AsianScientist

Issue 11
January 2022

SUPERCOMPUTING ASIA

POWERING THROUGH THE PANDEMIC WITH SUPERCOMPUTERS

TURNING THE TIDE WITH AI AND HPC

AVERTING ASIA'S WATER CRISIS

SUPERCOMPUTERS TO THE RESCUE

SECURING BETTER FUTURES IN A CHANGING WORLD

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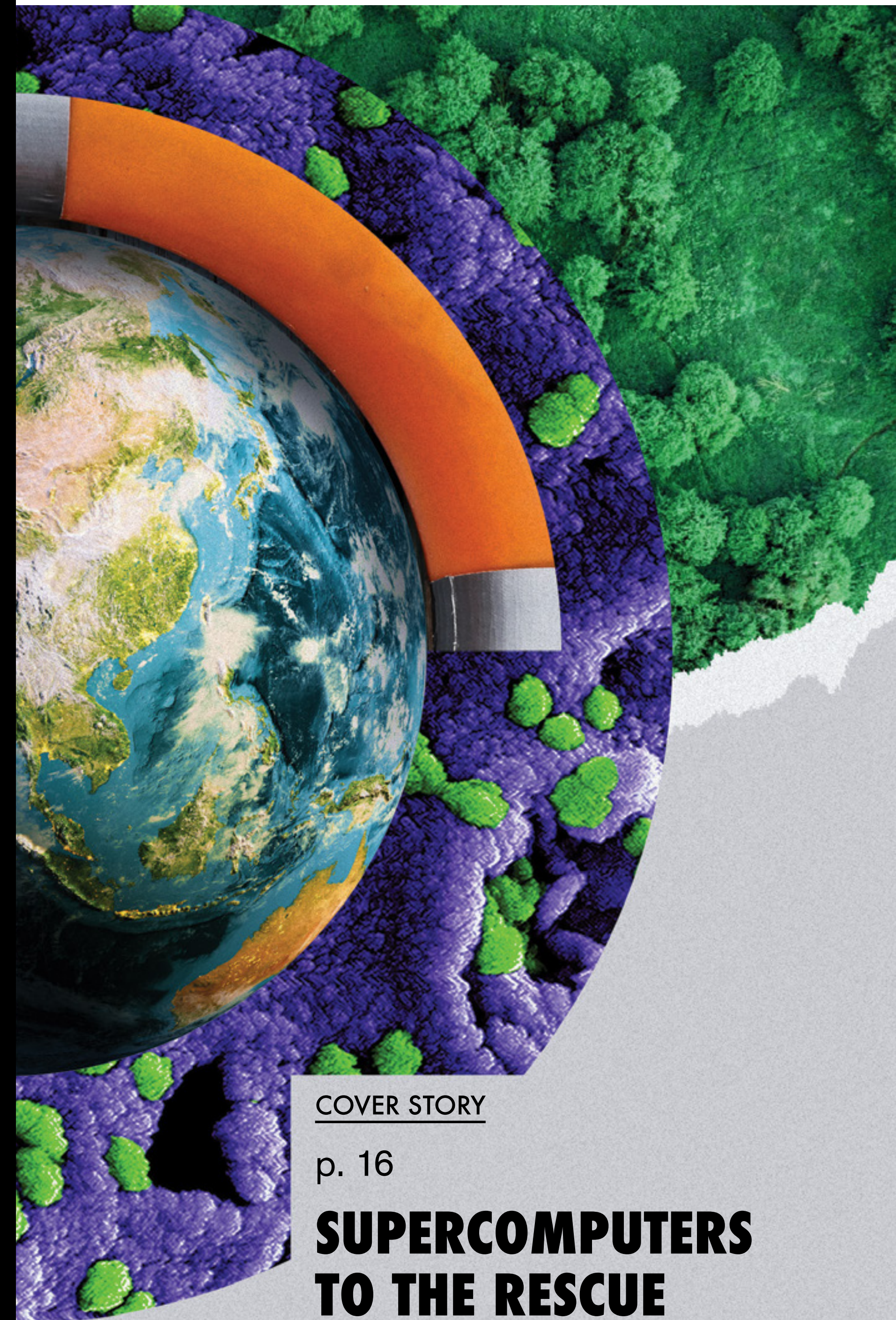

COVER STORY

EDITOR'S NOTE

The year 2021 has been defined by the new realities presented by COVID-19 and the mounting climate crisis. As we turn to 2022, we are proud to highlight the remarkable scientists in Asia who have risen to face these global challenges with human ingenuity and grit.

Harnessing the power of high performance computing (HPC), these brilliant minds have found solutions to some of the biggest challenges facing humanity.

In the cover story (*Supercomputers To The Rescue*, p.16), find out how Singapore is bolstering its efforts against the current pandemic and future outbreaks using HPC tools.

Asia also faces many climate issues that supercomputers are poised to address. Read about how scientists from Japan are taking real-time tsunami predictions to the next level, through combining artificial intelligence and HPC (*Turning the Tide with AI and HPC*, p.22).

Rivers and seas are lifelines for many communities in Asia; however, the region is facing an escalating water scarcity crisis due to rapid urbanization and declining freshwater sources. In *Averting Asia's Water Crisis* (p.28), we showcase the potential of exascale computing to uncover better ways of treating water and monitoring its flow.

Rounding out this issue, we acknowledge gender disparities in the scientific system. Against this backdrop, we hear from the women who beat the odds to make a mark in the field, while remaining committed to realizing an inclusive future in HPC (*The Women Changing The Face Of HPC*, p.34).

Enjoy the read and have an amazing 2022!

Julian Tang, Ph.D.
Managing Editor
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Digital Dispatch

BOOSTING SINGAPORE'S QUANTUM CAPABILITIES

The National University of Singapore's (NUS) Quantum Engineering Programme (QEP) is partnering up with Amazon Web Services (AWS) to accelerate innovations in quantum communication and computing. By harnessing quantum's potential to process complex computations and protecting data, the collaborative effort aims to translate quantum research into commercial applications that can deliver practical value.

The QEP is a national initiative launched by National Research Foundation Singapore in 2018 with the vision of devising quantum technologies that can solve real-world problems, such as modeling vast amounts of climate data and simulating the characteristics of industrial compounds for materials engineering. Such solutions will be made possible by scalable quantum algorithms and error-free hardware. To achieve this, the new memorandum of understanding between AWS and QEP entails pursuing new quantum computing research projects and integration with the National Quantum-Safe Network for quantum communications.

Moreover, it will open opportunities to engage local and international companies, supporting democratized access to quantum computing resources to spur rapid advancement in this sector. Ultimately, the partnership aims to bolster Singapore's status as a leading hub for revolutionary technological innovation, ushering the nation's digital transformation in a quantum-enabled future.

JAPAN'S MOST POWERFUL QUANTUM COMPUTER AWAKENS

The new IBM Quantum System One computer is set to advance quantum innovation in Japan.

Credit: IBM Research

The University of Tokyo (UTokyo) and tech giant IBM have unveiled the IBM Quantum System One, Japan's most powerful quantum computer to date. It is the latest advancement in their ongoing collaboration to boost Japan's quantum innovation ecosystem and realize IBM's ambitious global quantum roadmap.

The state-of-the-art computer is readily assembled and operates stably at client sites, thanks to cryogenic engineering technologies that maintain the extremely cold temperatures needed by quantum states to operate. Quantum System One's hardware provides predictable high-quality qubits—the quantum building blocks that facilitate high-speed computing—alongside high-precision electronics to tightly control the behavior of up to 27 qubits.

