BEYOND the SIMULATION

Where is Computational Science Today?
Beyond the Simulation

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Computational science technology enables computer simulations to run by setting desirable conditions such as combinations of atoms and temperatures.

But even with the power of computational science, it was difficult to reproduce real-world phenomena. For example, a reproduction of even a small experimental chemical reaction requires computations taking into account the simultaneous movements of hundreds of millions of atoms occurring in hundreds of millions of steps.

And yet, computational science is rapidly becoming capable of simulating real-world phenomena owing to recent advancement in computer technology. Using the computational science approach, we are aiming to estimate the structures of materials with new functions, and reproduce them in experiments.

In this issue, we look at the current status of computational science, which has been evolving from a tool to merely reproduce empirical experiments to a tool that suggests plans to develop new materials.

How Far Has Computational Science Come?

In all areas of science, computation is now one of the most important and advanced research means, along with theory and experiment. The area of materials science is no exception. Computational science is expected to go beyond its conventional function of "explaining the experimental results" and to play a greater role in "forecasting" revolutionary new materials. What is the current status of computational science in the area of materials science, and what will become of it in the future? Two figures representative of different spheres of science, computational and experimental, discuss these issues extensively.
Beginning of collaboration among theoretical, experimental and computational sciences

Nishimura: Computational science has established its presence as the third pillar of science. I am in experimental science, but from day to day, I am feeling the presence of computational science becoming greater. I am curious about how theoretical and experimental sciences will unite together in the future, so I have been looking forward to talking with you today on the current status and future prospects of this topic. First, let us look back at the history of computational science. What was computational science like when you joined the National Research Institute for Metals (NRIM), NIMS’s predecessor, in 1987?

Sasaki: At that time, computational science began to be introduced in some disciplines, such as fluid dynamics which is indispensable for the design of aircraft, but it was rarely observed or analyzed the results of their experiments on an atomic scale. However, in the 1990s, high-spec electronic microscopes were too expensive and not widely available, so experimental scientists were not easily observed or analyzed the results of their experiments on an atomic scale. This probably caused a rift between theoretical and experimental scientists. I think they began to engage in research on an equal footing. Nanotechnology started to attract public attention.

Nishimura: Accordingly, findings were obtained at the nano-scale through experiments, and at the same time, the K computer development project was launched and the performance of computers dramatically improved. Along with this, useful calculation techniques were established.

Sasaki: As a result, an environment has been set in place where theoretical, computational and experimental scientists can discuss the characteristics of materials all on an atomic scale. As collaboration among those three moves on to the next stage toward solving diverse social problems, such as environmental and energy-related problems, progress is expected to be made in the development of new scientific and innovative technologies that will change our industrial structure and lifestyles. As a scientist who actually deals with computational sciences, such as fluid dynamics which is indispensable for the design of aircraft, but it was rarely observed or analyzed the results of their experiments on an atomic scale. However, in the 1990s, high-spec electronic microscopes were too expensive and not widely available, so experimental scientists were not easily observed or analyzed the results of their experiments on an atomic scale. This probably caused a rift between theoretical and experimental scientists. I think they began to engage in research on an equal footing. Nanotechnology started to attract public attention.

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Sasaki: By setting a goal precisely and creating a model of a high degree of perfection through mutual feedback of results, experimental science and computational science will start to be recognized as something that can be used by research units which are not in experimental science, such as MANA and NIMS. When I joined the institute, among about 300 researchers, only four researchers were including me dealt with computational science. I feel the trend of the times that led to today’s rise of computational science.

Nishimura: Moreover, the progress of computational science will lead to the progress of computational science itself and bring about new ideas. Seven years ago, when I was present at the scene where GREEN was in the final stage to be selected as a MEXT-sponsored project, one of the judges, a great professor, said that he didn’t think computational science would be of any use. I still clearly remember this harsh comment. But the situation has greatly changed since then. Now I feel that the day the development of revolutionary materials will be achieved under the initiative of computational science is approaching.

Our mission is to be the light of the lighthouse.

Taizo Sasaki

Development of new calculation techniques will be the key to practical application of innovative materials.

Nishimura: Among the areas of materials science, which area would you cite as where computational science currently demonstrates its advantage?

Sasaki: Depending on their functional features, materials can be largely divided into structural materials and functional materials. In this respect, computational science is really fit for the experiment. My reason is that the dramatic improvement in the performance of supercomputers has made it possible to reproduce the behavior of each atom fairly faithfully through computer simulation. Conversely, computational science may not be good at handling structural materials because it is difficult to grasp phenomena at the nano-scale.

