HPCI magazine FUGAKU HYAKKEI Vol.1 - Vol.15

HPCI magazine

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FUGAKU HYAKKEI

Vol.1 - Vol.15

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HPCI magazine FUGAKU HYAKKEI

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This booklet is a reprint of interview articles about research achievements from the web PR magazine "HPCI magazine FUGAKU HYAKKEI" Vol.1-Vol.15.

Using Simulations to Search Existing Drugs for Possible COVID-19 Treatments

The COVID-19 pandemic has upended our way of life. Pharmaceutical companies and research institutes around the world are laboring away to develop drugs to fight it. Running precision simulations with innovative High Performance Computing Infrastructure centered on supercomputer Fugaku, researcher Yasushi Okuno was able to find promising candidate drugs that are potential treatments for COVID-19 from among 2,128 existing drugs already being used against other diseases.

Yasushi Okuno
Deputy Program Director, Medical Sciences Innovation Hub Program, RCSTI, RIKEN
Professor, Department of Biomedical Data Intelligence, Graduate School of Medicine, Kyoto University

“Surprising Results” from Precision Simulations

Vaccines and pharmaceutical treatments for COVID-19 are being developed at a breakneck pace in order to limit the disease's impact and hasten social and economic recovery. A lot of this activity is focused on identifying drugs that are potentially effective against this new coronavirus from among existing drugs, including antivirals. Since they've already been proven safe in clinical trials, the time required to develop treatments based on existing drugs should be significantly shorter. Yet, despite all the research underway worldwide, from experiments at the cellular level to clinical trials, effective therapeutics remain elusive.

Given this state of affairs, a lot of hope is riding on supercomputer-based simulations.

“That's because we can examine the efficacies of many medications in much less time than it takes for experimental evaluations, and we can also understand how these medications work,” explains Yasushi Okuno. In April 2020, Okuno began his search for therapeutic drug candidates among existing drugs. Under the “Fugaku Preliminary Use Projects” program, he used the supercomputer Fugaku, developed and maintained by RIKEN and other institutes, and under the “High-Performance Computing Infrastructure COVID-19 Research Access Projects” program, he used the supercomputer Cygnus at the University of Tsukuba.

The Fugaku research project searched for drug candidates among 2,128 existing drugs. It targeted the “Non-Structural Protein 5” (NSP5) main protease of the coronavirus, which is critical to coronavirus replication in infected cells. Okuno's research team constructed models of the main protease and existing drug molecules in Fugaku, and ran molecular dynamics simulations to investigate their behaviors. “These computations allowed us to faithfully reproduce the molecular behaviors, showing the conformational transition of the protein’s active site pocket*1 between the closed and open states, and the transition of the drug from an unbound state to a bound state at the active site pocket or other sites on the molecular surface (Fig.1).”

Then, sorting by how long the drug molecules being evaluated remain in the main protease active pocket and other factors, they were able to find dozens of promising candidates from the existing drugs studied (Fig.2). “These drugs are expected to have a strong binding affinity to the main protease, and may be effective in fighting the new coronavirus. Before we ran the simulations, I was concerned that we might not find enough promising drugs like these, or might even find too many. But we found a suitable number of candidates. And 12 of these are being used in clinical studies and clinical trials as new coronavirus treatments in other countries. I was surprised how good the results were,” said Okuno. The fact that 12 of the drug candidates discovered through these simulations are already at the clinical study or clinical trial stages for COVID-19 speaks well to the reliability of the simulations.

*1 Active site pocket: Some proteins have pocket-like indentations on their surface where certain molecules bind to them to start working. These indentations are called “active site pockets” or “active pockets”. A molecule that occupies the active pocket instead of the usual molecule can prevent that protein from functioning. Thus, discovering such a molecule is the first step in drug development.

Fig. 1 **Molecular Dynamics Simulated on Fugaku**

This is a still from a movie based on the Fugaku simulations investigating the molecular interactions between the main protease critical to the coronavirus replication (gray) and the existing drug Niclosamide (pink). One of the drug molecules has settled into an active site pocket (yellow), others have bound elsewhere, and still others have not bound to the protein. These simulations were performed on 2,128 existing drugs.

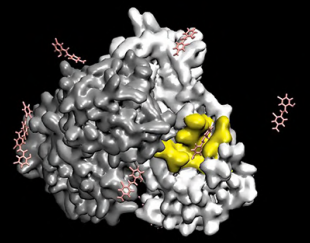
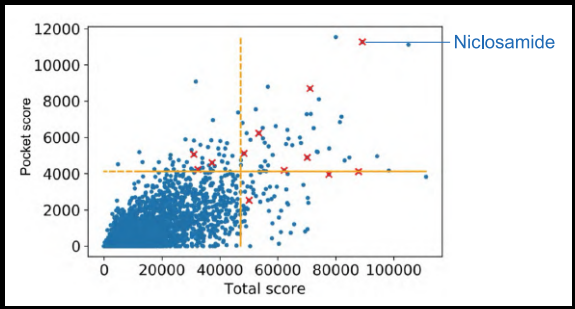


Fig. 2 **Identifying Therapeutic Drug Candidates**

The simulations shown in Fig. 1 examined how long a drug molecule stays in the active pocket of the protein (vertical axis) and how long it stays anywhere along the surface of the protein (horizontal axis). Each dot in Fig. 2 represents one of the 2,128 existing drugs evaluated in this research. Drugs undergoing clinical studies or clinical trials in other countries are marked with a red “X”. The closer to the upper right a drug is located, the better its expected ability to bind with the protein. Those in the upper right quadrant were considered suitable candidates for COVID-19 therapeutic drugs.



Among the 12 candidates, the drug Niclosamide is expected to have a particularly strong tendency to bind to the active site pocket. Not yet approved in Japan, it is inexpensive and has been confirmed safe overseas, where it is used to treat parasitic infections. Given these results, clinical research is expected to gain momentum.

Taking Full Advantage of Fugaku's Processing Capabilities

Okuno and his team began running simulations on Fugaku at the end of April 2020. Despite having less than a month to prepare, everything went smoothly and they had treatment candidates in hand by the end of June. He says they pulled this off thanks to “previous experience on the K computer, and because Fugaku was very easy to use.”

Okuno and his team had previously run drug discovery simulations on the K computer. But for simulations at this level of detail, the K computer was only able to examine a few dozen existing drug types. “In the early stages of drug discovery, it's important to ‘choose from many’. Although a huge number of candidates is evaluated at this stage in the experimental approach, the K

computer hadn't quite reached the point where it's realistic to fully simulate those processes. But, Fugaku could run calculations for more than 2,000 kinds of drugs, which is much more practicable.” Identifying viable drug candidates from over 2,000 types of existing drugs through these precise molecular dynamics simulations was a ‘world's first’ achievement. It was of great significance both as a computational technique and from an academic perspective. What's more, these simulations were done using only 5,500 nodes, which are a fraction of Fugaku's total processing power.

In addition to Fugaku's raw calculating power, this achievement was also the result of several endeavors and innovations in the computational approach. One of those is running each simulation with hundreds more drug molecules present, so interactions with the proteins become a more common occurrence. This can reduce the run time needed for the simulations. Too many drug molecules, on the other hand, could prevent the simulations from executing properly. Thus, the number of drug molecules present had to be carefully controlled. The team also confirmed that the length of time the virtual drug molecules remained in the active pockets was consistent with actual laboratory test results. Because the Fugaku simulations can produce such massive amounts of data, they also needed to devise ways to analyze all that data.

Using the Power of Cygnus to Simulate Another Protein

Using the University of Tsukuba's Cygnus supercomputer, the team investigated whether the therapeutic drug candidates selected from the Fugaku simulations would also bind to NSP16, another protein produced by the new coronavirus. NSP16 inhibitors, which bind to NSP16 to suppress its function, haven't been studied as much as the main protease inhibitors. Running simulations to explore the therapeutic potential of existing drugs against NSP16 is an ambitious experiment.

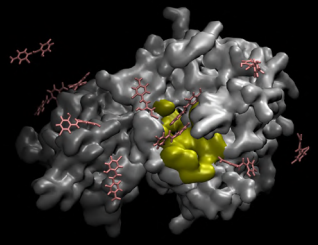
The Cygnus computer is outfitted with an abundance of modern GPUs[*2], which are often used for artificial intelligence research, and can quickly execute molecular dynamics simulations. “Since Cygnus was already fully up and running, it didn't take as long to pre-process the data for these simulations, and they ran reliably.”

Cygnus ran simulations with higher concentrations of the drug molecules to efficiently capture the molecular interactions (Fig.3), like those run on the Fugaku, evaluating each drug molecule's ability to bind to the NSP16 active site pockets. The results are still being analyzed, but different drugs are expected to bind more easily to different proteins. It will be interesting to see if the findings bear that out.

*2 GPU: Short for “Graphics Processing Unit”, a special type of computer chip optimized in design for image processing. For certain types of calculations, GPUs can be much faster than the CPUs (Central Processing Unit) commonly used for doing math.

Fig. 3 **Molecular Dynamics Simulated on Cygnus**

The interactions between the main protease-targeting candidate drug Niclosamide and NSP16 were computed on Cygnus the same way Niclosamide and main protease interactions were computed on Fugaku.



About the

Researcher

The approach that Yasushi Okuno took in this battle against COVID-19 can be applied in the search for drugs for other diseases. In fact, with Fugaku operating at full capacity, Okuno intends to search for drug candidates for cancer and other challenging diseases. His research work places the priority on the patients. “I hope to use the power of Fugaku to quickly identify a suitable drug for each patient’s particular cancer, and to search existing drugs for those effective against diseases that currently lack medications.” In addition to his supercomputing work, he is also involved in a consortium that brings together pharmaceutical companies and researchers from different fields to accelerate drug discovery. Driven to provide the patients he encounters with suitable medications as soon as possible, Okuno continues to lead in the field of computational drug discovery.

Associated Research Projects

- “Promotion of Innovative Drug Discovery Infrastructure for Acceleration of Precision Medicine” (hp200129)
- “MD-based Screening of Drugs with Novel Action Mechanism Against COVID-19” (hp200155)

Fugaku's Record-breaking Computations Enable More Accurate Weather Forecasting

Although weather forecasts are steadily improving, it is still difficult to accurately predict the paths of tropical cyclones and where heavy rains will occur. More accurate weather forecasts require detailed simulations on supercomputers with more processing power, and also applications designed to utilize that power. To help address this issue, Hisashi Yashiro, a member of a research project[*1] under the "Program for Promoting Research on the Supercomputer Fugaku", carried out the largest-ever meteorological computations for weather forecasting use.

Hisashi Yashiro
Senior Researcher
Satellite Remote Sensing Research Section, Earth System Division,
National Institute for Environmental Studies

Better Weather Forecasts Require Massive Computations

Modern weather forecasting is based on supercomputer simulations. As supercomputers have become more powerful, the forecasts have become more accurate over the last two decades, but nevertheless sometimes fall short. Moreover, it is quite difficult to accurately predict the paths of tropical cyclones and where heavy rains may occur. Improving these simulations will require processing colossal amounts of meteorological data points known as "state values" in the weather model.

Looking back on 2014, when the development work on Fugaku first got underway, Yashiro says, "I wanted to make use of the computing power of Fugaku to help contribute to more accurate weather predictions." It was decided

that Fugaku would undergo a “co-design” approach, where the hardware and software developers would collaborate in determining specifications. Yashiro contributed to this co-design effort, overseeing the weather and climate software perspective. The co-design team began work on a project, “to develop an application that could address the challenges of massive-scale calculations at a practical level when a supercomputer with the power of Fugaku became available to national meteorological organizations in the future.”

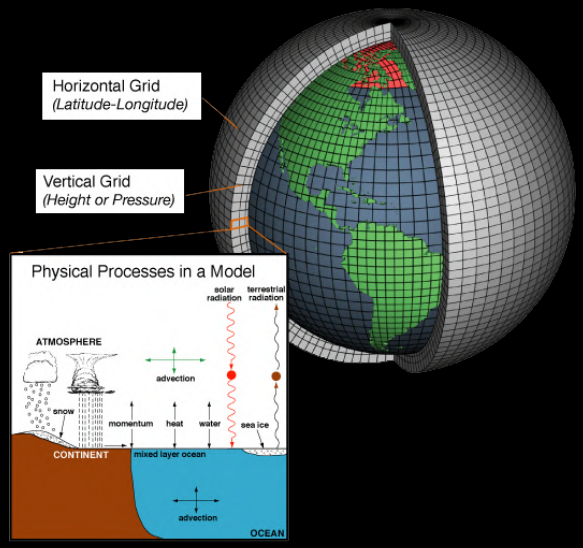
Better Forecasts Start with Better Replication of Current Weather Conditions

Weather patterns, such as clouds, rain, and snow, are the result of atmospheric conditions, such as temperature, humidity, pressure, and wind. To model these conditions for the entire planet, scientists divide the globe into a 3-dimensional grid and compute the changes expected at each grid point (or box) according to the laws of physics (Fig.1a). The challenge is choosing initial values for each grid point that accurately reflect the atmospheric conditions there. Weather pattern developments are sensitive to initial conditions. If the initial values used in the computations don't match the actual state of the atmosphere, the predictions will suffer. But, there are far more grid points in the model than actual observation points measuring atmospheric conditions. So to begin running a simulation, researchers need a way to calculate a suitable starting value for each grid point where no direct measurement data is available. Many meteorologists have been working on ways to compensate for this incomplete initial data.

Yashiro and his colleagues used an approach called “ensemble-based data assimilation”. First, they assign a temporary initial value for each grid point. Next, they run weather forecast simulations for a while to see how those values change over time. They then check those values against values acquired from actual observations, and update the value for

Fig. 1a **Atmospheric Simulations and Data Assimilation**

In this model, the Earth's atmosphere is divided into a grid. Changes to the atmospheric conditions at each grid point are computed according to the laws of physics. In this example, the grid is divided horizontally by latitude and longitude, and vertically by altitude with corresponding barometric pressure. The finer the mesh of the grid, the more accurate the simulation becomes, but the longer the computations and data processing take. This model is used both for weather forecasting and for data assimilation. The lower left diagram shows the physical processes modeled for each grid point, including how atmospheric heat and water interact over land and sea.



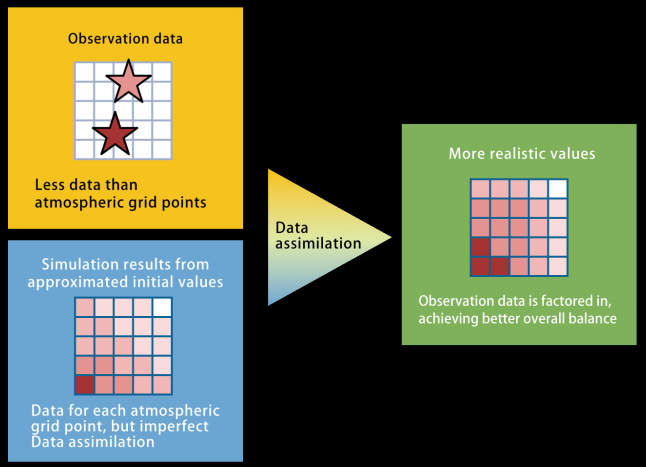
Source: National Oceanic and Atmospheric Administration

Fig. 1b

Atmospheric Simulations and Data Assimilation

Observational data is assimilated into the results of atmospheric simulations that began with approximated initial values. Each grid point is updated to more realistic values based on statistical estimates.

— Graphics based on JMA data



each grid point based on statistics and probability theory (Fig.1b). This is “data assimilation”. “Ensemble” means running multiple meteorological simulations at the same time with slightly different states. Like real weather, atmospheric simulations evolve non-linearly over time. If the weather model is incomplete, the longer the simulation runs, the more the results deviate from real-world observations. To address this problem, a number of simulations are run in parallel with different initial values. Comparing the results of multiple simulations tells the researchers which particular grid point locations are more sensitive to the initial values, and therefore more likely to contribute to a forecasting error. Those more sensitive grid points (areas) are then weighted with greater importance when the observation data is assimilated.

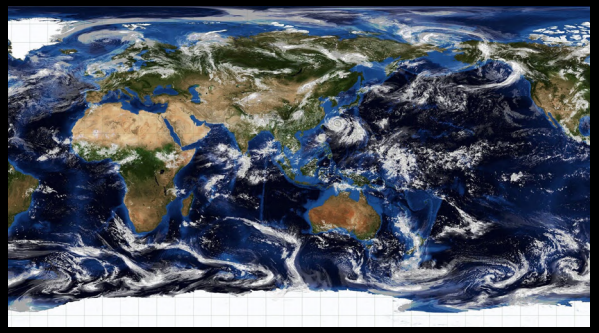
“How well data assimilation can reproduce the real atmospheric conditions will greatly affect the accuracy of the prediction results,” explains Yashiro. For this reason, meteorological agencies worldwide are attempting to assimilate data using ensembles with more members, and grids with finer meshes. Application performance and supercomputer processing power have typically allowed only dozens to hundreds of members per ensemble, with each grid point representing 10 to 50 kilometers of the Earth's surface.

The ensemble data assimilation done by Yashiro's team for this project used about 80% of Fugaku's total node count to perform computations with 1024-member ensembles, and a mesh size of approximately 3.5 kilometers. They were able to execute large-scale computations, about 500 times larger than those performed by meteorological agencies, with run times fast enough for use in weather forecasting systems.

Developing more Computationally Efficient Applications that Make Use of Fugaku's Performance

The application that Yashiro and his colleagues ran for atmospheric simulations featured optimizations by RIKEN research teams. Team Leader Hirofumi Tomita oversaw optimizations using the “Non-hydrostatic Icosahedral Atmospheric Model” (NICAM), a very high-resolution global atmospheric model. Team Leader Takemasa Miyoshi directed optimizations of the data assimilation system using a “Local Ensemble Transform Kalman Filter” (LETKF). In 2013, Tomita's team, which then included Yashiro, ran the world's highest-resolution model simulation of the global atmosphere, with a horizontal mesh

Fig. 2 **Atmospheric Simulation with NICAM**



The 6-hour later forecast produced by a global atmosphere simulation with a grid mesh size of 870 meters and with observation data from midnight August 25, 2012, as the initial values. Using one-quarter of the K computer's 80,000+ nodes allowed accurate reproductions of atmospheric flow and typhoon development.

— Joint research by RIKEN, the Japan Agency for Marine-Earth Science and Technology, and the University of Tokyo's Atmosphere and Ocean Research Institute (HPCI Strategic Programs for Innovative Research, Area 3).

— Visualization: Ryuji Yoshida

size of approximately 870 meters, using the K computer (Fig. 2).

This time, the mesh was less dense, with grid points every 3.5 kilometers, but with 1024 parallel NICAM calculations for each, and data assimilation throughout, making these historically intense computations. For these calculations to be practical in actual weather forecasting, however, they have to run faster than time elapses in real life. Even with the power of Fugaku, that is no simple task. Yashiro and his associates had to devise a number of modifications to make the application run faster.

In particular, a large amount of data needs to be transferred whenever shifting from the atmospheric simulation process to the data assimilation process. They therefore modified the program to minimize the time required for data transfers. They also tried to make maximum use of the solid-state drives (SSD) attached to Fugaku's computation nodes to speed up data reading and writing. SSDs have very high performance for reading and writing files. For this project, the team designed the software to take advantage of Fugaku's hardware, which was designed to include SSDs.

Explaining the significance of co-design, Yashiro says, “Fugaku is a world-class supercomputer that inherits the best features of the K computer. And because it was co-designed by hardware and software engineers, we could come up with ways to make full use of its performance. I think co-design will improve the results for a number of scientific fields, not only ours.” There are plans for future calculations to

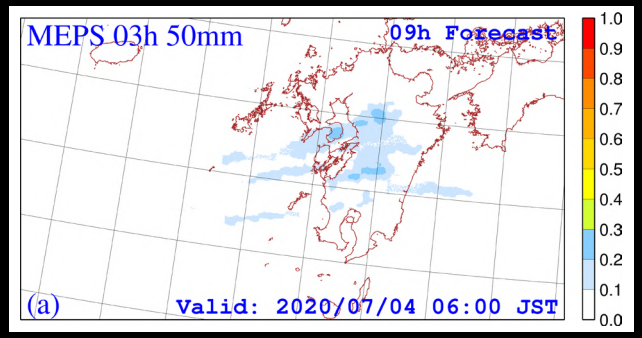
Fig. 3

Increasing the number of ensemble members to improve weather forecasting.

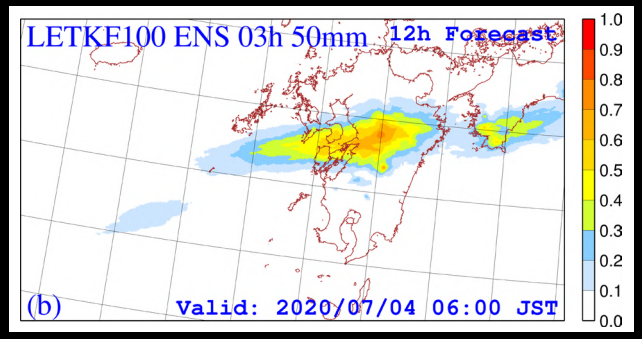
Results from Fugaku calculations using observation data from torrential rains in July 2020 by a research project team under the “Program for Promoting Research on the Supercomputer Fugaku”. After data assimilation, the team ran ongoing ensemble calculations to produce a 12-hour later forecast predicting the likelihood of heavy rains (more than 50 mm of rain in 3 hours). The closer to red, the higher the probability. The 21-member ensemble used by the JMA's meso-ensemble prediction system did not clearly identify which locations could expect heavy rains. The research team's 1,000-member ensemble, however, was able to identify those locations, making the prediction results a strong contender for use in providing emergency sheltering advisories. The areas that the 1,000-member ensemble predicted were very likely to, did actually experience heavy rains.

— Le Duc et al. (2021): Forecasts of the July 2020 Kyushu heavy rain using a 1000-member ensemble Kalman filter, SOLA

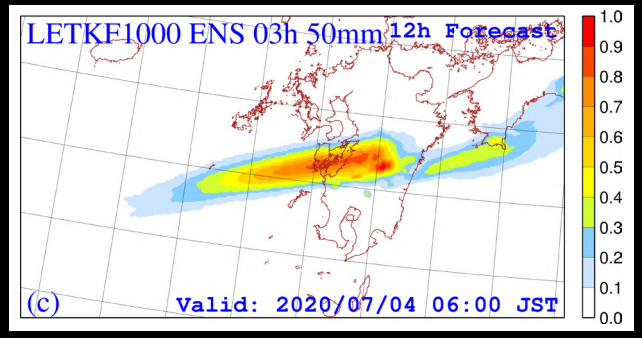
21-Member Ensemble



100-Member Ensemble



1,000-Member Ensemble



assess the accuracy of weather forecasts based on these ensemble data assimilation results. Yashiro, however, is confident. “Seeing the results (Fig. 3) of other teams working under the 'Program for Promoting Research on the Supercomputer Fugaku', we expect the accuracy will improve considerably.” As meteorological agencies around the world develop and use software incorporating our techniques over the next ten to twenty years, they will surely be able to more accurately forecast the paths of tropical cyclones and where heavy rains will occur, which will help minimize the damage they cause.

The “Large Ensemble Atmospheric and Environmental Prediction for Disaster Prevention and Mitigation” research project received enhancement support from RIST.

The long execution time for the parallel pre-processing program for the JMA's non-hydrostatic model (NHM) was made significantly faster with enhancement support from RIST. This made it possible to execute computations including pre-processing at higher speeds with up to 10,656 Fugaku nodes, calculations not possible on the K computer.

*1 Research project name: “Large Ensemble Atmospheric and Environmental Prediction for Disaster Prevention and Mitigation”
(Principal Investigator: Professor Masaki Satoh, Atmosphere and Ocean Research Institute, The University of Tokyo)
• Theme 1: “Short-range Regional Prediction”
(Principal Investigator: Takuya Kawabata, Head, Meteorological Research Institute)
• Theme 2: “Global-scale Prediction”
(Principal Investigator: Associate Professor Tomoki Miyakawa, Atmosphere and Ocean Research Institute, The University of Tokyo)
• Theme 3: “Advanced Technology of Data Assimilation”
(Principal Investigator: Hisashi Yashiro)

About the

Researcher

Hisashi Yashiro did not originally intend to become a researcher. While still a master's student, he spoke passionately about his research during a job interview. The interviewer asked him why he wasn't continuing his research, which put the idea in his head of becoming a researcher. As a student, he specialized in monitoring greenhouse gases, working with simulations only as a user of the resulting data. His research shifted to simulation-based studies and atmospheric modeling, and then to application development. In July 2019, he moved from RIKEN to the National Institute for Environmental Studies (NIES), where he is involved in research that integrates data received from the Ibuki greenhouse gas monitoring satellite into model simulations. A choral singer since his school days, he's a member of the institute's choral singing club.

Associated Research Projects

• “Large Ensemble Atmospheric and Environmental Prediction for Disaster Prevention and Mitigation” (hp200128)
Principal Investigator: Masaki Satoh, Atmosphere and Ocean Research Institute, The University of Tokyo
A paper reporting on the findings of this project was selected as a 2020 ACM Gordon Bell Prize finalist.

High-precision Fluid Flow Simulations to Revolutionize Manufacturing

One of the crucial final steps in designing ships and cars is to produce a scale model or a prototype to evaluate real-world performance. These tests often require large facilities to reproduce the environments in which the vessel or vehicle will actually be used. If those tests could instead be carried out by computer simulations, it could make the design process much faster and less expensive. At present, however, both of the simulation software and the processing speed of even supercomputers are not enough to run such simulations with the required accuracy. As the principal investigator on a project under the "Program for Promoting Research on the Supercomputer Fugaku",*1 Chisachi Kato intends to overcome these limitations. He has achieved simulations that could alter the performance testing conventionally done in ship design, and that can run within a feasible time during the design process.

Chisachi Kato
Center Director / Professor
Center for Research on Innovative Simulation Software,
Institute of Industrial Science, The University of Tokyo

The Simulations Needed for Ship Design

Manufacturing vehicles or watercraft begins with a "concept design" that determines the basic shape, functions, and so forth of the product to be made. This is followed by a "basic design" that lays out the basic specifications of the product, a "detail design" that refines the detailed specifications, and finally performance tests using ship models or prototypes (Fig.1). Explaining the significance of his team's performance test simulations, Kato says, "a large ship model is built and tested in a big long 'towing tank' filled with water. The testing for a single ship design costs about 10 to 20 million yen and takes about a week. Our goal is to replace this real-world testing with computer simulations. If we can run simulations instead of the

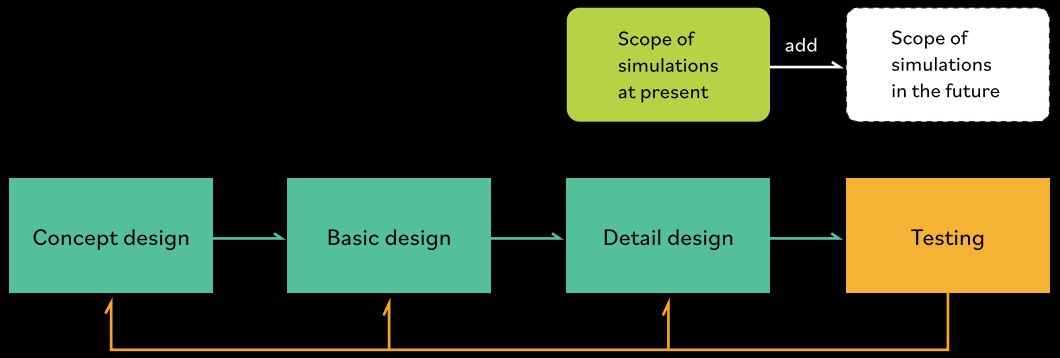
towing-tank tests, we can reduce the costs because we won't need to build a model ship to test. And if we find a performance problem, we can immediately modify the hull design to address it, which also saves time."

There are two main performance tests for ships: resistance testing and self-propulsion testing. In the resistance tests, a model ship is towed, without the propeller installed, to ascertain what resistance the hull encounters from the surrounding water. In the self-propulsion tests, the model is towed, with the propeller installed, to evaluate the interference effects between the hull and the propeller. A computational method known as "finite element analysis" is used to reproduce on computer the flow of water around the hull and propeller in simulations that aspire to completely replace the resistance and propulsion tests. In this method, the water around the hull is divided into a number of small segments called "elements", and the flow of water through these elements is computed according to the laws of physics.

To replace the towing-tank tests, the hydrodynamic modeling must be highly precise and accurate. This means it is necessary to replicate swirling eddies*2 less than 1 millimeter in size near the hull exterior. With conventional computations, however, the number of elements around the hull was at most tens to hundreds of millions, not enough to reproduce such small eddies. Kato and his team ran simulations 1,000 times more detailed, using

Fig. 1 Expanding the use of simulations in manufacturing.

The design of a ship or automobile progresses through several stages: concept design, basic design, detail design, and finally, performance testing with models and prototypes. If a problem is detected in the performance tests, the designer must step back through the previous stages and start over, sometimes all the way back to the concept design stage. So far, simulations have mainly been used at the detail design stage. Replacing the prototyping and testing stages with simulations also could save time and money. Moreover, it could dramatically reduce the overall design time, since required changes detected at the performance testing stage could immediately be reflected in the design.



*1 The "Research and Development of Innovative Fluid-dynamics Simulations for Aerodynamic/Hydrodynamic Performance Predictions by using Fugaku (Principal Investigator: Chisachi Kato)" research project consists of five research topics:
• Topic 1: "Realization of Numerical Towing Tanks and Improvements in Propulsion Efficiency with Energy Saving Devices"
• Topic 2: "Wall-Resolved Large Eddy Simulation of Internal Flow in a Multi-Stage Centrifugal Pump with Narrow Gaps"
• Topic 3: "Direct Analysis of Compressor Surge"
• Topic 4: "Prediction of Real-World Automotive Aerodynamic Performance"
• Topic 5: "Real-World Automotive Aerodynamic Sound Prediction"

*2 Includes a range of eddy sizes in temporally and spatially irregular flows.

from tens of billions to 100 billion elements, which could reproduce eddies less than 1 millimeter in size. Their simulations produced results that very closely matched the towing-tank test results (Fig.2).

Kato explains, “We had, in fact, done the same simulations before on the K computer. But they were so intensive that, even using around 25,000 of its compute nodes, the computations took about two days to complete. That's not fast enough for the actual design process. So, we've been doing research and development work on Fugaku with the goal of executing those computations in less than 1/30th the time.”

Fig. 2

The precision needed for computer simulations to replace towing-tank performance tests in ship design.

When testing a ship hull design, a scale model of the ship is towed in a long water tank, as shown in the photo at the top. The three graphs below compare waterflow velocities near the stern as obtained with: resistance testing in the water tank (top), conventional simulations (middle), and the new Fugaku simulations (bottom). The conventional simulations weren't able to reproduce the small turbulent eddies. But the new simulations use grids with 1,000 times as many grid points, allowing them to closely replicate the test results down to the small eddies. This is the level of precision that will be needed for simulations to replace the towing-tank performance tests.

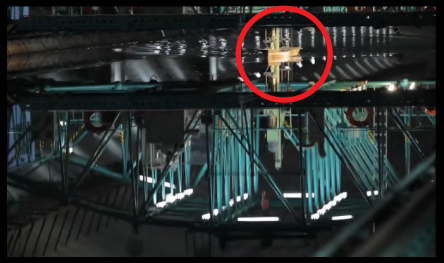


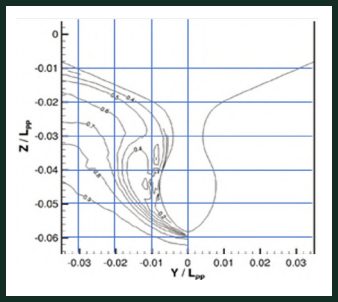
Image courtesy: Shipbuilding Research Center of Japan

Testing a model ship
(circled in red)

- Tank size: 400 x 18 m
- Water depth: 8 m
- Model length: 6 m
- Max. towing speed: 15 m/s (54 km/h)

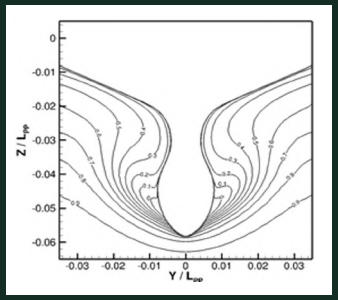
Flow velocities at ship rear
(Vertical cross-section)

Towing tank test results



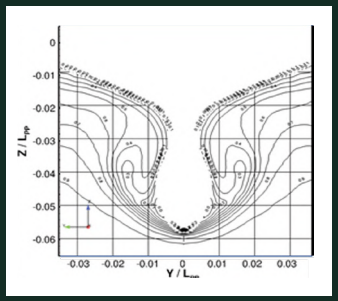
Conventional simulation results

Grid points (elements):
Tens to hundreds of millions



Simulation results in this study

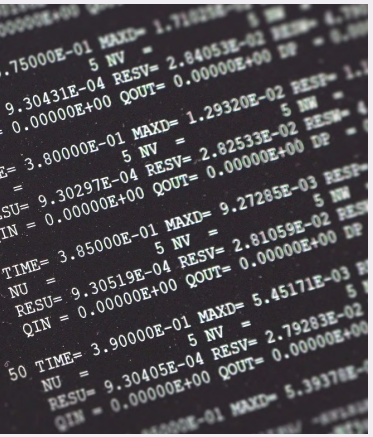
Grid points (elements):
Tens of billions to 100 billion



Faster Data Transfer Rates Speeded Up Computations

Kato and his team are developing a “flow solver” software based on the finite element method. It is called “FrontFlow/blue” (FFB). After completing his master's degree program in 1984, Kato joined a manufacturing company, where he wrote the software that served as a prototype for FFB. Since moving to a position in academia, he has been upgrading the FFB software, with the support of projects sponsored by MEXT, to achieve ever-better performance as supercomputers have grown more powerful.

