

Title	Contributing to monozukuri manufacturing through numerical simulations : an extensive field of study that encompasses prosthetic limb defect detection, apps that recommend metallographic structures, quantum computing, and more
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Contributing to *Monozukuri* Manufacturing through Numerical Simulations

An extensive field of study that encompasses prosthetic limb defect detection, apps that recommend metallographic structures, quantum computing, and more

Muramatsu is blazing new trails as she works to expand the capabilities and possibilities of numerical simulations, combining them with other methodologies and thinking how to implement them in quantum computing. In our interview, we asked her about the unique results she has achieved on her journey, such as her technology for detecting defects in prosthetic limbs, developing an app to recommend metallographic structures, and proposing methods that bridge different types of numerical simulations.

Using the “Finite Element Method” to Investigate How Objects Deform

How much load can an airplane wing withstand? How do the bodies of cars crumple upon collision? How do we know if there are any foreign substances mixed into the materials of a prosthetic limb? In order to live our lives safely, there are myriad things we need to know about manufacturing materials. However, conducting real experiments can be prohibitive both in terms of time and cost. In these situations, “numerical simulations” can be incredibly powerful tools. They are computer renderings of experiments that use numerical models (equations) to express targeted physical phenomena.

The methodology changes with scale, but for Muramatsu’s work with materials

that are used to build airplanes and other vehicles, the main approach is to use the “finite element method (FEM)” which can handle phenomena ranging from millimeters to kilometers in size (Fig. 1). FEM divides the target materials into smaller polygons (see front cover), solves for the equations of motions for those individual pieces, and integrates this information to analyze how the object as a whole will react or deform. FEM is already being used to design structures such as roads and buildings.

When asked about her research, Muramatsu said, “I would say that the finite element method is the main theme of my research, but I want to be able to analyze materials in greater detail, so I am working to combine a variety of methodologies together.” Diving from one outside academic field to the next, Muramatsu is intent upon improving

numerical simulations, taking the field to new heights by using these simulations to develop materials.

I Want to Find Defects in Prosthetic Limbs

Using machine learning, FEM, and application experiments

Muramatsu’s lab is currently developing an application that can detect defects in prosthetic limbs. The technology combines FEM with machine learning (a type of AI) and application experiments. Prosthetic limbs are made of an incredibly strong and light material known as carbon fiber reinforced plastic (CFRP). CFRP is also used in airplane wings and motorcycle bodies, but because it is created by overlapping multiple sheets of carbon fiber cloth, foreign substances may be inadvertently introduced to the material and affect its strength. This means that for quality assurance and user safety, two people have to conduct a full ultrasound inspection on the completed product where it is assembled. Muramatsu’s goal is to reduce time and labor by replacing one of these technicians with an AI.

“When you apply force to a material and make it deform, they have a property that