Following another IBM system in Germany, Japan's Quantum System One installed at the Kawasaki Business Center now stands as the second system to be built outside the United States.

Through a web portal administered by UTokyo, researchers from academia to industry can now access these high-performance quantum resources and solve problems from drug design to energy storage. Moreover, the system is coupled with conventional processing systems, ensuring security over the internet and repeatability when running quantum algorithms.

JOINING FORCES FOR EU'S QUANTUM COMMUNICATION INFRASTRUCTURE

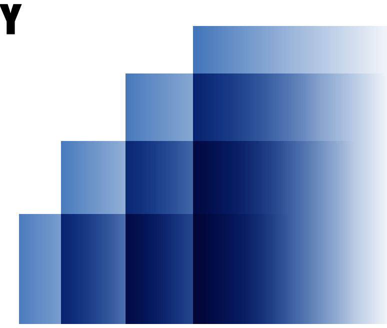
All 27 member states of the European Union have committed to building a secure quantum communication infrastructure that will span the entire region. The project, dubbed EuroQCI, will be developed in collaboration with the European Commission and the European Space Agency.

The quantum-based system is envisioned to deliver high-speed yet secure data transfer all over Europe, and enhance the reliability and cost-effectiveness of communications networks. EuroQCI will consist of a land segment involving national and cross-border fiber communication links and a space segment using satellites to establish quantum-based communication networks across the region and globally.

To safeguard Europe's critical infrastructures like hospital records and energy grids, the EuroQCI will double down on security by implementing quantum cryptography technologies. This highly secure form of encryption involves quantum keys, which are patternless passwords that are known only to interconnected members in the network. Any tampering attempts will cause the keys to collapse, automatically catching any intruders in the system.

While early rumblings of the EuroQCI plan began in mid-2019, the earliest that countries can expect a high-speed broadband in place will be in 2027.

SCALING UP DATA STORAGE THE COST-EFFECTIVE WAY



Australia's Pawsey Supercomputing Center is introducing one of the world's largest yet cost-effective object storage systems to power high performance computing tasks at the facility. It will house a total of 130 petabytes (PB)—that is, 130 quadrillion bytes—of online and offline storage.

Pawsey granted A$7 million to tech giants Dell and Xenon to build the multi-tier storage system. The offline storage component carries two 70-PB libraries, which act as duplicates of each other to improve data security. Meanwhile, the disk-based component provides 60 PB of object storage that hosts data online and separates data types to minimize delays in accessing data.

Besides accelerating data transfer, the multi-tier system's object storage technologies will enable greater flexibility in data management. The online infrastructure was also designed with scalability and cost efficiency in mind, supporting stable and high-performance storage even when more servers are added.

"An important part of this long-term storage upgrade was to demonstrate how it can be done in a financially scalable way," said Mark Gray, head of scientific platforms at Pawsey. "This system is now not only fit for purpose, but is also flexible and scales easily in capacity and performance to grow with our needs into the future."

FIGHTING QUANTUM WITH QUANTUM

Blockchain has changed the game for storing and distributing data over a shared digital ledger, enabling transparent record-keeping for applications like supply chain logistics. However, their promise of security is threatened by another emerging technology—quantum computing.

Because of quantum's ability to rapidly manipulate data and run several simulations in parallel, it can find cracks or weak points in the encryption layers protecting blockchain infrastructure. To resolve these vulnerabilities, a team from the Inter-American Development Bank (IDB) Laboratory, Cambridge Quantum (CQ) and Tecnologico de Monterrey has developed a novel cryptography layer to block out quantum hacking threats—with quantum tech itself.

The cryptography layer was tested and developed for IDB Lab's blockchain network, used by over 50 entities in the Latin America and the Caribbean region. To ensure the integrity of digital transactions, the team implemented quantum-proof keys generated from CQ's certified quantum entropy technology.

By measuring the randomness or uncertainty in a system, quantum entropy enables distinguishing between different quantum states, thanks to another quantum principle called entanglement. Since entangled entities mirror each other's properties, the keys to access data will be kept secret between blockchain nodes, with any breaches being detected right away.

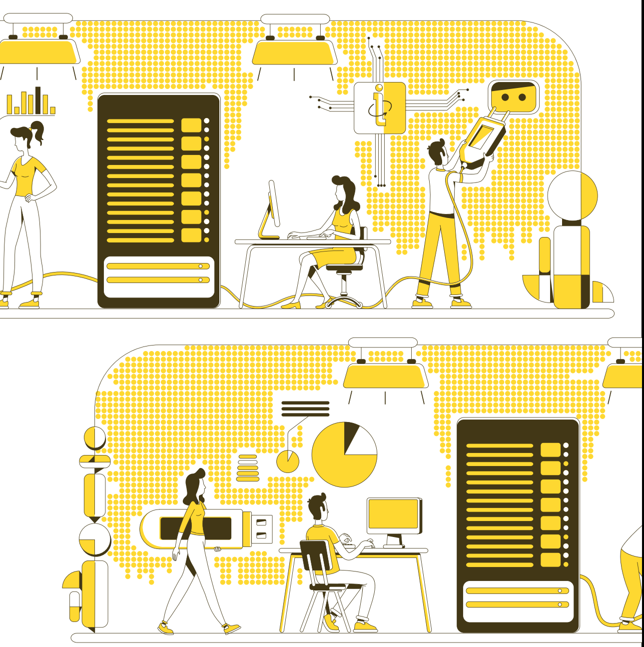
Digital Dispatch

SUPPORTING GLOBAL DIGITALIZATION

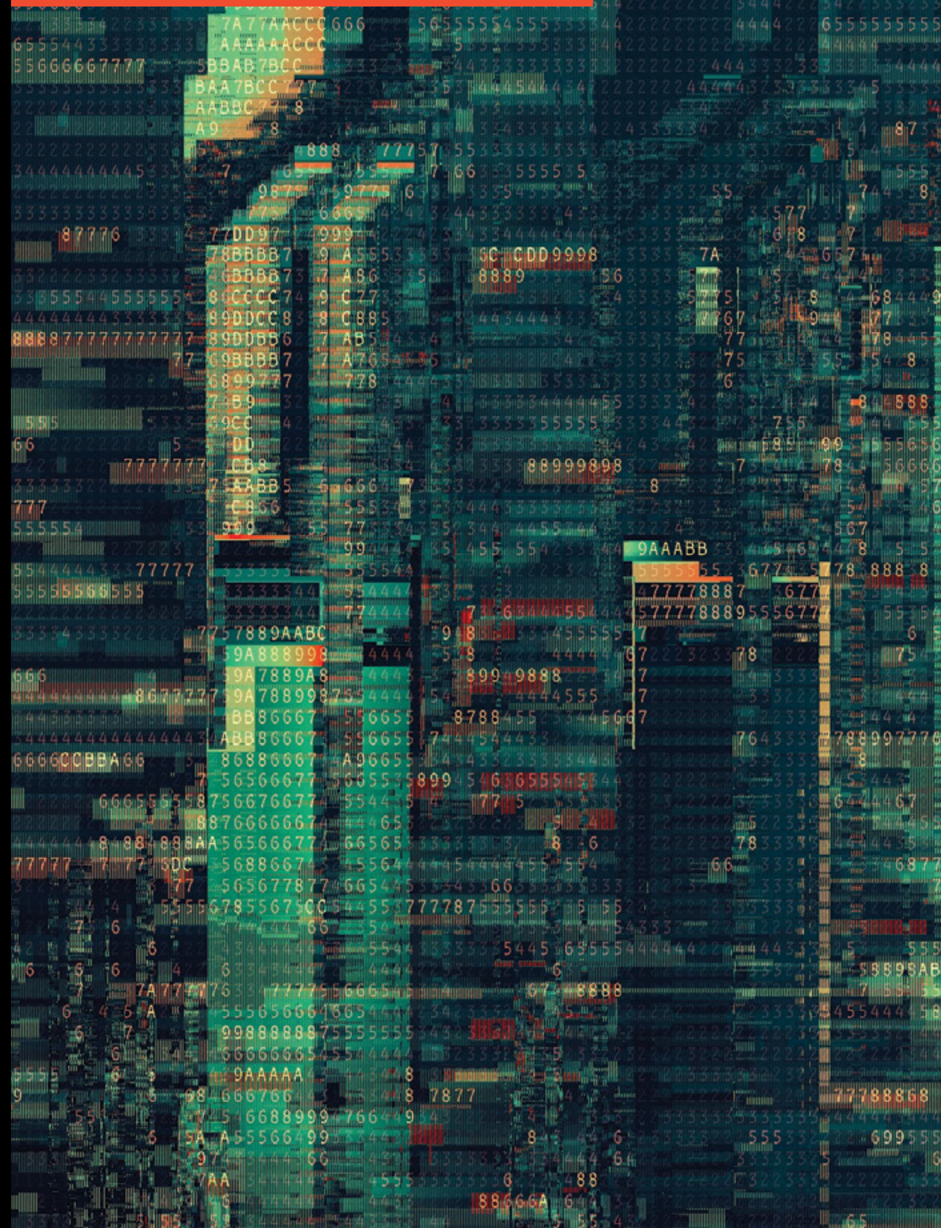
Talk about going global—cloud service provider Tencent Cloud has recently launched in four cities, namely Bangkok, Hong Kong, Tokyo and Frankfurt. With the addition of these internet data centers (IDCs), it now has operations in 27 regions and 66 availability zones across the globe.