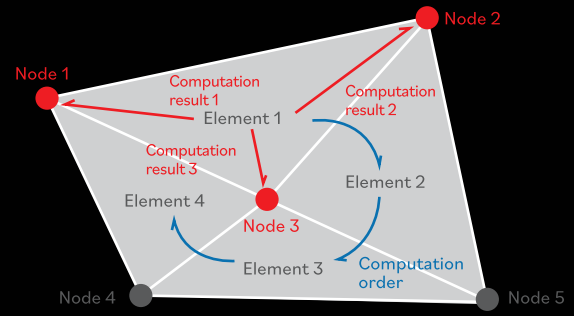
Taking advantage of the distinctive design features of Fugaku, his team devised yet another way to reduce FFB's run time. They leveraged the faster rate at which data is transferred between the memory and the arithmetic logic unit in a CPU. FFB's computations require large amounts of data to be read from memory. The improved data transfer rate means faster execution.



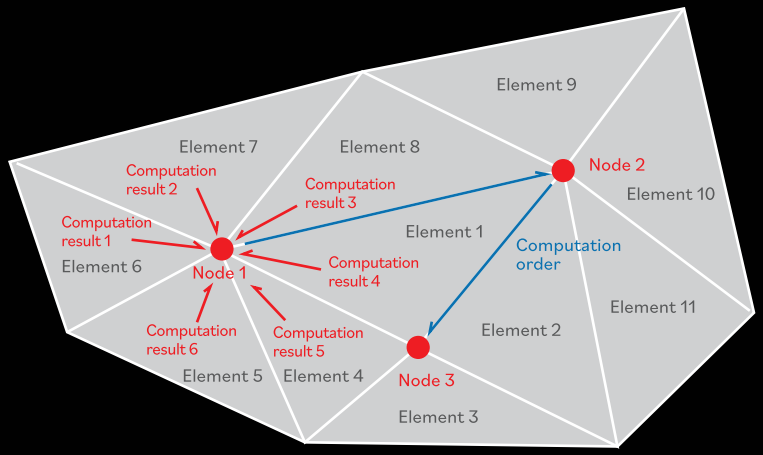
“One of our innovations was to arrange the data as carefully as possible when placing data into memory. This makes it possible to quickly retrieve the data to be used in computations. Another is that we have devised an algorithm with a modified finite element method (Fig. 3). Conventionally, element values are computed in order by element. But we decided to compute element values by node, in the order of the nodes that delineate the elements.”

Fig. 3 **A new algorithm utilizing Fugaku’s fast memory transfer.**

Conventional finite element algorithms compute in order by *element*. The value for Element 1 is computed first, then Element 2, and so on. FFB's new algorithm computes in order by *node*. All the elements sharing a common node are computed at once, and then those resulting values are used to update the value for that particular node, and so on. Changing the basic execution order of these computations takes full advantage of the performance offered by Fugaku's state-of-the-art CPU design.



Conventional finite element computation method

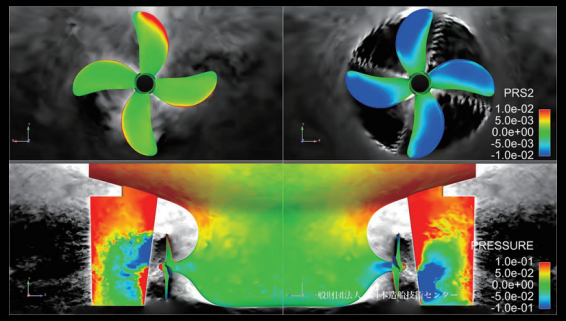


Computation method devised in this study

This increased the memory data transfer rate, nearing Fugaku's effective maximum memory bandwidth.*3 The computations were executed 70 times faster on Fugaku than on the K computer. Computations that had taken around two days with the K computer were completed in less than an hour, a success far exceeding the team's goals.

*3 The actual maximum memory bandwidth performance according to benchmark software, rather than a theoretical memory bandwidth according to memory specifications.

Fig. 4 **Simulations to evaluate waterflow interference effects near the propeller.**



— Image courtesy: Shipbuilding Research Center of Japan.

The flow of water around the hull and the rotation of the propeller cause interference, which affects the propulsion performance of the ship. Self-propelled ship models are used in water tank tests to measure these interference effects. But these towing-tank tests are limited in how much detailed data they can provide. The new simulations, however, can provide much more detailed data, which is expected to lead to improved ship hull and propeller designs. Pressure is shown in color, and waterflow is shown in black and white.

Working with End Users to Make Simulations more Practical

Kato and his team have run simulations, with detail down to small eddies, on several ship hull designs. They check the water-flow around the hull during resistance testing, the interference effects between the hull and propeller during self-propelled testing (Fig.4), and the resistance caused by waves. The results have closely matched those of the towing-tank testing. The simulations are getting to a level where they can replace real-world tests.

Speaking about future plans, Kato says, "Our main goal is putting these simulations to actual use. So, we want to move forward with computations for various ship designs and other conditions to demonstrate that these simulations are usable in the design stages."

But this is not limited to ships. The "Program for Promoting Research on the Supercomputer Fugaku" project that Kato oversees aims to make the use of supercomputer simulations feasible in the design of automobiles, pumps, compressors, and more. To facilitate industrial adoption, they have formed a consortium of 150 people from 54 organizations. They include the makers of ships, turbo-chargers, and hydraulic

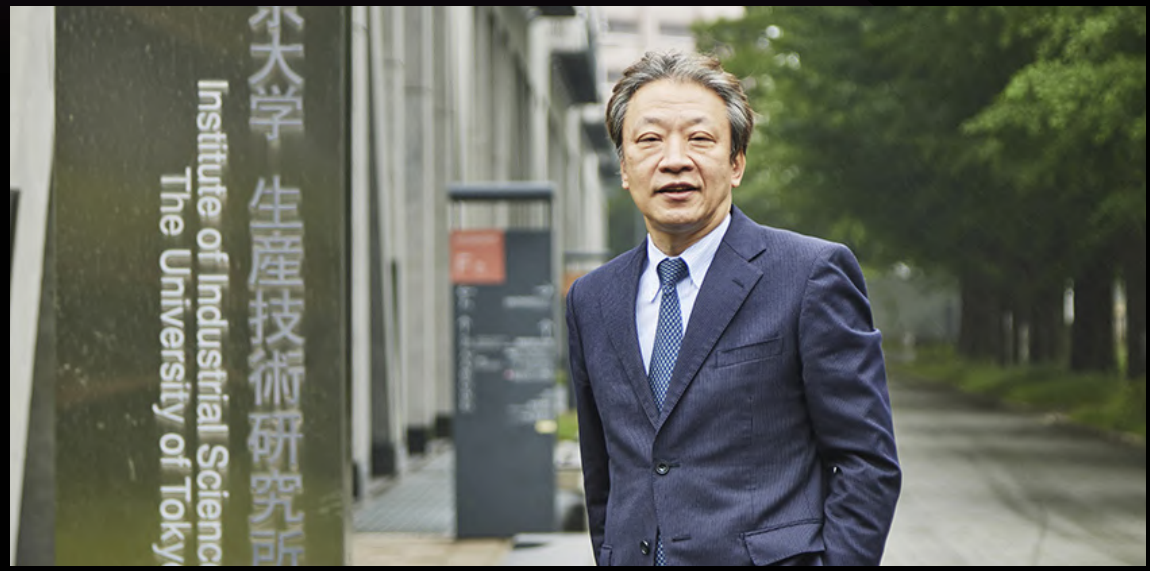
devices, as well as hardware and software vendors, who will work together to solve problems that manufacturers might encounter when implementing these computer models.

Kato has been working on software for fluid dynamics modeling since the dawn of supercomputers in Japan. The day when his efforts toward the practical use of simulations will bear fruit is just around the corner.

About the

Researcher

Chisachi Kato says as an elementary school student, he had a paper route to earn money to buy plastic models. At university, he majored in Mechanical Engineering and ran real-world experiments. But when he encountered computer-based simulations in his workplace after graduating, he became fascinated and has worked with simulations ever since. Having picked up organizational skills while working part-time as a mover and a party organizer, and with his attention to grammatical detail when preparing English manuscripts, computer simulation work seems to be his dream job. The research work doesn't seem to cause him stress. For fun, he plays golf with friends. He looks forward to playing again, once the COVID-19 crisis has ended.



Associated Research Projects

• “Research and Development of Innovative Fluid-dynamics Simulations for Aerodynamic/Hydrodynamic Performance Predictions by using Fugaku (Research and Development of a Turbomachinery Design Simulation System)” (hp200133)
Principal Investigator: Chisachi Kato, Institute of Industrial Science, The University of Tokyo
2020 ACM Gordon Bell Prize finalist for Research Findings

Innovative Materials Development with Computer Science, Data Science, and HPC

Materials Informatics (MI) is an attempt to improve the efficiency and sophistication of materials development by incorporating data science methods. While the use of MI in materials development is making headway thanks to advances in machine learning, a major obstacle that remains is a lack of data about the properties of the countless different materials known to exist. To tackle this problem, a team at Sumitomo Chemical lead by Shinya Nishino is using large-scale simulations to create a materials database suitable for machine learning. In this article, we look at this new materials development approach that combines computer science with data science and high performance computing.

Shinya Nishino
Team Leader
Digital & Data Science Innovation Department,
Sumitomo Chemical Co., Ltd.

Materials Informatics (MI): Transforming How Materials are Developed

Until recently, the development of materials for various industrial uses has mostly relied on the wisdom and intuition of experienced researchers and engineers. But, as customers' needs have grown more diverse and R&D time has been curtailed, it is becoming more and more difficult to address these needs with traditional approaches.

Enter Materials Informatics (MI), which brings AI and data science to materials development to drastically shorten development times and discover innovative materials with novel properties. Shinya Nishino at materials maker Sumitomo Chemical has striven to make

Explanation 1 How MI is being used in Materials Development

Materials Informatics can improve common development tasks:

High Throughput Screening

MI can quickly find the most suitable from a group of candidate materials.

Case 1: Using machine learning to screen 1.6 billion molecules to find OLED (Organic Light Emitting Diode) materials with 22% external quantum efficiency.

— R Gómez-Bombarelli, et al., *Nature Materials* 15, 1120-1127 (2016)

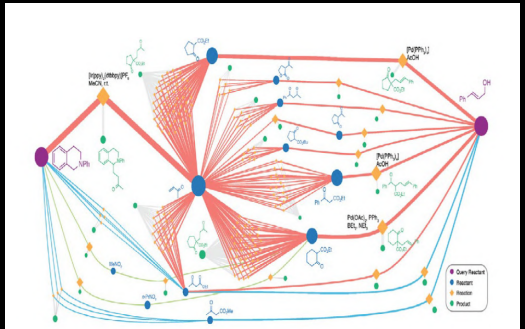
Inverse Problem Approaches

MI can start with the desired properties and work backwards to find the materials that have those properties.

Case 2: Using Bayesian inference to solve an inverse problem and successfully build a system that suggests molecular structures with the targeted properties.

— H. Ikebata, et al., *J. Computer Aided Molecular Design* (2017) 31: 379-391

Retrosynthesis

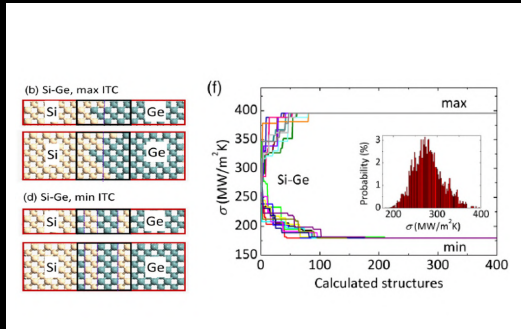


MI can learn from existing data to predict the most efficient pathways (processes) to synthesize the desired molecules.

Case 3: Learning documented synthetic pathways to predict new synthetic pathways with greater than 50% accuracy.

— M. H.S. Segler, M. P. Waller, "Modelling Chemical Reasoning to Predict and Invent Reactions", *Chem. Eur. J.* 2017, 23, 6118, Copyright Wiley-VCH GmbH

Efficient Experiment Design



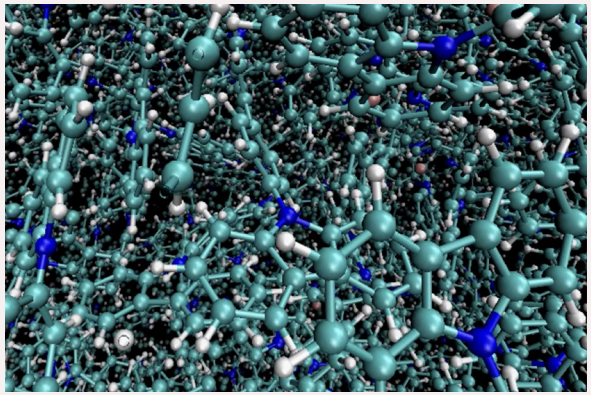
MI can help plan the most efficient experimental approach when investigating a particular property of materials.

Case 4: Using Bayesian optimization on existing data to minimize the number of physical tests in discovering optimal structures for thermoelectric materials.

— S. Ju, et al., *Phys. Rev.* X 7, 021024 (2017)

practical use of MI in the development of materials.

"When a new smartphone model comes out, for example, materials manufacturers have to provide new materials for a better-looking display or a longer battery life. Responding to these requirements with conventional approaches to materials development is time consuming, and finding new materials is becoming ever more difficult. Materials manufacturers are becoming increasingly aware of the need for a different approach to materials development, and MI is one of the answers."



The Bottleneck is a Lack of Data on Materials

In Materials Informatics, a prediction model is created through machine learning. That model is then used to predict the synthetic pathways and other properties of candidate materials. What is important here is that the prediction model can replace the intuition and experience of researchers and engineers, and that a database of material properties can be used to create the model. According to Nishino, however, the availability of such materials databases lags far behind those for other fields, such as drug discovery.

“Big data approaches are currently focused on fields with data that is more readily available. Unfortunately, there is very little data in the field of materials. If you try to find materials data with the features and process conditions you want for a particular development target, you may find that there are only 100 data sets at most. This lack of materials data is the biggest hurdle to implementing Materials Informatics.”

To address this problem, Nishino had the idea of running large-scale computer simulations to automatically create a database of materials and their predicted properties. First, they run computer simulations to understand the mechanism behind a particular property of a material. Next, they map that property to a numeric value known as a “descriptor”. Those descriptors can then be used to predict the properties of other materials at a lower computational cost. And then machine learning is applied to the materials data generated from those descriptors.

“If large-scale simulations on high performance computers can be used to generate materials data that was previously unavailable, we can get a competitive advantage in development. Combining Materials Informatics with that data can make it much more valuable. I expected that a combination of computer science, data science, and HPC could revolutionize materials development.”

A Combination of Large-scale Computer Simulations and Machine Learning

Nishino applied this “materials data from simulations” approach to research on organic light emitting diode (OLED) materials, which are commonly used to illuminate the displays of modern smart-phones and televisions. An OLED material’s ability to emit light is a property known as its “luminescence”. The luminescence is determined by how certain electrons move or “hop” within the molecular structure of a given material, an important phenomenon known as “charge transfer”. To better understand how charge transfer occurs in various OLED materials, Nishino ran large-scale simulations of quantum wave packet dynamics in collaboration with

Takeo Hoshi, an Associate Professor at the Tottori University Graduate School of Engineering. Because these calculations require advanced algorithms and powerful computing resources, they used the Oakforest-PACS supercomputer at the Japan Center for Advanced High Performance Computing, which was the fastest computer available in 2019.

These were “numerical simulations”, mathematical models of physical systems that allowed Nishino to analyze how electrical charges move around inside OLED materials. He discovered that the electrical charge transfers in an OLED material can be predicted using a “physical quantity” called the “inverse participation ratio” (IPR) as a molecular descriptor that indicates the material's properties. Using this IPR descriptor to sort the materials according to their charge transfer property allowed the research team to generate a materials database suitable for use as input for machine learning.

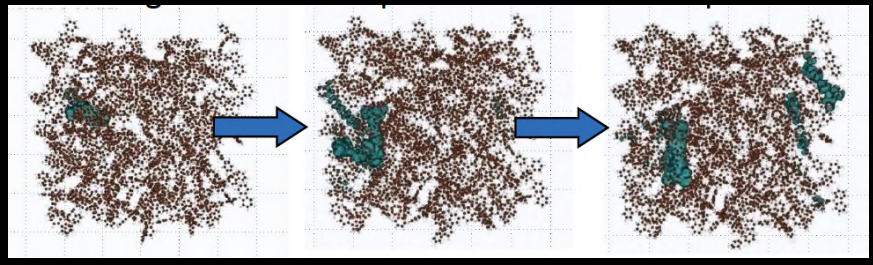
“It’s often better to use a particular property of a material as the machine learning input, rather than just the material's molecular structure. This is because models based on an underlying principle are generally more versatile. At this point, it's important to know what kind of descriptors to put into the model, which is hard to know with pure data science alone. It requires a knowledge of physics and chemistry, or experience working with the material. With that kind of knowledge and experience, it's easier to recognize that a particular section can be reduced to a feature (a physical quantity suitable for machine learning), and that it can be quantified.”

Explanation 2 Large-scale quantum simulations of charge transfers in OLED materials

The so-called “hopping” transfer of electrical charge within a molecule is the crucial physical phenomenon that determines the luminescent properties of a given OLED material. In this study, Nishino used numerical simulations of quantum wave packet dynamics to investigate how electrical charge propagates through the molecules of more than a dozen OLED materials with different combinations of host molecules and guest molecules, known as “host-guest complexes”. These numerical simulations were run by Tottori University Graduate School of Engineering Associate Professor Takeo Hoshi, an expert in large-scale high-performance computing simulations.

The figure below illustrates a charge transfer that occurs in OLED molecules as revealed by these numerical simulations. The simulations showed how the wavefunctions of two complexes overlap when a charge jumps from one complex to the other. This research demonstrated that the charge transfer property for a given OLED material can be predicted by a physical quantity called the “inverse participation ratio” (IPR). Calculating this IPR descriptor is much less computationally expensive than running quantum simulations, thereby lightening the computational load for predicting a material's properties. Nishino says his familiarity and experience with condensed matter physics theory was very helpful in discovering the IPR's usefulness a descriptor.

This series of images taken from the wave packet dynamics simulations shows how the wave packets move. The blue regions show the “hole” wave packets, the location of the charge. We can see that the charge jumps from place to place.



The IPR descriptor that Nishino found in this research is a physical quantity that is covered in the basic theory of condensed matter physics. But he says it has rarely been used in the field of materials science.

“I used to do research in theoretical condensed matter physics, which is how I determined the IPR could be used as a descriptor. The team members on this project include specialists in materials development, computer science, and data science. Plus, we have support from RIST, which is a leading organization for HPCI work. I think that diversity of expertise helped lead to this achievement.”

From Materials Informatics to the Cyber-Physical Systems Loop

Nishino says he wants to use HPCI resources like Fugaku to further apply this new “computer science meets data science meets HPC” approach to materials development.

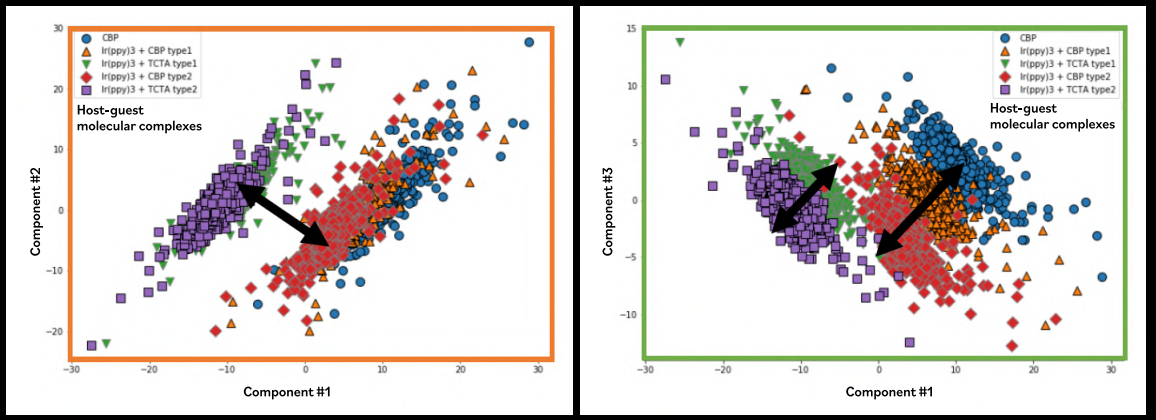
“It's increasingly vital to create data that others can't get, and to understand mechanisms that haven't been understood thus far. So, I think advanced simulations using HPC and data generation via those simulations will become even more important. What I want to work on in the future is a way to create machine learning models for the kinds of materials that are relatively easy to simulate, and then using those models even in areas where it's difficult to acquire data. This is called 'transfer learning'. It's often used in image analysis. But I think it could also be of use in materials development.”

Nishino hopes to create a more advanced and data-driven approach to materials development, one that combines theory, experimentation, simulations, and data science.

Explanation 3

Verifying the categories of materials produced with the IPR descriptor

The figures below show the results of tests to verify whether using the IPR as a descriptor accurately categorized the OLED materials simulated. The IPR is a multi-dimensional parameter, so the “principal component analysis” technique was used to reduce the number of dimensions when verifying the results. The left figure shows changes in the molecular host-guest pair complexes. The right figure shows changes in the concentration of these complexes. Both results show distinct differences for materials with different host-guest complex compositions. This suggests that a machine learning model that uses the IPR descriptor data to categorize materials should be effective in predicting the luminescence properties of OLED materials.



“At this stage, we've combined theory, computer science, and data science. But our goal is to add experimentation to this, generate new theories and new models based on the findings of those experiments, and then generate new data through simulations based on those models. The goal for the next iteration of Materials Informatics is realizing a materials development cycle called the 'cyber-physical systems loop'. And I think my role is in building a system that can sustainably create value by developing human resources who can master MI and the cyber-physical systems loop.”

About the

Researcher

Shinya Nishino says he studied the basic theory of physical properties at university, and worked in materials research which combined that basic theory with computer simulations as a graduate student and post-doctoral researcher. At that time, he and Takeo Hoshi at Tottori University developed the software that was used for these numerical simulations.

Nishino first became interested in Materials Informatics as a postdoctoral researcher. When running numerical simulations of materials for lithium-ion batteries at the request of a Japanese auto maker, he saw how Materials Informatics was being used by competitors abroad to examine candidate materials, and sensed the great potential of this field.

Nishino's comprehensive experience with materials theory, large-scale computer simulations, and actual materials development in practice is likely the key to his success as a pacesetter in Materials Informatics.

Associated Research Projects

- “Organic Semiconductor Material Design using Large-Scale Quantum Simulations and Machine Learning” (hp190066)
- “Design of Organic Semiconductor Materials by Machine Learning Model built from Big Data Generated by Large Scale Quantum Chemical Calculations” (hp200049)

Computational and Data Science for Next-generation Batteries with Safety and High Performance

To address the threat of climate change, Japan and other countries have embraced the goal of becoming carbon neutral and reducing their greenhouse gas emissions to zero by 2050. High-performance rechargeable batteries are expected to provide a decisive advantage in achieving this goal. Solid-state batteries in particular are expected to be widely used in electric vehicles, and the race to develop them is taking off around the world. To use the powers of computer science and data science to help develop solid-state batteries, Yoshitaka Tateyama's research group has been making steady progress in the quest to understand the underlying mechanisms of suitable materials for these new batteries. Their "Fugaku Battery & Fuel Cell"*1 project falls under the "Program for Promoting Research on the Supercomputer Fugaku" rubric.

Yoshitaka Tateyama
Group Leader
Interface Computational Science Group,
Center for Green Research on Energy and Environmental Materials,
National Institute for Materials Science

*1 Research project name:
"Computational and Data Science Study for ET Revolution by Development of Next-Generation Battery and Fuel Cell" (Principal Investigator: Yoshitaka Tateyama)

Solid-state Batteries to Make Electric Vehicles Mainstream

Electric vehicles themselves do not emit carbon dioxide while running. So, if the electricity used to charge them is obtained from renewable energy sources, the total carbon dioxide emissions should be drastically less than with gasoline-powered vehicles. One of the key factors in the adoption of electric vehicles is developing safe, efficient batteries. At present, electric vehicles are equipped with lithium-ion batteries similar to those used in smartphones and other portable devices. But the liquid electrolytes used in these lithium-ion batteries are flammable and require strict safety measures. To mitigate these problems, both academic and industrial researchers are working on battery designs

with solid electrolytes instead of the liquid ones.

“Solid-state batteries are not only safer; they can also be more efficient. With energy and power densities greater than those of conventional lithium-ion batteries, solid-state batteries are expected to extend the cruising range of electric vehicles, improve acceleration, and shorten recharging times,” says Tateyama.

But developing solid-state batteries is not an easy task. The biggest challenge is the need for a solid electrolyte material that conducts lithium ions well. In both conventional and solid-state batteries, lithium ions travel between the positive and negative electrodes during charging and discharging (Fig.1). The organic liquid electrolyte in a conventional battery allows lithium ions to flow through freely. But the solid electrolyte particles in a solid-state battery impede the lithium ions' ability to pass through, limiting the battery's charge-discharge performance.

Researchers are therefore investigating a range of candidate materials to find a solid electrolyte that will allow lithium ions to pass through faster. Physically testing the immense number of candidate materials, however, would require enormous time and effort. That's where Tateyama and his team come in. They are using supercomputers like Fugaku to search for solid electrolyte material candidates.

Using Machine Learning to Search for Promising Solid Electrolytes

To efficiently search for materials that can pass lithium ions very quickly, Randy Jalem of Tateyama's group devised a new approach to the calculations (Fig. 2). First, based on structures found in a database of known materials, tens of thousands of hitherto unknown materials are generated on a computer. Next, using clues such as the shape of the pathway for lithium ions and the types of elements around the pathway, promising candidates are selected from among the many materials generated. Then, machine learning with

Fig. 1 Lithium-ion Battery Designs

In solid-state batteries, the conventional organic liquid electrolyte (a) between the positive and negative electrodes is replaced with a solid electrolyte material (b). Both designs operate the same way, with lithium ions transfering back and forth between the positive and negative electrodes when charging or discharging the battery.

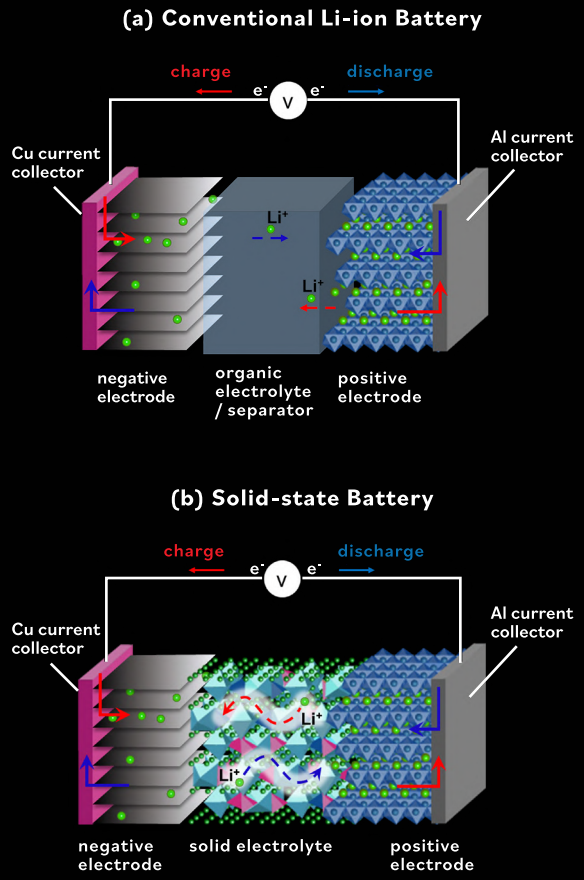
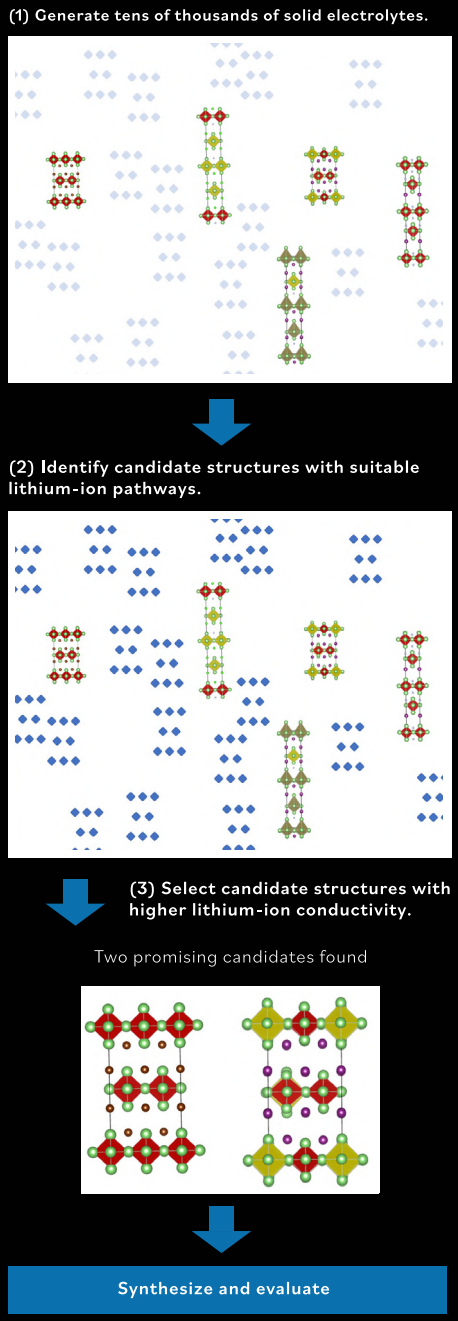


Fig. 2

The computational process for discovering solid electrolyte candidates and its inventor, Randy Jalem.

The Steps to Discovery:
(1) Rearrange the atoms of known crystal structures to generate tens of thousands of solid electrolyte candidates.
(2) Narrow down the candidates based their lithium ion pathways and the types of elements around the pathways.
(3) Use Bayesian optimization to select the remaining candidates with higher lithium ion conductivity.
The remaining candidate materials discovered through this process were actually synthesized in the laboratories of the Tokyo Institute of Technology.

Randy Jalem
Senior Researcher
Interface Computational Science Group,
Center for Green Research on Energy and Environmental Materials



Bayesian optimization is used to select the materials that should allow the lithium ions to pass through the fastest.

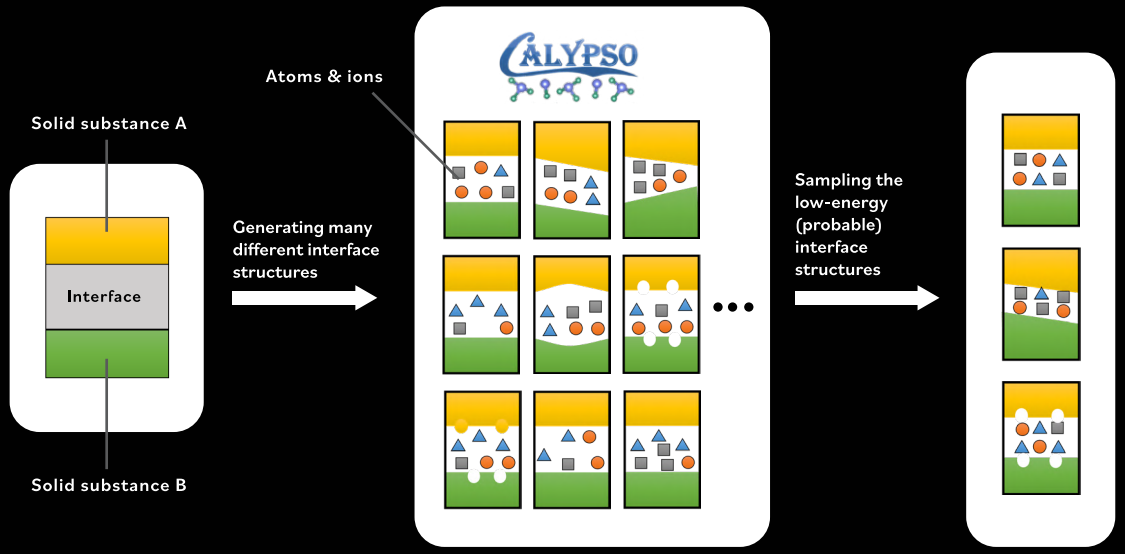
Jalem says, “With this approach, I found two promising candidates. Those two will be synthesized in a lab and tested for their performance.” The results show that large-scale computations can speed up research by selecting candidate materials logically.