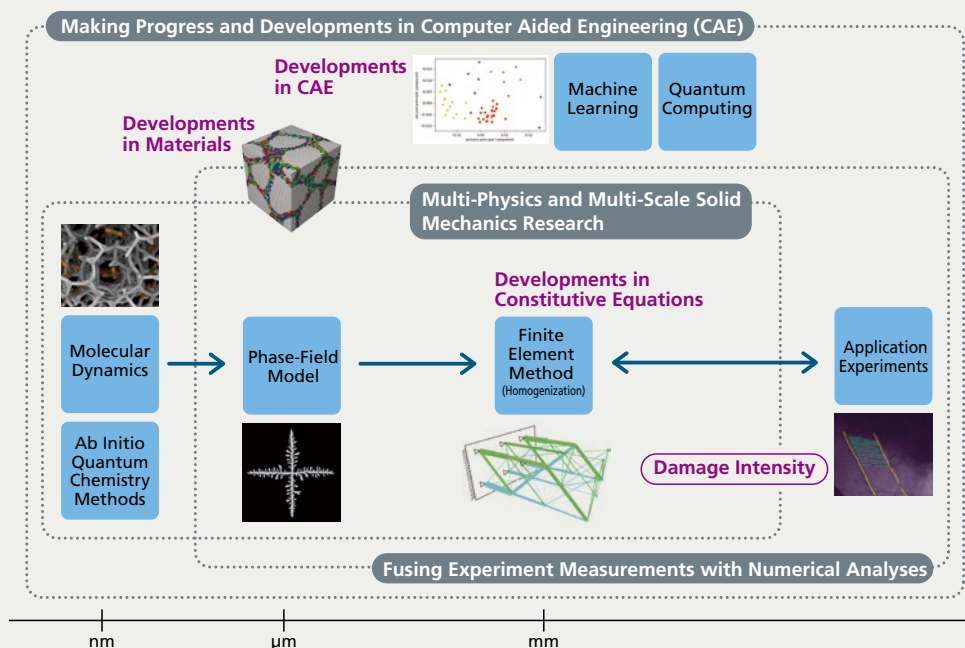


Fig.1 Overview of Muramatsu’s research on materials

Incorporating numerical simulations at multiple scales, machine learning, and quantum computing with the “finite element method (FEM)” at the core of an experiment, opens up new possibilities for numerical simulation as a research method (marked in the gray dotted boxes). “Multi-physics and multi-scale simulation” refers to how Muramatsu’s material analyses examine multiple combined phenomena such as heat and deformation over a range of scales. The scale at the bottom corresponds to the size covered by each numerical simulation. The images in this diagram show the types of findings obtained using each research method.

The simulations listed are as follows: Molecular dynamics: method for analyzing the physical movements of atoms and molecules; Ab initio quantum chemistry: method which only uses experimental values of fundamental physical constants; Phase-field model: method to calculate crystal growth; FEM: method to work with complex shapes or materials.

makes them release heat. This means that it is possible to capture a force distribution on a material by using a thermal camera. My idea was that it would be possible to use AI to determine where foreign matter had gotten mixed into the material based on whether irregularities appeared in the temperature distribution.”

To make this technology into a reality, it is necessary to train the AI with immense amounts of data showing foreign matter being introduced to a material and the corresponding temperatures when this happens. However, since CFRP is an expensive material, it is not possible to actually put together enough experiments that can show data for all of the relevant types of contaminants. This is where numerical simulation comes into play. Based on a limited amount of real experimental data, a computer can postulate other scenarios in which other contaminants are present. This is the basic idea that formed the application which can assess whether foreign objects are present in a prosthetic leg (Fig. 2).

I Want to Know Which Structures Determine a Material's Properties
Using machine learning, FEM, and phase-field modeling

“A material's internal microstructure (how it separates) determines its strength, workability, and the way it will deform. This means there is a great need to identify the patterns of potential structures for different materials. You also will want to know how the material deforms when force is applied to this structure.” This type of calculation can be done using conventional numerical simulations, but it is very time consuming. Muramatsu, thinking that the current approach was useless for actually trying to develop new materials, solved this problem by using machine learning two times over.

“The first round of machine learning looks at patterns in the material's structure. The second round of machine learning predicts how strong the material

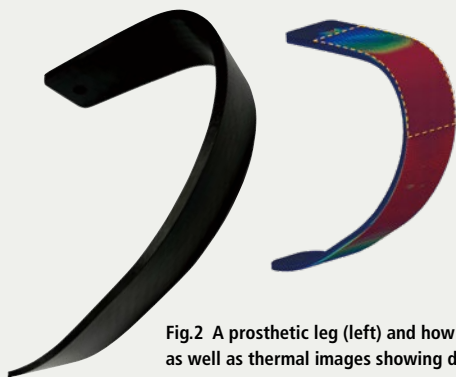


Fig.2 A prosthetic leg (left) and how it compresses (middle) as well as thermal images showing difference between material with and without foreign contaminants (right)
The dark blue patch in the left portion of the bottom image depicts a square foreign substance. There are no foreign substances in the top image.