Nishimura: It seems so. But even in such area, computational science may have a potential in developing designs of new materials through the integration of simulation and data science and reducing the time required from discovery until practical use of innovative materials.

In order to ensure that computational science will play a more active role in areas of materials science, do you think that improvement of the performance of supercomputers will be the key?

Sasaki: No, I can’t simply say so. Of course, it is better that a computer has greater performance. But, when dealing with materials that have an irregular or irregular structure, even a supercomputer would be unable to do a complete calculation by the conventional method of the first-principles calculation, because the volume of data would be massive. This situation will basically remain unchanged even when an advanced version of the K computer becomes available. Therefore, we have also been working on the development of a new calculation technique that we call Order N (see p.6). This has enabled, for the first time in the world, the first-principles calculation of a system having tens of thousands of atoms. As a result, it is now possible to do calculations regarding nanostuctured materials having a complex grain boundary and biological materials such as proteins.

In the areas of materials science, the subjects of study cover a very wide range, and researchers wish to do as many calculations as possible under various conditions. So, not only supercomputers but also distributed computing systems consisting of multiple PCs connected together and small or medium-scale computers are assuming an important role.

Expections for further advance ment in computational science and a Nobel-prize class discovery

Nishimura: These days, personal computational scientists are seeing serious improvement in performance and a lot of versatile software programs are available, so it is common that researchers who mainly engage in experiments do simple calculations using their PCs at hand.

Sasaki: Yes. This means that we, computational scientists, will have to do more than just doing calculations in the future. We have to be more creative.

At present, NIMS has a one-petabyte supercomputer. It operates at about 90% capacity, of which only about 20% is used by the members of the Computational Materials Science Unit, and the remaining portion is used by research units which are not in computational science, such as MANA and GREEN. When I joined the institute, among about 300 researchers, only four researchers were including me dealt with computational science. I feel the trend of the times that led to today’s rise of computational science.

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What do you think will be demanded of computational science in the future?

Sasaki: My ultimate goal is to make proposals and give advice to materials researchers based on computational science. I would be happy if my proposal or advice would lead them to develop new materials that smash conventional ideas.

Nishimura: Theoretical scientists have predicted the existence of new materials based on their own theories, and then experimental scientists have proved it through their experiments. You mean, in the same way, computational scientists may predict the development of new materials based on their own theories.

Sasaki: I remember an interesting comment by a professor at Osaka University. “Theoretical scientists will discover a revolutionary material and make a prediction, if they serve as the light of a lighthouse to guide a ship which experimental scientists are astern. But only a handful of theoretical scientists can be as brilliant as a lighthouse and most of them act as nothing more than the dim light of lanterns.” I really agreed with him. As he said, the mission we have as computational scientists is to be the light of the lighthouse.

Nishimura: I hope that in the near future, computational science will pave the way toward a Nobel Prize-class discovery and the development of new materials that no one has ever imagined.

(by Kumi Yamada)

Interdisciplinary development of computational science will bring about new ideas.

Chikashi Nishimura

* The first-principles calculation is a calculation technique for elucidating laws of physics and estimating physical properties on the basis of quantum mechanics (first principles), which is the fundamental law for materials on an atomic or nano-scale.
Creating a dream device through fusion of computational science and experimental science

Tsuyoshi Miyazaki, the leader of the First-Principles Simulation Group, studies the behavior of atoms and electrons in materials by performing the world’s largest-scale calculations: he deals with 10,000-1,000,000 atoms. Meanwhile, Naoki Fukata, a leader of the Nanostructured Semiconductor Materials Group, is working to develop highly-functional devices using nanostructured silicon materials. Through collaboration, Miyazaki and Fukata are hoping to create a ground-breaking device.

To perform calculations that take into account a large number of atoms

“It was only five or ten years ago when computational scientists and experimental scientists were able to engage in constructive discussions about materials on the nanoscale,” says Tsuyoshi Miyazaki of the First-Principles Simulation Group. This progress was made partly because Miyazaki’s group developed an order-N first-principles calculation program called “CONQUEST.”

First-principles calculations allow for computation of interatomic forces and the behavior of electrons based on quantum mechanics, the most fundamental principle in atomic physics. If you know the state of electrons in a material, you can reveal the properties of the material. However, this process requires very complex calculations, made worse as the computational complexity increases proportionally to the number of atoms in the material (N). For example, if N doubles, the computational complexity increases eight times. As such, the number of atoms that can be calculated is limited.