Jalem enthuses, “When we were using the K computer, the materials search calculations took weeks, because we have to iterate through loop statements so many times. With Fugaku's huge number of high-performance nodes, we can run the calculations much faster. So, we could run a search with many more candidate materials.”

Fig. 3

Heterogeneous Interface CALYPSO Method

First, in the interface section between the two different types of solids (A and B), various arrangements of atoms and ions from these two solids are used to generate tens of thousands of different interface structures. While the energy of each candidate interface structure is being calculated, the positions of its atoms and ions are optimized. From these, the structures with the lower energies, meaning more probable structures, are selected.



Massive Searches for Interfaces to Maximize Battery Performance

Another major issue in the development of solid-state batteries is controlling the interface between the solid electrolyte and each electrode material. Researching and developing the coating layers is particularly important. “Actually, solid-state battery performance tends to degrade over time with repeated charging and discharging. We know that a thin coating of a different material applied to the surface of the electrode material can effectively prevent this degradation, but we don't exactly know how that works. So, the strategy has not been quite established which material is best to use or how thick that coating should be,” explains Tateyama. To make the best use of lab testing resources, he is using computer science to better understand how lithium ions and electrons travel through the materials that comprise the electrodes, the coating layer, and the solid electrolyte.

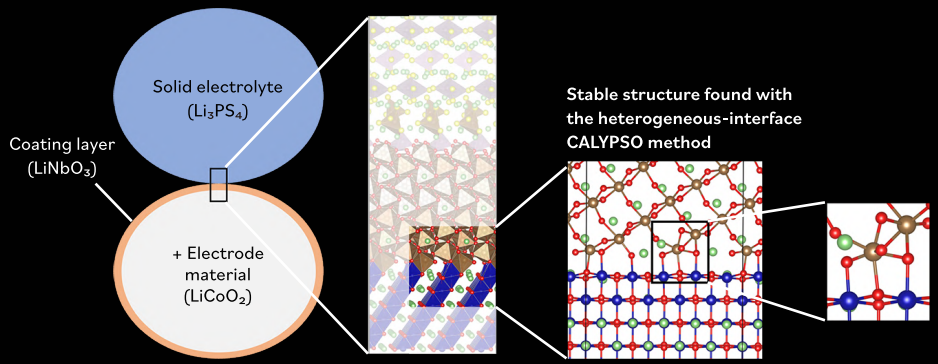
Tateyama's group developed an AI-based CALYPSO (Crystal structure AnaLYsis by Particle Swarm Optimization, Fig. 3) method to predict the structures at the “heterogeneous interface” where the atoms and ions of two different materials adjoin in structures with varying arrangements. The CALYPSO method generates tens of thousands of these atomic interface structures, and efficiently calculates the energy of each to predict which structures are more stable and therefore more likely to occur. Using this method, Tateyama was able to find stable structures for both the electrode-to-coating interface and the

coating-to-solid electrolyte interface (Fig. 4). This was Tateyama and his team's game changing work with computer simulations to automate searches for stable interface structures. The computing power of Fugaku enabled them to search an enormous number of these structures. The team is now studying the behavior of the lithium ions and electrons in the structures they discovered to better understand how the coating layer suppresses degradation.

“Controlling the interface as well as the coating is key to developing solid-state batteries. So, we'd like to help formulate guidelines for interface design by showing what's actually happening at the interface. To calculate the energy of the interface structure, we use a precise method called “first-principles calculations”,*2 which requires a huge amount of calculating for even a single structure. But with Fugaku, we can compute the energies of many structures at once in parallel, so our research can move quickly,” says Tateyama. The combination

*2 First-principles calculation: A calculation that follows the fundamental laws of physics without the use of empirical parameters. In this case, it refers to calculating a property such as the energy of a material according to quantum mechanics.

Fig. 4 Coating Layer Research



The coating layer is sandwiched between an electrode material on one side (in this example, the positive electrode material), and the solid electrolyte material on the other. The particles comprising the electrode material and the solid electrolyte material are a few micrometers in size, but the coating layer is much thinner, only a few nanometers. The heterogeneous interface CALYPSO method was used to find possible interface materials with a stable structure on both the electrode-facing side and the solid electrolyte-facing side. The conductivity of the structures in those candidate interface materials was then studied to determine how easily lithium ions and electrons could pass through them. The right side of the figure shows an example of the calculated interface structures between the solid electrolyte material and the coating layer. In practice, the interfaces between many different materials were studied.

of laboratory testing and Fugaku's calculations will greatly accelerate the research and development of solid-state batteries. Computer science and data science will help create high-performance solid-state batteries, which in turn will help us achieve carbon neutrality as electric vehicles become the norm.

About the

Researcher

Yoshitaka Tateyama decided to become a scientist in elementary school upon reading the biography of physicist Lev Landau and being captivated by his forthright attitude toward science. Tateyama says his motto concerning work is “to do groundbreaking research”. To that end, he values actively communicating with people from all walks of life. There is a lot to be learned from conversations, and sometimes the seeds of future research can be found through interactions with experimenters. A nice drink or an enjoyable meal can grease the wheels of communication. But for now, the COVID-19 pandemic has put such opportunities on hold.

Associated Research Projects

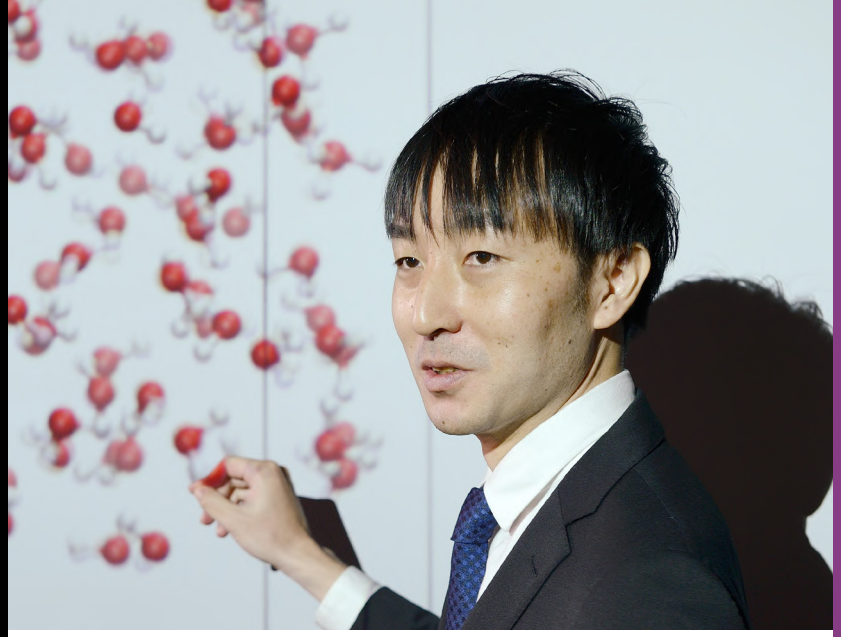
• “Computational and Data Science Study for ET Revolution by Development of Next-Generation Battery and Fuel Cell” (hp200131/hp210173)
Principal Investigator: Yoshitaka Tateyama, National Institute for Materials Science

First-Principles Molecular Dynamics Simulations for Water Interface Science

When water comes in direct contact with another substance, the “water interface” describes the area where their respective molecules meet. It is a place rich with peculiar chemical interactions whose underlying mechanisms are not well understood. Tatsuhiko Ohto at Osaka University is exploring the mysteries of the water interface. He uses first principles molecular dynamics (FPMD) simulations based on "density-functional theory”. These FPMD simulations compute the interactions of individual molecules based on their electronic states. Using a combination of massive simulations on high performance computers (HPC)*1 and verification testing, his research is expanding the frontiers of FPMD, elucidating photo-catalytic reactions and finding the computational methods most suitable for simulating the water interface.

Tatsuhiko Ohto
Assistant Professor
Division of Frontier Materials Science
Department of Materials Engineering Science
Graduate School of Engineering Science, Osaka University

*1 High Performance Computing uses supercomputers to perform massive-scale calculations, typically to simulate complex real-world interactions for research and development work.



The Water Interface: Where Chemical Interactions Get Interesting

The “water interface” is the molecular boundary between water and the other substances that water comes in contact with. Some of the phenomena that occur here are unique to the water interface, and not seen in either substance by itself. The surface tension between the legs of an insect that walks on water and the water surface, and the ability of lotus flower leaves to repel water, are examples of water interface phenomena.

The interface between water and solids is also where the electrochemical and catalytic reactions needed for industrial technologies

take place. The chemical properties where an electrode meets the electrolyte in a battery, for example, can significantly impact battery performance. And understanding the interface between catalysts and water molecules is important for generating clean hydrogen energy more efficiently.

Tatsuhiko Ohto at Osaka University is using first principles molecular dynamics simulations to elucidate the chemical interactions at the water interface.

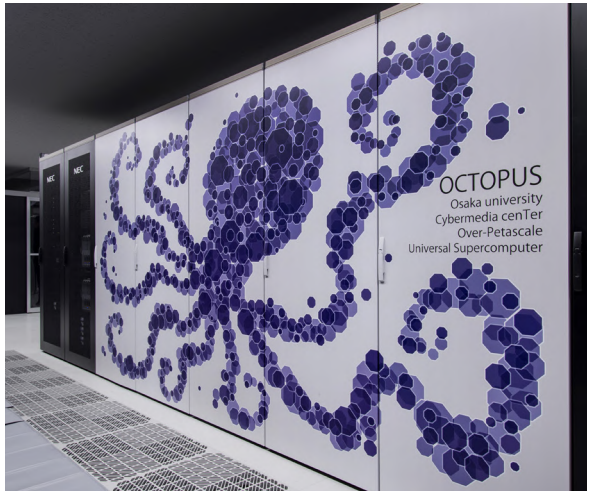
“The interface region is no more than a few water molecules thick. That very narrow region is extremely difficult to observe through experiments. But computer simulations allow us to reproduce those interactions down to the movement of molecules and even individual atoms. These simulations are proving to be an extremely powerful tool for studying what occurs at the interface.” says Ohto.

Simulations Track the Movement of Individual Molecules

Most molecular dynamics simulations to date have approximated these atomic interactions by relying on simple functions, such as that of a spring-like force. These are approximations of *classical force fields*. However, these spring constants and other known parameters might only apply to water molecules away from the interface. There was no guarantee that these values would also hold true for the peculiar place where water interfaces with another material.

Ohto therefore ran “first principles molecular dynamics” (FPMD) simulations based on deeper fundamentals, specifically the force values obtained through “density-functional theory” *quantum mechanical* modelling of the molecules’ electronic structures, rather than parameters obtained through experiments.

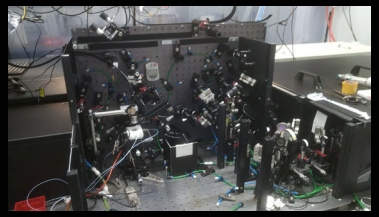
“Even if the simulations tell us what the molecular structure of an interface should be, it’s still just a theory until it’s proven through real world observations. So, we ran experiments using ‘sum frequency

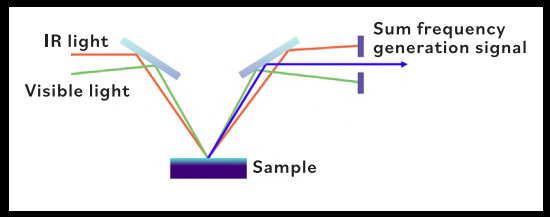


generation’ spectroscopy, which measures how the molecules vibrate at the interface. We then confirmed the interface properties predicted by our computations by comparing them to the experimental results.”

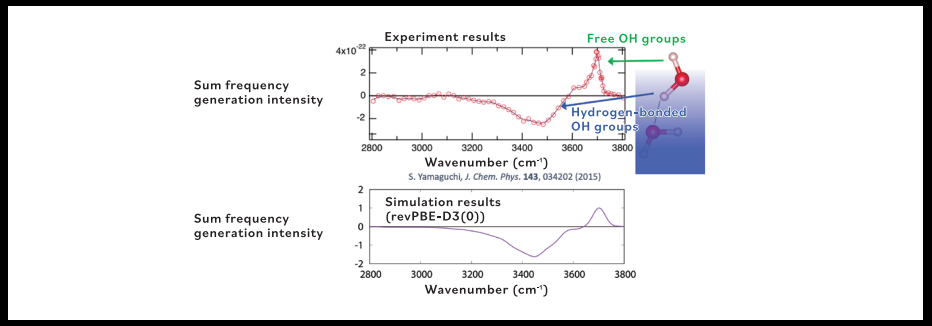
Explanation 1 Sum Frequency Generation Spectroscopy Experiments

Ohto used “sum frequency generation” spectroscopy to verify the results of his FPMD simulations. In sum frequency generation, visible light and infrared light are directed onto the same water interface sample at the same time. The light reflected back from that interface is measured. When the frequency of the infrared light matches the vibration frequency of molecules at the interface, the interface *generates* light at a third *frequency*, which is the *sum* of the original two frequencies, hence “sum frequency generation”. The frequency of the infrared light is varied to obtain the shape and intensity of the reflected light spectrum. He then compared those results with the computer simulation findings.





Photograph (left) and diagram (right) of the experimental setup for the sum frequency generation spectroscopy measurements. The measurements were conducted by Ohto’s collaborators at the Max Planck Institute for Polymer Research in Germany.

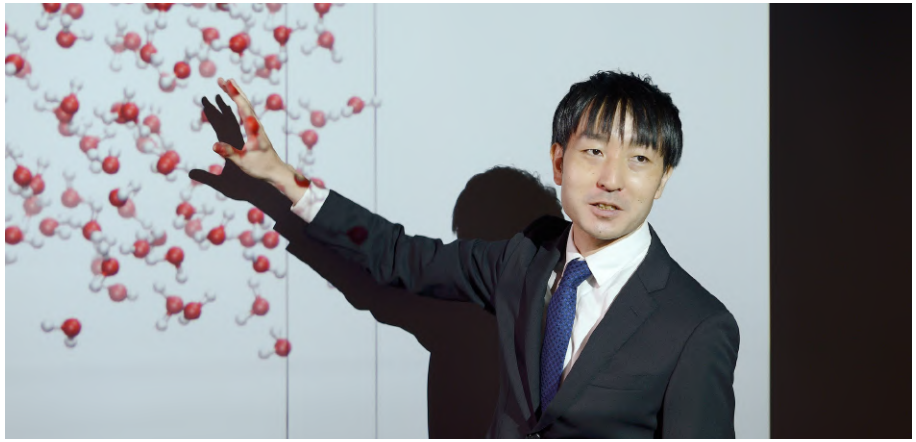


Comparison of the sum frequency generation spectra of the water-air interface from the measurements (above) and the FPMD simulations (below). Both show peaks at frequencies around 3500 and 3700 cm^{-1}. These frequencies are thought to correspond to the stretching vibrations of the hydrogen-oxygen bonds in the water molecules at the interface (positive and negative peaks representing the upward and downward orientations of the OH bonds).

Explaining the Mysteries of Photo-catalyst Interfaces

Titanium dioxide is a commonly used photo-catalytic material. Under normal conditions, titanium dioxide is “hydrophobic”, meaning it repels water. But when exposed to ultraviolet light, it becomes “hydrophilic”, attracting water. This change was thought to be caused by “OH groups” (bonded pairs of oxygen and hydrogen atoms) dangling on the surface of the titanium dioxide at the interface. But it had yet to be confirmed.

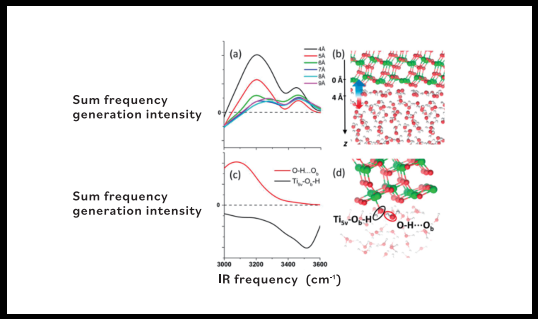
This prompted Ohto to run FPMD computations simulating titanium dioxide with and without OH groups dangling on its surface, and compare those results with the actual sum frequency generation spectra obtained through experiments. The results showed that the hydrophilic or hydrophobic properties correlate strongly to the presence or absence of OH groups. This gives us a better understanding of the photo-catalytic reactions occurring at this interface, and may allow us to produce more effective photo-catalysts in the future.



Explanation 2

First-Principles MD Simulations of the Titanium Dioxide/Water Interface

Ohto performed FPMD simulations with and without OH groups dangling on the surface of the titanium dioxide (see figure below). The measured spectra more closely matched the computer simulations with OH groups present (figure c) than without (figure a). This suggests that OH groups are present on the surface of UV-irradiated titanium dioxide.



Results of FPMD simulations of the titanium dioxide/water interface.
(a) Depth-dependent sum frequency generation spectra of the OH bonds calculated with FPMD trajectories at the nonhydroxylated titanium dioxide/water interface. (b) A snapshot of the nonhydroxylated titanium dioxide/water interface. (c) Individual contributions of the O–H hydrogen bonded to O_b atom and the O_b–H group chemisorbed on the five coordinated Ti atom to the sum frequency generation spectrum at the hydroxylated titanium dioxide/water interface.
(d) A snapshot of the hydroxylated titanium dioxide/water interface.

— S. Hosseinpour, T. Ohto et al., *J. Phys. Chem.* Lett. 8, 2195 (2017).

The University of Tokyo's massively parallel Oakbridge-CX supercomputer and the Osaka University Cybermedia Center's OCTOPUS supercomputer were used for these FPMD simulations. "HPC is essential for the enormous and complex computations that FPMD requires," says Ohto.

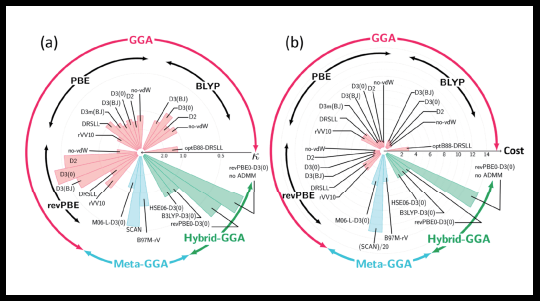
Finding Cost-Effective Calculation Methods

Because it is not possible to get an exact solution for a "many-body problem", first principles calculations require some amount of approximation. "Density functional theory" is used for this purpose. While the exact expression of the "exchange-correlation functional" that describes the interaction between the electrons of interest is not known, various approximations have been proposed. In general, the more accurate the approximation, the higher its computational cost. So, cost performance is of particular importance for FPMD simulations, which can require tens of thousands of calculation steps. However, it was not well known which approximation formula would provide the most cost-effective calculations for such a distinctive subject of study as material interfaces.

Ohto ran water interface simulations to compare the accuracy and computation time of different approximation formulas. He found that some approximation methods with relatively small computational cost can provide highly accurate results. "Moving forward, we intend to apply these findings to our water interface research," says Ohto.

Explanation 3

Comparing Approximation Methods for Exchange-Correlation Functionals



(a) Accuracy in approximating the water-air interface

(b) Computational cost

Comparing various approximations of the exchange-correlation functional for FPMD computations of the water interface. Figure (a) on the left shows the accuracy of the calculations (the longer the radius, the more accurate). Figure (b) on the right shows the computational cost (the longer the radius, the longer the calculation time). For example, "revPBE" was found to provide highly accurate approximations with relatively short computation times.

— T. Ohto et al., *J. Phys. Chem.* Lett. 10, 4914 (2019).

Toward More Realistic Water Interface Simulations

The findings of this research provided insights regarding the special properties of the water interface, and also showed the enormous potential of high performance computing for first principles molecular dynamics simulations. Ohto says he hopes to further develop these methods for more complex and more realistic studies of the physical phenomena that occur at the interface.

“We were able to find good calculation methods for the interface between water and air this time,” said Ohto. “In the future, I’d like to apply these methods to more complex water interfaces. In real world chemical reactions, the pH level varies according to the ions, and there are numerous impurities and defects on the surface of a solid. I’ d like to run simulations of water interfaces that are even closer to reality and take those effects into account.”

About the

Researcher

Tatsuhiko Ohto says he’s been interested in the natural sciences since childhood. He became curious about astronomy in elementary school, and environmental issues in junior high and high school. An internship at Germany’s world-leading chemical manufacturer BASF during his master’s program led to his interest in research work. Having experienced R&D work in BASF’s computing department, he says he felt that, “there was still a lot left to do in academia”. Upon returning to his university laboratory, and wanting to do research on bigger issues that could be verified experimentally, he decided to pursue his long-standing interest in catalytic reactions. “There aren’t a lot of people working on first principles molecular dynamics, but Fugaku and the rest of Japan’s high-performance computing infrastructure have helped make it available to more people. I think it’s fascinating to be able to trace the movement of molecules and atoms. I hope more people will join in this field.”

Associated Research Projects

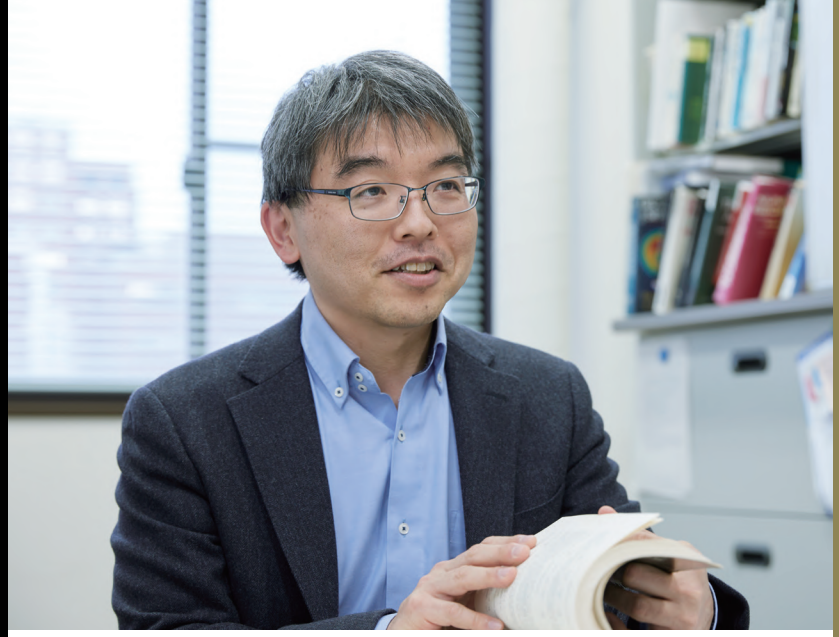
- “Development of an Exchange-correlation Functional to Describe Solid-Liquid Interfaces” (hp200081)

High-Precision Simulations of the Evolving Universe to Weigh Cosmic Neutrinos

In July 2021, a six-dimensional Vlasov simulation was executed using nearly all the nodes of supercomputer Fugaku. Researcher Kohji Yoshikawa became the first person in the world to develop software that could successfully perform such a computation. His results showed, with much greater precision than previously possible, how the distribution of neutrinos throughout the universe has changed from the Big Bang up to the present day. How did he arrive at this achievement? And what is the scientific significance of these results?

Kohji Yoshikawa

Associate Professor
Center for Computational Sciences
University of Tsukuba



Neutrinos Influence the Formation of the Large-Scale Structure of the Universe

The countless galaxies throughout the universe are known to not be distributed uniformly but rather have a structure similar to sticking bubbles. Our current understanding is that galaxies are clustered along the surfaces of many enormous structures conceived as “bubbles”, with relatively few galaxies residing inside these bubbles. In the very early days of our universe, matter was distributed mostly uniformly, albeit with some slight fluctuation variations in density. We think the gravity of the slightly denser regions attracted nearby matter, thereby causing them to grow and attract ever more matter.

This difference in density gradually increased, creating the *large-scale structure of the universe* as it now exists.

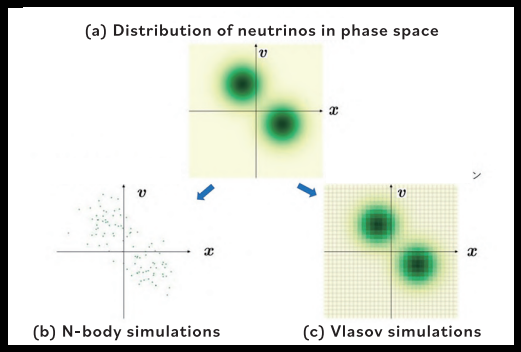
"Dark matter" is believed to have played a major role in the evolution of the universe. Dark matter is an unidentified and invisible component of the universe, only known for exerting gravity on surrounding matter. Although we can't see dark matter, we believe it makes up *most of the mass in the universe* and that its distribution throughout the universe corresponds to the observed distribution of galaxies. To better understand how the large-scale structure of our universe came to be, researchers run "time evolution" simulations and study how the distribution of dark matter *evolves over time*. In such simulations, researchers have adopted a well-established method called "N-body" simulation, in which the distribution of matter in the universe is represented by a very large number of particles mutually interacting via gravity.

Around the year 2000, it was discovered that even tiny neutrinos have some amount of mass. Scientists then began to include neutrinos in their simulations of the evolving universe. "Neutrinos are extremely light, but they're quite abundant in the universe. They zip around at tremendous speeds in the universe, which interferes with the dark matter's ability to attract mass gravitationally. So, scientists started running N-body simulations that include neutrinos, but they weren't accurate enough," explains Yoshikawa.

Fig. 1

Vlasov Simulations and N-body Simulations of Neutrino Distribution in the Universe

Simulations of the evolving universe compute the motion of matter in a virtual "phase space" in the form of 3D coordinates for both position and velocity. Real-world neutrinos are smoothly distributed in the phase space (a). In N-body simulations (b), however, these distributions are represented by discrete particles. In Vlasov simulations (c), the neutrino distribution represented in the form of a distribution function mapped onto the fine mesh grids is very smooth. So, the Vlasov simulations produce less noisy, more accurate results than the N-body simulations.



Taking on an Equation Once Thought Unsolvable

Rather than N-body simulations, Yoshikawa opted for Vlasov simulations, which solve the "Vlasov equation". Here's how they differ.

Neutrinos hurtle through the universe at various speeds and directions. In computer simulations, the positions and velocities of these neutrinos are represented by coordinates of a virtual "phase space" which consists of a 3D position space and a 3D velocity space, meaning six dimensions in total. This is the case in both of N-body and Vlasov simulations (Fig. 1a). The difference is that in N-body simulations, the virtual "particles" are placed in a neutrino-dense area and then their changes in position and velocity over time are computed (Fig. 1b). In Vlasov simulations, on the other hand, the phase space is divided into fine mesh grids and the *time evolution* of the neutrino distribution within those mesh grids is computed (Fig. 1c). Whereas real-world neutrino distributions are quite smooth

(Fig. 1a), the scattered particle images produced by the N-body simulations contain a significant amount of random noise. The Vlasov simulations can properly compute even low-density areas, allowing for more accurate results.

The actual results of Yoshikawa's simulations (Figure 2) show that Vlasov simulations can reproduce the smooth distribution of neutrinos. But, solving six-dimensional Vlasov equations requires a supercomputer with enormous memory capacity and exceptional performance, not to mention a numerical algorithm that is both very efficient and very accurate. Yoshikawa's results overturned commonly-held long-standing assumptions that such computations were impossible.

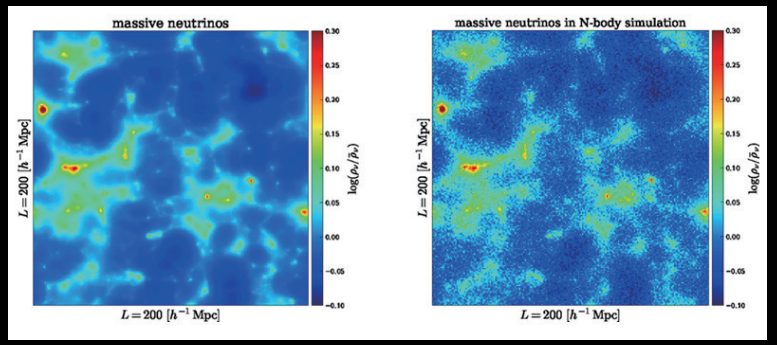
Yoshikawa began developing the numerical code for these simulations in 2007, when he started working at the University of Tsukuba. After several years of trial and error, in 2013 he successfully demonstrated that six-dimensional Vlasov equations could be solved on the university's "T2K-Tsukuba" supercomputer. This was a world's first achievement. Next, at the suggestion of Naoki Yoshida at the University of Tokyo, Yoshikawa decided to use his simulation code to tackle the real-world problem of neutrino distribution in the universe over time.

However, developing a "numerical scheme" to solve these 6D Vlasov equations for the expanding universe with sufficient numerical accuracy was not easy.

Yoshikawa reflects "I thought about quitting it many times." Takashi Minoshima at the Japan Agency for Marine-Earth Science and Technology provided him with an important clue to overcoming the difficulty. The two promptly began working together. By 2017, their numerical schemes had been improved and become much more accurate. Yoshikawa performed numerical simulations with the improved numerical scheme on a variety of supercomputers, including the K computer. Then in the fall of

Fig. 2 **Comparing Vlasov Simulations with N-body Simulations**

Comparison of neutrino distributions obtained with a Vlasov simulation (a) and an N-body simulation with a similar computational cost (b).
In the Vlasov simulation, the neutrino distribution is smooth, whereas the counterpart in the N-body simulation appears somewhat pixelated, making the subtleties of the structures harder to be discerned.



(a) Vlasov simulation (b) N-body simulation

2019, he was given permission to run his simulations on an early access system of Fugaku.

All-node Calculations Get Maximum Performance out of Fugaku

Fugaku's huge memory space, a fast interconnect and high parallelization efficiency make it ideal for Vlasov simulations, in which calculations on a large number of mesh grids are performed in parallel. However, since Fugaku has a SIMD (Single Instruction Multiple Data) instruction set different from previous supercomputers, the code has to be refactored to match the Fugaku's instruction set for the maximum performance on Fugaku. Yoshikawa devised an idea for speeding up the calculations, and postdoctoral researcher Satoshi Tanaka (currently a research fellow at the Yukawa Institute for Theoretical Physics, Kyoto University) implemented it in the program.

In July 2021, a Vlasov simulation of cosmic neutrinos adopting about 400 trillion mesh grids was successfully performed using 147,456 nodes, or about 93% of the total 158,976 nodes on Fugaku (Fig. 3a).

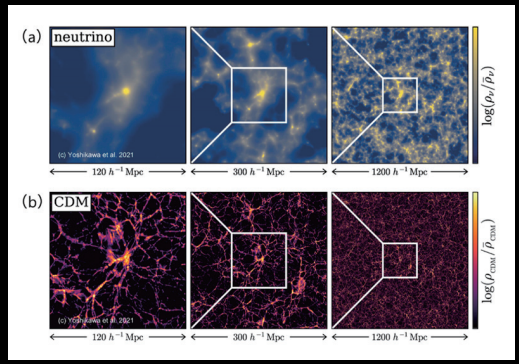
This was, of course, the largest Vlasov simulation ever conducted in the world. It was also 10 times faster than a comparable N-body simulation previously performed on a Chinese supercomputer.

The distributions of neutrinos and dark matter are computed with Vlasov and N-body simulations, respectively (Fig 3b). "We can constrain the possible range of yet-to-be-known neutrino mass by analyzing the simulated data and comparing them with observational data.", explains Yoshikawa about the scientific significance of these simulations. Weighing the neutrino mass directly leads to the understanding of the dynamical effect of neutrinos on the large-scale structure formation in the universe. Furthermore, the Vlasov simulations are expected to be successfully applied to the numerical simulations of magnetic plasma such as "accretion disks" formed around the astrophysical black holes and magnetic storms in the inter-planetary space.

Yoshikawa reflects, "This time, the simulations used practically all the nodes of Fugaku, and also used up nearly all the memory space. There were various issues both in the software and hardware sides.We believe that lots of valuable experiences to overcome such issues will

Fig. 3 **The Results of Simulations Using 147,456 Nodes on Fugaku**

The time evolution of neutrinos and dark matter was computed using a Vlasov simulation (a) and an N-body simulation (b), respectively. The matter distribution at the very beginning of the universe (about 200 million years after the Big Bang) obtained from actual observations was adopted as the initial condition and evolved into the present-day universe (after the 13.8 billion years after its birth). A timestep of the simulation corresponds to about 2 million years. The size of the simulated volume is 5.6 billion light-years (1200 Mpc/*h* per) side, which covers nearly all of the observable universe.
[Mpc/*h* is a unit of length corresponding to about 466 million light years. The *h* is the Hubble parameter normalized by 100km/s/Mpc and observationally estimated to be around 0.7.]



be reflected in the future operation of Fugaku and be useful to bring the best performance it has." This substantial all-node run will be an encouraging impetus to the future utilization of Fugaku.

About the

Researcher

"I'll become a researcher because I can do what I love for a living." Yoshikawa has always thought so since he was a junior high school student. In 1995, when he was a junior in undergraduate school, he started to study astrophysics attracted by the emerging computer simulations which were not common yet at that time. There, he encountered the Vlasov equation and decided to numerically solve it himself one day. As a mentor, he encourages his students to conduct research with the attitude of doing what no one else is doing. As a native of Suzuka City, which is famous for holding Formula One Grand Prix in Japan, he loves watching motor sports, saying "I love the pursuit of pure speed."