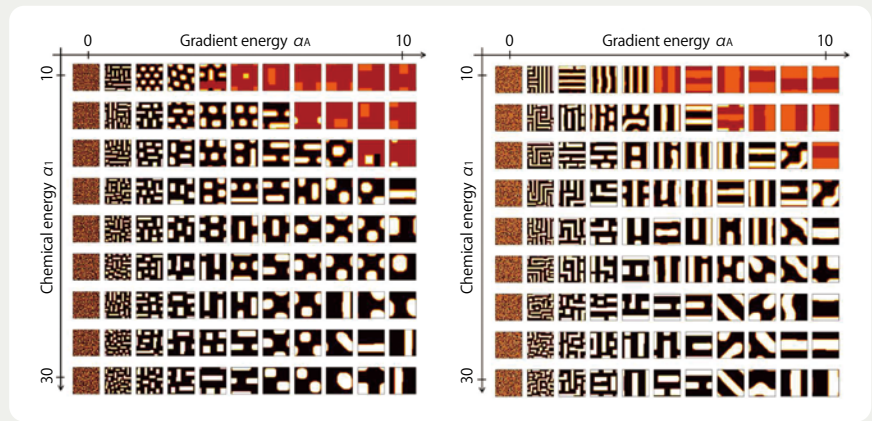


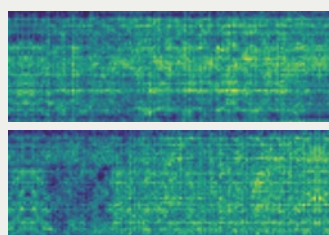
Fig.3 Patterns of material structures derived from quantum computers
Calculations of two different types of materials showing their structures (how they separate). Moving right shows when conditions allow for the materials to mix more easily due to higher temperatures, etc. Moving down shows when the materials are least likely to mix due to their different properties. The right image shows a ratio of 7:3 while the left image shows a ratio of 6:4.

is, looking at how much the material can stretch and how well it absorbs applied force. The program then recommends structural patterns with the desired characteristics.”

New Developments in Numerical Simulation

Both the technology to find defects in prosthetic legs and the technology to recommend material structures were created from the desire to apply data obtained from numerical simulations to monozukuri manufacturing.

Muramatsu's research, however, extends far beyond even these accomplishments. One such example is her goal of combining molecular dynamics with FEM. “When analyzing a material with FEM, you designate whether it is a metal, a plastic, or a ceramic. Different materials have different properties that require specialized constitutive equations to solve. This means that it is impossible to analyze new materials for which there are no known constitutive equations. However, constitutive equations are derived using molecular dynamic simulations which show movement on the molecular scale. I realized that if that was the case, why not just combine molecular dynamics directly with FEM?” Muramatsu's daring idea to bypass constitutive equations by combining different scales of simulations has already met with some success. Furthermore, Muramatsu is



working on developing an application that can run numerical simulations on what is regarded as the next generation of computing technology: quantum computers. Quantum computers use quantum mechanics and, because they function in a fundamentally different way than the traditional type of computers we use now, it is necessary to develop new applications to run on this type of system.

Muramatsu says that this is the type of challenge she is able to take on because she works at Keio University.

“First of all, President Kohei Itoh himself is a quantum computer research scientist. We also have an incredibly vigorous quantum computing program, with Keio University establishing the IBM Q Network Hub in 2018, becoming the only organization in Asia to have access to IBM's latest model of quantum computer from the United States (As covered in Issue No. 29 of the new Kyurizukai). I wondered whether it would be possible to use this technology for computational mechanics as well.”

Even when working with low-resolution input, quantum computers can calculate a pattern of a structure that is a blend of various materials in only a single second. This type of computer can put out a low-resolution pattern of a structure made up of a blend of materials in only a single second. Previous attempts on traditional computers would take approximately twenty minutes, making this a huge step forward. Researchers are just waiting for quantum computers to become more precise and practical (Fig. 3).

Muramatsu's research ranges from so many different areas and subjects that it cannot be covered in just one article. It is hard to take our eyes off Muramatsu and her work, and impossible to guess what she might embark on next.

(Interview and text writer: Akiko Ikeda)