“The number of atoms that can be computed by first-principles calculations used to be only several hundred. Even a cube that has only 10 atoms on each side contains a total of 1,000 atoms. Standard computational methods cannot handle even such a tiny object. On the other hand, a material consisting of several hundred atoms is too small to handle in experimental science. So, experimental scientists had urged us to make progress in computational science, so that it could deal with much greater numbers of atoms. Of course, we ourselves were well aware of the issue, and therefore, we spent more than 15 years developing a first-principles calculations method capable of executing large-scale computations. Then, Miyazaki and Professor David Bowler (affiliated with both the University College London, and the London Centre for Nanotechnology in the UK) is he also a NIMS-MANA member) succeeded in developing a new computational method called the order-N method. This is a ground-breaking method as it removes the cubic increase in computational complexity when N increases, replacing it with a linear increase. For instance, when the value of N doubles, the computational complexity also doubles based on the relationship that the computational complexity increases proportionally to N. In conventional first-principles calculations, a wave function needs to be calculated for every single electron. In contrast, in order-N first-principles calculations, the computational complexity is minimized by dividing the whole material into localized small units and calculating density matrices. There are different types of order-N methods, and many groups worldwide are competing with each other in developing superior methods. CONQUEST has the advantages of conducting stable and accurate calculations and being efficiently compatible with a massively parallel computer. Because of these features, CONQUEST is capable of carrying out calculations involving more than 30,000 atoms routinely, and has been shown to handle as many as over 1 million atoms (Figure 1). This means that the computational power has been boosted by two orders of magnitude or more in CONQUEST compared to previously developed programs. “The first-principles molecular dynamics simulations involving 30,000 atoms are the world’s largest scale, and our method has many features that other codes do not have,” Miyazaki says.

Perfect timing for collaboration between computational and experimental sciences

Miyazaki always had in mind that, “it is vital for us to develop a practical computational method that is applicable to actual materials, instead of merely developing a theoretical computational method for the sake of publication.” Accordingly, he started searching for a target material to be simulated using CONQUEST. “A material consisting of 30,000 atoms is about 10 nm in size. Nanostructured materials sometimes exhibit unique functions, which regular-sized materials do not possess. So I looked for nanostructures with interesting features in literature worldwide. I was excited to find a paper on a very interesting material: silicon (Si)/germanium (Ge) core-shell nanowires. And to my surprise, the author of the paper was a NIMS researcher. I immediately contacted and met with him.”

The author was Naoki Fukata in the Nanostructured Semiconductor Materials Group. “I first thought that Dr. Miyazaki contacted me because he was looking for a research partner within NIMS. But I was told just today that he contacted me because he was intrigued by my research while conducting an extensive worldwide literature review. That is an honor to me,” says Fukata smiling. “Before I gained acquaintance with Dr. Miyazaki, I was also considering teaming up with a computational scientist in pursuit of conducting joint research. The problem was that computational scientists and experimental scientists dealt with different materials sometimes exhibit unique functions, but we spent more than 15 years developing a first-principles calculations method capable of executing large-scale computations. Then, Miyazaki and Professor David Bowler (affiliated with both the University College London, and the London Centre for Nanotechnology in the UK) is he also a NIMS-MANA member) succeeded in developing a new computational method called the order-N method. This is a ground-breaking method as it removes the cubic increase in computational complexity when N increases, replacing it with a linear increase. For instance, when the value of N doubles, the computational complexity also doubles based on the relationship that the computational complexity increases proportionally to N. In conventional first-principles calculations, a wave function needs to be calculated for every single electron. In contrast, in order-N first-principles calculations, the computational complexity is minimized by dividing the whole material into localized small units and calculating density matrices. There are different types of order-N methods, and many groups worldwide are competing with each other in developing superior methods. CONQUEST has the advantages of conducting stable and accurate calculations and being efficiently compatible with a massively parallel computer. Because of these features, CONQUEST is capable of carrying out calculations involving more than 30,000 atoms routinely, and has been shown to handle as many as over 1 million atoms (Figure 1). This means that the computational power has been boosted by two orders of magnitude or more in CONQUEST compared to previously developed programs. “The first-principles molecular dynamics simulations involving 30,000 atoms are the world’s largest scale, and our method has many features that other codes do not have,” Miyazaki says.

