on Computational Physics 2012 that was held in Kobe from October 14 to October 18, 2012. The moderator was Professor Hideaki Takabe of Osaka University, who also chaired the conference.)

Moderator: Thank you Ms. Tsuji. Ms. Tsuji has brought our attention to a number of issues from the media perspective. I am sure that there are many computational scientists here at this conference who would like to comment. However, I suggest that the discussion focuses on the four points pointed out by Ms. Tsuji in the final viewgraph. I welcome comments from the floor.

Floor: I would like to comment on the second item regarding development strategy. Ms. Tsuji suggested that, a supercomputer is expensive because it is uniquely developed and, therefore, it should be purchased because it is merely a tool. That is one opinion. Ms. Tsuji, at the same time, also mentioned the Fukushima Daiichi nuclear power station. When nuclear energy first began in Japan, physicists in Japan such as Dr. Hideki Yukawa were not essentially opposed to it. However, their view was that nuclear energy technology should be developed independently. But what actually happened was that we bought it because it was cheap, fast and part of the U.S. global strategy. Thus, the Fukushima Daiichi nuclear power station was made possible by introducing technology from abroad. One of the causes of the recent accident was, I believe, that they bought equipment that could be activated at the flick of a switch. Installing emergency generators underground was the U.S. design and the fact that the equipment was installed that way is a lesson. Therefore, I have my doubts about how cheap and fast purchased technology is. Prior to this, I was relegated to the Old Guard by your correspondent Komiyama but the fact remains that we must develop much of the key technology ourselves because of
its very nature. For this reason, I am inclined to think that we will still need to use budgets to some extent.

![Figure 5. Ms. A. Tsuji responding a question from Floor.](image)

Tsuji: I don't believe that we should buy everything either. Development is needed in key aspects. For example, we should buy the chips if we cannot make them in Japan but we need to develop key software. Given the age that we live in, I think that we should use those items that are used around the world and develop key items ourselves. The crux of my argument is that we have persisted with pure domestic products and that is why it has been expensive. Now, with the Fukushima nuclear plant as well, when we have the nuclear power from a country with a focus on natural disasters such as hurricanes and tornadoes in a country like Japan which is affected by tsunamis, even if we use it as it is initially, there is no doubt that we failed to make modifications using Japanese technology.

Floor: When nuclear reactors were supplied by the U.S., Japan should have revised the design. In my view, something in the nature of a committee should have been set up to examine this. If it were my country, India, there would be special committees to review the designs. Therefore, the problem was not buying from the U.S.; it was probably the fact that there should have been a study by a committee to ensure that they were appropriate for the location.

Floor: First of all, I would like to thank Ms. Tsuji for a wonderful keynote address. My name is Eric Rimenda. I used to head up one of the laboratories at Cray Research. When we are thinking about supercomputers, we must not forget software. The software for designing the new materials we use today was created 30 years ago for the supercomputers of that time. When it comes to that
software being used by the younger generations, it must be upgraded for the supercomputers of today or even 10 or 20 years into the future. The key is to consider the hardware and software together and focus on the point that the K supercomputer is presenting new concepts for software.

Floor: On the question concerning why you need to be the best, I think the importance lies in not having the fastest but creating something that is faster than what we have today. For example, it may not be possible to make predictions about earthquakes. I don't believe it is possible to predict other natural disasters either. But, I do think it is possible to make limited predictions. For example, when strong wind and rain is initially not too violent and then unexpectedly worsens causing more deaths, it may become possible to predict developments like that with a faster supercomputer than K.

Tsuiji: Typhoons can be predicted with considerable accuracy in Japan today. But with the recent changes in meteorological phenomena, there have been some fairly strange events. We have even seen tornadoes in Japan. Speaking of tornadoes, I understand that they can be predicted with fairly high accuracy in the US. However, the accuracy of tornado prediction in Japan is totally inadequate and I think we need to have better performing computers. This is my perception and I have no objections.