Associated Research Projects

• "Toward a Unified View of the Universe: From Large-scale Structures to Planets" (hp200124/hp210164)
Principal Investigator: Junichiro Makino, Kobe University
2021 ACM Gordon Bell Prize finalist for Research Findings

High-Fidelity Simulation of Airflow Ushering in a New Round of Innovation in Aircraft Design

Air and water constantly flow around us. Although we are not usually aware of it, technologies and products that make good use of these flows make our lives more convenient and prosperous. A typical example is airplanes. Recently, Prof. Kawai and his team succeeded in numerically simulating the airflow around an aircraft using a computer with overwhelmingly higher fidelity than ever before. This achievement was realized by combining the performance of the supercomputer Fugaku with the fundamental research that Prof. Kawai and his team have conducted over many years, and is expected to bring about a revolution in aircraft design.

Soshi Kawai
Professor, Department of Aerospace Engineering,
Graduate School of Engineering, Tohoku University

“I Was Able to Realize Part of a Dream I Have Had Since My Graduate School Days.”

Prof. Kawai discussed the history and current status of aircraft aerodynamic design as follows. “Computational fluid dynamics simulations have been used in aircraft aerodynamic design since the 1980s. Before that, until the Boeing 767, design relied on wind tunnel testing, which was costly and time-consuming. The introduction of numerical simulation has revolutionized aircraft design, but simulation can still only predict the flow around the aircraft with smooth geometry and under less-turbulent cruise conditions. Therefore, aircraft manufacturers expect the second round of innovation to occur when it becomes possible to simulate the flow around the entire aircraft (whole-aircraft simulation) during

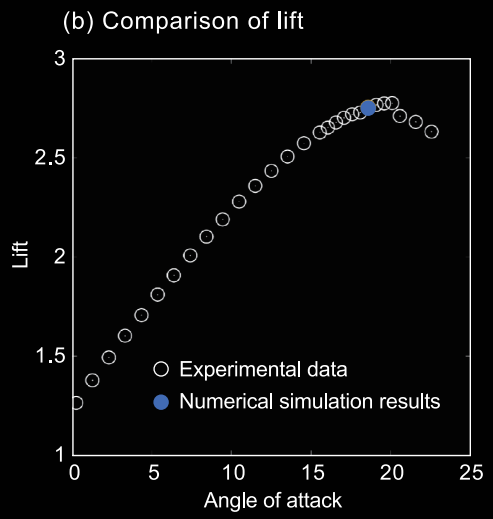
takeoff and landing, which involves complex geometries and highly turbulent flow."

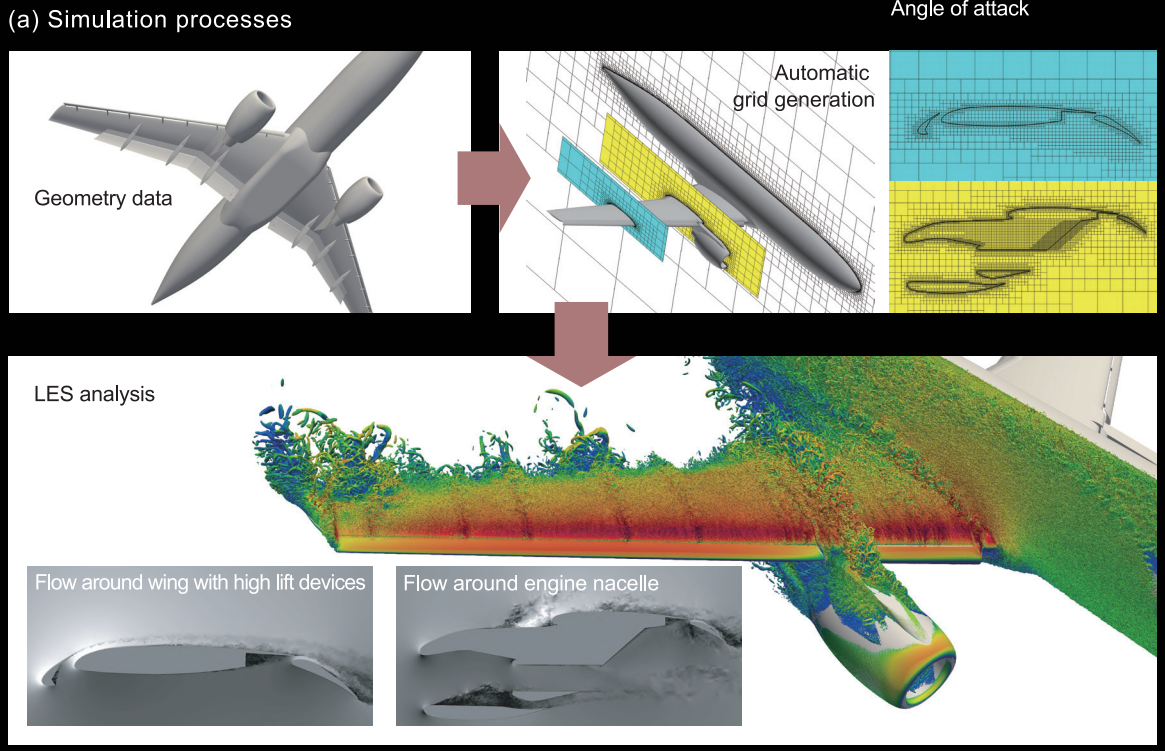
Since an aircraft raises its nose to obtain more lift during takeoff and landing, it is crucial to predict the relationship between the aircraft's inclination (angle of attack) and lift in aircraft design. In particular, the maximum lift value significantly affects takeoff and landing performance, such as how much runway is required, and safety. Therefore, it is expected that a whole-aircraft simulation that can obtain lift values with high accuracy and can replace actual flight tests can be developed. However, this is not easy to achieve.

The flow follows the Navier-Stokes equations, which are solved numerically in Large Eddy Simulation (LES), where the space around the object is divided by a grid and the eddies (turbulence) with large energy are calculated directly on the grid. Prof. Kawai began researching LES in 2002, when he entered his doctoral program. In 2005, when he received his doctorate, he decided he wanted to use LES to analyze the flow around an entire aircraft. At the time, there was no one working on LES in the aerospace field in Japan. Since then, Prof. Kawai and his collaborators have conducted fundamental research and

Fig. 1 **Example of aircraft simulation using FFVHC-ACE**

(a) JSM (JAXA Standard Model) was used as the aircraft geometry model, and the flow was calculated with approximately 12 billion grid points around the aircraft. The minimum grid spacing is 250 μm, and it took about two days to obtain the results of flow using 3,456 nodes of Fugaku for this calculation. The flow eddies (turbulence) around the wing and the longitudinal vortex from the engine nacelle are well reproduced. (b) The blue circle shows the lift near the maximum lift obtained from this simulation. It is in good agreement with the experimental data.

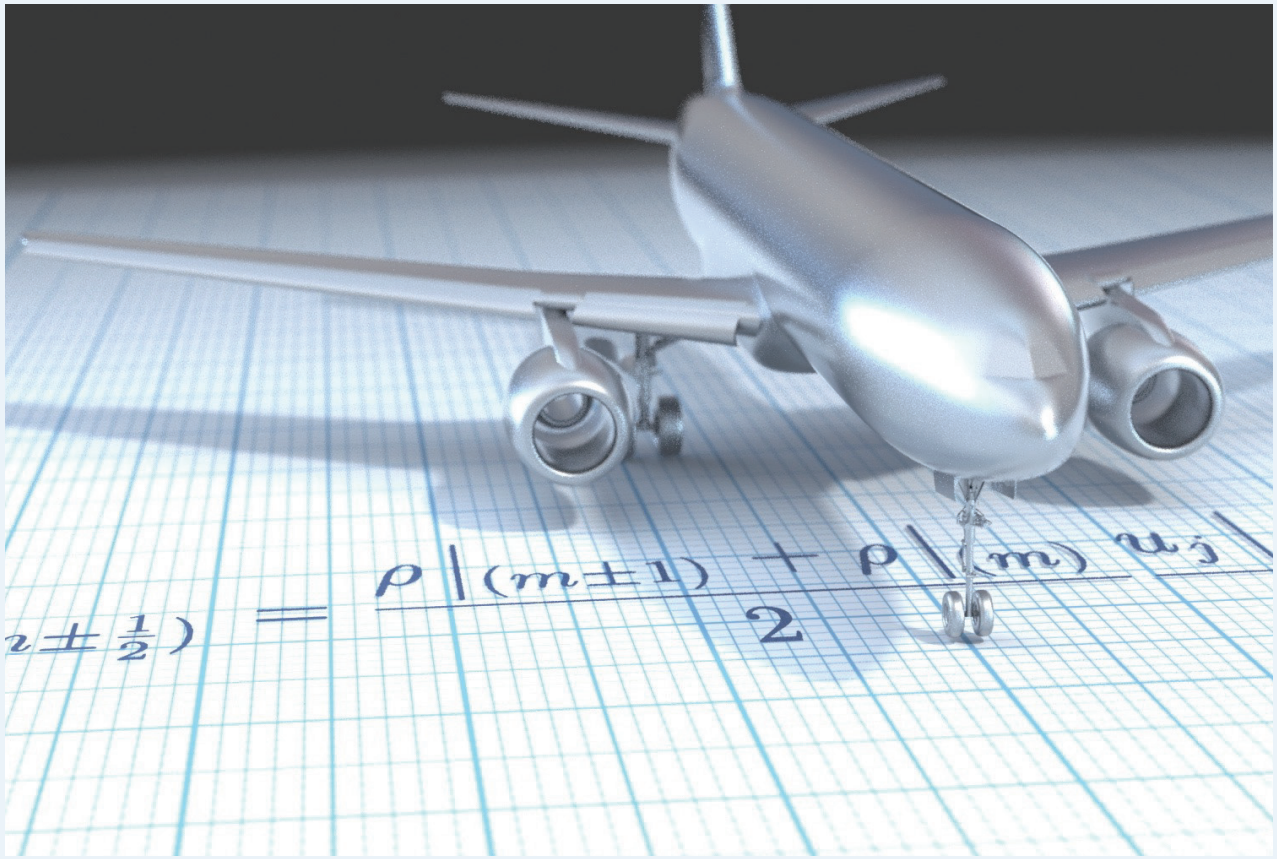




developed the “FFVHC-ACE” software, and recently succeeded in a high-fidelity (physically more accurate) simulation of the flow around an entire aircraft by using this software on Fugaku (Fig.1). Furthermore, the maximum lift obtained from these simulation results agreed well with experimental data. The results are beginning to meet the expectations of aircraft manufacturers.

Fundamental Research and Fugaku Made Difficult Simulations Possible

Why has it been so difficult to perform high-fidelity simulations of the flow around an aircraft? One reason is that the Reynolds number of the flow is very high, about 10 million. The Reynolds number is the ratio of the flow effect (inertial force) and viscous effect (viscous force) of the flow. When this number exceeds a certain value, eddies (turbulence) occur in the flow; the higher the value, the smaller the eddies. “LES is a method that simulates turbulent phenomena almost directly, so the prediction accuracy is high. However, to calculate small eddies, the grid size must be reduced, so the number of grid points required for the calculation becomes enormous, and the calculation cost jumps,” Prof. Kawai says.



In particular, the vortices are smaller near the walls of the aircraft, so Prof. Kawai has developed a physical model that accurately reflects the effects of small vortices near the walls (Fig. 2a). “Only very close to the surface of the aircraft, we replaced the LES calculations with calculations based on this model. This reduced the computation time by a factor of about 10,000. Without this modeling, we would not have been able to calculate for the entire aircraft even with all the nodes in Fugaku,” Prof. Kawai says, explaining the significance of the modeling.

Another reason why high-fidelity simulations are difficult is that the flow around the aircraft must be treated as a compressible flow. Computations of compressible flow are prone to instability, so existing software stabilizes the calculations with mathematical

manipulations that provide artificial diffusion. However, this manipulation causes turbulence to decay in a way that is contrary to physics, and thus does not yield correct results.

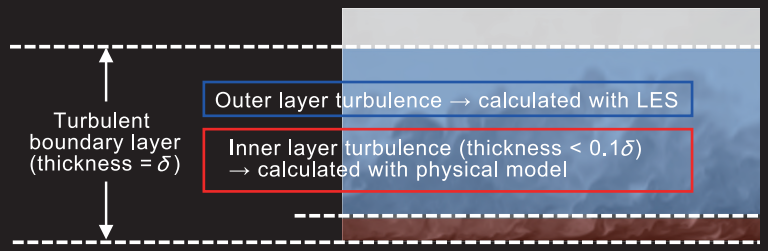
To counter this problem, Prof. Kawai and his colleagues established a calculation method named the KEEP (Kinetic-Energy and Entropy Preserving) scheme in their fundamental research. In compressible flow simulations, the flow is usually calculated under the condition that it satisfies the mass conservation law, momentum conservation law, and energy conservation law. In addition to them, the kinetic energy equation and entropy conservation law are satisfied when calculating with the KEEP scheme (Fig. 2b). The KEEP scheme allows researchers to conduct stable calculations without adding artificial diffusion and to obtain more physically correct results.

"In flow simulation, which requires large-scale calculations, the use of supercomputers has always been promoted, but Fugaku is very easy to use, and I think it is a good computer in terms of smoothly conducting large-scale computations. I believe that the results of this project have come out of a well-timed encounter between the fundamental research we have been conducting for many years and Fugaku, and the multiplication of the two," Prof. Kawai says.

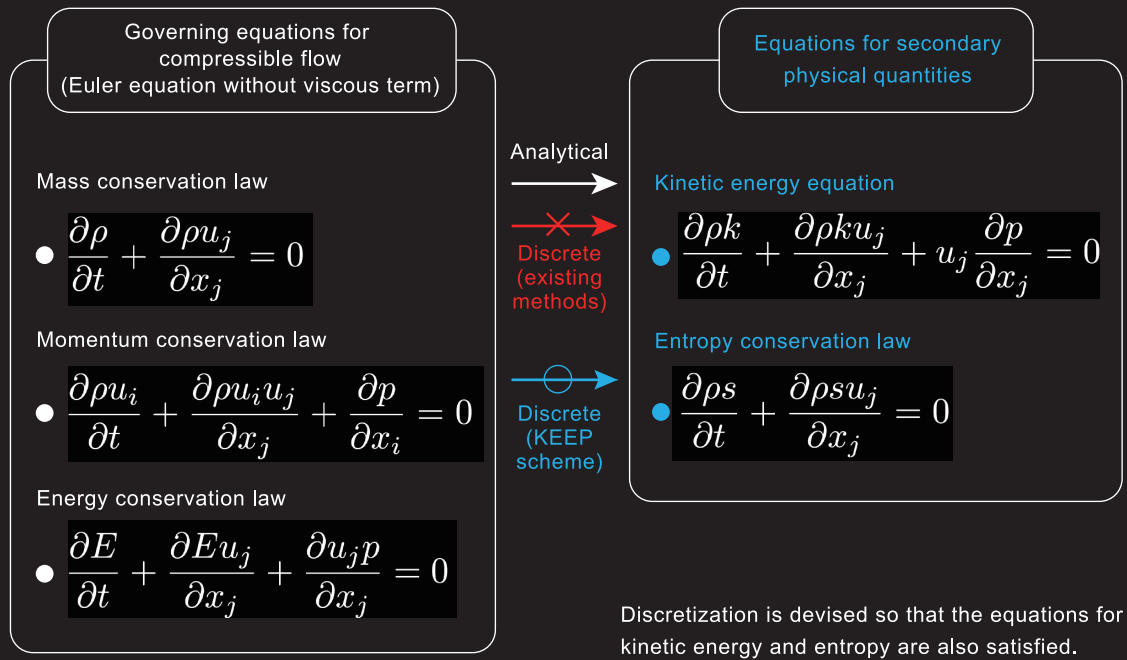
Fig. 2 **Two fundamental researches that enable high-fidelity simulations**

(a) The thickness (δ) of the turbulent boundary layer that develops on the surface of the aircraft is about 3.5 mm at 10% of the position from the leading edge of the wing. An area less than one-tenth of this thickness (shown by the red shading) is modeled, and the rest is calculated using LES. This results in a speedup of about 10,000 times faster than when all of the boundary layer thickness is calculated with LES. (b) The usual compressible flow simulation is performed under the condition that the mass conservation law, momentum conservation law, and energy conservation law are satisfied, but in this calculation, a discretization method is devised to satisfy the kinetic energy equation and entropy conservation law. This enables stable and high-fidelity LES calculations.

(a) Wall-modeled LES



(b) KEEP (Kinetic Energy and Entropy Preserving) scheme



Discretization is devised so that the equations for kinetic energy and entropy are also satisfied.

A Dream that Extends Beyond the Sky

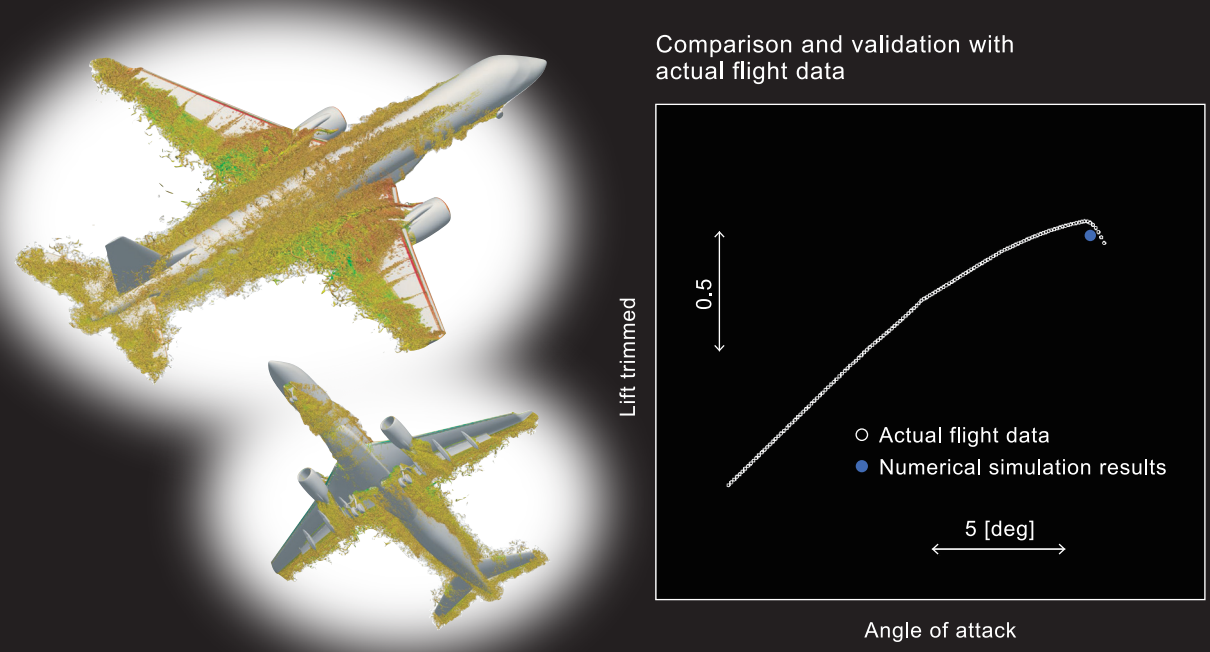
Prof. Kawai and his colleagues have applied FFVHC-ACE to several aircraft geometry models, and have confirmed that the maximum lift and other parameters agree well with experiments. “We are proud that FFVHC-ACE is the world’s most powerful compressible flow LES analysis software,” he says. “Moreover, industrial users only need to prepare geometry data to perform complex geometry LES calculations with high speed, ease, and high quality. In fact, the Mitsubishi Heavy Industries Group has successfully conducted a simulation using FFVHC-ACE and the geometry data of the SpaceJet and obtained good agreement with actual flight test data (Fig. 3).”

However, Prof. Kawai is not satisfied with this achievement. “We will continue our research to predict not only takeoff and landing performance, but also high-speed flight limits, aerodynamic noise during the landing approach, and flutter phenomenon (severe vibration of the wings caused by flow), with the aim of using the FFVHC-ACE in aircraft design,” he says enthusiastically.

Prof. Kawai has a dream beyond this kind of success of the FFVHC-ACE. “Aerodynamic design of aircraft until now has relied heavily on experience, so it has been risky to develop an aircraft that looks different from past aircraft,” he says. “But that will become possible when various performance of an aircraft is accurately predicted through simulation. I would be happy if we can turn the ‘imagination’ of having an airplane of a desired geometry into an actual ‘creation’.” (Prof. Kawai used the Japanese word *souzou*, which means both “imagination” and “creation.”)

Fig. 3 **Industrial applications of FFVHC-ACE**

The Mitsubishi Heavy Industries Group (Mitsubishi Heavy Industries and Mitsubishi Aircraft) applied FFVHC-ACE to geometry data of the aircraft SpaceJet and conducted a simulation with Fugaku. Although Prof. Kawai was not directly involved in the calculations, only giving advice, the simulation was successful. The maximum lift was in good agreement with the actual flight test data, demonstrating that FFVHC-ACE is a high-fidelity compressible flow LES analysis software that can withstand use in academic research to industrial applications. Image courtesy of Mitsubishi Heavy Industries Group.



He also hopes to release FFVHC-ACE as a basic software that can be used for all kinds of compressible flow analysis, not restricted to aircraft, so that it can be used widely from academia to industry. The engineering fields involving compressible flow range from high-speed railroads and turbines for power generation to nozzles and diffusers, jet engines, and rockets. Since compressible flow simulations can directly determine the sound, which is the coarse and dense waves of air, simulations can also be used to find ways to reduce noise, which is a common problem in the industry.

The dream Prof. Kawai had 20 years ago is now becoming a reality through steady fundamental research and the advent of Fugaku. And now, it is about to expand beyond the framework of aircraft to the industrial world and bring about major innovations.

About the

Researcher

Prof. Kawai entered the Department of Aerospace Engineering at his university because of his childhood dream of becoming a pilot. Because of this, he enjoyed his student life so much that when he was assigned to a laboratory in his fourth year, he was astonished at the limitations of his knowledge. To become a responsible member of society, he studied hard and took a doctor's course, where he was fascinated by the fun of research and became a researcher. His path was not smooth, however. For example, the place he was supposed to go as a postdoctoral researcher in the U.S. had to be changed due to the 9/11 terrorist attacks. "I have been blessed to meet many people, including a researcher I met at the new place and developed compressible flow calculation methods and a wall-modeled LES," he says. Prof. Kawai loves spending time in nature and frequently visited national parks when he was studying abroad in the U.S. Now that he is in Sendai, he regrets that he does not have much time to spend in Tohoku's nature.

Associated Research Projects

"Leading Research on Innovative Aircraft Design Technologies to Replace Flight Test" (hp200137, hp210168, hp220160)
Principal Investigator: Soshi Kawai, Graduate School of Engineering, Tohoku University

Computing Crustal Deformation with Uncertainty Quantification

– Large-Scale Earthquake Simulation beyond Common Sense

“In an ideal simulation, I would like to do this calculation, but the number of calculations is huge, so it is impossible.” Overcoming problems like this is a showcase for simulation researchers. Prof. Ichimura, who studies earthquake simulation, has released many computational technologies that enable ideal calculations with existing computational resources. “Five or 10 years from now, when computational resources such as the supercomputer Fugaku become available to more people, we will be able to make improvements based on our achievements for their own purposes. We are pursuing methods that can be used with modifications that suit each purpose based on our results,” Prof. Ichimura said, introducing his research.

Tsuyoshi Ichimura
Professor/Head of Center, Research Center for Computational Earth Science,
Earthquake Research Institute, The University of Tokyo

Large-Scale Earthquake Simulation – A Pressing Need for Society

To allow the government to decide how to prepare for future major earthquakes, such as a direct hit on the Tokyo Metropolitan Area or a Nankai Trough earthquake, more accurate earthquake assessments are required. It is not possible to predict when an earthquake will strike, but better assessments will enable disaster prevention professionals to make better measurements and decisions. To construct an integrated prediction system for quantitative assessments of earthquakes, in April 2020, one of the Programs for Promoting Research on the supercomputer Fugaku was launched. The name of the study is “Large-scale numerical simulation

of earthquake generation, wave propagation and soil amplification" (Principal Investigator: Dr. Takane Hori, Japan Agency for Marine-Earth Science and Technology).

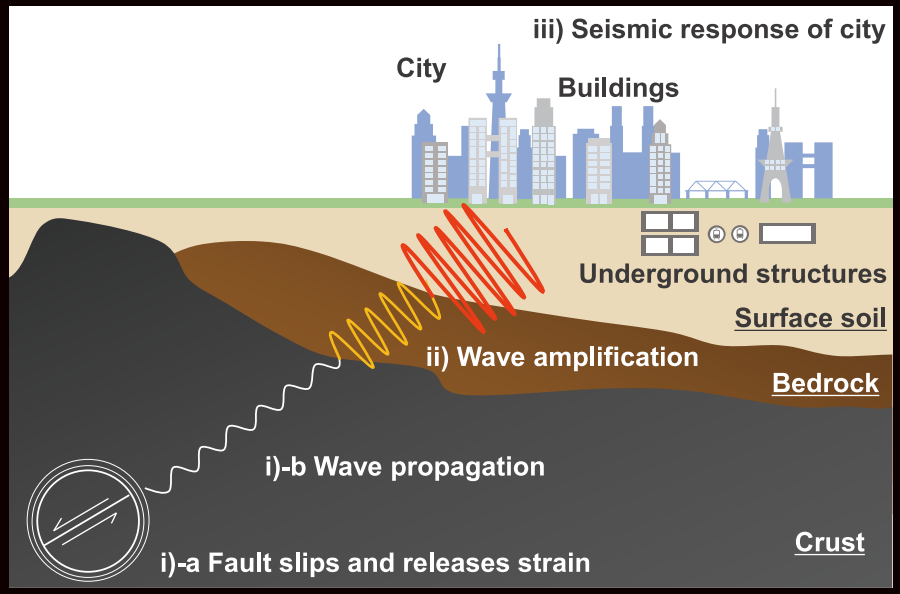
Prof. Ichimura is creating a series of innovative earthquake simulation methods in this program. Here we introduce two representative simulations from his results.

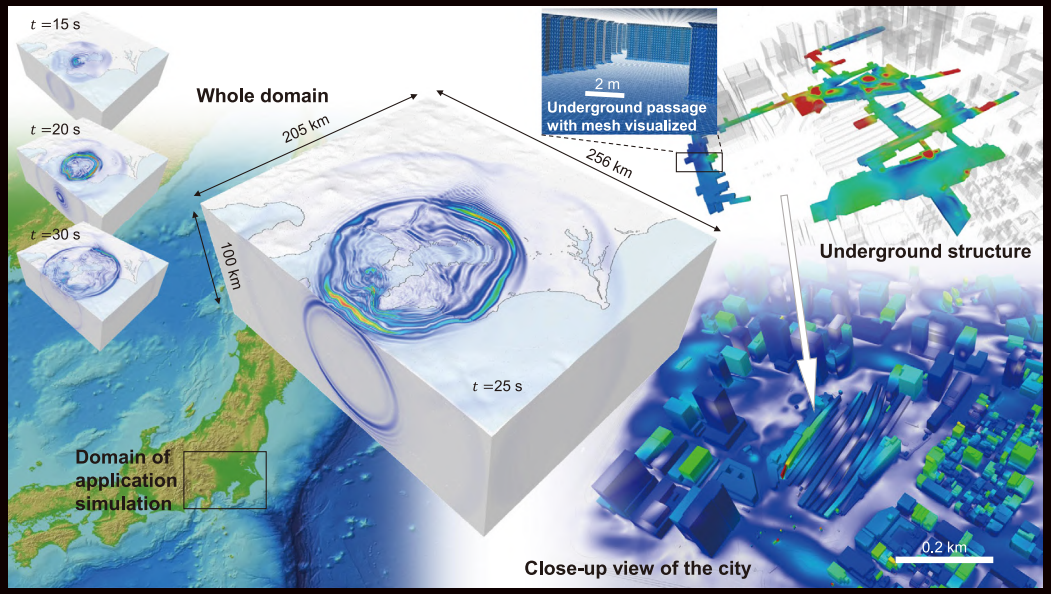
A Comprehensive Simulation from the Fault to the Structures, Which Has Been a Long-Standing Issue*1

In an earthquake simulation, researchers calculate how the waves generated at the fault propagate through the earth's crust and soil, until they meet structures such as buildings and houses and make them shake. However, to accurately simulate wave propagation, the crust and soil must be calculated on a fine grid. Furthermore, simulating the shaking of structures due to transmitted waves requires a huge number of calculations. That makes it difficult to analyze everything from the fault to the structures at the same time, targeting a wide area.

Fig. 1 **A comprehensive simulation from the occurrence of an earthquake to the shaking of structures on the entire Kanto Plain**

They simulated a model consisting of the crust and ground in an area including the Kanto Plain (256 km east-west x 205 km north-south x 100 km depth) and a highly concentrated city around a terminal train station. The size of the lattice ranges from about 0.125 to 64m, and the scale of calculation is 320 billion degrees of freedom. The calculated area consists of soft soil layers on heterogeneous crust, as well as above-ground and underground structures. The complex geometry of the structure is modeled in detail with a very fine mesh of minimum 0.125m.





Tsuyoshi Ichimura, Kohei Fujita, Kentaro Koyama, Ryota Kusakabe, Yuma Kikuchi, Takane Hori, Muneo Hori, Lalith Maddegedara, Noriyuki Ohi, Tatsuo Nishiki, Hikaru Inoue, Kazuo Minami, Seiya Nishizawa, Miwako Tsuji, and Naonori Ueda. 2022. 152K-computer-node parallel scalable implicit solver for dynamic nonlinear earthquake simulation. In International Conference on High Performance Computing in Asia-Pacific Region (HPCAsia2022). Association for Computing Machinery, New York, NY, USA, 18 -29. https://doi.org/10.1145/3492805.3492814. Fig. 1 and 2.

"Therefore, we usually divide the domain from the fault to the structure into several stages and perform calculations," Prof. Ichimura says. "Is it possible to obtain correct calculation results with this method? Aren't there any ways to calculate all of them at once continuously?"

Using Fugaku, Prof. Ichimura and his colleagues took on the challenge and succeeded in conducting a comprehensive simulation from the fault to the structures, targeting an area including the Kanto Plain around Tokyo (Fig. 1). It took a lot of ingenuity to make full use of the characteristics of Fugaku as a computer suitable for the fusion of data science and simulation. Prof. Ichimura had previously developed a learning method[*2] using artificial intelligence (AI), and this time he developed this into a revolutionary data learning method. By accumulating the calculation results during the simulation and learning the data in real time, the initial value of the subsequent calculation called the iterative method can be estimated with high accuracy. This reduces the amount of computation and speeds up the simulation. As a result, he and his team achieved a calculation speed 1,070 times faster than the maximum performance of RIKEN's K computer.

A Large-Scale Simulation with 32 Trillion Degrees of Freedom that Surprised the World[*3]

Prof. Ichimura and others also took up the challenge of simulating the Nankai Trough. This is a large-scale simulation of the ground surface deformation that occurs immediately after a large earthquake caused by the slip of the fault. The feature of this simulation is that it handles a wide area and includes "ambiguity." Ordinarily, this is such a huge problem they would not even attempt it because the number of calculations required is enormous.

What do they mean by "ambiguity"? The hardness of the earth's crust is not actually directly measured by digging, so its hardness cannot be determined as a single value. It is more reliable to express it as "this kind of crustal deformation occurs with this probability" with a certain distribution.