To realize the practical use of nanowires as transistors, it is critical to control charge carriers (i.e., electrons and holes) that flow in nanowires. One way of controlling charge carriers is to dope with impurities. However, in nanowires, this method has an issue that scattering by ionized dopant impurities may reduce the mobility of charge carriers. “This won’t be an issue if Si/Ge core-shell nanowires are used,” says Fukata. If the Si shell is doped with boron atoms (B), holes in the shell migrate to the Ge core, allowing charge carriers to flow only in the core (Figure 4). In this procedure, the doped area and the area in...
which charge carriers are mobile are completely separated, and this arrangement prevents reduction of charge carrier mobility.

Computational science gives guidance and experimental science embodies a new device

“...for the first time in the world in measuring the state and behavior of impurities in nanowires using spectroscopic techniques. Furthermore, we observed holes migrating from the doped Si shell to the Ge core like water seeping out. In the future, we are hoping to observe phenomena taking place at the interface between Si and Ge. Unfortunately, spectroscopic techniques do not allow us to observe such phenomena due to their small scale. We need the aid of computational science to achieve this objective. The way of conducting research based solely on empirical experiments is a thing of the past.”

Using CONQUEST, Miyazaki calculated atomic and electronic states at Si/Ge interfaces in Si/Ge core-shell nanowires (Figure 5). While they are not ready to tell us their findings in detail yet, the results are astonishing, to say the least. Fukata says, “I was shocked, and sparks ran through me, by the fact that the results of the computations were totally different from my expectations in terms of electronic state. The great thing about computational science is that it is able to show us the kind of phenomena due to their small scale. We are able to see phenomena in the actual materials. In such cases, we correct the models and calculations based on empirical data. Or, we sometimes even need to develop a new computational technique. Incorporating feedback from computational science and experimental science in a back-and-forth manner, we improve the prediction accuracy of our models and calculations, thereby contributing to the successful development of a new transistor consisting of Si/Ge core-shell nanowires. We may also discover a nanostructure with a function unknown to science.”

Discussion is essential for the fusion of computational and experimental sciences

What needs to happen for fusion between computational science and experimental science in a manner that will produce innovative results? Miyazaki and Fukata answered simultaneously, “That’s discussion.” Then Miyazaki continues, “The two disciplines use different languages and are partially incompatible. Even so, I enjoy explaining my calculations to my partner as much as possible. I also want to understand my partner’s experiment in detail. It is vital for both of us to understand each other’s work.”

Fukata says, “I want to create materials and devices with new functions using silicon, which is the second most abundant substance in the earth’s crust, and thus is inexpensive and easily available. For example, using silicon nanowires, I am aiming to develop new solar cells that are superior to conventional silicon solar cells in terms of conversion efficiency from solar energy to electric power. I would very much like to team up with Dr. Miyazaki for this project as well.” In response to Fukata’s passionate request, Miyazaki responds, “I believe that a solar cell’s power generation efficiency can be improved through the optimization of the structure and arrangement of nanowires. I am sure that computational science will be able to make great contribution to that problem.”

The fusion of computational and experimental sciences is becoming key to the advancement of science and technological development. It is expected that the fusion of the two disciplines will continue to evolve and lead to many ground-breaking achievements and discoveries.

(by Shino Suzuki, PhotonCreate)
or less. Steel strength of 800 MPa means that permanent deformation of the steel does not occur unless a load of 800 N (about 82 kg) per 1 mm is applied to it.

Process parameters required to create 1 μm crystal grains identified

Inoue had expertise on theoretical science and computational science, carrying out research mainly on dissimilar materials and composite materials. “This was my first time dealing with steel, and I hadn’t even seen any steel structures manufactured.” Since I was new to this specific subject, I did a thorough literature review on miniaturization of grains of steel, and asked many questions to the project members from major steel manufacturers. After gathering information, I realized that there is no consistency among the different test results.”

It had been confirmed based on many experiments and published papers that when a great force is applied to a steel material, strain energy builds up internally, which in turn facilitate grain miniaturization and strengthening of steel. The test results, which later documented the relationship among the processing rate (i.e., % reduction in steel thickness), grain diameter, and the degree of hardness were increased. What did Inoue mean by “there is no consistency among the different test results?”