Floor: First of all, thank you for your presentation. I have listened with great interest. At the same time, it made me think from a different perspective. I disagree on one point in your address. That is where you said that computational science is the third mode of science. I think this is incorrect. Computational science is a modern science. Theoretical physics cannot be debated with pen and paper. It is not even possible to subject it to a simple analysis. A hundred years ago it was possible to analyze the atom but in this age, we need computers to conduct experimental analysis on subatomic particles. Computational science is a theoretical science, and supercomputers should be utilized to use this in making advances in science. The following is a comment. It was mentioned that computational science challenges the problems of humankind. But this is a fairly difficult problem. The computational science that I deal with has many theoretical aspects and areas in which we are not sure how they relate to humanity. But, let's consider this mobile phone. It functions beautifully through two theoretical developments. The first is Fourier analysis. Fourier was a mathematician who lived 200 years ago. I imagine he could not even conceive things like mobile phones. The other is GPS. GPS works on the basis of Einstein's theory of general relativity. We carry out our work without really knowing how our research will contribute to society but I think it is examples like those that motivate us.
Moderator: I thought your point that computational science is not the third mode of science was very persuasive. As Ms. Tsuji mentioned, computational science practiced by people with flexible thinking will lead to new discoveries. That is a very important point. If we allocate computational science to a place that is independent of theory, we will end up looking at technological aspects only. I think that what we are essentially looking for in computational science are new theoretical directions and such results. If the younger generation is taught that computational science is the third mode without being properly educated about this point, the key components of theoretical insights related to the results of this science are going to be incomplete.

Tsuji: Yet, in Japan, it is frequently stated that computational science is the third mode. Maybe this is an expression of the computational scientists' conviction that they are also part of the scientific world. Perhaps there are some here at this conference who disagree and believe that computational science is the third mode of science. If so, I would like to hear their views.

Floor: I would also like to comment. First, I think we should call it the "most powerful" computer rather than the "fastest". As the participant from Cray Research pointed out earlier, it becomes the fastest only when the hardware and software work well together. Second, on the subject of whether computational science is the third mode, I think that it emerged as a new form of science. It is led by hypotheses, but is also based on experiments and observations, as well as data. It is still in its early stage. In the past, it helped advance theoretical and experimental science. But I expect that it will become more independent in the future.

Floor: I would like to touch on an extremely significant point, if I may. But first, let me talk about three smaller points. First, the Fukushima nuclear plant. Japan did not buy the plant from the US. It was constructed in Fukushima in collaboration with U.S. parties. In addition, the blunder in Fukushima was the result of being unable to respond promptly in an intelligent manner. Supercomputers may have been able to help but they were not utilized. I think Japan could have modified the location of the emergency power supply themselves but this was neglected, which is the problem. So please stop accusing the U.S. unilaterally. Second, about the Sequoia. You say it is cheaper than the K supercomputer but it was produced in series and this is the 5th model. Therefore, the development expenses should be assessed as a whole, and such assessment would show that it is very expensive. Sequoia was cheap only because improvements were made over five successive models. My third and final point: insistence on purely domestic products. I read a very interesting Japanese book, a book by Yukichi Fukuzawa. He was the first Japanese to visit San Francisco. He walked down
the streets of San Francisco carrying a couple of swords at his side. Americans watched him with great curiosity because they had guns instead. However, he didn't come there to fight. He was there to learn. Besides, he was extremely observant, and perhaps much more intellectual than those he observed. He also visited Paris and other countries. This was 150 years ago but he learned that the technical and cultural revolutions were transforming the world. He wrote a book to give the Japanese public his advice. Sound advice for anyone, not just Japanese. In his book he says that the Meiji Restoration required two major changes in awareness. He used key words. One of which was "independence". He said Japan had to become independent of other countries and make its own decisions on national concerns. This also applies today and other countries should imitate this. Another word he mentioned was "numbers". When considering something, you must look at the numbers. This point is brought out in The Autobiography of Fukuzawa Yukichi. A large computer produced and programmed by Japanese people, functioning independently and handling numbers efficiently, embodies the spirit of Yukichi Fukuzawa.