These IDCs provide local communities with highly reliable and high-quality internet routing systems that are integrated with both local and international network operators. By allowing access to groundbreaking information technology tools, these centers serve as critical cores of communications networks, enabling their smooth daily operation.

The new infrastructure is also set to provide cloud services to a wide user platform, making resources such as data storage and high-performance computing power accessible on-demand. By distributing these functions over multiple locations and users, different sectors can easily leverage high-power computing to solve computational tasks or develop new applications, ultimately building communities empowered by digital transformation.



WHAT'S UP!



SUPERCOMPUTINGASIA 2022

To offer both in-person interactivity and a robust level of safety, the annual SupercomputingAsia (SCA) conference will return in 2022 as a hybrid event. From March 1–3, 2022, the onsite experience will take place at the Suntec Singapore Exhibition & Convention Centre, while other participants can opt to tune in to all the seminars and workshops via a virtual platform.

SCA22 is co-organized by high performance computing (HPC) institutes from Singapore, Japan and Australia with the vision of fostering a vibrant supercomputing ecosystem in Asia. With this year's theme "Towards Supercomputing for All," the event turns the spotlight on the growing accessibility of HPC resources across the globe and the rapidly evolving pace of society's digital transformation.

The Conference on Next Generation Arithmetic (CoNGA), the leading conference on emerging technologies for computer arithmetic, will be held in conjunction with SCA22. Get the latest updates on breakthroughs in next-generation data formats and their corresponding hardware, applications and services.

Book your ticket to SCA22 and don't miss out on the latest HPC trends, delivered straight from thought leaders in academia and industry!

For more information, visit https://www.sc-asia.org/

WHERE

SINGAPORE AND ONLINE

WHEN

MARCH 1–3, 2022

ISC HIGH PERFORMANCE 2022

After a successful digital event experienced by over 2,000 attendees last year, Europe's oldest HPC conference—the International Supercomputing Conference (ISC) High Performance—is heading back to the in-person format this 2022. For its 37th edition, the ISC High Performance will take place in Hamburg, Germany from May 29–June 2, 2022, with three days of the conference followed by a full day of workshops and other exhibitions.

The event aims to highlight the most critical developments in HPC, machine learning and high performance data analytics through a combination of keynote speeches, focus sessions and panel discussions, as well as research paper and poster presentations. As the world opens up, the global community including students, scholars and industry stakeholders are all invited to connect in-person and celebrate the HPC sector's continued advancements and evident impact across society.

From parallel programming to quantum computing, participants will enjoy a spectacular array of computing topics and trends, sparking ideas for more ways to leverage HPC to address pressing issues like climate change and chronic disease.

Save the date and get ready to gain visionary insights on emerging innovations and future opportunities in supercomputing!

For more information, visit https://www.isc-hpc.com/

WHERE

HAMBURG, GERMANY

WHEN

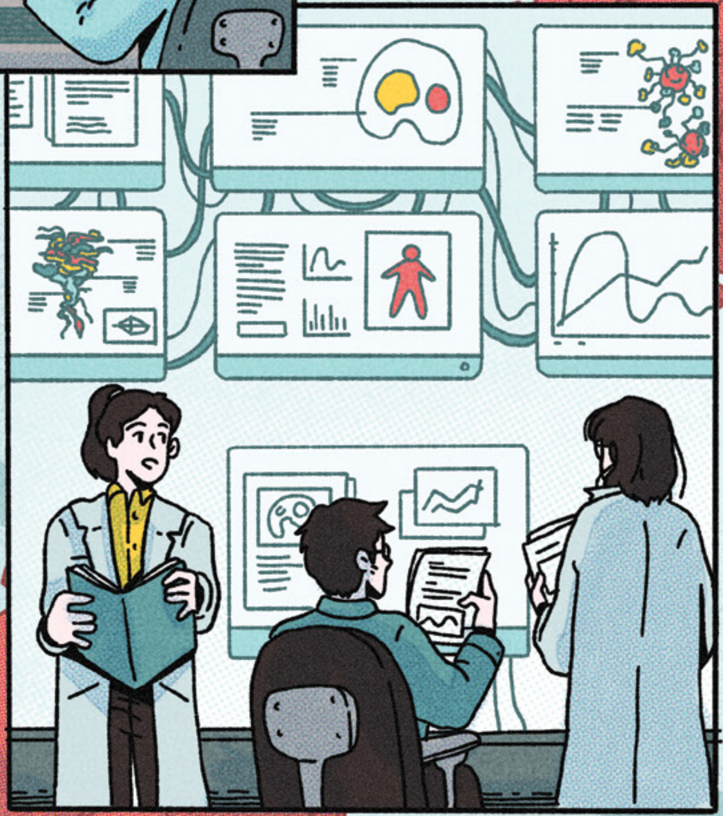
MAY 29–JUNE 2, 2022

POWERING THROUGH THE PANDEMIC WITH SUPERCOMPUTERS

By performing trillions of calculations per second, supercomputers are accelerating COVID-19 diagnosis and the development of test kits and vaccines to help scientists combat the pandemic.

By **Pecier Decierdo**

Illustrations by Danyel Maxin Santos



Almost two decades ago, countries across Asia were imperiled by a contagious and deadly disease caused by a coronavirus. In a matter of weeks, the severe acute respiratory syndrome (SARS) outbreak crossed international boundaries, resulting in thousands being infected and a death toll of nearly 800, coupled with severe pressure on Asia's interconnected systems.

In early 2020, the same systems, including healthcare, research, transportation and logistics, were once again tested by a coronavirus. Within a year, SARS-CoV-2, the virus behind COVID-19, had spread across the continent and the world, wreaking havoc on almost every economy.

While nations may have responded differently to the current pandemic, one common truth has stood out—those that take the opportunity to adapt and transform will emerge stronger.