“There are two methods of applying force to steel: rolling, in which steel is extended while going through rotating rolls, and forging, in which steel is hammered or compressed using dies.” Even if these two methods are applied to the same processing rate, the strengths of forces applied to steel are different. As a result, the ways steel is strained are different between the two methods. Furthermore, change in processing speeds either add or removes heat, causing the temperature of the steel to vary. Therefore, it is important to quantitatively understand the relationship between various process parameters, including the processing rate, and the microstructure of steel. If this relationship is understood, you can specify appropriate conditions to fabricate 1 μm crystal grains for the given processing rate and for the given size of steel to be processed.”

To practice this approach, Inoue measured key process parameters such as temperature, strain rate, strain and cooling rate using a very small steel test piece, and recorded the relationship between these parameters and the resulting microstructure of steel. At that time, other research groups both in Japan and overseas proposed a technique called the severe plastic deformation process, and they later announced that they succeeded in creating 0.1 μm grains and a steel material that is three times stronger than conventional steel by repeatedly compressing the steel. “These high-profile studies attracted much attention. On the other hand, we continued collecting data in a steady manner based on the belief that quantification of the relationship between process parameters and the microstructure of steel is absolutely critical in sounding out stronger steel through the creation of ultrafine grains.”

The next step was to test Inoue’s team finally quantified the process parameters necessary to create 1 μm grains.

Success in the production of rod material and 18 mm thick steel plate

Since the beginning of the project, Inoue had another issue addressed. “So far, we used very small steel test pieces smaller than 1 cm in most experiments. However, we are aiming at developing structural materials that will be used for the construction of buildings, bridges, automobiles and ships. For this reason, we need to fill the large gap between the test pieces and end products in terms of size.”

There was another research team engaging in the ultra-short steel project, and the team was steadily dealing with the issue. Based on the knowledge gained from basic studies conducted by Inoue’s team using very small test pieces, in 2000, the other team successfully produced steel rods that have an 18-mm-by-18-mm cross section, are about 20 m long, and consist of grains with diameters 1 μm or less that are uniformly distributed from the surface to the core of the material. Then, in 2001, the same team succeeded in the production of a steel plate that was 18 mm thick, 10 mm wide, and about 2 m long. The plate consisted of grains with diameters of 0.5 μm to 0.6 μm. Both the steel rods and plates were created using a rolling machine at an external facility after tests were conducted using a NIMS-owned rolling machine. While the rolling process is often performed at 800°C or higher so that the steel being processed becomes red hot, the NIMS team took a different approach for processing the steel at between 500 and 600°C. The use of lower temperatures facilitates buildup of strain energy and creation of ultrafine grains.

Aiming to create steel plates with 25 mm thickness, Inoue’s team focused on the production process. This is when Inoue’s expertise in computational science came in handy at last. The fundamental purpose of computational science is to interpret and apply to the production of steel plates using a new production procedure. To proceed with this plan, Inoue asked the JSW to allow them to use its 3,000-ton press machine at the JSW Muroran Plant. The request was granted.

Inoue immediately visited the plant taking the blueprint of the new production procedure he prepared based on the simulations. “The first trial was a complete failure. Due to my limited understanding of the specifications of the press machine, the precision of the simulation was very poor.”

“Remember feeling encouraged when we obtained study results that were consistent with the concept: the internal microstructure and the external shape of a material are interconnected to each other as evident from the fact that free forging produces uneven surfaces.”

There were many other parameters that could improve the precision of the simulation such as the shape of the dies that pound the steel, the pressing speed, changes in applied pressure, the load on the manipulator that holds the steel plate, and the movement of the manipulator. However, a forging plant is a place where machines and equipment are operated by craftsmen who rely on their experience and intuition. “Outsiders were told to observe the press machine only from a distance. Due to this restriction, I was not able to gather necessary information, so I desperately asked the plant workers to allow me to observe the machine more closely. Then, to my surprise, the plant manager allowed me to observe the press machine from the operator room, which is normally inaccessible to visitors. Moreover, I received permission to videotape steel processing in action using a fixed camera. Diligently looking through the on-camera monitor, I made sure to record all necessary information in detail on the press machine, manipulator, and the operator controlling the system.”

As soon as the experiment was completed, Inoue immediately flew back to Tsukuba for a reexamination of the new production technology. “Steel production technology itself is a vital tool in serving such purposes,” says Inoue. “That is because simulating technology may drastically speed up the steps from research planning to commercialization, thereby meeting the needs of society quickly.”