Figure 6. A participant said that Japan should follow the way indicated by Yukichi Fukuzawa 150 years ago, when Japan opened its gate to the US and European countries.

Moderator: Let me add to the comment from our attendee from the United States. Please take a look at a 10,000 yen note, if you have one. There you'll find a portrait of Yukichi Fukuzawa. He was the first person to introduce a psychological revolution, the concept of democracy, to Japan during the Meiji Restoration some 150 years ago. We just heard comment that the problem during the Fukushima nuclear accidents was not whether the nuclear reactors,
the hardware, were made in the U.S.A. or Japan, but rather if the Japanese government had sufficient software to enable it to take prompt action in response to the situation. He called to our attention the fact that Japanese politics had not yet been able to maintain a firm sense of independence in disclosing information, and to respond promptly as a democratic nation, trusting in the intellect of its people. Quoting Fukuzawa’s words from 150 years ago, the commenter pointed out that Japan should reflect more on its lack of software in the form of swiftness, rather than focus on whether the reactors were made in the U.S.A.

Moderator: Our discussion began with the question of whether computational science is the third mode of science. Is there anyone who is of the opinion that, as the third way, computational science can exist independently of experiments and theories?

Floor: Yes. I think they are clearly different. Documents sometimes contain theories, results of experiments proving those theories and things that were verified using mathematical models. In other words, numerical verification. With respect to the Nobel Prize, Kenneth G. Wilson won the Nobel Prize in Physics in 1982 for his "study of critical phenomena in connection with phase transitions". This achievement is known today as "Wilson's renormalization group." He is a professor at Cornell University and has contributed to the fields of theories, simulations, science and engineering. I think this is a good example. It is significant because he won the Nobel Prize and because it shows that theories and simulations are completely different. What is mentioned there cannot be proved using mathematical models alone, but can be visualized using computer in simulations.

Floor: That's mathematics. Theorems have nothing to do with physics. In physics, there are concepts as well as experiments to confirm them. Theories change constantly.

Floor: Is computational science the third mode of science or just a scientific tool? To answer this question, I think we need to look at science from various perspectives, especially in terms of what it will enable us to do. Firstly, it allows us to study complex systems. In other words, it can help us to encapsulate nature into laws. Through computational science we can study laws inherent in nature, and examine larger complex systems. It can also satisfy our needs for faster computer resources. It enables us to handle various complicated systems in real life using the computer. Moreover, we can perform experiments on the computer. Computational science makes it possible to study subjects which would be too costly to perform experiments on, or which do not allow for experiments at all.
Moderator: A very important point was just raised. Computational science exerts great potential when examining complex systems. With complex systems, we look not only at the results but the biggest elements affecting those results. Computational science really excels when used as a tool for performing calculations to remove various elements from the equation and identifying what the essence is. Whether scientists using the computer can achieve this is where the abilities and scientific instincts of the researchers, who we compared to Shi Huangdi earlier, come into play. It is important for computational science to continue elucidating governing mechanisms in complex systems in this way.

Figure 7. A snapshot of the discussion.

Moderator: There was another noteworthy comment. That was that computational science provided a means for simulating effects on the computer where experiments are not possible. I think that it is extremely important for computational science to keep venturing into these fields and seek to find new forms of science. Today's theme is "Computational science to address humankind's problems". As Ms. Tsuji explained, shouldn't young people be encouraged to tackle social science issues where experiments are not possible without adhering to the field of natural science, and senior researchers in the computational science field assist them in their pursuits? For instance, an easy-to-understand example would be to study how changes in the government's economic policies would affect economic activities. Simulated results of various changes in policies may be used by economic experts to implement policies that are considered to be the most logical. Wouldn't you agree that we need studies like that? I hope that young researchers in particular will be motivated to try their hands in new areas like these.