Responding quickly in the early days of the COVID-19 outbreak, scientists around the globe began tapping into the massive power of high performance computing (HPC). They were able to process large volumes of COVID-19 data and simulate biological and chemical processes by running complex mathematical models on supercomputers.

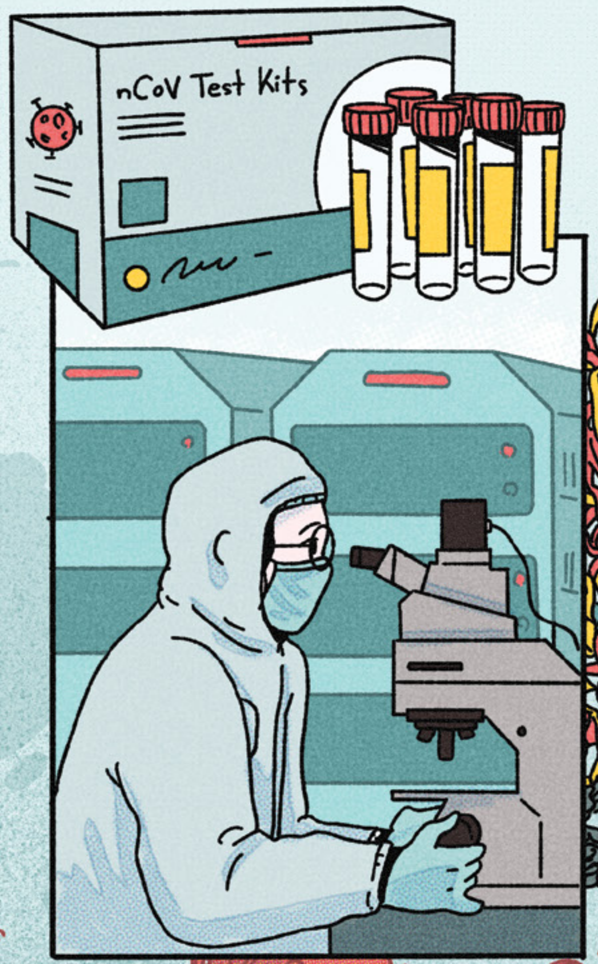
These simulations not only advanced our understanding of the evolving virus and how it causes human infection, but also paved the way for the rapid development of interventions against it. Read on to find out about how organizations, governments and universities in Asia have harnessed supercomputer solutions to power throughout the pandemic.

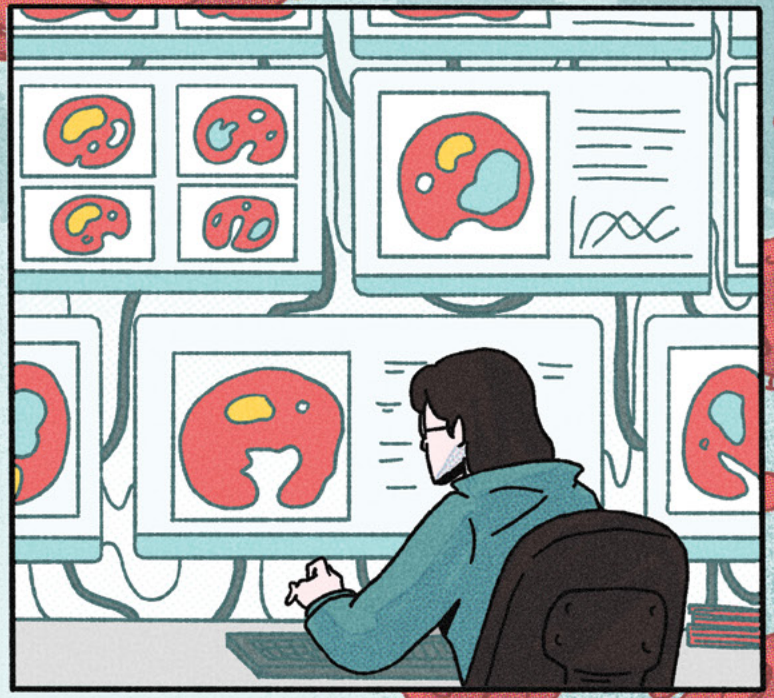
Supercharging test kit development

At a virtual press conference in March 2020, the director-general of the World Health Organization, Dr. Tedros Adhanom Ghebreyesus, gave clear advice to all nations, "Test, test, test. Test every suspected case."

But to roll out testing en masse, a country first needs test kits. Heeding the call, Seoul-based biotech company Seegene used their supercomputer to develop a test kit within a matter of weeks, rolling them out even before other countries confirmed their first cases of the new virus. The test kit, based on the real-time reverse transcription polymerase chain reaction (RT-PCR), could detect the presence of viral genes in suspected patient samples.

Despite the lack of physical samples from patients on hand, the team used artificial intelligence to analyze the molecular blueprint of SARS-CoV-2 and assemble the required reagents that would react with the virus' genetic material to create a highly sensitive test. Without the supercomputer, it would have taken the team two to three months to develop such a test, Dr. Chun Jong-yoon, founder and CEO of Seegene, told *CNN*.





Mission: infection detection

Diagnosing COVID-19 currently relies on RT-PCR testing, considered the gold standard for detecting viral genetic material from clinical samples. If initial RT-PCR testing delivers inconclusive results, though, chest computed tomography (CT), similar to X-ray scans, may be used instead.

However, doctors have to spend a considerable amount of time—at least 15 minutes—assessing CT images, proving a major bottleneck when these healthcare experts are in such short supply.

To bridge this gap, researchers at Tsinghua University in China devised an HPC-enabled artificial intelligence (AI) tool to perform the analysis in a significantly shorter timeframe, taking only a few minutes or even mere seconds. The supercomputer that was called in to help was the Elastic High-Performance Computing (E-HPC) Solution for Life Sciences by Chinese e-commerce and cloud giant Alibaba.

The E-HPC includes four Intel central processing unit-based configurations and one similar configuration with additional Tesla P100 graphical processing units, all with network speeds ranging from 10 to 25 Gbps. With such processing power, the E-HPC easily accommodated the algorithms and data requirements, allowing the AI program to quickly learn to pinpoint COVID-19 diagnoses from CT scans.

Beyond diagnosis, researchers at Sun Yat-Sen University also leveraged E-HPC's ability to accelerate data transfers to gain more detailed insights into the virus' evolution. Meanwhile, a Peking University team harnessed E-HPC's resources to speed up their molecular docking tests, which analyze how molecules fit together. Given their vast computational power, such supercomputers are valuable in advancing the discovery of antibody and drug candidates to target the virus where it's most vulnerable.

Unlike their conventional counterparts, HPC-powered models can look at tons of different molecules at once, simulating how they might latch onto and disable SARS-CoV-2's spike protein, the key to entering and infecting human cells.