When simulating uncertain events while considering probability like this, researchers usually use a method called the "Monte Carlo simulation." This calculation method

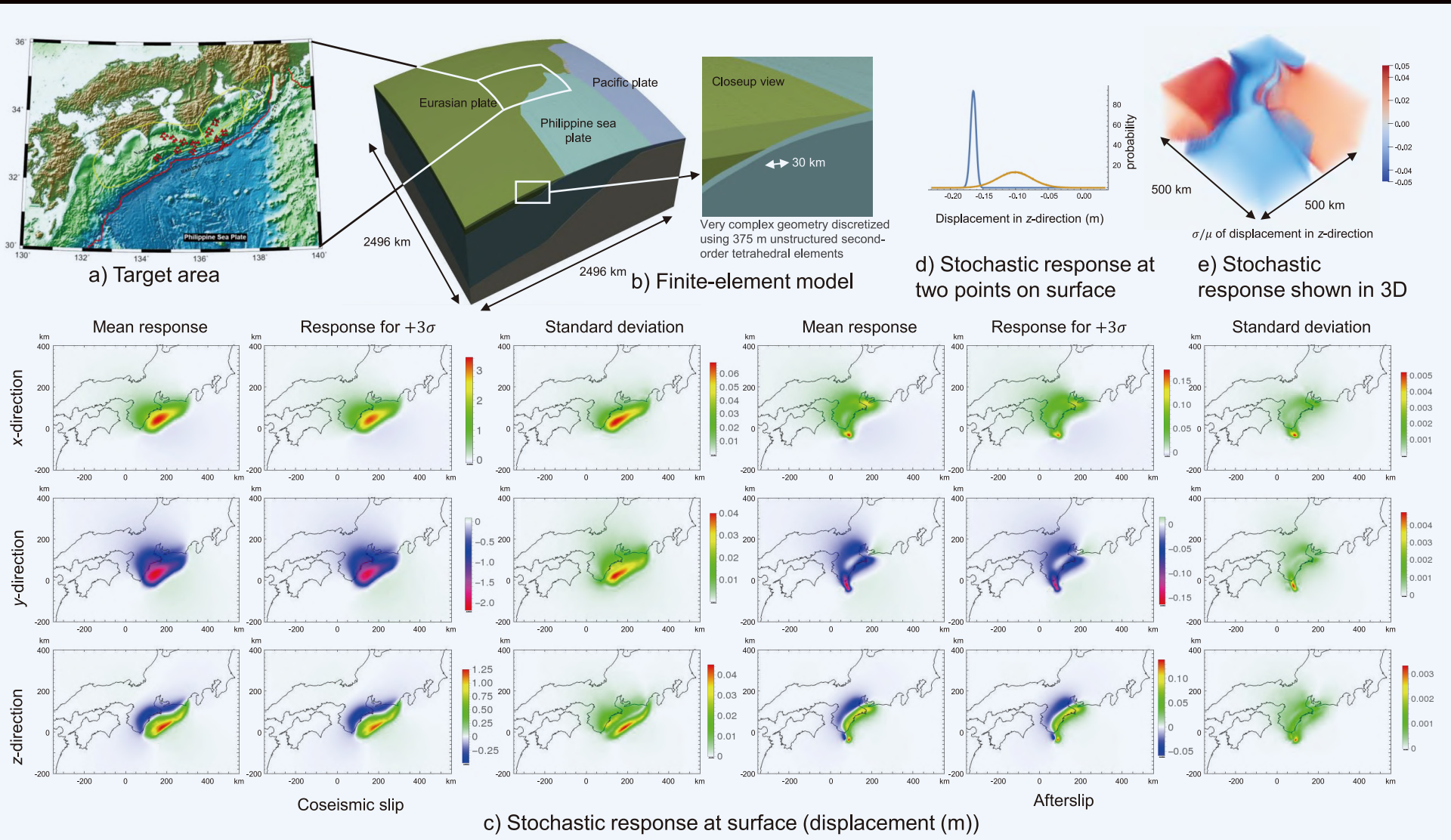


Fig. 2 **Simulation of Nankai Trough earthquake considering ambiguity**

The team simulated an area of 2,496 km x 2,496 km x 1,101 km centered on the Nankai Trough (which includes the entire Japanese archipelago). Maps in lower half represent the magnitude of deformation in the x, y, and z directions. Simulation results of "mean," "mean + 3σ (σ is the standard deviation; the probability of falling within this range is 99.7%)" and "standard deviation" are shown. This broad range of results enhances the quality of the simulation.

repeatedly selects one numerical value from the possible range of values and perform calculations with it, but in order to obtain highly accurate results, it is necessary to repeat the calculation more than 10,000 times. Therefore, doing a wide-area earthquake simulation is beyond even Fugaku's abilities.

Instead, Prof. Ichimura and his team performed a simulation using a calculation method called the stochastic finite element method. With this method, results with distribution can be obtained in a single calculation. The calculated area covers the entire Japanese archipelago, which measures 2,496 km east-west, 2,496 km north-south, and 1,101 km deep, with a scale of approximately 32 trillion degrees of freedom. The finite element method, which is the basis of the stochastic finite element method, is thought to be unsuitable for large-scale calculation. Even 10 million degrees of freedom was considered large, and only a billion could be calculated at most. So, researchers around the world were amazed at the 32 trillion degrees of freedom of the stochastic finite element method. What's more, Prof. Ichimura's calculation is 224 times faster than the previous record. The reason the team could perform such large-scale calculations so quickly was that they studied a method to execute calculations using Fugaku skillfully from the aspect of computational science and computer science.

However, the code to perform this calculation contains thousands-lines complex parts that would be prone to errors if written manually. Therefore, Prof. Ichimura and his colleagues created software to have a computer automatically write a complicated part of the code.

This achievement of a large-scale, precise simulation that considers the "quantification of uncertainties" has attracted attention from all over the world. Regarding this calculation method, Prof. Ichimura said, "People who had given up on considering ambiguity in large-scale problems would wonder, 'Is there such a solution?' If we can obtain information on the slip of the fault, we can use this research to understand the deformation of the ground surface. The value of the deformation can be used as data for post-earthquake predictions. Since this method can handle hard objects, it can be used in applications other than earthquakes."

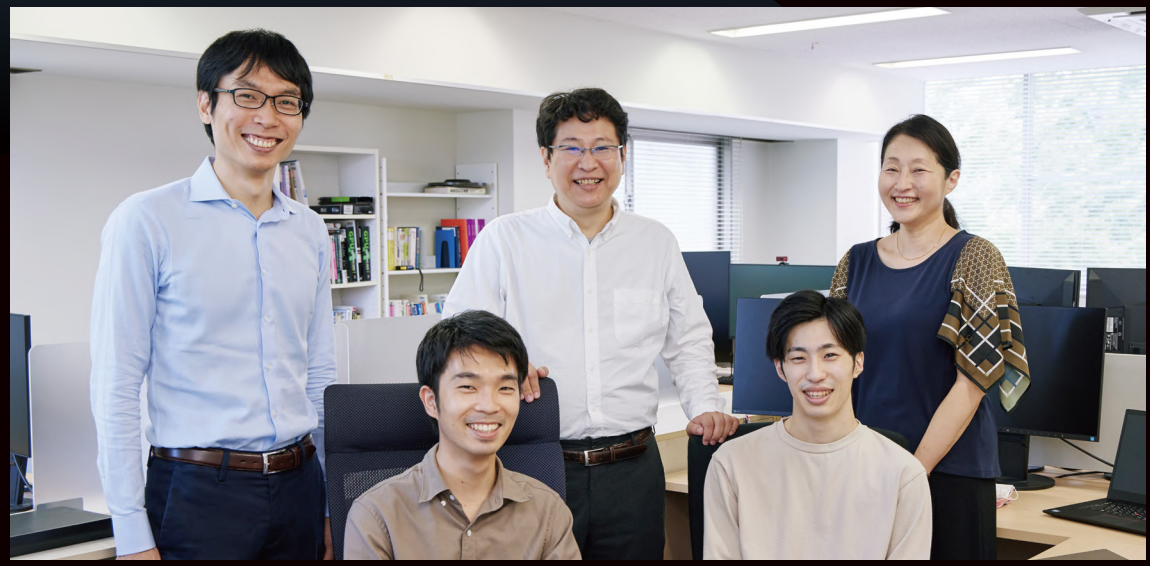
Prof. Ichimura continued, “In this simulation, we calculated the deformation immediately after the earthquake, but I would like to solve deformation over time and more complex nonlinear deformation.” He is excited at the prospect of tackling problems that are even more complex, with the computation amount increasing exponentially. He and his team will continue to create innovative methods to get closer to the “ideal simulation.” The team members have high hopes for the next move.

*1: HPC Asia 2022 Best Paper Award research results
*2: Workshop on Accelerator Programming Using Directives (WACCPD 2021) Honorable Mention award-winning research results
*3: 2022 ACM Gordon Bell Prize finalist research results

About the

Researcher

From novels to science texts, Prof. Ichimura as a child read books whenever he had free time. He liked to think, “What’s going to happen next?” When he entered the University of Tokyo, he chose to study science, but at the end of his sophomore year, he seriously considered going into the Faculty of Letters or the Faculty of Economics; he ended up choosing the path of Civil Engineering, where he could come into contact with a wide range of academic subjects. He began to devote himself to earthquake simulation research, which he started with his graduation thesis.



The members of the lab: from left in the back row, Associate Professor Kohei Fujita, Prof. Ichimura, and Project Academic Support Specialist Yumiko Nagasaki. From left in the front row, Ryota Kusakabe, a third-year doctoral student, and Souta Murakami, a second-year doctoral student.

Associated Research Projects

Large-scale numerical simulation of earthquake generation, wave propagation and soil amplification (hp200126/hp210171/hp220171)
Principal Investigator: Takane Hori, Japan Agency for Marine-Earth Science and Technology

Consortium for Industry-Academia-Government Collaboration and Fugaku Establish Advanced Platform for *In-Silico* Drug Discovery

The FMO Drug Design Consortium (FMODD) was formed at the end of 2014 by volunteers from industry, academia, and government. Currently, about 140 members are accessing the supercomputer Fugaku from all over the country. There are several ways to utilize Fugaku. In some cases, large-scale calculations are performed using a large number of nodes by a few people; in other cases many small calculations are done by a large number of members, like this consortium. The purpose of the FMODD is to develop the FMO method as a practical means of drug discovery. To that end, the FMODD is accumulating and disclosing basic data and is developing new methods to generate better results. We asked Prof. Fukuzawa, the group's chair, about the achievements and future developments.

Kaori Fukuzawa
Professor, Graduate School of Pharmaceutical Sciences, Osaka University

FMO Method for Rational Drug Design

Many new drugs are currently being developed that target disease-causing proteins. New drug development involves multiple stages. At the earlier stage, we must find a candidate compound that binds to the target protein and inhibits (or enhances) its function. After a candidate compound is found, researchers have to gradually modify its structure to improve its efficacy and safety. At these stages, it is necessary to actually synthesize and test candidate compounds, so the number of compounds synthesized before a single new drug hits the market can reach the tens of thousands, and is one of the factors driving up the time taken and cost of new drug development.

For this reason, "*in silico* drug discovery," in which researchers calculate on a computer how a compound binds to a target protein and use the results to design a candidate compound, is gaining popularity. "*In silico* drug discovery is efficient because it reduces the number of experiments, and it also has the advantage of being able to investigate the possibility of compounds that have not yet been synthesized," Prof. Fukuzawa explains.

There are several methods for calculating the binding state of a protein-compound complex. Prof. Fukuzawa and her colleagues use the "fragment molecular orbital" (FMO) method developed by Prof. Kazuo Kitaura of Osaka Prefecture University (currently Guest Professor of Osaka University) in 1999 (Fig.1). "We want to accurately understand the binding state of the protein-compound complex." To do this, quantum chemical calculations must be performed to reveal the electronic structure. However, the computational cost is too high for macromolecules such as proteins. The FMO method was devised to overcome this problem.

In the FMO method, a macromolecule is divided into small fragments. Quan-

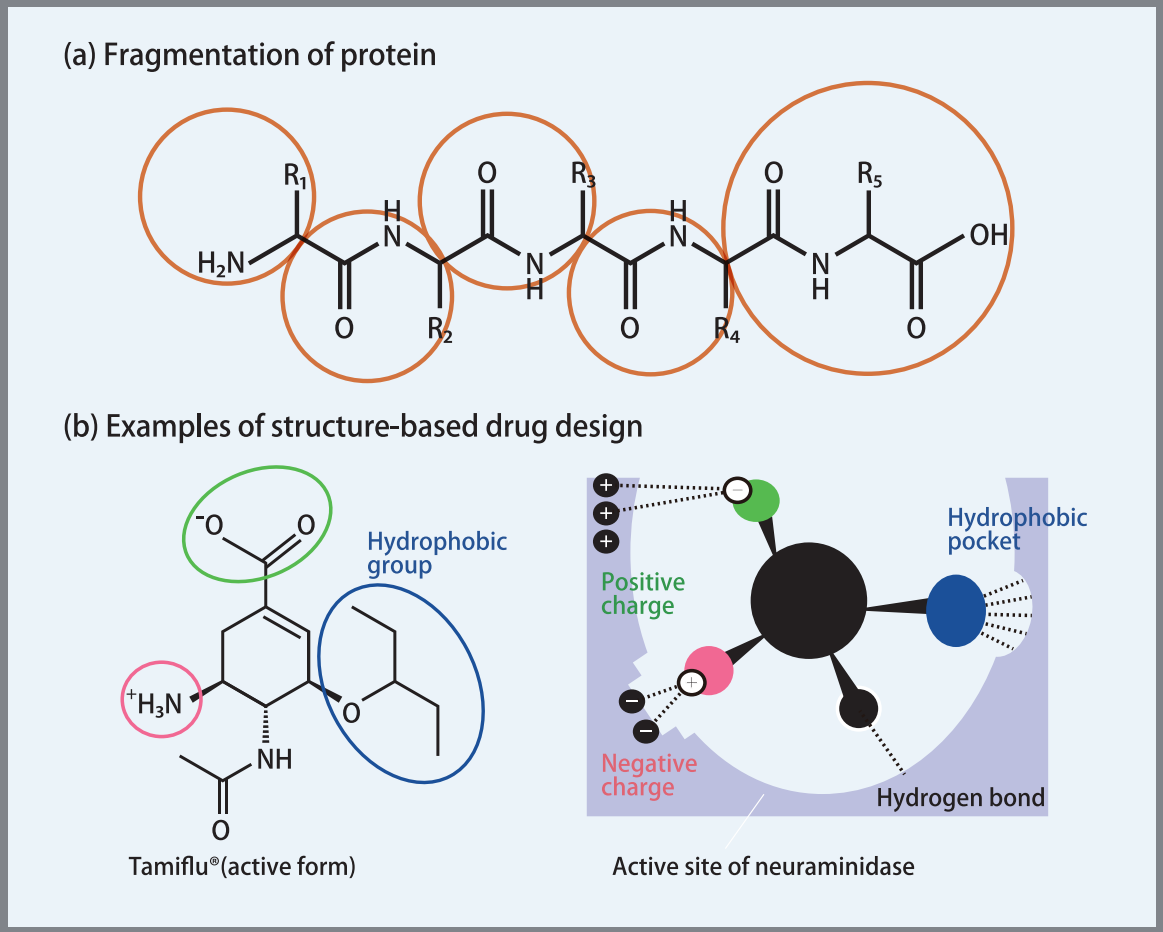


Fig. 1

Fragment molecular orbital (FMO) method and structure-based drug design

(a) In the FMO method, a macromolecule is divided into small fragments. A protein is divided into amino acid units, as circled. A compound that binds to a protein is often treated as a single fragment, but can also be divided into functional moieties.
(b) Tamiflu® (generic name: oseltamivir), which is used to treat influenza, binds to the active site of neuraminidase, an enzyme necessary for the replication of influenza viruses, and suppresses its action. Tamiflu® is designed to bind to the active site through various interactions, such as electrostatic interactions where positive and negative charges attract and hydrogen bonding. This strategy is called "structure-based drug design." When the FMO method is applied to structure-based drug design, it is possible to precisely know which fragments of the protein the drug candidate compound interacts with and how strong the interactions are. That allows researchers to construct a candidate compound that interacts more strongly with the target protein at the appropriate parts.

tum chemical calculation is done for each fragment or fragment pair, and the calculation results are used to reconstruct the electronic structure of the whole protein. By taking the influence of surrounding fragments into account when calculating each one, the electronic structure can be calculated efficiently and precisely.

More importantly, the FMO method provides a quantitative understanding of various interactions between a protein and a compound. “When interactions are well understood, candidate compounds can be designed rationally. For this reason, the FMO method is increasingly being used in drug discovery by pharmaceutical companies, although it is rarely clearly disclosed,” says Prof. Fukuzawa, explaining the significance of using the FMO method.

Steadily Accumulating Data Using Large-Scale Computational Resources

“However, no matter how good the FMO method is, it will not develop into a practical drug discovery method if researchers in academia and pharmaceutical companies are working on their calculations independently,” Prof. Fukuzawa says. “We thought it necessary to use large-scale computational resources through industry - academia - government collaboration, and to develop and disseminate databases and methodologies.”

At the end of 2014, she and her colleagues called on industry, academia, and government researchers to launch a consortium to apply the FMO method project to the K computer. “Just around that time, the HPCI network began to be used, so members from all over Japan could access the K computer and perform calculations with the same quality in the same environment. I think it helped us establish the consortium's foundation,” Prof. Fukuzawa recalls.

The consortium focused on proteins such as enzymes and receptors, which are likely targets for drug discovery, and calculated the binding states of protein-compound complexes one after another. Then, the “FMO database (FMODB)” was constructed, and in February 2019, the data calculated up to that point was made publicly available for anyone to use. Since then, more and more data has been added, and as of Oct. 14, 2022, there are 15,653 public data points -- 17,625, including private data points.

Considering Fluctuations to Obtain More Realistic Data

FMODD not only accumulated data but also developed new methods for drug discovery. The background is, "*in vivo*, the structures of proteins and compounds are always fluctuating, but the FMO calculation consider only a single 'static' structure, so dynamic interactions that should be occurring *in vivo* are not known." To incorporate protein fluctuations, Prof. Fukuzawa and her colleagues came up with the idea of combining the FMO method with the molecular dynamics (MD) method, which simulates the movement of molecules (Fig. 2). First, the team generates a "movie" of the fluctuating protein-compound complex by the MD method, and obtains "snapshots" at a regular time interval. Then the FMO calculations are performed for each structure, and the results are averaged. By this method, the team is trying to examine the interactions taking into account molecular fluctuation.

"We started this calculation on the K computer around 2017," Prof. Fukuzawa said. "Regarding the MD method, we received the cooperation of the consortium (KBDD) headed by Prof. Yasushi Okuno of Kyoto University. The calculations didn't go very

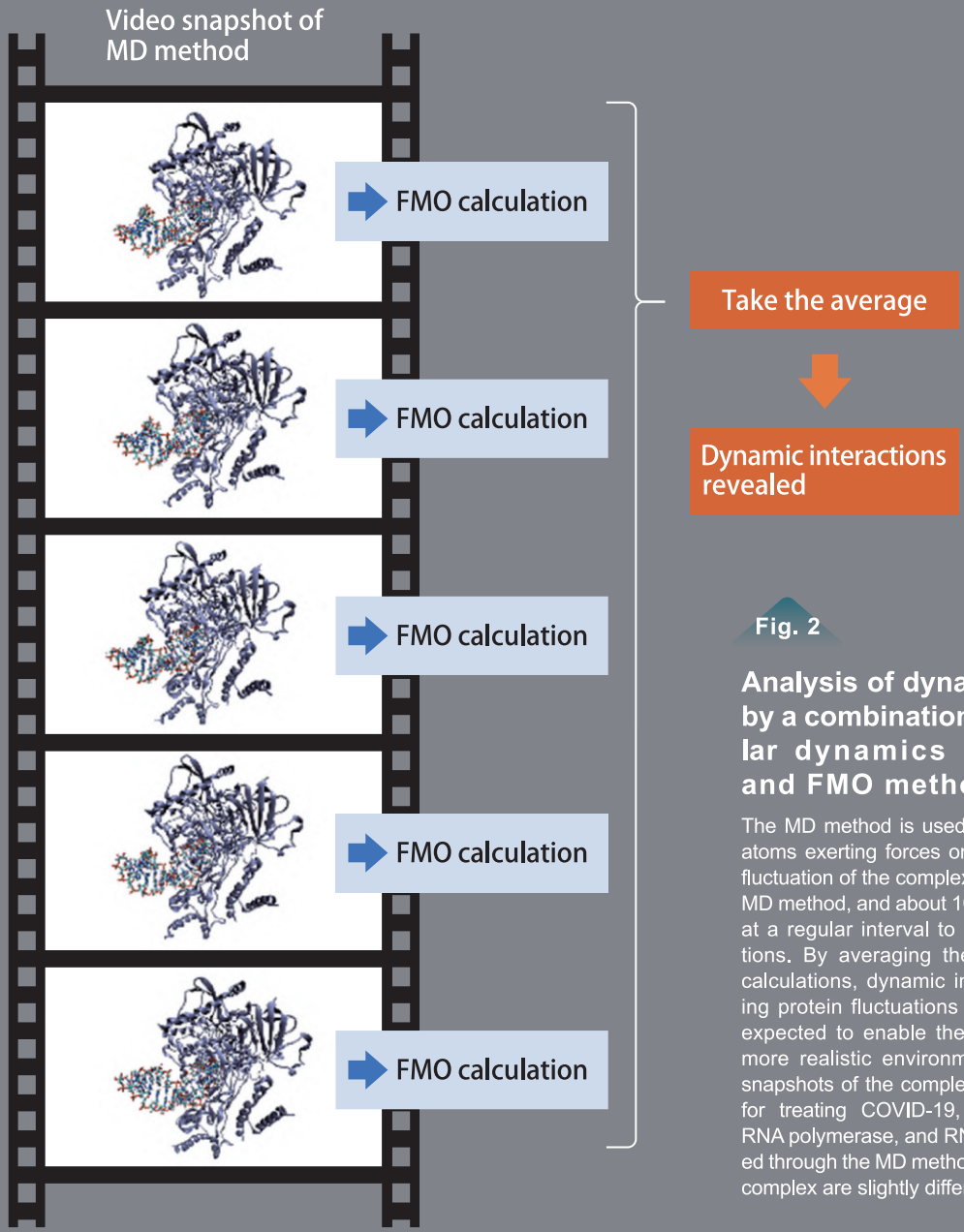


Fig. 2

Analysis of dynamic interaction by a combination of the molecular dynamics (MD) method and FMO method

The MD method is used to track the motion of atoms exerting forces on each other. First, the fluctuation of the complex is simulated using the MD method, and about 100 snapshots are taken at a regular interval to perform FMO calculations. By averaging the results of the FMO calculations, dynamic interactions incorporating protein fluctuations become clear. This is expected to enable the design of drugs in a more realistic environment. Shown here are snapshots of the complex of remdesivir, a drug for treating COVID-19, viral RNA-dependent RNA polymerase, and RNA, which was generated through the MD method. The structures of the complex are slightly different from one other.

smoothly, partly because we were unfamiliar with MD," she added.

"After the K computer ended its operation, we were able to use the HPCI computational resources TSUBAME3.0 and Oakforest-PACS, and finally completed the calculation." The method they established with a struggle at that time is now demonstrating its power in Fugaku. They have elucidated in detail the action of therapeutic drugs for COVID-19 (see Fig. 2). They are also studying membrane proteins, which are important drug discovery targets, and nucleic acid drugs*1, which are expected to become new types of drugs, using this method.

"Now, members from all over the country are accessing Fugaku and performing calculations just as they were in the project with the K computer. Fugaku's computational power is huge, and I feel that it's about 100 times more powerful than the K computer. FMO calculations of 100 structures obtained by an MD simulation can be done in about 30 hours using one rack of Fugaku, and then, we can immediately start scientific discussions to further improve the quality of the calculations," Prof. Fukuzawa says. As the next step, she plans to spread the MD-FMO combination method to young researchers and apply it to various complexes.

I Want to Elucidate Life Phenomena with Quantum Chemical Calculations

Meanwhile, Prof. Fukuzawa and her colleagues are also working on utilizing the huge amount of data they have accumulated. One example is prediction of interaction strength by machine learning. "There are several types of interactions between fragments, such as electrostatic interactions where positive and negative charges attract each other, and hydrogen bonds (see Fig. 1b). By learning the data for each interaction type, we can get information on the strengths of the interactions depending on the distance between fragments. By accumulating such information, we want to eventually predict the strength of the interaction without performing FMO calculations," she explains.

In this way, the FMODD has accumulated FMO calculation data that forms the interaction information basis of *in silico* drug

discovery, and has developed new methods and achieved excellent results. However, this is not Prof. Fukuzawa's goal. She has a dream as an expert in quantum chemical calculations. "Quantum chemical calculations are first-principles calculations that do not use assumptions or empirical parameters. So as long as the calculations are performed correctly, correct results can be obtained. I want to use those quantum chemical calculations to understand all life phenomena."

To realize this dream, Prof. Fukuzawa advances her research step by step, by setting goals to be achieved using the next supercomputer after Fugaku and the one after that, such as more accurate calculation of thermal fluctuations, FMO calculation of enzyme reactions and metalloproteins, and RNA kinetics.

*1: Artificially produced DNA and RNA used as pharmaceuticals. Practical application is progressing, particularly for drugs for the treatment of genetic diseases.

About the

Researcher

Prof. Fukuzawa believes it is important to lead a fulfilling life as a person, not to sacrifice everything other than research. In fact, she loves cooking and has taken lessons from a Michelin-starred Japanese chef, and she also interacts with artists. Through communication with people other than scientists, she learned "it is not necessary to cook exactly following a recipe, but enough to grasp the flow between the lines with my five senses." She also became aware that when doing research as well as playing music we begin with the interpretation of what our predecessors left behind, and then deepen it. "As a result of seeking a post that would allow me to do the research I wanted, I am currently working in Osaka without my family. I'm worried about my two children, a second-grade junior high and a sixth-grade elementary school student whom I left behind in Tokyo, so I return home on weekends as much as possible," says Prof. Fukuzawa, showing her mother's face. Her multifaceted nature seems to attract people and has helped bring together the people in the consortium.

Associated Research Projects

Construction of platform of FMO-based drug design using HPCI system
(hp190133/hp200101/hp210130/hp220143)
Principal Investigator: Kaori Fukuzawa, Graduate School of Pharmaceutical Sciences, Osaka University
(Current affiliation from April 2022, Hoshi University until March 2022)

Flying with Both Wings and Body – A Supercomputer Analysis of Butterflies' Complex Flight

Imagine butterflies fluttering about in a flower garden. Despite their fluttering, joyful appearance, butterflies use very complex movements to generate lift and thrust. Dr. Kosuke Suzuki says, "The more complex the phenomenon, the more I want to understand it." He uses numerical simulations to understand how butterflies fly in the air. Here, we introduce his research, which has a variety of potential applications, from Mars exploration to highly efficient refrigerants.

Kosuke Suzuki
Associate Professor, Department of Mechanical Systems Engineering,
Faculty of Engineering, Shinshu University

Calculating the Unique Flying Style of Butterflies

In order to develop micro air vehicles such as drones, many studies are being conducted around the world to understand how flies and mosquitoes fly. "In contrast to these insects, which do not move their bodies in order to fly, butterflies move their abdomen and thorax (Fig. 1). In other words, to model the flight of butterflies, we must account for the movement of not only their wings, but also their abdomen and thorax. It is a very complex and challenging study," Dr. Suzuki explains.

Butterflies gain lift by flapping their wings downward and thrust by flapping backward. At that time, the movement of the body is linked to the movement of the wings, and it is believed that

the angle of the thorax controls the direction the wings move, but the details have not been clarified.

Immersed Boundary-Lattice Boltzmann Method (IB-LBM) with Good Balance of Accuracy and Computational Complexity

To understand the flight of a butterfly, it is not enough to simulate the motion of the fluid (air) and the motion of the object (butterfly). The interaction between the fluid and the object must also be calculated because they mutually affect each other – when the butterfly flaps its wings, it induces an air flow, which affects the motion of the butterfly.

Since he was a graduate student, Dr. Suzuki has been researching methods to accurately simulate systems in which the fluid and the object affect each other's motion while minimizing the amount of computation needed. There are several numerical methods for systems in which the fluid and the object interact (Fig. 2), and among them, Dr. Suzuki has been developing and improving the "immersed boundary-lattice Boltzmann method (IB-LBM)" (Fig. 2e), which is a combination of the immersed boundary method, which has been known since about 50 years ago, and the lattice Boltzmann method, which has been rapidly developing in recent years .

The immersed boundary method represents a moving object in a fluid by applying a force called a body force around the object (the red area in Fig. 2e). The body force makes the velocity of the fluid the same as the velocity of the object's surface, thus preparing a field in which the moving object can be embedded. When applied to the flight of a

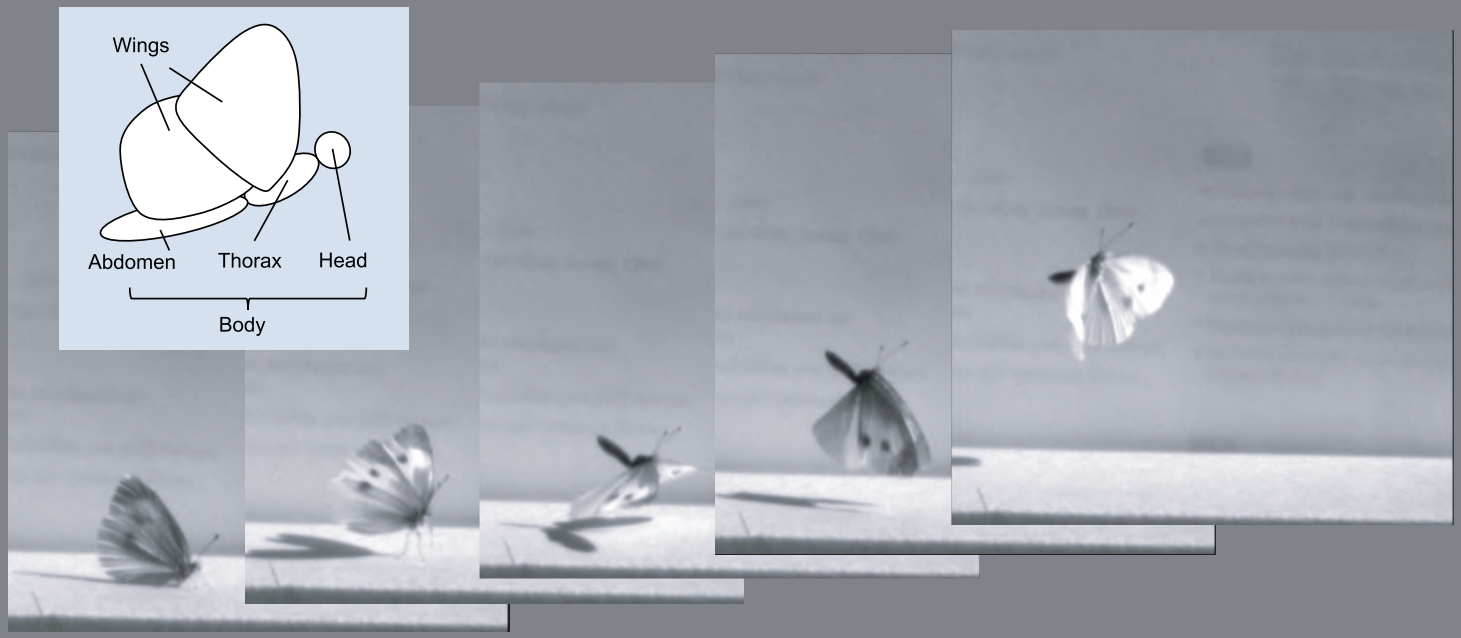


Fig. 1

A cabbage butterfly in flight

Captured from a video taken by Dr. Suzuki and his colleagues. It can be seen that when the butterfly flaps its wings downward, its body is flexed and it raises its abdomen significantly. The wings are raised and lowered 10 times per second while the wings, abdomen, and thorax move simultaneously.

butterfly, the butterfly is placed in this field and is moved according to the equations of motion.

On the other hand, the “lattice Boltzmann method” is a flow simulation technique that treats the fluid as a collection of fictitious particles that can only exist at the intersections of orthogonal lattices (lattice points). Each particle is assumed to move between the lattice points at some fixed velocity, and to collide with other particles. The density, velocity and pressure of the fluid can be obtained by averaging the mass and momentum of the particles that are distributed in a space according to the rule above-mentioned.

The lattice Boltzmann method, when applied to incompressible flows such as water and low-speed air flows, has been mathematically proven to result in the Navier-Stokes equations that describe the motion of fluids. The lattice Boltzmann method does not require solving Poisson equation to calculate the pressure, thus allowing for highly accurate calculations with low computational cost. It is also suitable for parallel computing because it uses only the information of particles on adjacent lattice points for the calculation of a particle on one lattice point and does not require information on faraway particles.

“Both the immersed boundary method and the lattice Boltzmann method use orthogonal lattices, so they are well suited for use in combination. The relative simplicity of the algorithms and the ease of writing program code for both are also favorable for research,”

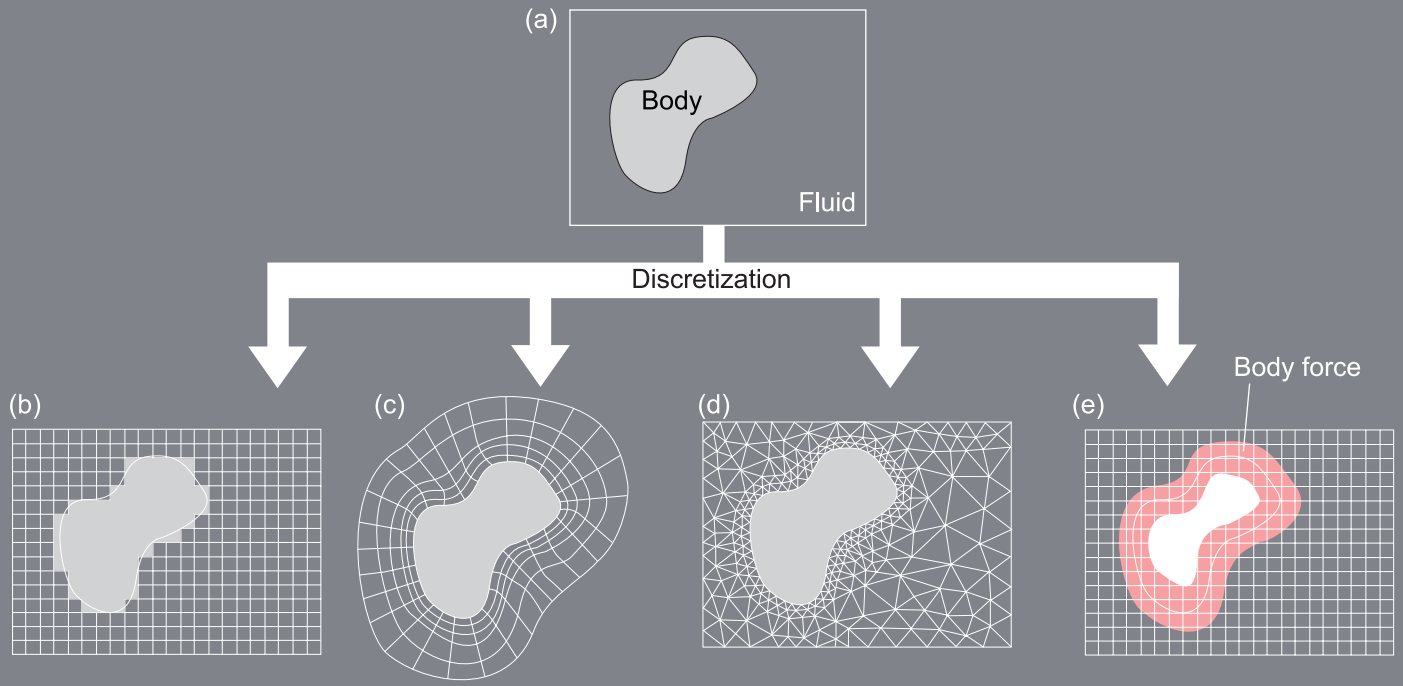


Fig. 2

Comparison of numerical computing methods for fluid-object interaction

(a)The fluid and the object (body) to be calculated. (b) A method of stepwise approximation of the space around an object. (c) Boundary-fitted grid method. Creating a grid along the object. (d) Unstructured grid method. Using small and large triangles. (e) IB-LBM. In the methods in (b), (c) and (d), the computational load is high because the grid is recreated each time the object moves. In (e), it is only necessary to move the body force field, so the motion of the object can be expressed with the suppressed computational load.