Floor: Computers are a tool, a means to an end. They lead to swift decision
making and everyone reaps the benefits. Therefore, everyone in Japan should be proud to have the K computer. It was mentioned that high-performance computers play an important part in national defense, but isn't it also important to protect a country in the area of science, without using weapons and ammunition? As an international research consortium, we are grateful that the Japanese government has directed efforts into developing an infrastructure for computational science. I wish my country, Russia, would do more.

Floor: I want to stress one point. That is that it doesn't necessarily have to be supercomputers that solve humankind's problems. To give you a short example, the project I am involved in is funded by the EU. We analyze how much customers are being informed of the contents of food and other products, and also look at to what extent package labeling has filtered through among customers. A PC is sufficiently adequate for handling numerical databases for this analysis. At times, solving small problems can benefit the entire human race. Supercomputers will be used to solve larger issues. This requires hardware, software and humanware. I do not see the costs of the K supercomputer as being such a big problem. People in Japan pay three to four times as much as people in Europe for a bottle of beer.

Moderator: That is a valid point. We are not saying that supercomputers are essential if we are to tackle new issues facing humankind. As pointed out earlier, it is the software that is important. This software becomes increasingly complicated with time. But we must pass on these assets to the next generation. For that, education is required. Problems that started off manageable on a personal computer may become complicated and more widespread due to historical developments. It is then that we need supercomputers and the challenge of passing on technologies to the next generation arises. That's why the question of how to foster human resources mentioned by Ms. Tsuji becomes a major issue.

Floor: I would like to make a brief comment. I think large computers are necessary for fields such as astrophysics. We cannot control data on the evolution of the universe. Therefore to follow the evolution of the universe over billions of years, sometimes we have no choice but to rely on computers. On the other hand, CERN's LHC (Large Hadron Collider) experiment on the Higgs boson is a large-scale experiment in which everything appears to be controlled, and it requires a large-scale computer. It has 150 million sensors and countless instruments binding these together, and data needs to be accumulated every millisecond. It is no longer possible to perform theoretical analysis of this data manually. Performing computer simulations in conjunction will lead to discoveries of new particles. We are already in an age when we cannot engage
in leading-edge research in this field without using a large computer.

Moderator: You touched on an important point and I think it leads on nicely to the subject of "big data" which has become a hot topic recently. Traditionally, in statistics, data collected by individuals is used for statistical analysis. Personally, I think it is inevitable that the accumulated data will eventually exceed that which can be handled on individual levels and will have to be analyzed by computer. Ms. Tsuji, what are your thoughts on this?

Tsuji: As things stand, in the U.S., President Obama announced a national project on "big data." In Japan, although the issue is being discussed by various parties, we have not seen the kind of progress that the US has had regarding national initiatives due to the vertically-divided structure of the government ministries and agencies. Even when we talk of big data, usually, those held by individuals are very small compared to those handled by organizations such as CERN. Also, there are many types of "big" data. Therefore, we must look at multiple types to consider the hardware requirements, but such discussion is yet to be held. Things are still in a state of disarray. It has been pointed out that the matter should be examined scientifically and that a consensus reached within the scientific community should be incorporated into government policies. This has not yet materialized. I think that we need to formulate a grand design, a map as it were, for this process.

Figure 8. Many attendants joined the discussion on the important subject of the special session.

Moderator: Again, perhaps it is necessary for us to take the initiative in making inroads into the areas of statistics and big data from the computational science
side. We must promote joint research while passing on computational science's progress in hardware and techniques in the development of software for handling complex problems. Take huge volumes of data that would not fit inside a person's head, store it inside a computer and use exceptional software to ensure consistency. Actions like this are what we really need, right now.