→

Breaking infection chains

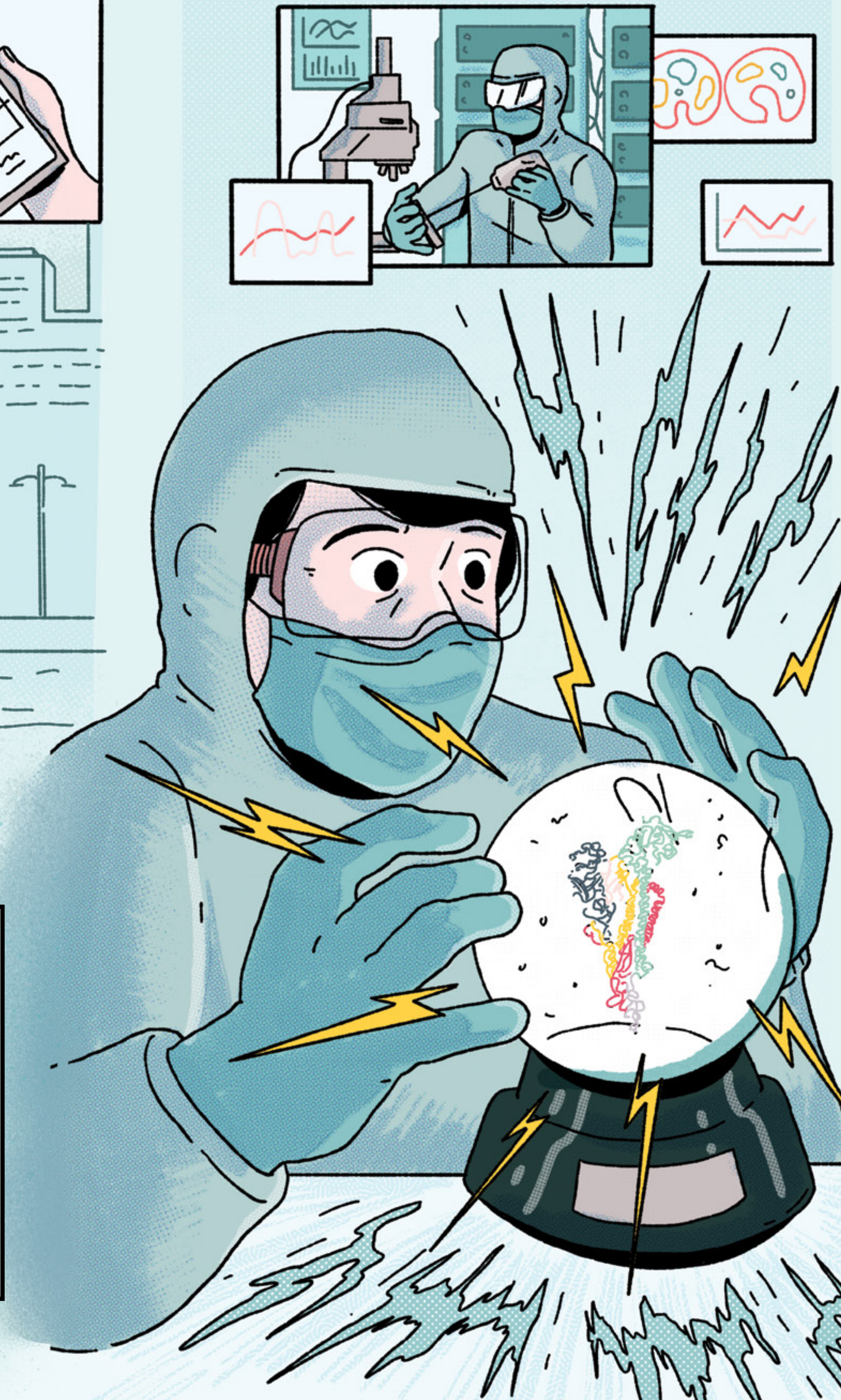
Within a year since the first reported COVID-19 case in December 2019, nearly 250 million cases were recorded, with Asia accounting for over a fifth of that number. Key to stemming the virus' spread is tracing the chains of infection, including asymptomatic cases, so that health officials can promptly identify and reach out to those who come into contact with potential carriers.

Supercomputers have a crucial role to play in stamping out these transmission chains, thanks to their ability to streamline contact tracing processes.

In the earlier stages of the pandemic when case counts were surging in South Korea, the Korea Institute of Science and Technology (KIST) and the Korean Ministry of Science and ICT jointly established the KIST's Individual-based Simulation Toolkit for Transfer phenomena. The tool leverages HPC to simulate the movement of people across the country, collating data on the location of almost 50 million individuals in South Korea.

By tracing infections stemming from specific 'nodes' or points of contact, health officials can notify suspected COVID-19 cases to undergo testing or self-quarantine protocols, helping to snap potential transmission chains.

In Hong Kong, meanwhile, the Department of Health worked with the police to deploy the Major Incident Investigation and Disaster Support System, using a supercomputer to map out the relations among infected patients. Through these visualizations, authorities easily identified clusters where cases were flaring up, leading to data-driven policy decisions for mobility restrictions and other interventions.



Peering into the SARS-CoV-2 crystal ball

As a virus spreads, it amasses mutations that can give rise to new variants—ones that can be more contagious and deadly. SARS-CoV-2 is no different, with the Delta variant and now Omicron variant evolving to become at least twice as contagious as the original strain.

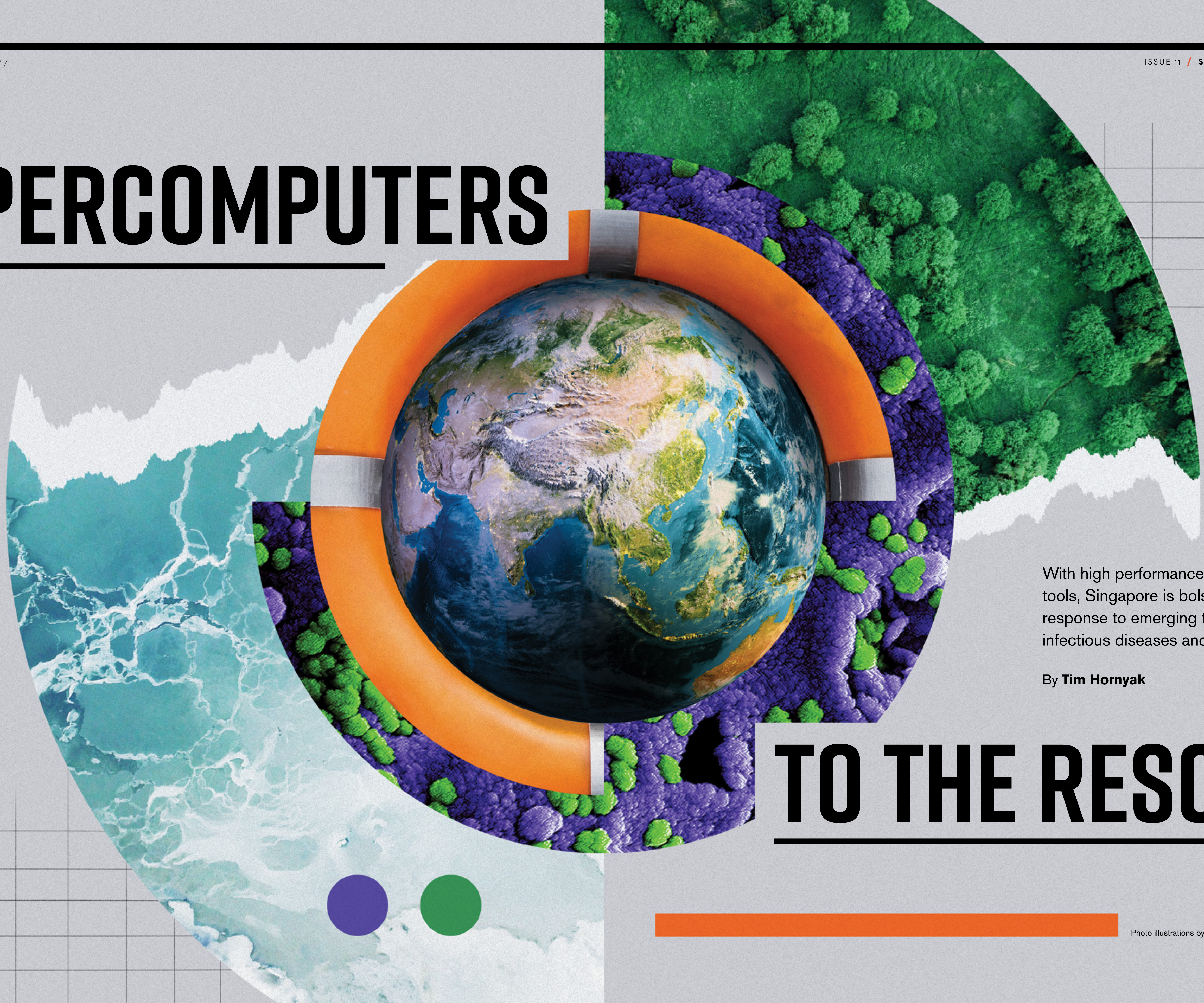
To ensure that the emerging variants are accurately detected and that vaccines and treatments still remain effective, scientists are rushing to grasp the changing characteristics of the virus, such as its genetic composition and the expression of proteins essential for host cell invasion.