Suzuki, K.: “Development of an immersed boundary-lattice Boltzmann method for moving boundary flows and its application to flapping flight.” *NAGARE* (Journal of the Japan Society of Fluid Mechanics) 37 (2018) 215-220.

Dr. Suzuki says, explaining the advantages of combining the two methods.

Dr. Suzuki's team was the first in the world to apply IB-LBM to butterfly flight in 2012, and in 2013 they succeeded in creating a simulation of a butterfly in flight. "At first, the butterfly did not fly like a real butterfly because it flipped over or ran in reverse," Dr. Suzuki says. "Other researchers are working on butterfly flight research, but we are the only team in the world that has solved the equations of motion by linking the motion of the butterfly, including its body, with the motion of the fluid," he added proudly.

Two Approaches to Understanding Flight

"We use two approaches to analysis: top-down and bottom-up," Dr. Suzuki explains (Fig. 3).

The top-down approach incorporates the actual movements of butterflies into the computational model. A cabbage butterfly caught on a riverbank is filmed from three directions with a high-speed camera, and its shape and movement are recorded using motion capture. From this data, a computational model of the butterfly is created and made to fly in a fluid. The result is shown in Fig. 3a.

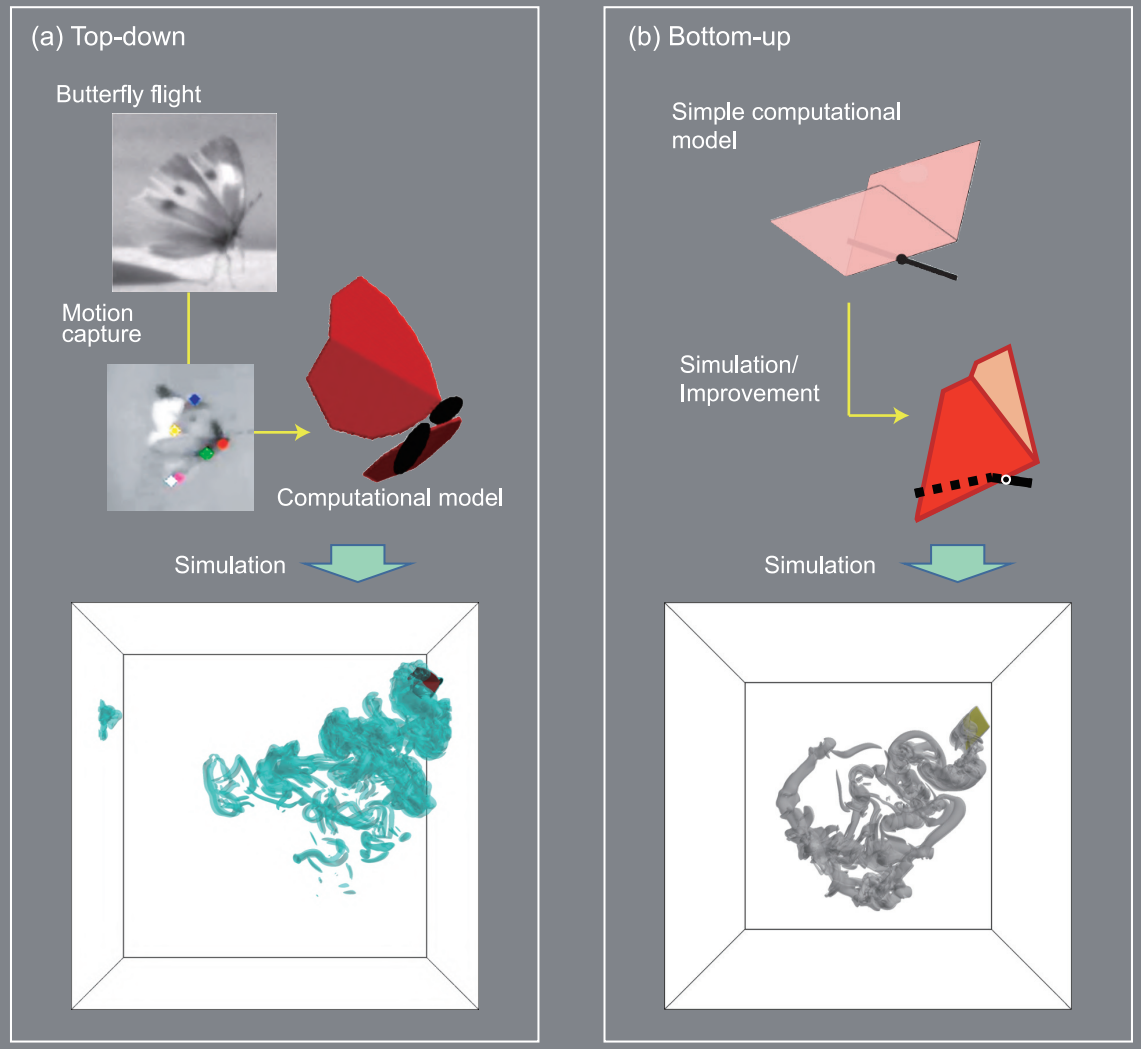


Fig. 3

Butterfly flight as elucidated by the supercomputer

(a) Top-down approach. Butterfly flight was simulated using a computational model of a butterfly that faithfully simulates the shape and behavior of an actual butterfly. (b) The simulation was performed using a computational model created in the bottom-up approach. The figures in (a) and (b) obtained from the simulations trace the changes in the vortex behind the butterfly.

Conversely, the bottom-up approach starts with a simple model and improves it through repeated simulations. First, Dr. Suzuki considered the flight of a simplified model of a butterfly on a computer, consisting of a pair of square wings and a stick with no thickness. Based on the results, he examined how factors such as the shape and mass of the wings affected the butterfly's flight, and improved the model to make it fly more like a butterfly. Fig. 3b shows a simulation of the model he created in this way.

Comparing the two simulations shown in Fig. 3, the butterfly calculated by the bottom-up approach flutters in the same way as the butterfly calculated by the top-down approach, and a stepped vortex structure forms behind the wings. The bottom-up approach also reproduces the butterfly's movement quite well (Fig. 3b). However, there are still some challenges. There is a hypothesis that butterflies adjust the angle of their thorax by moving their abdomen up and down, but if we include this adjustment in the calculation using the bottom-up approach, the abdomen swings at an angle that is impossible in reality. Therefore, in the calculation shown in Fig. 3b, the thorax angle is calculated by inputting the value obtained from the experimental data, and the control of the thorax movement by the movement of the abdomen is not included in the calculation.

"In the bottom-up approach, our goal is to identify the minimum elements necessary to reproduce the butterfly's flight as we refine the model," Dr. Suzuki says. By bringing the bottom-up and top-down flying manners closer together, he is trying to elucidate "what is butterfly flight?"

To perform these calculations, Dr. Suzuki and his team have been using two of HPCI's supercomputers, System A (CRAY XC40) at Kyoto University and the "Flow" Type I subsystem (FUJITSU FX1000) at Nagoya University *1. They also use their own computer cluster, but as the number of elements to be calculated increases, they need the computing power and large memory of a supercomputer.

One of the reasons they chose the "Flow" is that it is compatible with the supercomputer Fugaku. What kind of calculations would he like to perform if he had the chance to use the methods developed on Fugaku, which has enormous computational power? Dr. Suzuki says, "Currently, in order to reduce the amount of calculations, we are slightly lowering the Reynolds number*2 and making the butterfly's wings flap more slowly than they actually do, but eventually we would like to do calculations at the actual Reynolds number. It is also believed that the streaks and scales on a butterfly's wings also affect its flight. We do not include these factors in our calculations at this time, but we would like to include them in our calculations as well."

Potential Applications Range from Small Ice Pellets to Mars Exploration

Dr. Suzuki is also working on applying IB-LBM to phenomena other than butterfly flight. One such application is "ice slurry" (tiny ice particles dispersed in water), which is expected to find use as an excellent refrigerant. "We are applying IB-LBM to calculate the interaction between ice flow and water flow, and studying what kind of ice slurry is suitable for efficient heat exchange," he says.

Meanwhile, he is also looking to develop his butterfly flight research. Micro air vehicles such as drones that imitate the flight of flies are not good at recovering their correct attitude instantly once they lose it. If Dr. Suzuki

can elucidate a flight model of a butterfly that recovers its attitude while swinging its body, he may be able to develop a flying object that can instantly recover and continue to fly even if it loses its attitude.

The Martian atmosphere is much less dense than Earth's and gives a lower Reynolds number, so it is difficult to fly on Mars for the fixed-wing aircrafts used on Earth, which are designed for high Reynolds number conditions. This is why insect flight is attracting so much attention. "I would like to develop my research and make large-scale calculations on how to fly in a Mars environment," Dr. Suzuki says, expanding on his dreams for the future.

*1 System A (CRAY XC40) was used in FY2021 and the "Flow" Type I subsystem (FUJITSU FX1000) in FY2022.
*2 Reynolds number: Ratio of inertial force to viscous force. A small value indicates a regular flow (laminar flow), while a large value indicates an irregularly turbulent flow (turbulent flow).

About the

Researcher

Dr. Suzuki was fascinated by the shape of insects and used to collect them in his childhood. He fell in love with mathematics and physics, and majored in aerospace engineering at university. "I wanted to know what kind of theory could explain what it means to fly," he says. "I was impressed by the depth of understanding that could be achieved using fluid engineering, plasma engineering, and electromagnetics," he says. Once he began his research, he wanted to unravel complex things that could not be explained by simple fluid engineering, and his application was to flying insects, specifically butterflies. He and his students go to the riverbank early in the morning to collect cabbage butterflies sleeping on the underside of leaves. His hobby is sake tasting. In Nagano, where there are many sake breweries, he enjoys drinking sake while thinking about the brewer and the production process.

Associated Research Projects
Numerical analysis of flapping flights of insects by IB-LBM using a massive parallel computer (hp210037/hp220037)
Principal Investigator: Kosuke Suzuki, Department of Mechanical Systems Engineering, Faculty of Engineering, Shinshu University

A Supercomputer Reveals the True Nature of the ‘Disappearing Magic Ball’

Takayuki Aoki
Deputy Director (Advanced Computing Research Division) / Professor
Global Scientific Information and Computing Center
Tokyo Institute of Technology

One of the most exciting aspects of baseball is the interaction between the pitcher and the batter. The main players in this interaction are the various breaking pitches that pitchers have developed, but the reasons why their trajectories change are not well understood. In particular, there is a theory as to why the forkball falls so sharply, but it has never been properly demonstrated. A joint research team of the Tokyo Institute of Technology, Kyushu University, and Keio University, led by Dr. Aoki, took on the challenge of elucidating the “fall mechanism” by using a supercomputer and thus discovered a previously unknown mechanism.

Does Forkball Fall Due to the Action of Gravity?

The first person to throw a forkball in Japan was Chunichi Dragons pitcher Shigeru Sugishita, some 70 years ago and it took the world by storm. It was called the “disappearing magic ball” because of its large drop and the fact that it seemed to disappear from the batter’s view. Since then, many famous pitchers have used the forkball as a trump card when facing batters. “For many years, it has been said that gravity is the reason that the forkball falls so rapidly. However, I have always believed that there must be other factors besides gravity,” Dr. Aoki recalls. In April 2020, the research team led by Dr. Aoki (Photo 1) began studying forkballs using hydrodynamic simulations.

Photo 1 :
The research team that has been working to elucidate the breaking balls

Back row, from left: Dr. Seiya Watanabe (Assistant Professor, Research Institute for Applied Mechanics, Kyushu University), Dr. Hiromichi Kobayashi (Professor, Faculty of Law, Keio University), Yuwei Yin (2nd-year master’s student, Tokyo Institute of Technology). In the front row is Dr. Aoki. In the lower right circle is Ryoga Ohashi, who completed his master’s degree at Tokyo Institute of Technology in 2021.

Normally, a thrown ball follows gravity and falls in a parabolic curve, but a fastball thrown by a pitcher flies in a straight line. This is due to the “Magnus effect” working on the ball. When a pitcher throws a fastball, he applies a strong backspin to the ball. Backspin means that the upper side of the ball rotates in the opposite direction of the direction the ball is going.

The air around a flying ball has a layer that flows along the ball, so-called boundary layer, but when it separates from the surface of the ball, in the process it creates turbulence behind the ball. As shown in Fig. 1, in the case of a ball with backspin, the airflow above the ball is dragged by the rotation of the ball, and the point where the layer flowing along the ball separates is shifted backward. Conversely, on the underside of the ball, the rotation of the ball and the surrounding flow oppose each other, causing the separation point to shift forward. As a result, the airflow behind the ball is biased downward. This adds an upward force to the ball, weakening the downward force generated by gravity. This phenomenon of a force (lift force) perpendicular to the direction of motion acting on a rotating object is called the “Magnus effect.” This effect increases with the number of rotations of the object. In other words, a ball with a strong backspin will be lifted by the Magnus effect, resulting in a fastball.

On the other hand, in the case of a forkball, the pitcher throws the ball with as little rotation as possible. This reduces the Magnus effect and makes the ball more susceptible to gravity, so it has been thought that the ball falls rapidly before reaching the bat.

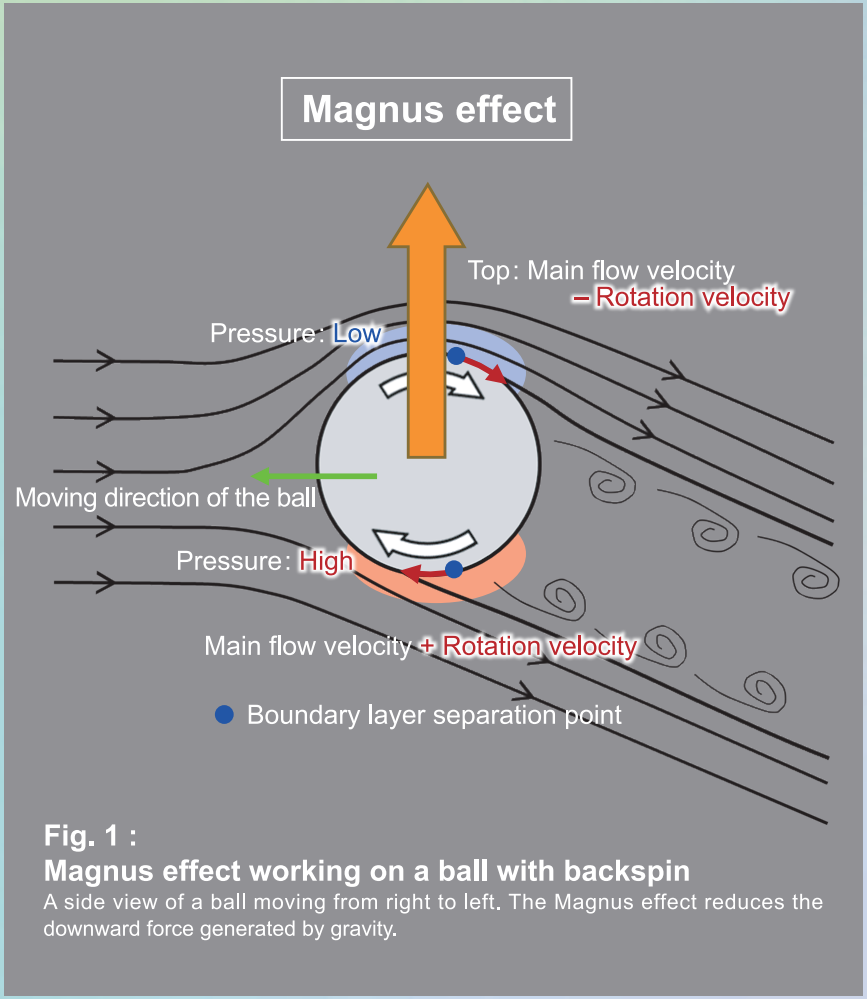


Fig. 1 :
Magnus effect working on a ball with backspin
A side view of a ball moving from right to left. The Magnus effect reduces the downward force generated by gravity.

Flow Simulation around a Ball with Seams

Dr. Aoki, who has been questioning the commonly accepted forkball theory, focused his attention on the seams of the ball. The surface of a baseball has a seam only 0.9 mm high. It has long been known that these seams affect the airflow. However, it was not well understood how it affected the ball. As the ball rotates at high speed, the position of the seam changes from moment to moment. It was impossible to evaluate the impact of the stitches on the ball without the help of advanced computational technology and high-performance supercomputers.

In recent years, however, the performance of supercomputers has improved dramatically. Furthermore, Dr. Aoki and his team have developed methods to perform state-of-the-art fluid calculations utilizing the capabilities of such supercomputers, which allowed them to achieve their results. At the same time, the development of accurate sport measurement devices has made it possible to measure detailed data about a pitcher's ball, such as its velocity, rotation speed, and trajectory drop. Recently, the Major League Baseball has begun publishing these measurements, which has made it possible to compare and verify the results of supercomputer simulations with actual data.

In fact, it was found that the direction of the ball's seam differs between a fastball and a forkball. When looking at a fastball from the batter's side, the seam appears four times per rotation of the ball, while on a forkball, the seam appears only twice (Fig. 2). For this reason, the rotation of the fastball is called "four-seam rotation," while the rotation of the forkball is called "two-seam rotation."

Dr. Aoki and his team used the TSUBAME3.0 GPU supercomputer at the Tokyo Institute of Technology to determine the difference in the way the ball falls between four-seam and two-seam rotations. For the numerical calculations, they used the cumulant lattice Boltzmann method, which is optimal for performing turbulence calculations. They set the same values for ball velocity and rotation number for four-seam

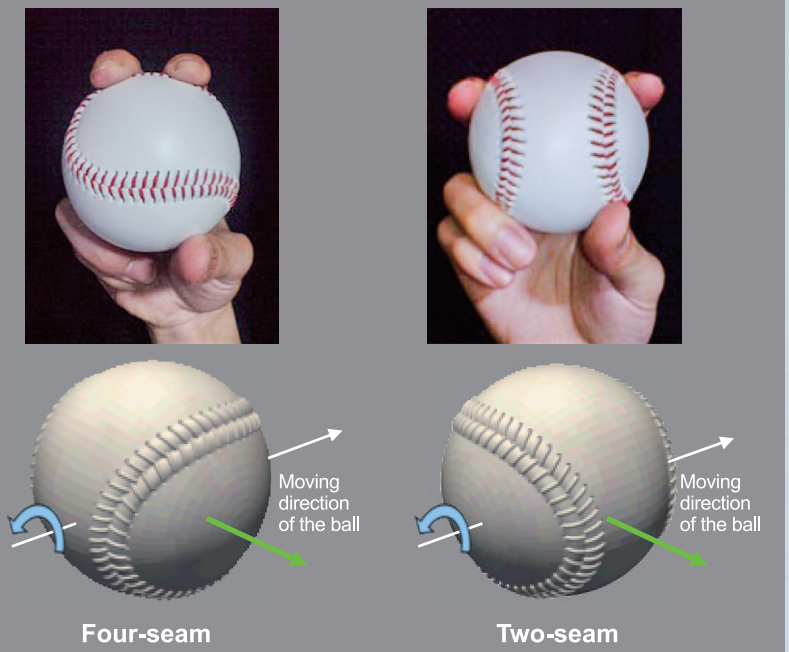


Fig. 2 : Four-seam rotation and two-seam rotation

and two-seam rotations. The space around the ball was then divided into approximately 370 million grids to simulate how the airflow was generated and how this flow affected the ball.

The simulation code was developed mainly by Dr. Seiya Watanabe, a graduate of Dr. Aoki's laboratory who is now an Assistant Professor at Kyushu University. "In the beginning, the calculation time needed to complete the process of a pitcher throwing a ball to a catcher was estimated at 200 days, even using TSUBAME3.0. We succeeded in reducing the time to about one week by improving the efficiency of parallel distributed processing and reducing the number of unnecessary grids," said Dr. Watanabe, looking back on the development efforts.

Discovery of the "Negative Magnus Effect"

The main results obtained from the simulation are as follows.

First, in the case of a four-seam rotation it was found that the point where the boundary layer separates from the surface of the ball shifted backward each time the seam came up, and conversely, on the underside of the ball, the point where the boundary layer separates was pulled forward by the appearance of the seam. Lift forces were also always positive. In other words, it was confirmed that the seam enhances the Magnus effect described above.

Second, in the case of a two-seam rotation (Fig. 3), when the seam was at the top, it was confirmed that on the upper side, as in the four-seam case, the boundary layer was less likely to detach and a downward flow behind the ball was generated. However, when the smooth part of the ball with no seam was on the pitcher side of the ball, the airflow behind the ball changed to an upward direction. Then, when the ball rotates and the seam was on top again, the flow changed downward again. When the airflow behind the ball turns upward, the ball is considered to be subjected to a force in the opposite direction of the lift force.

Mr. Ryoga Ohashi, then a second-year master's student in Dr. Aoki's laboratory, and Dr. Hiromichi Kobayashi, Professor at Keio University specializing in turbulence analysis, worked with colleagues in Dr. Aoki's laboratory to analyze in detail a large number of images obtained through simulations. As a result, they found that the lift force was always positive in the four-seam rotation, whereas in the two-seam rotation, the lift force

Lift characteristics of two-seam

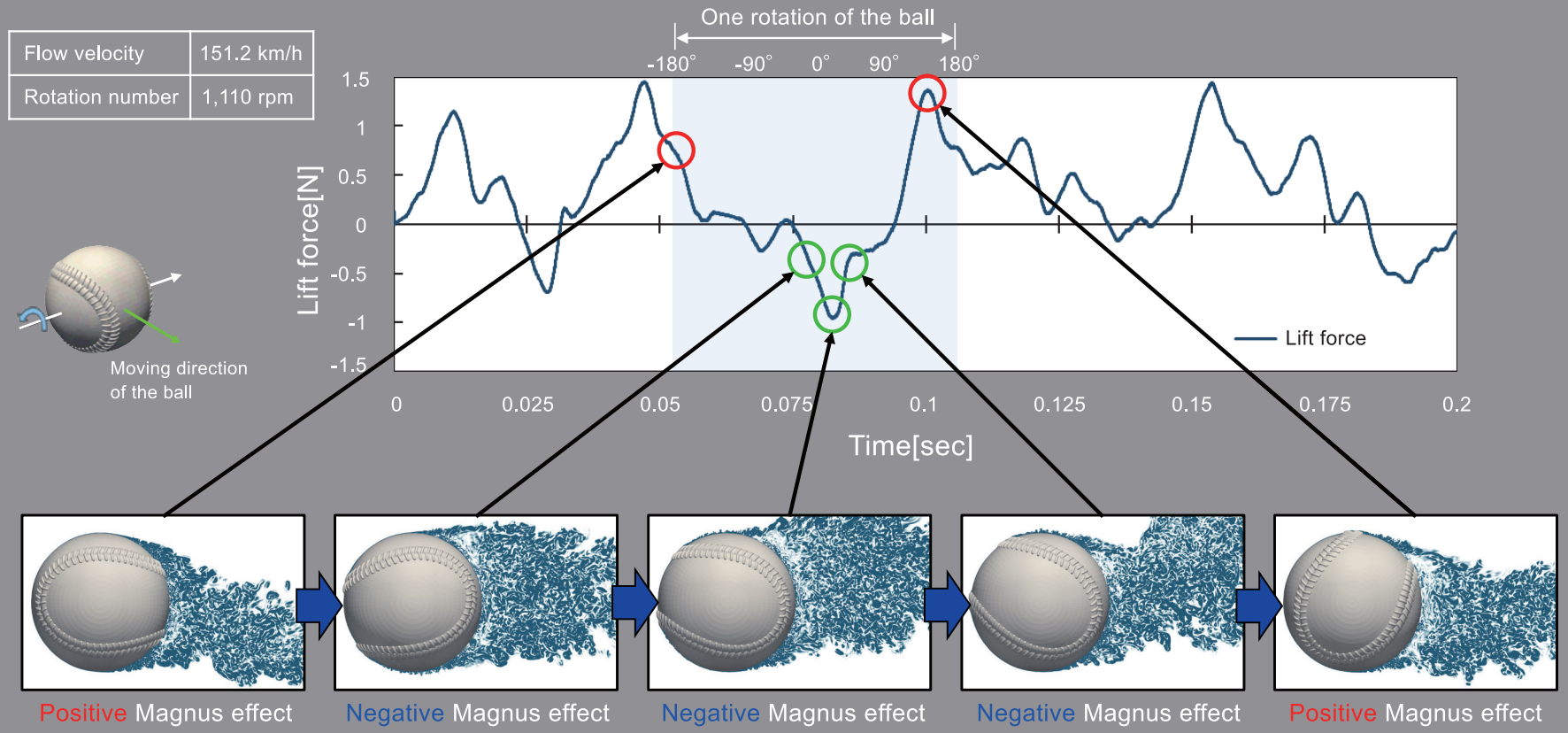


Fig. 3 : Analysis of two-seam turbulence
When the smooth part of the ball is on the pitcher side, a “negative Magnus effect” occurs, in which the lift force is negative, working to make the ball fall.

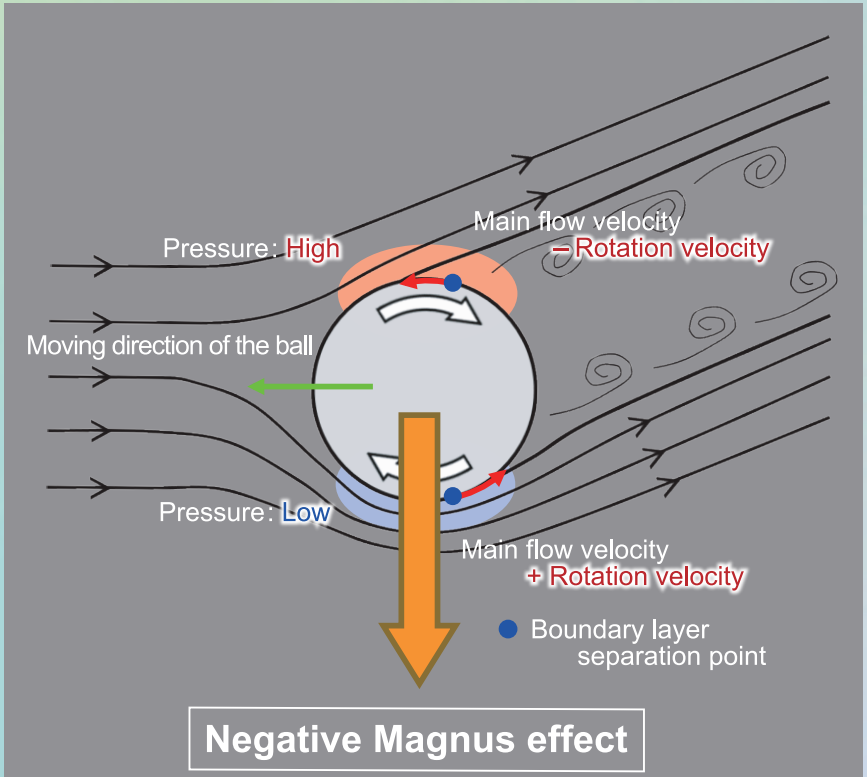


Fig. 4 : Negative Magnus effect

was negative at moments, as shown in Fig. 3. They found that when the stitch angle of a two-seam ball is in the range of -30 to 90 degrees, the force is in the opposite direction of the lift force.

It is known that on a slippery (no seam) ball, turbulence in the layers flowing along the surface causes a “negative Magnus effect” in the opposite direction of the “positive Magnus effect” that acts as a lift force (Fig. 4). Dr. Aoki recalled, “Mr. Ohashi pointed out that the negative Magnus effect might also occur on the slippery surface in two-seam rotation.” As a result of the calculations and analysis, it was found that the forkball with two-seam rotation falls sharply not only due to gravity but also due to the negative Magnus effect. Furthermore, when the velocity and rotation number of the ball were set to the same value, the two-seam forkball fell about 19 cm lower on the home base than the four-seam forkball.

“This result shows how much the stitching affects the ball. This was the first time in the world that a negative Magnus effect was shown to occur on a baseball, and it was the moment when my long-held question was answered. This was also made possible by the fact that the supercomputer was able to capture the air changes around a ball with seams from moment to moment,” Dr. Aoki explained.

The Mystery of Ohtani’s Forkball Unraveled, Too

Next, Dr. Aoki and his team took on the mystery of the forkball thrown by Shohei Ohtani of the Los Angeles Angels and Roki Sasaki of the Chiba Lotte Marines, who achieved a perfect game in 2022. This was because the forkball they threw was said to have a sharper drop, even though it was spinning faster.

Dr. Aoki explained, “As the speed of the ball increases, the number of rotations of the ball increases. As the number of rotations increases, the frequency of the appearance of the seam increases, and the positive Magnus effect increases, so the ball’s fall should decrease. However, it falls more sharply. I speculated that this was due to gyro-rotation rather than backspin.” Gyro-rotation is a rotation in which the moving direction and the axis of rotation coincide (Fig. 5). Unlike backspin, when the ball

makes one rotation, the forces received from the top, bottom, left, and right are canceled, so the Magnus effect does not occur.

“However, in the case of gyro-rotation, the airflow around the ball is more complex than in backspin, so the space around the ball must be divided into smaller grids and analyzed in several different patterns, including ball speed, number of rotations, and direction of the axis of rotation,” said Dr. Aoki. Therefore, Mr. Yuwei Yin, a graduate student in the Aoki Lab, conducted the simulation using Nagoya University’s “Flow” Type II subsystem (CX2570), a GPU supercomputer. In addition, Dr. Watanabe rewrote the code for CPUs and conducted detailed simulations on the supercomputer Fugaku. In this research, Mr. Yin played a major role by creating shape data from a 3D scan of an official MLB ball and analyzing turbulence together with Dr. Kobayashi.

The simulation results confirm that when the ball makes one rotation, the forces due to the airflow are canceled out in the vertical and horizontal directions, and only gravity remains. It is now clear that a forkball due to backspin receives lift forces, albeit with a negative Magnus effect, whereas a gyro-rotating forkball falls sharply because only gravity is at work.

Furthermore, Dr. Aoki and his team are gaining new knowledge by trying to elucidate Ohtani’s sweeper, a pitch that makes a big curve across the home base.

Thus, Dr. Aoki’s research team’s simulations have revealed that baseball breaking pitches are produced by the ball’s velocity, number of rotations, angle of the axis of rotation, and the effect of the ball’s seams. “In the future, I would be happy if we could combine the results of this research with virtual reality (VR) and augmented reality (AR) to create a device that would allow anyone to experience Ohtani’s magic ball. We may even see the emergence of a second or third Ohtani among the children who have practiced with such a device,” said Dr. Aoki with a smile.

