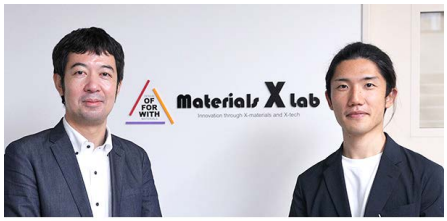
Department of Materials Engineering, The University of Tokyo Material Modelling Lab

Making the most of supercomputers as a driving force for creative thinking as well as for molecular dynamics calculations

"Supercomputers can play a big role in molecular simulations and other applications that require huge amounts of computation. Also, I value their role in education. I hope we can nurture those proficient in both material science and digital technology by having students in materials science use the supercomputer whenever they wish. I would love to see student-led research that begins with the PRIMEHPC FX700 and develops to use the Fugaku. In addition to expanding existing simulations, we aim to discover new research seeds by encouraging students to think creatively and seek new ways to use the supercomputer. Specifically, I hope to deploy the supercomputer in new research that utilizes simulations and materials data. This will be a new way of using it, but I think it will be effective in various universities and fields of research."

Yasushi Shibuta, Associate Professor
The University of Tokyo Department of Materials Engineering



Summary of Case Study

- **Hardware** FUJITSU Supercomputer PRIMEHPC FX700
- **Software** HPC Middleware / FUJITSU Software Compiler Package, VT-HPC Package

The Material Modelling Lab in the Department of Materials Engineering at the University of Tokyo specializes in material modeling and molecular dynamics, aiming to design and develop new materials with the aid of computers. In order to understand and simulate the structure and changes of materials at the atomic and molecular level, massive amounts of data needs to be processed. AI and data-driven methods have seen great advancements in recent years, and how they make use of high-performance computers greatly impacts their research.

Against this background, the Material Modelling Lab has introduced the FUJITSU Supercomputer PRIMEHPC FX700. In addition to using this high-performance supercomputer, which utilizes the same CPU (A64FX) as the Fugaku, for the lab's research, Associate Professor Shibuta who heads the laboratory hopes to create an environment in which students can freely use the supercomputer to help train students and discover research seeds.

Challenge	Selection Key Point
In materials science research, molecular dynamics simulations and data-driven methods are actively utilized, leading to an increasingly large amount of mandatory computing.	Having a supercomputer on hand at the lab makes it possible to process a huge amount of computing quickly.
Personnel who has a good understanding of both material and digital technology are necessary. It is also important for scientific studies not only to solve known problems, but also to discover new, unknown problems.	Creates an environment in which students can freely use the PRIMEHPC FX700 to develop skills to utilize digital technologies in the field of materials science. Also, it may help in discovering new seeds for research.

Background

Computers are essential tools for simulations and data-driven processes

For a long time, science and technology have been developed through two primary methods, experiments and theory. A third method, simulation, then joined them; more recently, the so-called data-driven method began to be used as a fourth method. Materials science is no exception to this trend.

The molecular dynamics (MD) simulate the dynamics of matters at the atomic level, observe the motion of each atom, and elucidate their structures and properties. "The size of one atom is about one billionth to ten-billionth of a meter, so if we attempt to capture what happens in the materials at a visible size, the number of atoms involved becomes huge," explains Shibuta.

The Department of Materials Engineering handles all kinds of materials, including metals, ceramics, semiconductors, and polymers. Shibuta mainly focuses on metallic and semiconductor materials. "Traditionally, in the field of metallic materials, solidification and microstructure formulation were controlled based on empirical knowledge. However, it is impossible to understand what is actually happening without observation at the atomic level. The more precise the simulation we aim for, the more atoms and molecules we need to handle. We have even been performing large-scale molecular dynamics simulations with 10 billion atoms. This makes us one of the top labs in the world in terms of large-scale calculations, yet we wanted to perform efficient calculations beyond this level in the future." (Shibuta)

Furthermore, the application of AI and data science has become more and more popular recently. Good examples are the effective visualization of simulations, post-processing, such as physical property extraction, and data assimilation. "If we handle the coordinates of 10 billion atoms through post-processing, the amount of computing can amount to 20 terabytes. The data assimilation method improves accuracy by reflecting actual measurement data in simulations. However, since it needs more than 100 parallel simulations, it also requires a huge amount of computing." (Shibuta) Therefore, high-performance computers are indispensable for this research.