At CMKL University, established as a collaboration between Carnegie Mellon University in the US and King Mongkut's Institute of Technology Ladkrabang in Thailand, researchers are using the Apex-Goliath supercomputer to stay ahead of SARS-CoV-2's mutational curve. With a processing speed around a million times faster than a typical household computer, Apex-Goliath can sift through viral genomic data collected from patients and identify mutation points.

Moreover, the AI-powered system automatically raises an alert if the genetic codes show a propensity for harboring dangerous mutations. By predicting possible mutations and variants quicker than ever before, healthcare experts and state authorities can take proactive measures to stop COVID-19's spread.

As supercomputers empower novel solutions from detection to drug development, scientists and governments are striving to realize a future where the pandemic is finally under control. In the same way that the effects of COVID-19 are widespread, the interventions against the viral disease have arisen from multidisciplinary efforts bridging fundamental science and technological innovation.

SUPERCOMPUTERS TO THE RESCUE



With high performance computing tools, Singapore is bolstering its response to emerging threats such as infectious diseases and climate change.

By **Tim Hornyak**

Photo illustrations by Lam Oi Keat / Supercomputing Asia

As the world enters year three of the COVID-19 pandemic, it continues to face the threat of other infectious diseases as well as the multifaceted crisis of climate change. At first glance, the two may sound like important yet disparate challenges. Deeper investigations, however, have increasingly revealed that human health and environmental health are heavily entangled.

For instance, several contagious diseases such as hepatitis A and parasitic infections spread easily in areas with poor sanitation, while air pollution exposure is associated with lung and cardiovascular disorders. Meanwhile, ecosystem destruction and habitat loss can degrade the ability of the environment to control outbreaks, potentially leading to disease-causing agents spilling over from animals to humans.

Losing sight of any of these looming threats could spell grave disaster both in local and global contexts. To understand the intricacies of these emerging hazards, supercomputers are vital tools that could make a big difference to reverse this ominous narrative in Singapore and the world.

THE BATTLE AGAINST INFECTIOUS DISEASES

Singapore has faced a surge in COVID-19 cases in the past year, underlining the danger of infectious diseases in the tropical nation. To help the country fight the current pandemic and future outbreaks, scientists have harnessed the power of high performance computing (HPC) in deciphering disease characteristics and enabling better healthcare interventions.

Keeping a close eye on these emerging threats, the Institute of High Performance Computing (IHPC) at the Agency for Science, Technology and Research (A*STAR) closely collaborates with the National Supercomputing Centre (NSCC) Singapore, whose resources include the petascale ASPIRE 1 HPC system. ASPIRE 1 carries 1,288 central processing unit (CPU) nodes and accelerator nodes with NVIDIA K40 graphical processing units (GPUs), capable of performing the high-speed and complex calculations needed to model the spread of the coronavirus.

As droplet behavior may vary across climate conditions, IHPC researchers examined the role of coughing in COVID-19 transmission, modeling how far virus droplets can travel in an outdoor tropical environment. Reporting in the journal *Physics of Fluids*, they found that small-droplet dispersal is "relatively insensitive" to humidity.

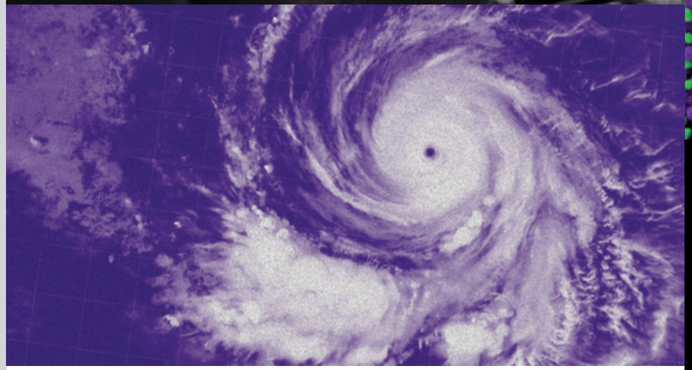
On the contrary, large droplets are a force to be reckoned with, traveling farther distances and posing a serious infective threat. By better understanding infection routes, scientists and their supercomputers are supporting government agencies in the development of data-driven solutions to reduce the risks of virus transmission.

Besides simulating disease transmission, HPC solutions have also revolutionized COVID-19 diagnosis. IHPC partnered with Tan Tock Seng Hospital, a large public hospital in Singapore, to leverage HPC-powered artificial intelligence (AI) to detect signs of pneumonia from chest X-ray scans. By accelerating the hospital's screening process, AI-based image analysis helps doctors identify urgent cases and deliver interventions much earlier. Moving forward, IHPC is working with other local hospitals to apply AI technologies for the detection of other diseases, ushering in a new dawn in digital healthcare.

"As the world becomes more digitalized and interconnected, HPC plays a crucial role in powering societies to overcome threats and create opportunities," said Dr. Lim Huck Hui, executive director of IHPC, in an interview with *Supercomputing Asia*. "HPC enables advanced modeling and AI solutions to be developed, which could positively impact not only healthcare, but also diverse areas including food security, urban solutions and climate change."

Just as how the coronavirus can evolve into separate variants, another rampant pathogen known to come in several forms is the dengue virus. Strikingly, researchers at the Environmental Health Institute Singapore (EHI), Nanyang Technological University, Singapore and the National University of Singapore (NUS) discovered that the dengue virus type 2's Indian subcontinent lineage is maturing into a new genotype.

The researchers used standalone high-performance desktops and NSCC HPC resources to deftly analyze virus dispersal and genetic characterization, detailing the dengue virus' evolution in *Scientific Reports*. These valuable insights could improve the mitigation of dengue and potentially other infectious diseases as well.



"Unlike conventional approaches, current epidemiological research utilizes HPC to gain deeper insights into disease patterns, including the contribution of potential genetic and environmental risk factors," said Hapuarachchige Chanditha Hapuarachchi, study co-author and a senior scientist at EHI. "As big data analytics is becoming a common practice in modeling and genomics, supercomputers are indispensable to this field."

> **"HPC enables advanced modeling and AI solutions to be developed, which could positively impact not only healthcare, but also diverse areas including food security, urban solutions and climate change."**
>
> **Dr. Lim Keng Hui**
> Executive Director
> Institute of High Performance Computing
> Agency for Science, Technology and Research

FIGHTING CHANGES IN THE CLIMATE

Regardless of how the pandemic unfolds, climate issues loom as a tremendous and persistent danger. Singapore's government calls it an existential threat—and rightly so. The various interactions between the atmosphere, ocean and land constitute an extremely intricate and massive system, one that could leave far-reaching consequences if urgent action is not taken.