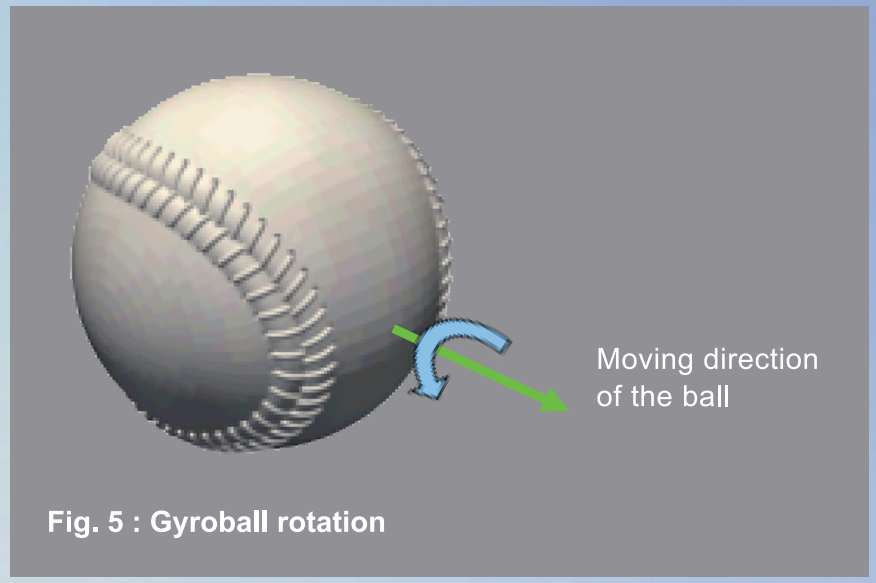
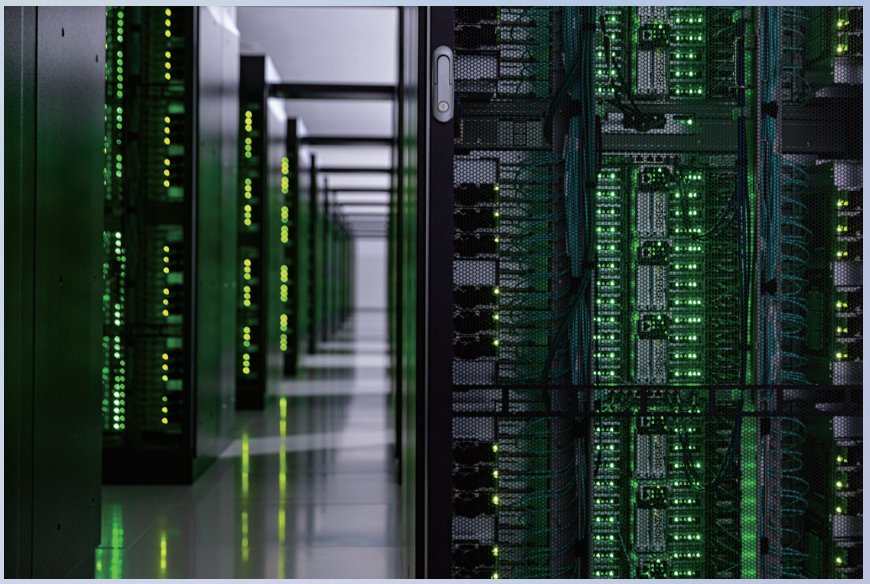


Fig. 5 : Gyroball rotation



About the

Researcher

Dr. Aoki specializes in fluid dynamics. As an undergraduate, he studied in the Department of Applied Physics, where he began researching the dream energy, nuclear fusion, in his graduation project. In graduate school, he went on to the Department of Energy Science, where he began conducting research using theory and simulation. It was during this time that the Tokyo Institute of Technology developed the world's first GPU supercomputer, TSUBAME. Dr. Aoki started hydrodynamic simulations using TSUBAME and received the Gordon Bell Prize Special Achievements for his numerical simulation of dendritic solidification of metallic crystals using TSUBAME2.0 in 2011. He is currently working on a wide range of topics from dolphin swimming to torrential rain disasters and tsunamis containing large amounts of debris and driftwood. Why did Dr. Aoki choose the theme of "breaking ball" for this project? "I thought that if I could do numerical calculations for complex torrential rain disasters, I would also be able to do so for breaking balls," he said. Working on this theme has changed the way he watches baseball games, which used to be a hobby of his. "I started to think, 'They should put in more slow motion so you can see the stitching on the ball'," he said. He hopes to continue to enjoy watching baseball games in between research projects.

Associated Research Projects:
Aerodynamics of Rotating High-speed Baseball (hp200070)
Aerodynamics of Gyro-rotating Baseball (hp220063)
Principal Investigator: Takayuki Aoki, International Research and Information Center, Tokyo Institute of Technology

Boosting Novel Materials Discovery
—mVMC Software Accurately Simulates Strongly Correlated Electron Systems

In May 2023, the first HPCI Software Award was announced. In the development category, the software named mVMC was selected for the Grand Prize, and the development team received recognition. mVMC is capable of efficiently and accurately calculating structures of interacting electrons that strongly influence each other. “Utilizing this feature, it becomes possible to explore novel materials,” said Dr. Kota Ido, one of the key members involved in developing mVMC. He hopes people aiming to evaluate and develop new materials will make use of it. We recently sat down with Dr. Ido to discuss the software’s development process and its distinctive features. Dr. Takahiro Misawa, Project Associate Professor at the Institute for Solid State Physics (ISSP), The University of Tokyo, who has been a close collaborator in Dr. Ido’s research and has contributed to making mVMC open-source, joined the conversation.

Kota Ido
Research Associate
The Institute for Solid State Physics (ISSP), The University of Tokyo

Capable of Simulating Strongly Correlated Electron Systems with Up to 1,000 Particles

“mVMC, in a nutshell, is a ‘simulator for accurately predicting the structures of electrons in materials’,” explains Dr. Ido. Many properties of substances are closely related to the structures of electrons within them. As an everyday example, electric current flows through metals due to the presence of freely moving electrons, and the direction a magnet points is determined by the alignment of the electron’s spin. Therefore, in the field of quantum condensed matter physics, which investigates the macroscopic properties of materials based on the behavior of microscopic particles, understanding the movement of electrons is of paramount importance.

Particularly in “strongly correlated electron systems,” where electron-electron interactions are much stronger compared to typical materials, unique phenomena such as superconductivity and quantum entanglement arise. Given the ongoing development of materials like superconductors with minimal energy loss for efficient wiring or materials indicating strong quantum entanglement crucial for realizing quantum computers, the significance of simulating the underlying strongly correlated electron systems has increased.

However, when calculating electronic structure in strongly correlated systems, the computational complexity increases exponentially with the number of electrons. As a result, the exact treatment of a larger number of electrons has been limited to around 20 electrons, requiring the use of approximations to handle more electrons. While approximations can yield reasonably accurate results when electron interactions are weak, introducing approximations to calculate the electronic structure in strongly correlated systems significantly compromises accuracy. Addressing this challenge and enabling accurate treatment of structures involving around 1,000 electrons is the achievement of the mVMC software.

mVMC is an application implementing the many-variable variational Monte Carlo method, which also serves as the inspiration for its name. It has been under development for a long time. Recently, with the contributions of Dr. Ido, Dr. Misawa and others, the software has been extended to efficiently represent structures of around 1,000 electrons. Additionally, user-friendly features such as a refined user interface and result visualization have been incorporated, transforming it into an open-source tool accessible to everyone. Looking ahead, mVMC is expected to be widely used by researchers aiming to discover and develop novel materials like high-temperature superconductors and quantum materials. Recognizing its contribution to quantum condensed matter physics, mVMC was awarded the 2023 HPCI Software Award (Photo 1).

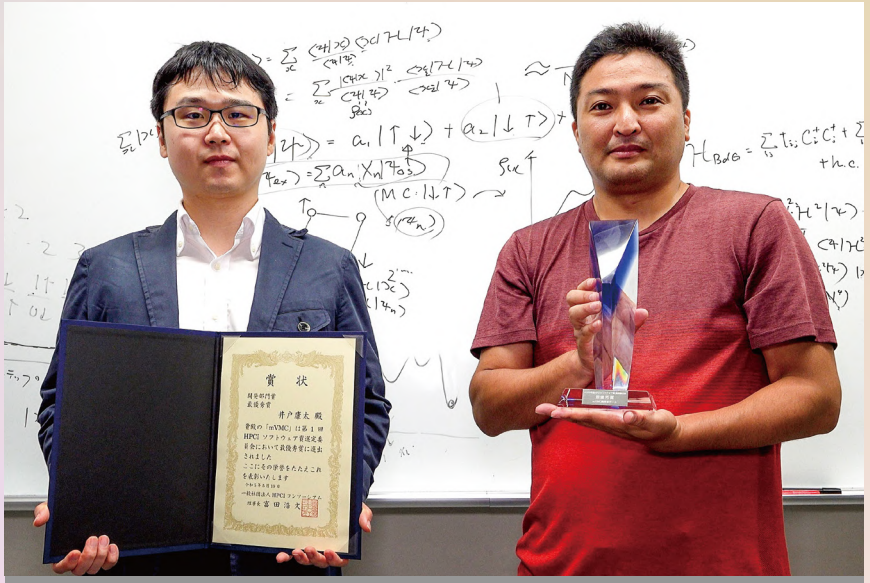


Photo 1 :
Dr. Ido holds the certificate for the HPCI Software Award (Development Category, Grand Prize), accompanied by Dr. Misawa holding the trophy.

Software Blossoming on the Foundation of Previous Generations' Efforts

First of all, how do we go about calculating the structure of electrons? The structure of electrons is represented by something called a wave function (Ψ) that spreads out like a wave. This wave function is determined by solving the Schrödinger equation (Fig. 1). In this equation, the environment in which the electrons are situated (for example, how atoms are arranged in a solid) is represented by an operator called the Hamiltonian (*H*). Solving this equation also yields the energy (*E*) of the wave function.

However, it should be noted that solving the Schrödinger equation exactly is limited to special cases, such as the hydrogen atom with a single electron. As a result, in fields like condensed matter physics that deal with a large number of electrons in materials, researchers have resorted to approximations to solve this equation. However, as mentioned earlier, in the case of strongly correlated electron systems, applying approximations while dealing with a large number of electrons severely compromises accuracy, making it challenging to obtain calculation results that could be useful for designing new materials.

One of the solutions to this challenge is mVMC, but the journey to Dr. Ido and his team's recognition was quite difficult.

$$H\Psi = E\Psi$$

Fig.1 : Schrödinger equation
The micro world, like electrons, follows the rules of quantum mechanics. The Schrödinger equation is an equation based on quantum mechanics used to calculate the structures of micro particles such as electrons.

The HPCI Software Award

The HPCI Software Award was established in 2023 by the High Performance Computing Infrastructure (HPCI) Consortium, a general incorporated association. The award is intended to recognize and honor organizations, particularly those led by young developers, that have made significant contributions to the advancement of computational science and have developed software that is deemed especially beneficial. It also acknowledges entities that have contributed to the dissemination of such software. The award is divided into two categories: the Development Award and the Dissemination Award. Among these, our consortium honored mVMC development team with the top prize in the Development Award category.

Hirofumi Tomita,
President of the HPCI Consortium

A method that has been used for a long time to represent the structures of many electrons is the "variational Monte Carlo method," which combines the concepts of a "trial wave function" and the "Monte Carlo method." In this approach, one starts by assuming an electron's structure and constructs a trial wave function to represent it. Then, through repeated calculations, the energy is determined while adjusting the parameters of the trial wave function to optimize it, aiming to find the wave function that yields the lowest energy. However, depending on the shape of the trial wave function, it's sometimes impossible to calculate energy exactly. Therefore, the Monte Carlo method is employed to predict the expected values of quantities like energy. With advancements in computing, it has become possible to compute the structures of around 1,000 electrons. However, the accuracy of representing the structures of many electrons depends on the assumed trial wave function. Increasing the number of

parameters to improve accuracy also increases the computational effort, and the number of parameters that can be introduced in the trial wave function has been limited to maintain tractability.

Dr. Ido explains: “In 2001, Dr. Sandro Sorella from Italy proposed a good optimization method that allowed the introduction of more parameters. Furthermore, this approach was further developed by Mr. Daisuke Tahara and Dr. Masatoshi Imada*1 from The University of Tokyo in 2008, who introduced the ‘many-variable variational Monte Carlo method.’ This allowed the incorporation of many parameters, providing flexibility to the representation capability of the wave function and increasing accuracy. When the number of parameters was limited, we were restricted to trial wave functions that ‘forced’ certain aspects, like the alignment of spins. However, since 2008, it became possible to use trial wave functions that can represent various states using a single form, enabling the representation of more complex electronic structure flexibly.”

“However, at that time, it felt like an internally used computational code. In 2016, Dr. Misawa received support from the ISSP’s project for the advancement of software usability in materials science, and he shaped it into a form that could be publicly released as software. Thus, mVMC’s development involved the contributions of many individuals. Additionally, I aimed to enhance the accuracy of the trial wave function and functionality of the software. Without years of accumulated effort, we wouldn’t be here,” Dr. Ido modestly says. However, Dr. Misawa highlights, “The computational complexity to compute electronic structures among 1000 interacting electrons requires at least 2^{1000}. Even if we started running the supercomputer Fugaku from the moment the universe began, we still wouldn’t have completed such calculations. Dr. Ido devised a way to calculate this in a realistic timeframe without losing the essence of strongly correlated electron systems.” He freely praises Dr. Ido’s achievements (Photo 2).

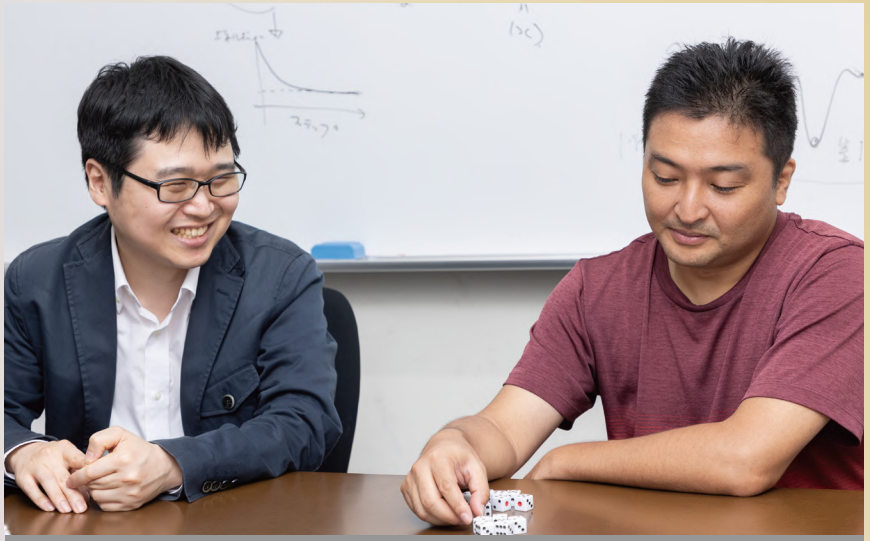


Photo 2 : Reflecting on the development of mVMC -- Drs. Ido and Misawa

Achieving Significant Results Using mVMC

In April 2022, Dr. Ido and his team issued a press release announcing their achievement of elucidating the unique properties of a quantum spin liquid that arises in organic solids using mVMC. Organic solids are materials in which organic compounds are regularly arranged. If the constituent organic compounds are complex molecules, the resulting organic solid will also have intricate structures. For instance, the organic solid $Pd(dmit)_2$ salt, which was the focus of this study, is composed of alternating layers of a metal complex layer ($Pd(dmit)_2$) and a cation layer (Fig. 2a). By altering the compounds in the cation layer, a transformation has been observed experimentally from a magnetic phase with ordered electron spin arrangements to a quantum spin liquid phase where the spin orientation remains undetermined.

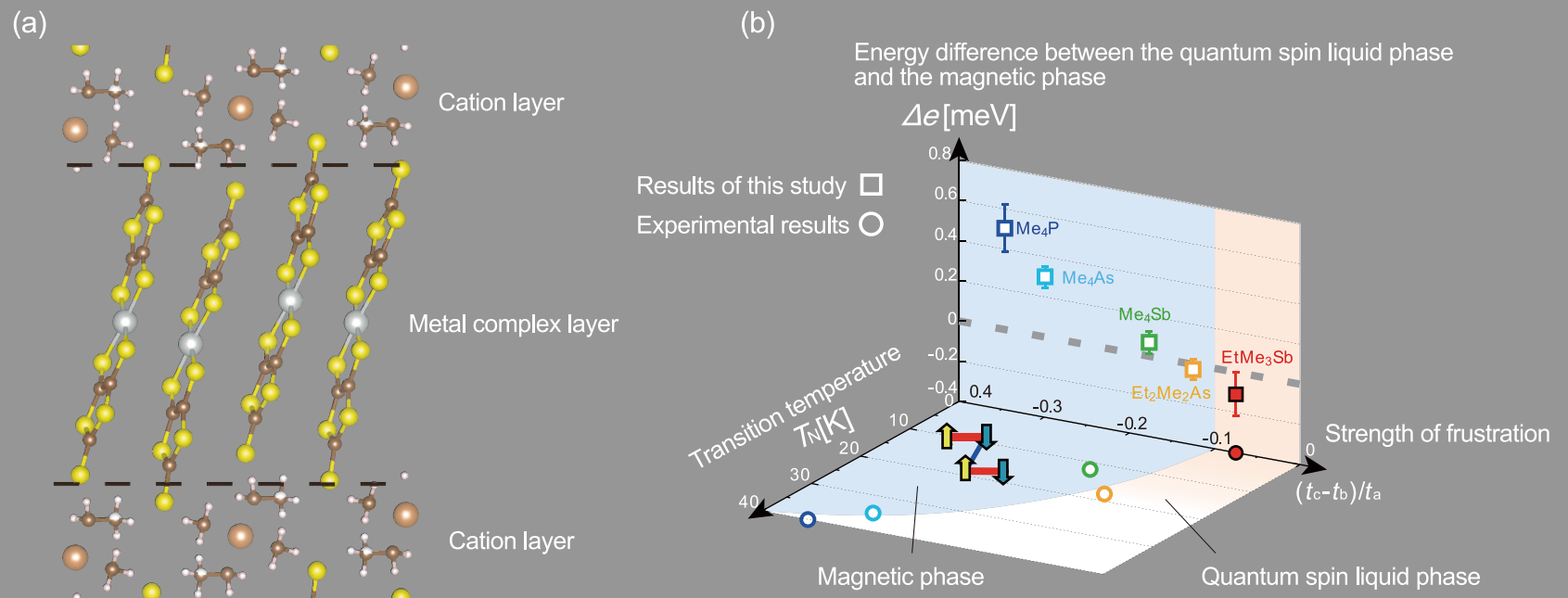


Fig. 2 : Expanded crystal structure of organic solid $EtMe_3Sb[Pd(dmit)_2]_2$ (a) and phase diagram of organic solid $Pd(dmit)_2$ salts (b)

(a) Crystal structure of the organic solid $EtMe_3Sb[Pd(dmit)_2]_2$, which is one of the $Pd(dmit)_2$ salts. The structure consists of alternating layers of the cation layer of $EtMe_3Sb$ and the metal complex layer $[Pd(dmit)_2]_2$. Here, Et stands for ethyl, Me for methyl, Sb for antimony, Pd for palladium, and dmit for 1,3-dithiole-2-thione-4,5-dithiolate. In the metal complex layer, two dmit molecules surround Pd (gray spheres).

(b) The vertical panel illustrates the dependence of the energy difference between the quantum spin liquid phase and the magnetic phase (vertical axis), calculated in this study, on the strength of frustration among electron spins (horizontal axis). When the value on the vertical axis is negative, the quantum spin liquid phase is realized. The lower panel plots the relationship between the temperature (transition temperature) observed in experiments for the onset of the magnetic phase and the strength of frustration. The blue and orange shaded regions indicate the experimentally observed regions where the magnetic phase and the quantum spin liquid phase appear, respectively. The color coding in the vertical panel is an extension of the color coding in the lower panel. Me_4P, Me_4As, Me_4Sb, Et_2Me_2Sb and $EtMe_3Sb$ are cation molecules present in each of the organic solid $Pd(dmit)_2$ salts. Changing the cation molecules results in variations in the plotted data. Only $EtMe_3Sb[Pd(dmit)_2]_2$ highlighted in red exhibits a quantum spin liquid, successfully reproducing experimental results

Source: Ido, K., Yoshimi, K., Misawa, T. and Imada, M. Unconventional dual 1D–2D quantum spin liquid revealed by ab initio studies on organic solids family. *npj Quantum Mater.* 7, 48 (2022). https://doi.org/10.1038/s41535-022-00452-8

Quantum spin liquids, known for exhibiting strong quantum entanglement[*2], are currently drawing attention due to potential applications in quantum computing. In the case of $Pd(dmit)_2$ salt, it was speculated that changing the type of cation layer would alter the frustration[*3] between electron spins and destabilize the electron spins responsible for the magnetic properties of the metal complex layer, leading to the emergence of a quantum spin liquid. However, the precise conditions and characteristics of this phenomenon remained largely unknown.

To address this, Dr. Ido's team selected five different types of $Pd(dmit)_2$ salts and conducted calculations using mVMC. By reproducing the structures of electrons within the substance on a computer, they clarified the conditions under which a quantum spin liquid appears. Their findings aligned with existing experimental results (Fig. 2b). Furthermore, a closer examination of the properties of the quantum spin liquid provided novel insights that could contribute to the development of quantum devices.

Aiming for Further Advancement of the Software

"In various fields, mVMC has been selected for the award, so I want to further develop mVMC in a way that lives up to the honor of the award," says Dr. Ido. He is already advancing the sophistication of mVMC. In fact, in the aforementioned press release study, artificial neural networks were employed during the optimization of trial wave functions. As a result, computational accuracy improved, leading to plans for integrating artificial neural network capabilities as a standard feature in the publicly available mVMC.

Furthermore, including the research described in the press release, they have previously focused on solving only the lowest-energy ground state as the wave function. However, experimental methods for understanding the electronic structure often involve irradiating materials with light or neutrons to gain information about excited states (states with higher energy than the ground state). To elucidate electronic structures through comparison between experiments and simulations, it's crucial to be able to compute excited structures of electrons. Therefore, enabling the representation of excited structures of electrons is a major future goal for Dr. Ido, and he's working on this challenge within a project (hp230213) of the Program for Promoting Research on the Supercomputer Fugaku for fiscal 2023.

In simulations of quantum condensed matter physics, researchers represent their target materials using Hamiltonians and solve the Schrödinger equation. Given that mVMC can flexibly represent electronic structures, it's applicable not only to the quantum spin liquid highlighted in the press release, but also to various strongly correlated electron systems. Additionally, since it's easy to input information about the target material, several research groups, both domestically and internationally, have already started using mVMC. Moreover, as Dr. Misawa points out, "You don't need a supercomputer like Fugaku to run this software. What matters is how you write a Hamiltonian to employ mVMC. Even with a small number of electrons, there's ample potential for revealing interesting phenomena."

Drs. Ido and Misawa have built upon the foundation laid by their predecessors, nurturing mVMC into an application that's freely available to many researchers. It's poised to continue blossoming with further improvements in performance and being employed on numerous computing platforms, not just within HPCI, contributing significantly to the field of quantum condensed matter physics.

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*1 Current affiliation: Waseda Research Institute for Science and Technology, Waseda University/ Faculty of Science and Technology, Sophia University
*2 Strong coupling phenomenon between two micro-particles. When the state of one is determined, the state of the other is also determined.
*3 Phenomenon in which the arrangement of electron spins becomes unstable due to the crystal structure.

About the
Researcher

“Even my hobbies are a form of research,” Dr. Ido says. He constantly juggles multiple research projects, finding diversion in some of them as a way to take a break. “If something seems interesting, even if there’s a high barrier, it becomes a way to unwind. When things go well, there’s that feeling of ‘Yes!’” During his student days, he never intended to become a researcher. It was with a light-hearted approach that he got involved in challenging simulation techniques to learn some technical skills before entering the workforce, and he got completely hooked. That passion from those days still burns bright, continuously driving him, and it’s what led to the development and achievements we’ve discussed here.

Associated Research Projects:

- AI numerical spectroscopy for analyzing emergent structures of quantum entanglement in correlated quantum materials (hp230213)
  Principal Investigator: Youhei Yamaji, National Institute for Materials Science
- Basic Science for Emergence and Functionality in Quantum Matter - Innovative Strongly-Correlated Electron Science by Integration of Fugaku and Frontier Experiments - (hp200132/ hp210163/ hp220166)
  Principal Investigator: Masatoshi Imada, School of Engineering, Waseda Research Institute for Science and Technology, Waseda University

Developing Generative AI Methods for a Secure, Safe, and Convenient Society with Fugaku

Rio Yokota
Professor, Global Scientific Information and Computing Center, Tokyo Institute of Technology

As of 2023, the proliferation of Generative AI is accelerating in Japan. Major IT companies such as Microsoft and Google in the United States have been aggressively investing substantial funds a few years prior to this, intensifying the competition in development. In this context, Dr. Yokota's research group is advancing the research and development of generative AI methods using the supercomputer Fugaku.

What is Generative AI?

Generative AI refers to Artificial Intelligence (AI) that generates new content such as text, images, audio, and videos based on input data. In contrast to traditional AI, which learns from given data to perform tasks like classification and detection, generative AI stands out for its ability to apply learned knowledge to generate images or text. Particularly noteworthy are “language-generative AI,” which produces fluent text, and “image-generative AI,” which creates images based on input text. OpenAI, an AI startup based in the United States, gained significant attention in November 2022 with the release of ChatGPT, a language-generative AI.

Generative AI generates text and images using a “model” that represents relationships between data. While there are various methods for constructing models, they often involve training on a large amount of labeled data, known as training data (e.g. a set of labels like “dog” and corresponding images of dogs). Deep learning requires training of layered connections of an artificial neural network, which models neural circuits in the brain, to input and learn from data. Such neural networks are commonly referred to as a “model.” For example, those used for image classification are called vision models, while those for language tasks are referred to as language models.

“In the past, people trained different models for tasks such as image classification, anomaly detection, summarizing text, and automatic translation. However, recently it has become common to train a single large model on various modes of data and then fine-tune it for different tasks. This approach, involving extensive training on a large dataset inadvance, is called ‘pre-training’,” Dr. Yokota explains.

Improving the Performance of Image Classification Models through Pre-training with Synthetic Images

The first challenge undertaken by Dr. Yokota and his team with Fugaku was the pre-training of image classification models. Dr. Yokota points out that the development of image classification models involves numerous challenges. “The performance of the model tends to increase empirically with the amount of data used in pre-training. For image classification models, it is necessary to input a large quantity of image data as training data. However, the task of collecting and labeling image data posted on the internet is inherently advantageous for companies operating search engines, such as Google. While Google has created several image datasets, they are not accessible to researchers from other companies or academia, posing a significant barrier to the advancement of image processing,” Dr. Yokota explains.

To overcome this situation, Dr. Yokota and his team took on the challenge of large-scale pre-training of image classification models using synthetic images. “Research on synthetic images was initially pioneered by the team at the National Institute of Advanced Industrial Science and Technology (AIST)*1. However, the scale of their work was relatively small. Therefore, in 2021, we started creating a large-scale dataset of synthetic images using only formulas, and in the 2022 Fugaku General Access (Super Large Scale Pre-training of Vision Transformers Using Synthetic Images, hp220028), we conducted pre-training of image classification models on Fugaku,” Dr. Yokota says.

The distinctive feature of Dr. Yokota’s synthetic images is that they are created solely using formulas without the use of real images, depicting

images such as fractals (Fig.1). Using this dataset of 21 million synthetic images, they performed pre-training on an image classification model called “Vision Transformer.” The effectiveness of this pre-training was nearly equivalent to the results obtained by Google when using their own dataset of 300 million real images. Furthermore, when compared to the commonly used real image dataset “ImageNet-21k” for pre-training (approximately 14 million images), their synthetic image dataset showed higher learning effectiveness. Dr. Yokota reflects on the success, stating, “The effectiveness of synthetic images in pre-training has been validated, giving us significant confidence.”

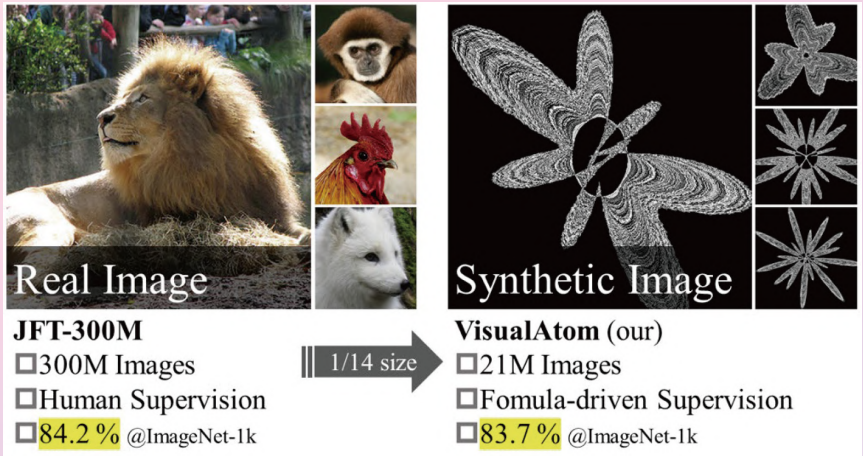

Fig 1 : Real vs. synthetic images
On the left are examples of real images, while on the right are examples of synthetic images. The learning effectiveness of the Vision Transformer using the JFT-300M dataset (Google’s private dataset of approximately 300 million real images) is shown, achieving an image recognition accuracy of 84.2%. The learning effectiveness using Visual Atom (the set of 21 million synthetic images created by Dr. Yokota and his team) is 83.7%, which is nearly equivalent. The “@ImageNet-1k” indicates the result of fine-tuning the pre-trained model on a small dataset of real images called ImageNet-1k.

Dr. Yokota highlights four advantages of synthetic images. The first is the ability to generate an unlimited quantity, the second is the absence of copyright concerns, the third is the lack of need to consider personally identifiable information, and the fourth is the avoidance of societal biases related to gender, race, etc.

“Currently, the internet is filled with biased images. For instance, if you search for ‘nurse,’ you might predominantly find images of women, creating gender biases based on professions. The use of such real images in pre-training poses significant problems. However, synthetic images completely sidestep these issues,” Dr. Yokota explains.

However, a question arises: Can synthetic images, which may not immediately convey their meaning, achieve the same learning effectiveness as real images? Yokota’s response to this question is intriguing: “This can be understood by comparing it to a fetus inside the mother’s womb. The fetal optic nerves react to light even within the mother’s womb. The fetus likely perceives vague shapes and forms even before birth. The rapid recognition of shapes after birth is attributed to the pre-training on light that occurred in the womb. In other words, synthetic images can be likened to what the fetus experiences as light inside the womb.”

Establishing the Research and Development Environment for AI with Fugaku

Why did Dr. Yokota choose Fugaku, which has all CPU nodes and no GPUs, for this large-scale pre-training? He explains: “Certainly, for deep learning, GPUs offer faster computational speed and are more suitable than CPUs. In fact, the ABCI supercomputer specialized for AI at AIST uses GPUs. However, Japanese AI researchers are flocking to ABCI, resulting in overcrowding and shortage of resources. Therefore, we

wanted to enable AI research and development even on supercomputers with only CPUs. Additionally, for the large-scale pre-training we conducted this time, having a large number of nodes available for an extended period was more important than computational speed. In this regard, Fugaku had a significant advantage in the allocated computational resources compared to ABCI (Fig. 2)."

On the other hand, Dr. Yokota acknowledges the challenges he faced with Fugaku as it was not originally designed for AI research and development. He explains, "First of all, the software infrastructure for performing deep learning quickly was not in place, and we had to develop it from scratch. When loading a large amount of image data, individually reading each image could impose a burden on input/output operations. Therefore, we implemented strategies such as compressing a large amount of image data into a single file to reduce input/output frequency. Additionally, to reduce memory consumption, we developed a new method for distributed parallel processing of image data and models. While we faced various challenges, this will enable many researchers to accelerate AI research and development using Fugaku in the future."

Fig 2 : Fugaku, left, and AIST's AI-devoted ABCI
The processing speed of one GPU on ABCI, specialized for AI, is 50 times that of one CPU on Fugaku. However, while ABCI has 4,000 GPUs, Fugaku boasts a massive 160,000 CPUs. Therefore, in a simple calculation, using all the CPUs on Fugaku would allow for computational capabilities nearly equivalent to ABCI. Furthermore, if Fugaku can be utilized for longer durations than ABCI, it holds a significant advantage

The Essential Need for the Development of Generative AI Methods

Building upon these achievements, Dr. Yokota has embarked on a new project, the Government-Initiated Category of Supercomputer Fugaku (Development of Distributed Training Method for Large Language Models on Fugaku, hp230254). In this project, a collaborative research team comprising the Tokyo Institute of Technology, Tohoku University, Fujitsu, RIKEN, CyberAgent, Kotoba Technologies, and Nagoya University aims to develop methods for large-scale distributed parallel processing on Fugaku to efficiently train large language models (models used in language generative AI).

“In the United States, massive investments are being made in generative AI. For instance, ChatGPT surpassed 100 million users in just two months, becoming an internationally adopted societal infrastructure. Given this situation, some argue that it may be too late to develop generative AI methods as we are already playing catch-up. However, the development of generative AI is primarily undertaken by startup companies, and there are concerns about the continuity of their businesses. Relying on such companies entails high risks. Additionally, generative AI is a foundational technology for Society 5.0*2, and it will be present in various fields such as healthcare, industry, and education. This is not a discussion about entering a specific industry after determining its ‘advantage.’ Just as Japan developed power and transportation networks during the high economic growth period not because Japanese power lines and road technologies had a global ‘advantage,’ but because investments in infrastructure with overwhelming productivity were imperative. Failure to invest in such infrastructure can have a devastating impact on the international competitiveness of the industries built on it,” Dr. Yokota emphasizes.

“As generative AI is expected to be widely utilized in various industrial sectors in Japan in the future, investments in computational resources, the accumulation of technical expertise and knowledge in AI, and the cultivation of advanced AI talent are becoming increasingly crucial,” he adds.

Aiming for Generative AI Capable of Handling Both Images and Language

Furthermore, Dr. Yokota and his team are actively involved in the development of generative AI itself. In the 2023 Fugaku General Access (Performance Optimization of Transformers and Their Application to Vision & Language, hp230119), they are working on optimizing the performance of Transformer on the A64FX processor developed by Fujitsu for Fugaku to make it capable of handling both images and language. Transformer is the neural network architecture that served as the basis for the Vision Transformer described above.