Floor: I am involved in the analysis of biological data. Perhaps some of you have heard of the term "personalized medicine". If you attend conferences on cancer research, you'll find that the major breakthrough at the moment is in genetic sequencing. This was originally very costly, but it is getting much cheaper. It is now becoming possible for cancer patients to have their genetic code sequenced. However, this requires a computer with terabytes of memory that can analyze cancer tumors at genomic levels. This data can then be used to determine the appropriate treatment for that particular patient. The costs will fall to around a half or a third of what they are. By the way, let me also comment on the question, "What's wrong with being No. 2?", raised earlier on in this discussion. A few years ago, I worked at SmithKline Beecham. I talked with various researchers in the company and was told that, as a pharmaceutical company, for example, you end up a loser if you come in second place and that's why you must always stay at the top. Unless you are the first one to have access to various resources, you are going to lose out. I think this is the kind of reasoning that goes through people's mind when they are investing on something.

Moderator: It is almost time to bring this session to a close. Mr. Alex Hansen, you are the Chair of the C20 Commission of IUPAP, the host of this event. Do you have any comments?

Floor: Allow me to share my views on whether computational science is the third mode of science. In regards to Kenneth G. Wilson who was awarded the Nobel Prize in 1982 (The Nobel Prize in Physics 1982 was awarded to Kenneth G. Wilson "for his theory for critical phenomena in connection with phase transitions"), his work began by examining the model described in Onsager's thesis of 1942. At the time, nobody understood the physics contained in this thesis because it was so complicated. So, in the 1960s, Wilson kept mulling over how to interpret it. In the 1970s, he created an algorithm to simulate the contents of the thesis, first by analyzing it on paper and then with the help of a computer. As a result, he was able to understand the physics through the algorithm. The important point here is that he was able to discover physics that had been concealed in the math, by using a computer. That was over 30 years ago.

Floor: As a second example, let's take fractal and other complex systems, which
is my area of expertise. The concept of fractal has existed for over 2,000 years but large volumes of data and calculation are required for it to come close to nature. I feel that looking at computer results gives rise to new concepts and new mathematical models. Structures you have never even thought of before sometimes emerge when you actually do the calculations. This, in turn, helps science on complex systems to evolve further. As illustrated in these examples, I think that computational science is the third mode of science. At the same time, I believe that it is a necessary element of science that is compatible with other scientific means.

Moderator: Listening to IUPAP-C20 Chairman Alex's comment, I felt that he gave us some hints on how to inform society of our study results, a point we have not dealt with yet in this discussion. We computational scientists tend to keep our wonderful results to ourselves and are not good at letting the public know in a way that they can understand. I think he used the word "fractal" to describe how we should always be mindful of this fact and strive to express ourselves. In recent years, large supercomputer development is fully funded by taxes. That is not to say that the funds come from beer tax alone. So we need to explain clearly, even to housewives who do not drink at all.

Moderator: Our time is up. Let me briefly summarize our discussion. Today we discussed the theme, "Computational science to address humankind's problems." On the second item, "Ideal style of supercomputer development", Dr. Koyanagi raised a number of issues. We could not discuss the third topic, "How to inform society," at great length but I think that this all begins with us being aware of our society and striving to convey the results of our individual and group research in a manner that is easy to understand. There is still much more to be implemented in this regard, particularly here in Japan. We must try harder. The fourth point pertaining to fostering human resources is linked to software development. No matter how fast the supercomputer is, its accomplishments depend on the software. The software will become increasingly sophisticated along with the hardware. This advancement will continue through successive generations and that is why it is so important to train up the next generation of scientists. In doing so, we must not only pass on the discipline, but also provide an environment in which knowledge can be passed down accompanied by an improvement in quality, by taking a broader view of, and collaborating with, other fields. Computational science should be able to contribute greatly to society if we continue to drive ahead with it, bearing in mind the issues that were raised in Ms. Tsuji's keynote address and the views expressed in this discussion.