Inoue concluded at the end, “The fundamental purpose of computational science is to make predictions. The discipline is not only a means to follow up empirical experiments, but also to contribute to the understanding of the results of basic research. Then we can propose, predict and verify new phenomena and experimental methods based on computations. That is the true integration between computational science and experimental science.”

(by Shino Suzuki, PhotonCreate)
Viewpoints of a theorist and computation and experiment specialists

In the scientific research community, there are experiment specialists, who conduct experiments using lab instruments on a daily basis, theorists, who work with mathematical formulas, typically scribbling notes on paper, and computation specialists, who carry out calculations or simulations using a supercomputer. These specialists are in a delicate relationship—they rely on each other’s expertise but at the same time, they tend to keep a certain distance.

On June 22, 2015, four materials science researchers, including a theorist, a computation specialist and an experiment specialist, took part in a roundtable session at the University of Tsukuba to have a frank talk on such topics as their impressions of each other and their passions for their own studies. Here is how the discussion went.

**Jun-ichi Inoue**
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Electron Microscopy Group
Environmental Remediation Materials Unit
Functional Geomaterials Group

**Round-table talks**

**Viewpoints of a theorist and computation and experiment specialists**

**Unexpectedly, these specialists get along well**

**Ono:** At this session, we are planning to hear the frank opinions of a theorist, a computation specialist and an experiment specialist. I believe that many people can easily imagine what experiment specialists generally do. On the other hand, I imagine it is difficult for them to understand the difference between theorists and computation specialists. What is your opinion on that?

**Inoue:** To me, it seems that theorists tend to reduce a phenomenon to a simple description by extracting the essence of the phenomenon. On the other hand, computation specialists try to reproduce the phenomenon in more realistic way with a mathematical approach using a computer.

**Sakuma:** I agree with Dr. Inoue. In other words, computation specialists take specific scientific approach to a phenomenon and use a computer in trying to understand its physical properties. However, the computations cannot be performed without theoretical bases. So, theorists play a role of developing the necessary theoretical bases.

**Aizawa:** I see theorists as experts dealing with something beyond my comprehension (laughing), whereas a computation specialist’s job is to explain the incomprehensible matter in an understandable manner. I guess the two parties take different approaches in their research.

**Inoue:** I suppose another way of saying “different approaches,” in more specific terms, is that theorists are interested in common features and universal properties, rather than differences, while computation specialists are more interested in differences and uniqueness than common features.

**Sakuma:** Like Dr. Inoue just said, I as a computation specialist, get more excited when I find different properties between materials.

**Ono:** I don’t have a feel for the difference in approaches taken by the two parties, owing to the fact that my mentor’s academic background was the particle theory. Since all researchers in this field aim to identify a universal law, I believe both theorists and computation specialists feel excitement in a similar manner when they come up with a theory explaining a phenomenon.

**Aizawa:** How about your impression of experiment specialists?

**Ono:** To me, experiment specialists are those who tirelessly carry out experiments, collect a huge amount of data, draw conclusions based on the data, and come up with a principle behind the phenomenon they studied. During this process, computation specialists play a role of data analysis for experiment specialists.

**Sakuma:** Supporting experiments is an important role of computation specialists, and as a computation specialist myself, I feel pleasure at experiment specialists finding my work useful. Also, I sometimes envy them when they discover new phenomena that had been unimaginable before through experiments. At the same time, I secretly perceive them as rivals due to the fact that I constantly pursue ways to predict new physical properties and phenomena based on computation results.

In addition, there are some instances where researchers can make predictions only with computation approaches, and not with theoretical approaches, so it is vital for the three parties to complement each other.

**Ono:** I am also a computation specialist and would like to make amazing discoveries. For example, I hope to obtain computation results that totally deviate from the expectations of experimental specialists. Then, I want them to verify the results by conducting experiments. On the other hand, it would be difficult for a computational approach to faithfully reproduce experimental results due to the insufficient performance level of the current computers. As such, computation specialists simplify their computations as much as possible by excluding factors with minor influence from their computations. My vision of skillful computation specialists is those who are able to draw significant results under a given set of constraints.

**Inoue:** I think there are different types of experiment specialists. There are roughly two types: the first type includes those who perform measurements first, then try to draw some sort of conclusion based on the measurement results. And the other type takes a completely opposite approach: they first determine the expected conclusion, and then they carefully design the experiment in an attempt to obtain the kind of data that is consistent with the expectations. The first type appears to be a good match with computation specialists while the second type seems to get along well with theorists.