“Image generative AI creates images based on text input. Images and language do not exist independently; both need to be learned. Therefore, we aim to develop a high-performance generative AI that can handle both images and language. The goal is to develop a generative AI that can generate correct images, not just amusing misinterpretations like a ramen bowl in the shape of a house, as seen in the ‘Family Ramen’*3 image (Fig. 3),” Dr. Yokota says with a smile.

Amusing images created by generative AI, not limited to family ramen, often appear on social media, becoming popular topics. Dr. Yokota points out, “The misunderstanding arises not because generative AI does not understand Japanese correctly, but because it lacks knowledge of Japanese culture and trends. In the future, we aim to develop generative AI that can accurately respond to Japanese society, not just the Japanese language.”

In the future, with the development of generative AI capable of

Fig 3 : Image of “Family Ramen” created by generative AI
(Note: This image is not the actual image posted on social media.)

handling both images and language, it will become possible, for example, for a cooking robot equipped with a camera to convert image data obtained through the camera into words. The robot can then ask the generative AI what to do next, and the generative AI responds. This enables the robot to autonomously cook without pre-instruction, bringing us closer to a society where such interactions are common.

Addressing the Growing Issue of Fake News, Regulation Is Crucial

In pursuing these challenges, Dr. Yokota and his team are advancing the development of generative AI methodologies while collaborating with other research groups in the country. However, as robots equipped with generative AI become more autonomous, capable of making judgments and taking actions without human intervention, some people may harbor concerns and fears. In response, Dr. Yokota says, “One thing I fear is the spread of fake images created by generative AI. Deepfakes in particular pose a significant problem. Deepfake is a portmanteau of ‘deep learning’ and ‘fake,’ originally a technology used in the film and gaming industries that has become widely accessible and is now being maliciously exploited for fake news and information manipulation. Consequently, leaders from various countries are convening conferences to discuss regulations.”

Indeed, during the G7 Hiroshima Summit held in May 2023, the creation of the “Hiroshima AI Process” was included. This framework aims to promote international rule-making regarding the use and development of generative AI, as well as its regulation, with a focus on technologies like ChatGPT. Furthermore, in November 2023, the world''s first international conference on the safe use of AI, the “AI Safety Summit,” took place in the U.K. High-ranking officials from governments, major AI companies, and leaders discussed the risks associated with the potential misuse and uncontrollable nature of advanced AI.

“In addition to these high-level meetings for regulations, I believe it is essential to hold gatherings that involve AI researchers and technologists. Through ongoing research and development of generative AI, I hope to contribute to the realization of a future society that is secure, safe, and convenient,” Dr. Yokota adds.

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*1 Reference for synthetic image creation and image distinction mechanism through pre-training on synthetic images (Japanese only): https://www.aist.go.jp/aist_j/magazine/20221130.html
*2 Society 5.0 was proposed in the 5th Science and Technology Basic Plan drawn up by Japanese government as a future society that Japan should aspire to. It envisions a human-centered society where the cyber (virtual) and physical (real-world) spaces are highly integrated, aiming to achieve both economic development and solutions to societal challenges.
*3 Family Ramen (家系ラーメン) refers to a style of ramen and a group of ramen shops often identified by names ending with “家” (“ya” or “house”). It gained the name “family” because many of these shops have “家” in their name.

About the
Researcher

Dr. Yokota was engaged in experimental research on fluid as an undergraduate student and undertook fluid simulation in his master's course. He started using GPUs for simulations during his doctoral program, when GPUs were just starting to become available. "At the time, we connected about 200 GPUs for gaming to create something like the world's cheapest supercomputer, and in 2009 we won the Association for Computing Machinery's (ACM) Gordon Bell Prize (Low Price / Performance Category)," Dr. Yokota says.

After this experience, he became seriously interested in supercomputers. He began researching machine learning using AI after arriving at Tokyo Institute of Technology in 2015, in response to his students' interest. Looking back, he says, "Although my research interests have changed, the focus on distributed parallel processing has remained consistent since my graduate school days."

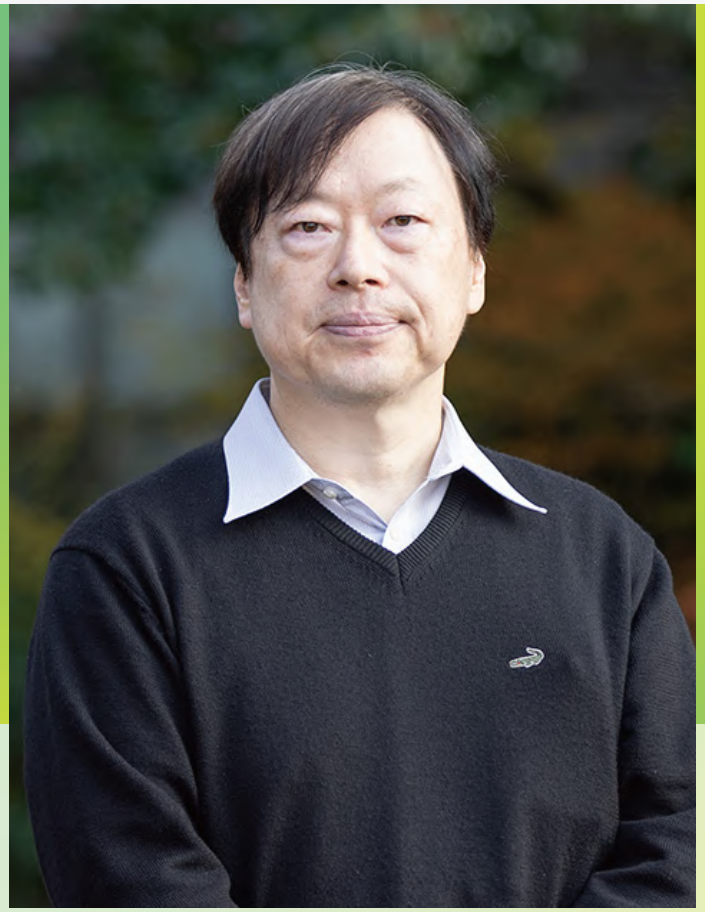
In his time off, Dr. Yokota pursues his hobbies, including diving and programming, and he is also a qualified diving instructor. "Recently I've been so busy that I haven't had time for any hobbies, so it's been a little tough," he laughs.

Associated Research Projects:

- Super Large Scale Pre-training of Vision Transformers Using Synthetic Images (hp220028)
- Performance Optimization of Transformers and Their Application to Vision & Language (hp230119)
  Principal Investigator: Rio Yokota, Global Scientific Information and Computing Center, Tokyo Institute of Technology
- Development of Distributed Training Method for Large Language Models on Fugaku (hp230254)
  Project Representative: Seiichi Shimasaki, Director of Research Promotion Bureau, Ministry of Education, Culture, Sports, Science and Technology (MEXT)

Challenging Decarbonization: Next-Generation Ammonia Fuel

Contributing to Burner Design through Ammonia Combustion Simulation



Yukihiko Okumura
Professor, Faculty of Engineering and Design, Kagawa University

Because ammonia does not emit carbon dioxide when burned, attention is turning to its potential as a fuel for achieving carbon neutrality by 2050. However, ammonia is generally a difficult substance to burn, and forcibly combusting it may result in the emission of harmful NOx exceeding environmental standards. To address these challenges through combustion methods, Dr. Yukihiko Okumura from Kagawa University is advancing research through a dual approach of experimentation and simulation. Obtaining insights unique to simulations that cannot be gained through experiments alone, Dr. Okumura arrived at a “tornado burner” that safely and efficiently burns pure ammonia.

Ammonia Fuel: More Cost-Effective and Energy-Efficient than Hydrogen

With an eye on achieving carbon neutrality by 2050, a movement is arising to realize a hydrogen society. Therefore, a method has been developed in which hydrogen (H_2) is converted into ammonia (NH_3) and transported from overseas, after which the hydrogen is extracted from the ammonia and used. This is done to transport hydrogen, which liquefies at minus 253°C, in a cost-effective and energy-efficient manner. However, Dr. Okumura, explaining the motivation for ammonia burner research, says, “Rather than extracting hydrogen from ammonia and using it as hydrogen fuel, burning ammonia itself allows us to obtain high calories without energy loss. Using additional energy for extracting the hydrogen is also unnecessary.”

However, ammonia is a fire-resistant substance that does not easily ignite even when exposed to flame. Additionally, forcibly burning it releases harmful nitrogen oxides (NOx). National environmental standards stipulate that “NOx emissions should be 150ppm or less for boilers and 600ppm or less for gas engines.” That is why, in 2017, Dr. Okumura began researching how to efficiently combust ammonia with minimal NOx emissions. Three years later, the Japanese government selected Hydrogen/Fuel Ammonia Industries as one of 14 fields in its Green Growth Strategy*1 in December 2020. Reflecting on the time he started studying ammonia combustion, Dr. Okumura says, “Finding a way to use inherently difficult-to-burn ammonia as fuel was a challenge itself. Little was known about ammonia combustion at that time.”

Having conducted combustion research on various substances since his student days, Dr. Okumura believed that understanding the combustion mechanism and flame structure of ammonia was crucial for developing an ammonia burner. Therefore, he decided to pursue combustion research using both experimentation and simulation.

Simulation of Ammonia Combustion

To burn ammonia, a mixed combustion method is commonly used that involves co-burning it with methane (CH_4), the main component of natural

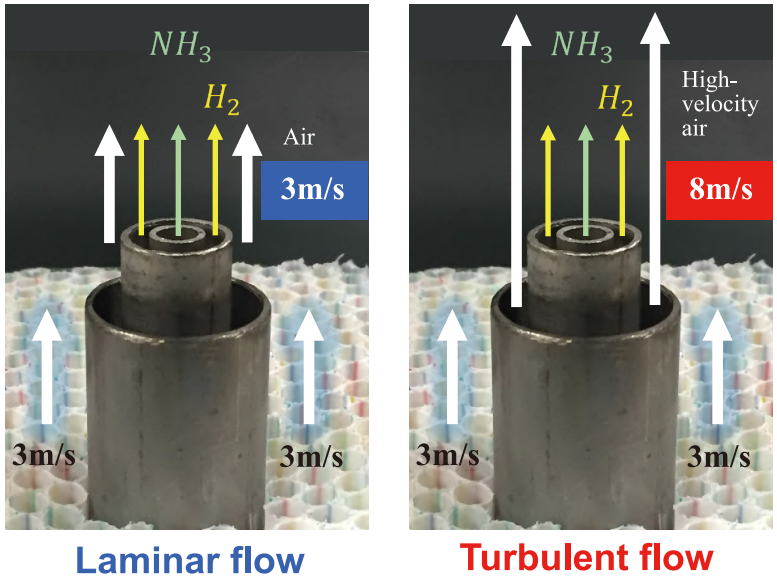


Fig.1 : Ammonia burner used in the research

The space between rims blows out ammonia, hydrogen and air. In the right diagram, turbulence is created by high-speed air (8m/s) flowing faster than ammonia and hydrogen. Generally, turbulent flow results in higher combustion efficiency per unit volume than laminar flow. To streamline the flow around the rim, students in the Okumura Laboratory laid cut straws and directed air at 3m/s. As a result, the calculation of the surrounding airflow was simplified.

gas. However, burning methane produces CO_2 emissions. So Dr. Okumura initiated research on a burner with hydrogen flame stabilizer to assist in the combustion of ammonia using hydrogen gas (Fig. 1). He designed and fabricated the burner so that it could create both laminar flows, in which the flame calmly rises, and turbulent flows, where the fuel is forcibly mixed with high-velocity air and becomes turbulent flame, by adjusting the amount of air sent along with the combustion gas. This allowed him to conduct experiments and simulations under the same conditions.

In experimental studies, temperature was measured at various locations in the flame. Gas measurements were also taken to determine the amounts of major chemical species (H_2, O_2, N_2, NH_3, NOx, H_2O) at those locations. Meanwhile, simulation studies utilized fluid dynamics software called “Advance/frontflow/red” to calculate in detail the distribution and reactions of all chemical species including radical species within the flame, determining how temperature changes with the progression of reactions.

No.	Reaction formula
1	$NH_3 \Leftrightarrow NH_2+H$
2	$NH_2+H \Leftrightarrow NH+H_2$
3	$NH_3+H \Leftrightarrow H_2+NH_2$
4	$NH_3+OH \Leftrightarrow H_2O+NH_2$
5	$NH_3+O \Leftrightarrow NH_2+OH$
6	$NH_3+HO_2 \Leftrightarrow NH_2+H_2O_2$
7	$NH_2+O \Leftrightarrow HNO+H$
8	$N+OH \Leftrightarrow NO+H$
9	$N+O_2 \Leftrightarrow NO+O$
10	$N+NO \Leftrightarrow O+N_2$

No.	Reaction formula
11	$NH_2+NH \Leftrightarrow NH_3+N$
12	$NH+NH \Leftrightarrow NH_2+N$
13	$NH_2+NH_2 \Leftrightarrow NH_3+NH$
14	$NH_2+NH_2 \Leftrightarrow N_2H_4$
15	$NH_2OH+H \Leftrightarrow HNOH+H_2$
•	•
•	•
•	•
202	$NO_3+OH=NO_2+HO_2$
203	$NO_3=NO+O_2$

Fig. 2 : Example of elementary reaction equations for ammonia combustion

The study utilized CRECK’s reaction mechanism (31 chemical species, 203 reaction equations).

The chemical reaction for ammonia combustion can be expressed as $4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O$, which is an equation summarizing all the reactions. In fact, within the flame, highly reactive and unstable radicals are produced, changing into other chemical species. There are 31 related chemical species and 203 reaction equations (Fig. 2). Considering all of them is crucial for understanding the details of combustion. Furthermore, the reactions with hydrogen and the surrounding air and flow fields also add complexity to the overall flame picture.

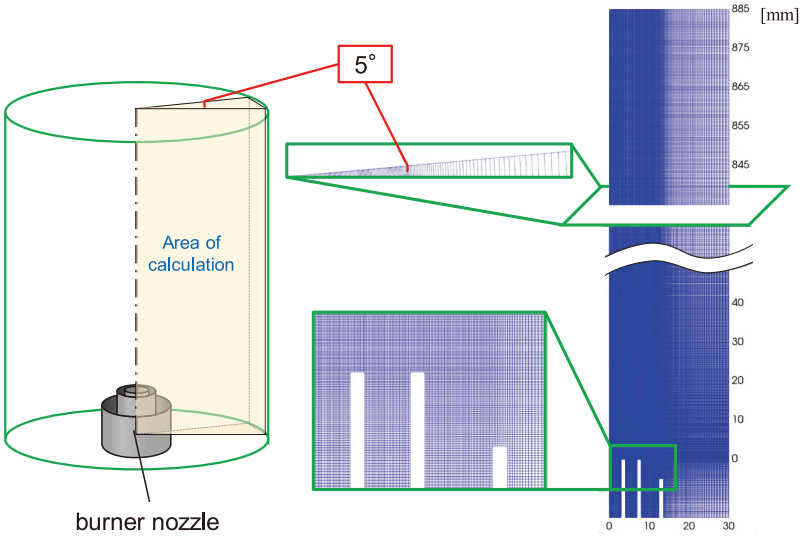
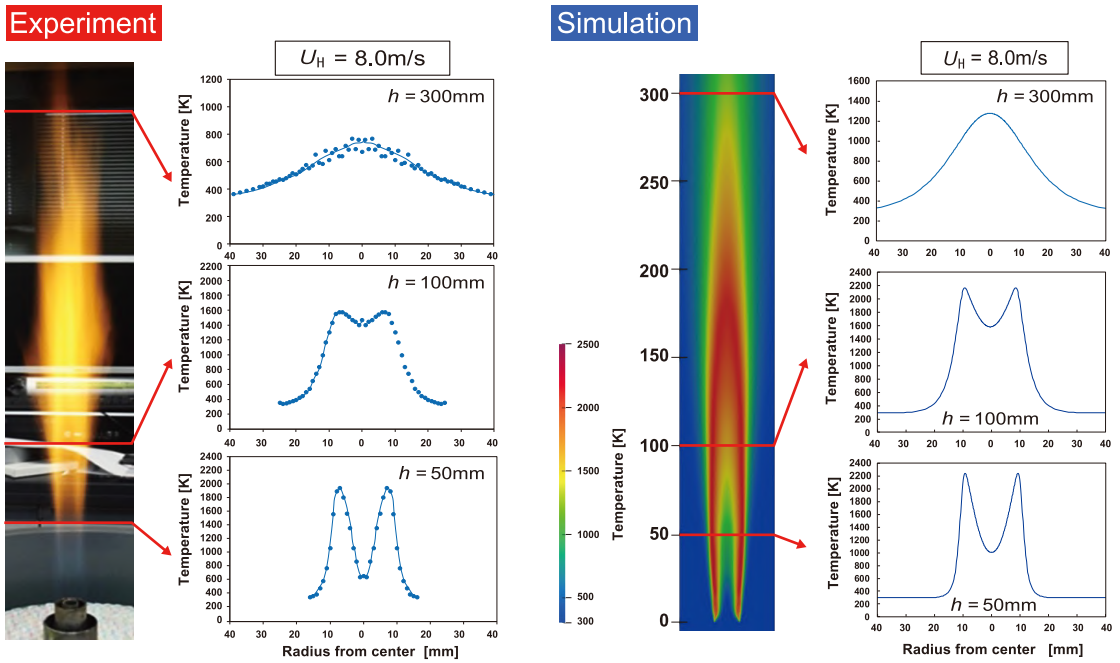


Fig. 3 : Simulation of a laboratory-scale ammonia burner

The area near the gas outlet (rim) employs a fine mesh with 0.1mm squares, while the part away from the rim is coarsely divided to reduce computational load. Assuming axial symmetry, the calculation range covers only 5 degrees rather than the entire circumference.

Fig. 3 - Fig. 6 : Reprinted from the Journal of the Combustion Society of Japan, Vol.64 No.208 (2022) 168-176, “Flame Structure and Reaction Analysis for Ammonia Turbulent Burner with Hydrogen Flame Stabilizer,” Okumura, Y., et al., with permission from the Combustion Society of Japan.



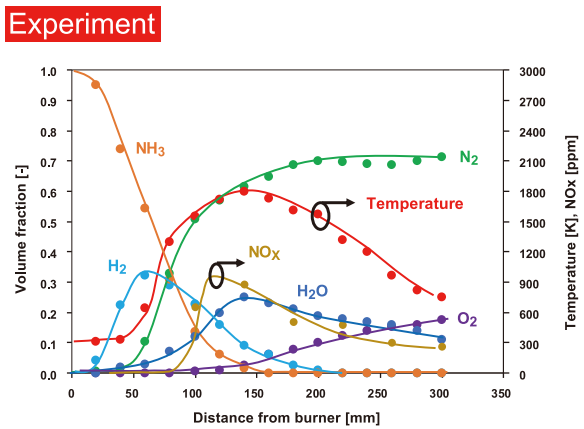


Fig. 4 : Comparison of experiment by using ammonia burner and simulation (turbulent flow)

The upper part shows the temperature distribution. The simulation closely aligns with experimental results, indicating the accuracy and precision of the simulation. The lower part illustrates the distribution of chemical species within the flame. Consistency with the simulation data is shown in the original paper. (In detail: the Journal of the Combustion Society of Japan, Vol.64 No.208 (2022) 168-176.) Although not shown here, simulations also match experimental results well for laminar flow.

"We divided the space occupied by the flame and surrounding air into a grid, solving a governing equations in reactive flow that included mass conservation, energy conservation, and momentum conservation, as well as the state equation of gases and the equation of mass conservation for chemical species (element conservation). Except for the equation of mass conservation for chemical species, this is the same as the atmospheric simulations used for weather forecasting. However, as soon as chemical reactions (elementary reaction groups) are included in the calculations, the computational load becomes enormous," Dr. Okumura says.

To reduce computational load, Dr. Okumura initially targeted laboratory-scale burners. He explored options to coarsen the grid while maintaining calculation accuracy, assuming axial symmetry and time-averaging turbulence (Fig. 3). For later turbulent calculations for the tornado ammonia burner and large burners, he transitioned to "Fugaku"-class computational resources capable of handling large-scale calculations (360° range and large spatial dimensions).

"At the beginning of the research, I had 69 elementary reaction equations for ammonia combustion. However, calculations at that

time, which used a scheme developed based on hydrocarbons, did not agree with the experimental results at all. Concurrently with my research, the elucidation of elementary reactions for ammonia combustion progressed, and the number of reactions related to ammonia increased. It was only when we included 203 elementary reaction equations that we finally obtained calculation results close to experimental results (Fig. 4). Performing calculations with 203 elementary reaction equations was made possible by the computational power of HPCI," Dr. Okumura says.

Simulation Is the Only Way to Understand the Mechanism of Ammonia Combustion in Detail

Dr. Okumura explains the simulation study strengths as follows. "There are limitations to the quantities that can be measured experimentally. Especially, it is almost impossible to determine the spatial distribution of essential radicals for combustion, such as H radicals, O radicals, and NH radicals. In contrast to that, simulation allows us to clarify reactions occurring at every location within the flame." Simulation results have revealed that OH radicals and H radicals move and mix due to turbulence, and that radicals and heat derived from hydrogen fuel particularly promote and sustain the combustion reaction of ammonia (Fig. 5).

Furthermore, Dr. Okumura believes that simulations could differentiate whether a nitrogen in a specific

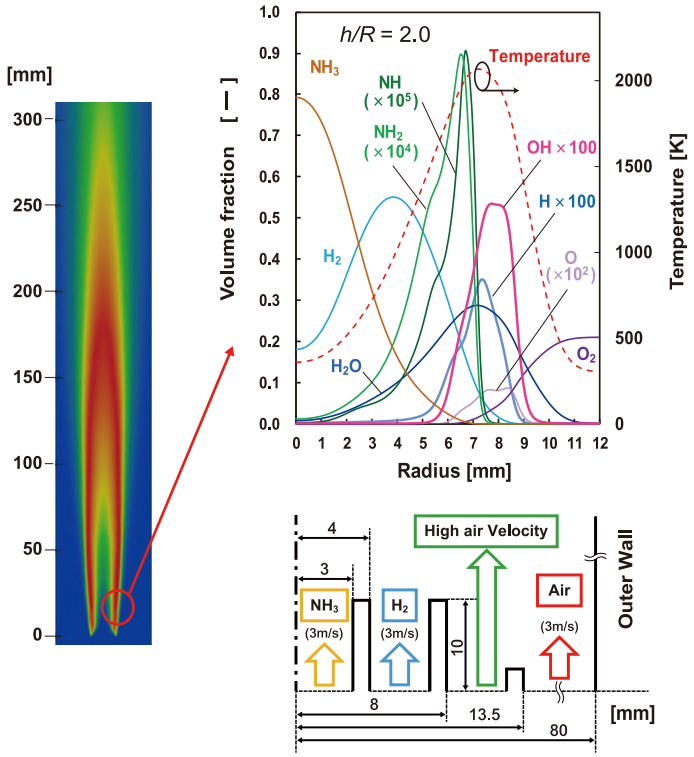


Fig. 5 : Radical concentrations in a turbulent burner with hydrogen flame stabilizer analyzed using the supercomputer "Fugaku"

At left is the temperature distribution of the flame. The upper-right graph shows the temperature and chemical species amounts at the red circle position (flame height of 14mm), and the lower-right indicates the locations where various gases are jetted. Looking at the upper-right graph, the highest temperature is observed in the region of 7<r<9 [mm] (where air is mixed), and OH radicals (pink line) and H radicals (blue line) that promote combustion reactions are generated more abundantly due to the combustion of supplementary hydrogen. In addition, the heat generated by burning hydrogen is transferred to the ammonia injection part, supplying energy to maintain the combustion chemical reactions of ammonia. The essential OH radicals and H radicals for combustion are diffused through turbulence and forcibly mixed in the region of 5<r<8 [mm], contributing to the stable maintenance of combustion.

NOx molecule formed from the air or the ammonia. He calculated the combustion process with distinguishing nitrogen atoms derived from ammonia and nitrogen molecules in the air, revealing that the majority of NOx emitted from the top of the flame into the atmosphere is derived from ammonia, with air-derived NOx existing only at the bottom of the flame and overwhelmingly minimal (Fig. 6 (1)).

Reflecting on the simulation, Dr. Okumura notes, “NOx did not reach extremely high levels.” The reason became apparent also through the simulation. Nitrogen atoms are oxidized to form NOx molecules, and they turn into N_2 molecules, when reduced. Analyzing where and how much of this oxidation-reduction reaction occurs, it was found that NOx is primarily generated in the slightly inner region of the high-temperature zone of the flame where fuel is abundant, and at almost the same location, reduction reactions also effectively eliminate NOx (Fig. 6 (2)). “It became clear that the contribution of the reduction reaction is significantly large, although the reaction rate of NOx generation is higher than that of NOx reduction. This knowledge, obtained through simulation, explains why there was no extreme increase in NOx concentration. It underscores the significance of simulation research in providing insights into reactions and flame structure,” Dr. Okumura says.

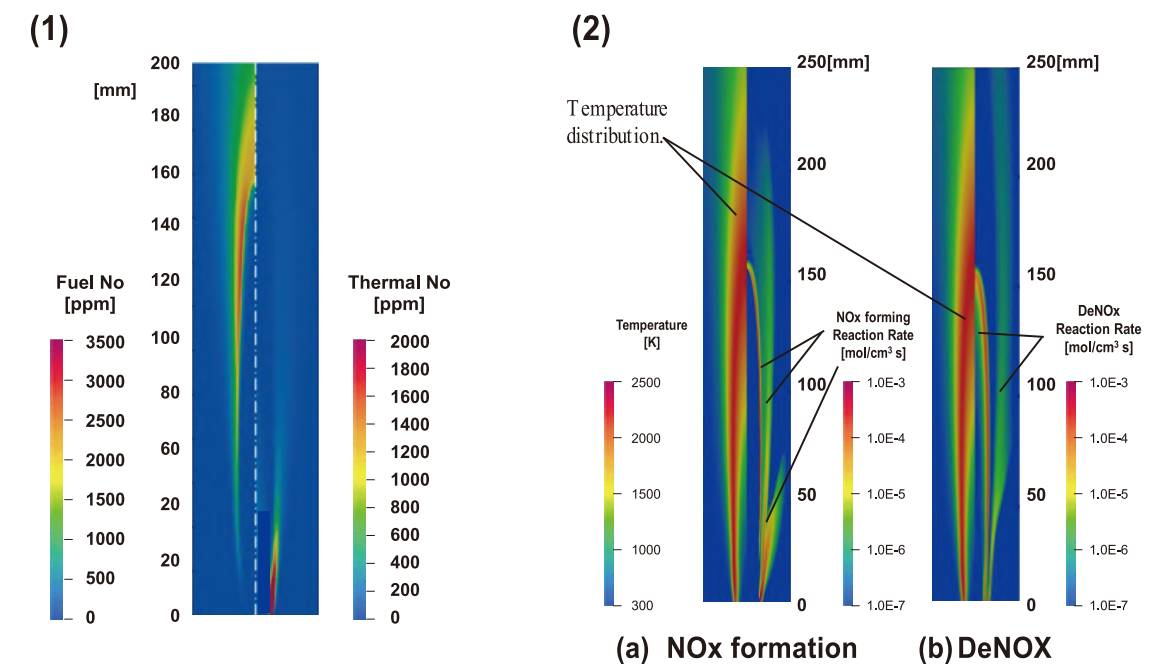


Fig. 6 : Mechanism of NOx formation

(1) The left half shows the distribution of NOx derived from ammonia (Fuel NO). The right half shows the distribution of NOx derived from nitrogen molecules in the air (Thermal NO).
(2) Reaction rates of NOx formation (a) and NOx reduction (b). NOx rapidly disappears in the region near its intense creation at a rate comparable to the formation rate.

Promoting Ammonia Burners in Industrial Settings and Achieving Carbon Neutrality by 2050

In the industrial sector, initiatives are already underway to replace burners, used in processes such as breaking down naphtha obtained from petroleum refining for plastic production and pottery kiln firing, with

ammonia burners. Dr. Okumura aims to popularize ammonia burners that can be used in industrial settings. To achieve industrial applications, it is crucial to realize ammonia combustion that meets environmental standards at low cost. Consequently, Dr. Okumura has also initiated research on an “ammonia dedicated burner,” which can combust ammonia without using expensive hydrogen.

Recognizing the importance of continuously generating active radicals to sustain ammonia combustion, Dr. Okumura devised the tornado burner. This burner releases a pre-mixed gas of ammonia and air from the bottom, and additionally injects it from the side of the cylinder, swirling the flame.

In this research, a combination of simulations using Oakbridge-CX at the University of Tokyo and experiments were employed to investigate the ratios of ammonia to air (equivalent ratio), flow velocities, and other factors for the main jet and swirling jets (Fig. 7). Successful results were achieved, showcasing the conditions for ammonia-dedicated combustion. The NOx emission level was also lowered, nearly reaching environmental standards due to the two-stage combustion method and tornado effect. Furthermore, technology has been developed to reduce unburned ammonia below environmental standards even with a large flow of ammonia injection.

Dr. Okumura emphasized the strength of experimental research in being able to cross-check simulation results, stating that experimental results are undeniable facts even if the combustion process is unstable or does not fit the theory. He highlighted the synergy between simulation and experimental research, describing them as the “two wheels” of a vehicle. Striving to introduce ammonia burners for industrial use promptly, Dr. Okumura is accelerating the research, leveraging both aspects. He expressed his aspirations, saying “My combustion technology (ammonia dedicated burner) has come very close to completion and I hope my technology will contribute to achieving carbon neutrality by 2050.”

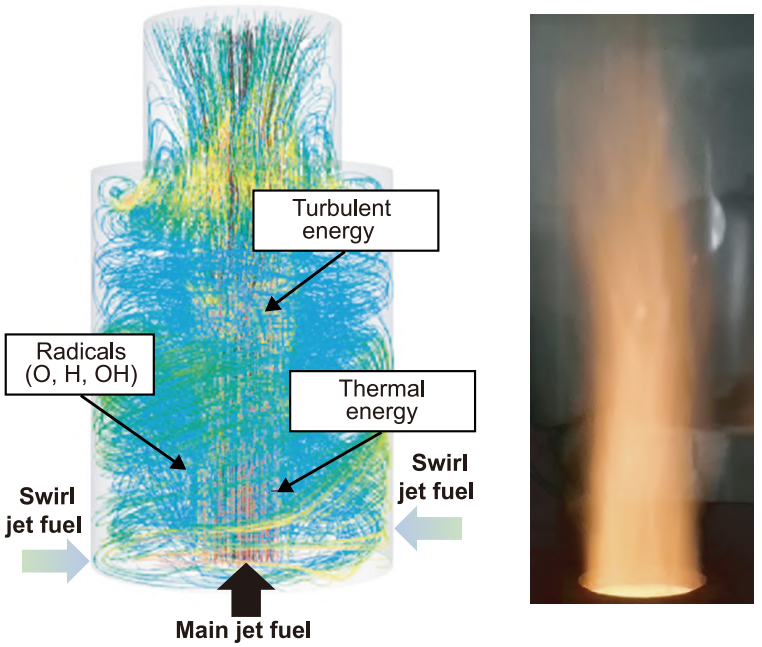


Fig. 7 : Simulation and actual combustion of tornado ammonia dedicated burner

The tornado burner enables combustion of the flame-retardant ammonia without the need for hydrogen. Simulation results revealed that the main jet and swirling jet mutually supply thermal energy, turbulent energy, and radicals. Numerous improvements have been made to the presented burner, bringing it closer to meeting the exhaust characteristics that comply with environmental standards.

*1 : Abbreviation for “Green Growth Strategy through Achieving Carbon Neutrality by 2050.” This refers to Japan’s industrial policy to connect the challenge of achieving “Carbon Neutrality by 2050” announced in October 2020 with the “virtuous cycle of the economy and the environment.” Among the 14 sectors expected to grow is the Hydrogen, Fuel Ammonia Industry.
https://www.meti.go.jp/english/policy/energy_environment/global_warming/ggs2050/index.html

About the

Researcher

Dr. Okumura is a longtime science enthusiast, having enjoyed experimenting since he was a child. He was fascinated by experiment kits that came with science magazines, often contemplating questions like, “Why does burning charcoal glow a bright orange color? Why does it keep burning?” Growing up during the period of Japan’s high economic growth, Dr. Okumura questioned environmental aspects, wondering, “Is it okay to emit so much CO_2? Can forests alone absorb it? Is the Earth large enough to dilute all this CO_2? Is it acceptable to leave Osaka’s rivers with their unpleasant odor and stagnation as they are?” With such thoughts, he chose to major in comprehensive energy engineering, focusing on research into combustion that does not produce pollutants. As he matured, Dr. Okumura learned about the adverse global effects of indiscriminate CO_2 emissions and, considering industrialization, dedicated himself to the research of CO_2-free burners. The background to his research approach reflects his childhood aspirations.

Associated Research Projects:

- Development of CO_2-free combustor for high intensity combustion and NOx reduction with simultaneous function (hp200033)
- Development of ammonia burner for high intensity combustion and NOx reduction with simultaneous function (hp200176)
- Optimization design of ammonia burner for CO_2-free combustion (hp210108)
- Optimization design of ammonia burner for a carbon-free society (hp220009)

Principal Investigator: Yukihiko Okumura, Kagawa University

You can watch the videos of the interviews featured in this booklet.

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