Key Points

Interest in Fugaku and PRIMEHPC FX700 arose from experience with the K computer

Yasushi Shibuta,
Associate Professor
The University of Tokyo
Department of Materials Engineering

There were two major motivations that made Shibuta decide to introduce the PRIMEHPC FX700 into the lab. One is that he wanted to make use of a supercomputer for his research. Shibuta had his first proper experience with a supercomputer in 2014 when he joined the post-K FLAGSHIP2020 Project (Note 1). In that project, he was involved in the development of large-scale computing methods for metallic materials. "Unlike semiconductor materials, metallic materials generally contain impurities and defects and form polycrystals, making it difficult to obtain a periodic structure, which requires a large number of calculations. For this purpose, I got the opportunity to use supercomputers including the K computer, and experienced their capability first hand." (Shibuta) After that project concluded, the computations in research continued to become larger. At the Material Modelling Lab, this trend was enhanced by the increase of the research utilizing data-driven methods.

This led to Shibuta's interest in the Fugaku, and when he learned about the release of the PRIMEHPC FX700, which utilizes the technology used in the Fugaku, he considered purchasing it. "When we wanted to use the Fugaku, we would need to apply for permission, but if we had the PRIMEHPC FX700 in our lab, we could use it whenever we wanted. This is what drew me to it." (Shibuta)

He then heard that Visual Technology Inc., a system integrator, sells the PRIMEHPC FX700 and so he began to consult with them. "Because I am not a specialist in computer science, my knowledge was limited. So I asked them to make it possible for me to use the PRIMEHPC FX700 as a user." (Shibuta) Visual Technology delivered the PRIMEHPC FX700 and peripherals, installed the OS and compiler, and performed network configuration and racking.

Note 1: A project led by the Ministry of Education, Culture, Sports, Science and Technology. The main development was conducted by RIKEN Advanced Institute for Computational Science. The projects aimed to develop a successor to the K computer and develop applications to solve nine social and scientific issues, called priority issues. The studies selected as priority issues were those that needed large-scale and high-precision simulations only possible with the high computational performance of the post-K supercomputer.

Having the PRIMEHEPC FX700 on hand is a huge draw for students

The second motivation was educational effect. Shibuta came to realize through his discussion with students that it is important for them to be able to freely use the supercomputer, and that the supercomputer may be one of the draws of his lab. As its footprint is equivalent to that of standard servers and it's air-cooled, the PRIMEHPC FX700 is easy to use and suitable for use at the laboratory level.

"Many students are interested in supercomputers, but there isn't a way for them to get hands-on learning experience with them unless their major is information technology or computer science. However, if a lab has its own supercomputer, they can use it readily. In addition, it's difficult to casually try things on supercomputers owned by others outside the lab, so in this lab, students can "play" freely with the PRIMEHPC FX700. This ease of access allows them to deepen their understanding while learning to use it." (Shibuta)

This policy is well received by the students, too. Aoi Watanabe, a graduate student says, "Having the supercomputer on hand means we can go through trial and error as many times as we want. There are a lot of things that we can only learn about on both the software and operation through hands-on experience.

Aoi Watanabe,
Postgraduate Student
The University of Tokyo
Department of Materials Engineering

Effect and Future Outlook

Utilizing supercomputers for seeds as well as needs

Although the software used in Material Modelling Lab, such as LAMMPS (an open-source molecular dynamics application), is yet to use the capabilities of the PRIMEHPC FX700 to their fullest, the supercomputer's effects on education are definitely being felt.

"In the three months after introducing the PRIMEHPC FX700 into the lab, we have learned quite a lot. We realized how challenging and fun it is to extract the best performance out of a supercomputer. It has been a great experience of learning to consider why something didn't work well and it has led us to the effective use of computing resources." (Watanabe)

Shibuta believes that free use of the PRIMEHPC FX700 will not only satisfy their research needs but will also lead to the discovery of research seeds. "In many cases, supercomputers have been used to perform calculations that have a clear goal and to conduct necessary computation for that goal. However, I believe it is also important to use them to produce new seeds that we never know what they will grow into. When we introduced the PRIMEHPC FX700, it gave us an opportunity to realize this idea."(Shibuta)

If the PRIMEHPC FX700 can act as the catalyst for unfettered, creative thinking, then we are confident it will spread further than just universities and research fields.

Profile

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Overview : As the improvement in computer performance expands the spatial-temporal scales that can be handled by numerical analysis, the lab has been applying this advantage to the investigation of materials processes using computational approaches such as molecular dynamics. Also, the lab are challenging the collaboration of materials science with data science-based methodology.
Website : http://www.mse.t.u-tokyo.ac.jp

VISUAL TECHNOLOGY, Inc.

Established in February 2009

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Overview : 1. Development, manufacturing, sales, and rental of computer systems for HPC, AI/DL and, imaging fields.
2. Engineering services related to the previous item
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