**Aizawa:** I think I am more likely to be the first NIMS NOW 2015 No.5 | 13
What kind of data do you use in your experiments? After all, you can’t make any sense out of the data without analyzing them. So it is natural for me to work with computer specialists, otherwise, my research won’t go anywhere. I choose a computer specialist whom I feel comfortable working with as a research partner.

In contrast, I only have a little interaction with theorists. Recently, new physical phenomena, such as topological insulation, have been discovered one after another, and it is required for us to develop new theories to explain these phenomena. When we try to reproduce these phenomena experimentally, we need a new theory for the analysis of experimental data. So this may be a good opportunity for me to start working with a theorist.

Inoue: I have an experience of working with an experiment specialist when he asked me to come up with a theory that explains his study results since the results appeared to be inconsistent (with existing theories). In this study, our attitude was: let’s solve the puzzle together, and this type of project is often carried out collaboratively. In contrast, it is difficult for me to take part in the type of research in which the researchers believe that the study is already thorough and completed. This kind of study is typically presented at conservative seminars.

Ono: When I am involved in experiments conducted by a group of researchers, I take charge of computations at first. Then later, experiment specialists often ask me to work with them. This is usually how I get involved in joint research. In addition, I sometimes get involved in collaborative research during a drinking party or other social gathering. Basically, I always get involved in joint research on casual occasions (laughing).

Sakuma: Up until recently, many experiment specialists did not appear to trust computer specialists very much. In fact, when I showed simulation models of material surface structures to an experiment specialist, they angrily told me, “Don’t talk to me as if you have seen the actual material.” Today, it is easier for me to work with experiment specialists as mutual understanding between us has been deepening. Lastly, I would like to ask all of you about your future vision. I personally hope that the three parties will build a stronger relationship of trust, complement each other and collaboratively contribute to materials science.

Ono: I want to be the type of computer specialist capable of predicting material physics and designing materials using a computer.

Azzawa: My goal is to make amazing discoveries through experiments. Then I would like theorists and computer specialists to prove my findings on a theoretical basis and establish a new theory. It would also be my pleasure to conduct a specific experiment and develop a new material at the instruction of a computer specialist.

Inoue: I think the true worth of theorists is represented by their ability to identify interesting problems to work on. Today, websites for internet-based retailers are capable of making customer-specific recommendations. Similarity, I have a wild idea that in the near future, scientific journal websites will become able to make recommendations to authors about their next research projects when their manuscripts are accepted for publication. However, I want to be the type of theorist capable of identifying my own creative research projects that the journal websites can’t recommend.

(by Kumi Yamada)

Round-table talks

Computer simulations

In this day and age of modern technology, computers have become very familiar tools to many of us. We use or benefit from various types of computers such as mobile phones, PCs, household electronics, products, car navigation systems and highly reliable weather forecasts on a daily basis.

However, the situation was much different 100 years ago; people then did not even dream that the computers would become reality. When they needed to calculate something, they used paper and pencil or an abacus as the most accessible calculation aids. Only few profession- als in need of sophisticated calculations such as scientists and architects were able to perform complex calculations using such tools as slide rules. At the beginning of the 20th century, new scientific and technological discoveries and developments were made in succession, which drastically transformed the ways in which people lived. People wondered how such scientific and technological development and popularization would further affect their lifestyles in the future. Then, some individuals around the world attempted to predict the future. Among them was a French novelist, Jules Verne, whose publication of a future-predicting novel attracted great attention at that time.

Similarly in Japan, one of the newspapers carried a special feature titled “Predictions for the 20th century” in its January 2 and 3 issues in 1901. There were 23 predictions in the feature regarding the kinds of inventions to be made and how they would change people’s lives by the end of the 20th century. Interestingly, some of them came true rather accurately. For example, they predicted, “The development of radio-telegraphy and telephones will enable free communications across the world.” “Invention of a new air conditioning machine will enable controlling the temperature of a room within a comfortable range.” “Electricity will become a primary energy source,” and “The advancement of railroad technology will enable people to travel between Tokyo and Kobe in two and a half hours.”

However, mysteriously enough, none of those predictions forecasted the invention of computers. In fact, there was no mention of the invention of rapid-calculating machines that would lead to the development of information society.

Our predecessors 100 years ago did not imagine the advent of computers. However, in reality, the world’s first computer came out in 1946 and computer technology has evolved very rapidly. Today, computers are indispensable not only as the heart of information society but also as the frontend tools in science and technology.