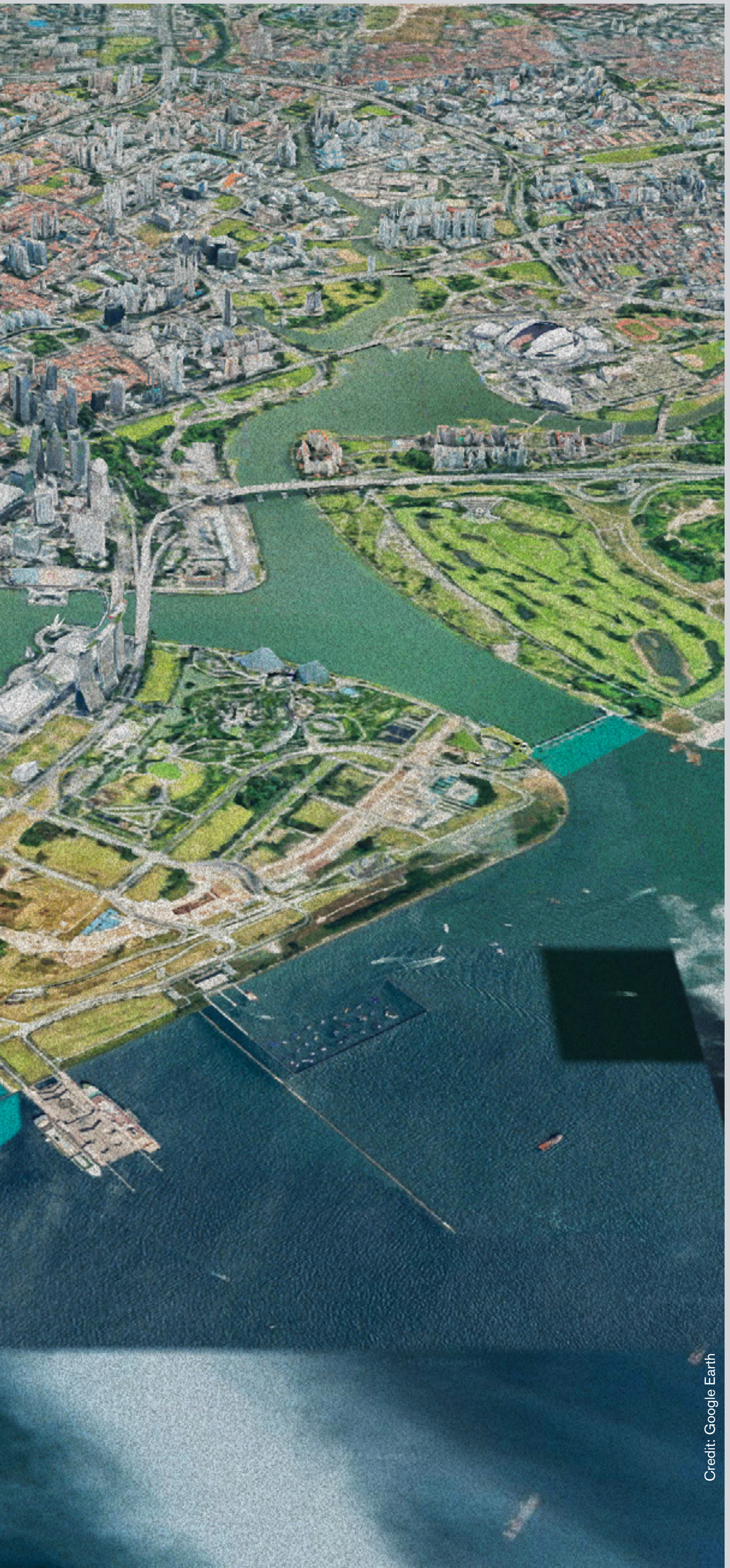
Under the National Environment Agency's Meteorological Service Singapore (MSS), scientists at the Centre for Climate Research Singapore (CCRS) tapped two supercomputing resources to confront climate change. Besides the supercomputing system at NSCC, the team also uses an in-house Cray XC-40 system named Athena for weather forecasting, operations, and research and development (R&D).

"HPC is essential to perform the trillions of calculations required to predict the impact of changing greenhouse gas levels on the climate system, which includes sea level rise, rainfall and temperature changes," said CCRS director Dale Barker, in an interview with *Supercomputing Asia*.

Despite significant strides toward creating high-accuracy simulations, current climate models are not perfect. To cope with the many uncertainties in predicting future scenarios, climate sciences need supercomputers to run 'ensembles' of multiple models all at once, solving equations that describe the physical interactions of various environmental factors.

"These models are run with different parameters and forcing—a technique for proving the consistency and independence of results—to provide a quantitative estimate of uncertainty," explained Barker. "Through such efforts, we can assign a likelihood statement, such as 'very likely' or 'unequivocal,' to inform risk assessments by decision-makers."

One threat that Singapore seems more than likely to face is flooding, with about a third of its territory found less than five meters above sea level. According to the MSS, the city-state's current sea level is around 14 centimeters higher than pre-1970 levels, while CCRS expects an average sea level rise of up to one meter by 2100.



To devise the best defense strategy against this looming hazard, the Coastal-Inland Flood Model is under development from the national water agency Public Utilities Board (PUB), NUS and water management company Hydroinformatics Institute. The model will simulate flooding in the country's coastal and inland areas, leading to more accurate risk projections during different weather and climate scenarios.

"In anticipating continued climate change, the development of such a model is critical to safeguard both our coastlines and our collective future against severe weather events and rising sea levels," said Professor Philip Liu, project team leader from NUS' Department of Civil and Environmental Engineering, in a press release.

But beyond all these proactive initiatives against the growing climate crisis, the fight entails much more than anticipating possible disasters. Singapore's researchers are also working on risk reduction and sustainability strategies.

IHPC, for instance, collaborated with the Housing and Development Board (HDB), a statutory board under the Ministry of National Development responsible for Singapore's public housing, to develop the Integrated Environmental Modeler for simulating urban conditions such as wind patterns and sunlight.

"In anticipating continued climate change, the development of such a model is critical to safeguard both our coastlines and our collective future against severe weather events and rising sea levels."

Professor Philip Liu
Project Team Leader
Department of Civil and Environmental Engineering, National University of Singapore

By analyzing environmental data captured by street sensors, the model can reproduce the interactions between building structures, urban heat and air flow across the island, helping to plan out more sustainable urban environments.

"This approach can be used to design green and livable urban new residential towns with good thermal comfort to promote the efficient use of energy," said Lim.

NEW TOOLS IN THE ARSENAL

While current supercomputers are already changing the game for climate modeling, new HPC techniques and hardware are constantly being brought to bear in the fight against emerging threats. Climate scientists are recognizing the need to update and refine their HPC strategies with the rising importance of GPUs, originally designed for graphics acceleration in video games.

"Many models have originally been developed and optimized on CPU architectures. But these days, HPC centers provide not only CPU resources but also increasingly, GPU resources," explained Dr. Heiko Aydt, R&D lead at the Singapore-ETH Centre for Global Environmental Sustainability, in an interview with *Supercomputing Asia*. "Unlike CPUs, which are general-purpose processors, the strength of GPUs is that they are highly specialized."

However, adapting the code of existing climate models to be compatible with GPUs is no easy feat. But if done right, it can significantly improve computing performance.

Barker similarly highlighted the importance of GPUs for innovative climate research, adding that these models are now being ported onto joint CPU-GPU clusters as well as distributed cloud computing technologies. The latter helps make HPC resources available to a broad range of users, hosting the service through the internet to enable access to data and running programs on-demand.