In particular, computer simulations are vital means of visualizing atomic behavior in chemical compounds and molecules, studying the structure of the universe, and measuring the resilience of buildings.

For instance, the universe had been thought to be made of matter, that is made up of atoms and molecules and energy. However, it has been discovered in recent years that most parts of the universe appear to be made of dark matter and dark energy, that are unknown to humans. Our understanding of the structure of the universe is making steady progress through computer simulation studies. Also, in the field of weather forecasting, the accuracy and precision of forecasting methods have dramatically improved with the evolution of computer simulations since when meteorologist Lewis Richardson attempted weather forecasting using manual calculations around 1920, and when mathematician John von Neumann succeeded in the first computer-based forecasting in 1950.

Computational science based primarily on computer simulations is probably the most advanced scientific procedure humans invented in the 20th century.

Written by Akio Etori
Title lettering and illustration by Shinsuke Yoshitake

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NIMS researchers awarded the 2015 Gottfried Wagenger Prize

(June 30) NIMS researcher Hossein Sepehri-Amin and Yoshitaka Tateyama won the German Innovation Award “Gottfried Wagenger Prize 2015”. This award provides support for young researchers in Japan and encourages collaboration between German and Japanese industry and academia. The award was established in 2008 by technology-innovation-focused German companies and the Japan-based German Chamber of Commerce and Industry. To be eligible for the award, researchers must be under 45 years of age and be affiliated with a Japanese university or research institute. The research has to fall within one of the categories of Mobility, Materials, Life Sciences, or Energy & Industry, and must be an applied study that provides innovative and creative solutions.

Sepehri-Amin and his team member Takahiro Akiya, postdoctoral research associate, jointly received the award in the Materials category for the research titled “Development of Dy-Free high performance Nd-Fe-B permanent magnets by engineering of grain boundary phase.”

Meanwhile, Tateyama, leader of the Nano-System Computational Science Group, and his team member Keitaro Sodeyama (project researcher, Kyoto University) jointly won the award in the Energy & Industry category for the study titled “Theoretical elucidation of reaction mechanism on electrolyte interface in lithium-ion battery with highly-efficient use of supercomputers.”

* Affiliations and positions of award recipients are those at the time of reception.

NIMS Researcher Awarded the IUPAP Young Scientist Prize in Magnetism

(July 7) Senior researcher of the Magnetic materials unit, Masamitsu Hayashi, was awarded the IUPAP Young Scientist Prize in Magnetism at the 20th International Conference on Magnetism (ICM) held at the Palau de Congressos de Catalunya in Barcelona, Spain. This award recognizes outstanding contributions to the areas of magnetism. Hayashi won the prize for “the pioneering work on domain wall dynamics in magnetic nanowires and contributions to the development of current controlled magnetism in magnetic heterostructures using spin orbit effects”. His work has contributed to advancing the understanding of electrical control of the magnetization direction of nanoscale magnets, which is a crucial technology for next generation information storage and computation devices.

Hello from NIMS

Hello, my name is Alexandre Fiori, I am French, and I love good food!

I really enjoy living in Tsukuba Science City. The city has a singular implantation of high-technology research centers in an agricultural plain, scattered with rice fields, forests, and residential places. Tsukuba City is a safe place, not too far from Tokyo, and very quiet at night.

Seven years ago, I joined NIMS for an internship under the supervision of Dr. Tokuyuki Teraj, at the wide bandgap semiconductors group, headed by Dr. Yasuo Koide. Since that, I have kept a strong interest in the synthesis of diamond and Japan. I came again to NIMS in 2011, during my Ph.D. course (Neel Institute, CNRS Grenoble). I experienced the big earthquake on March 11, the shortage of commodities, and a fast repatriation to France. Finally, in 2012, I joined NIMS a third time as a JSPS research fellow, and now as an ICYS-MANA researcher.

My research topic concerns the boron doping of synthetic diamond, superlattice architectures, and the study of metal/diamond interfaces.

Alex Fiori (French) 
Felt 2015-2017
ICYS-MANA researcher

Caption: Enjoying the transient beauty of flowers at NIMS Nanaki site. (from left to right : Toshie Mizuno, Alex Fiori, Suzuki Okamoto, Kuni Kurihara, Asuka Sakamoto, Tomoko Kudo, Mayu Narumi, Shoko Morakot}

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