FORGING AHEAD WITH THE BATTLE

NSCC is now building a powerful new tool as a successor to ASPIRE 1 to fortify Singapore's disaster resilience and response to emerging threats. The S$40 million system will be capable of up to 10 petaFLOPS of computing capacity, eight times that of ASPIRE 1.

Set to be operational in 2022, the next-generation supercomputer will be built with Hewlett Packard Enterprise's Cray EX supercomputer components, with close to 900 CPU and GPU computing nodes and more than 100,000 computing cores.

Researchers at the CCRS are eager to use the machine to estimate the extent and effects of changing rainfall patterns and sea level rise. The new resource will also help refine climate forecasts for Singapore, which barely registers on global climate models because of its small size.

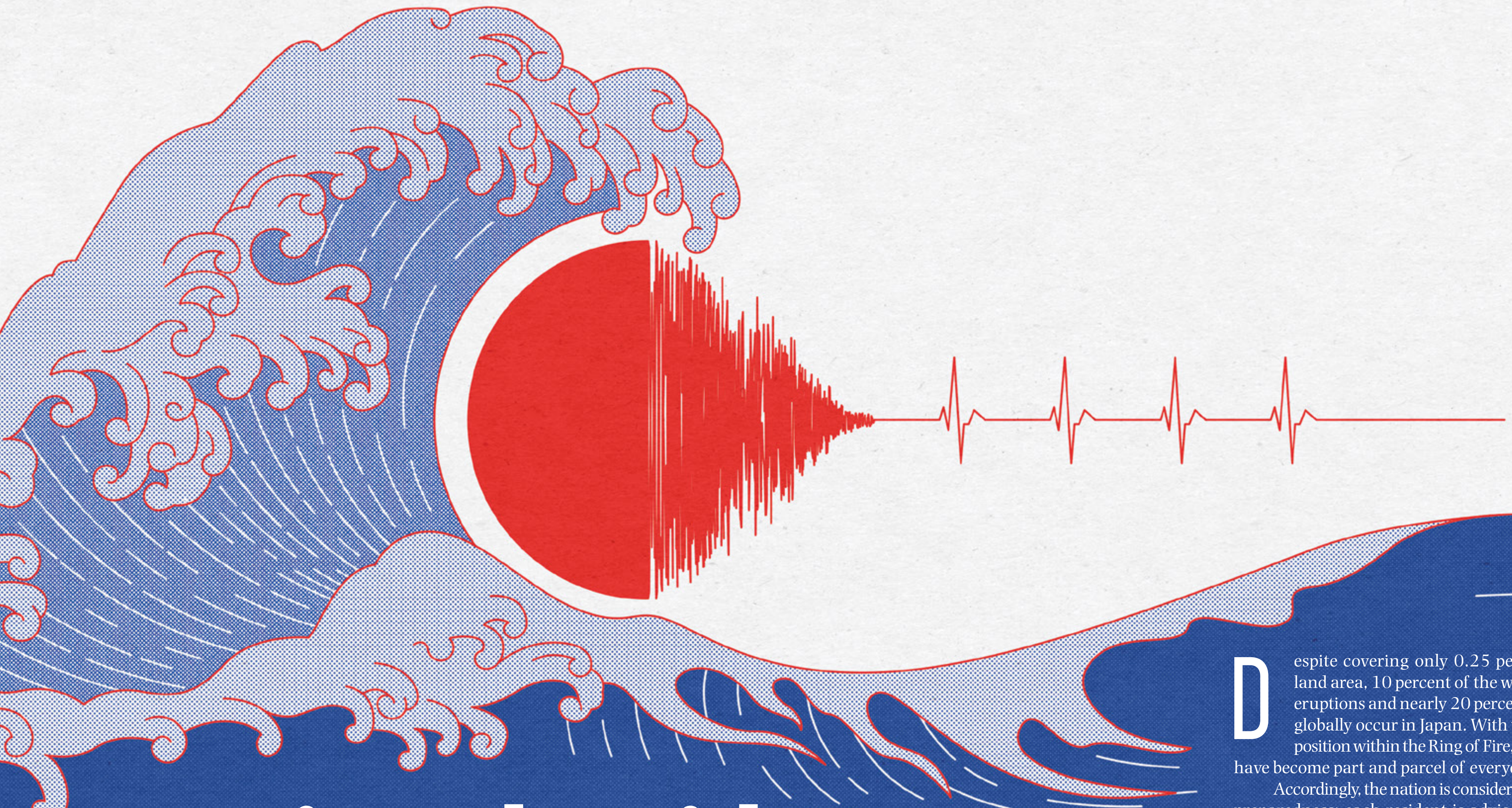
According to the team at CCRS, the system is set to run what is called a regional climate model that can help enhance predictions of large-scale climate variability across Asia.

Barker added that larger supercomputers can accommodate more sophisticated parameters, such as cloud-aerosol models, which are suspensions of fine particles in the air. These can also provide analytics at higher resolution, zooming into nitty-gritty details over more localized contexts.

Whether in weather forecasting or pandemic predictions driven by historical data, HPC applications are gearing up to combat emerging threats and weed out uncertainties. By providing more detailed risk projections and accurate assessments, supercomputing is in a prime position to direct the right interventions to mitigate damage and respond to hazards in real time—creating a safer and more resilient Singapore.

By harnessing both artificial intelligence and high performance computing in one powerful model, scientists from Japan are making real-time tsunami prediction more accessible.

By **Kamila Navarro**



The next wave of tsunami prediction

Turning the tide with AI and HPC

Illustrations by Shelly Liew / *Supercomputing Asia*

Despite covering only 0.25 percent of the Earth's land area, 10 percent of the world's active volcanic eruptions and nearly 20 percent of all earthquakes globally occur in Japan. With the country's unique position within the Ring of Fire, such natural hazards have become part and parcel of everyday life in Japan.

Accordingly, the nation is considered a model for disaster preparedness: each resident is advised to carry fireproof evacuation bags with first aid, sanitation products as well as food and water. Meanwhile, buildings constructed after 1981 are required to have earthquake-resistant structures, meaning thicker beams, pillars and walls as well as shock-absorbers to reduce shaking in taller buildings.

And yet, the 2011 Great East Japan Earthquake came as a huge shock—literally. On March 11, 2011, the Tohoku region along Japan's eastern coast was rocked by a magnitude 9.0 earthquake for six minutes; the strongest in the country's records so far. The massive upthrust in the seabed unleashed a tsunami that reached three stories high, sweeping away cars and bridges, flooding buildings and even toppling tsunami seawalls.

Notably, the tsunami also led to the Fukushima Daiichi nuclear disaster, with three nuclear reactors melting down and causing the discharge of dangerously radioactive water in Fukushima. Combined, the earthquake and tsunami led to nearly 20,000 deaths and an estimated US$235 billion in damages—the costliest natural disaster in history.

While earthquakes and tsunamis are bound to happen again, accurate forecasts could spell the difference between life and death. Consider the case of Costa Rica: in September 2012, the country's Nicoya Peninsula was struck by a magnitude 7.6 earthquake. Despite the quake's size, there was limited damage and no deaths as geoscientists had predicted the occurrence of such a hazard years prior, giving the government ample time to increase earthquake awareness and enforce building codes.

Technological advances in the decade since the 2011 Great East Japan Earthquake could ensure more accurate predictions and more resilient populations. With Japan home to the world's fastest supercomputer, Fugaku, the nation's best minds are leveraging its powerful resources to better prepare for when disaster strikes.

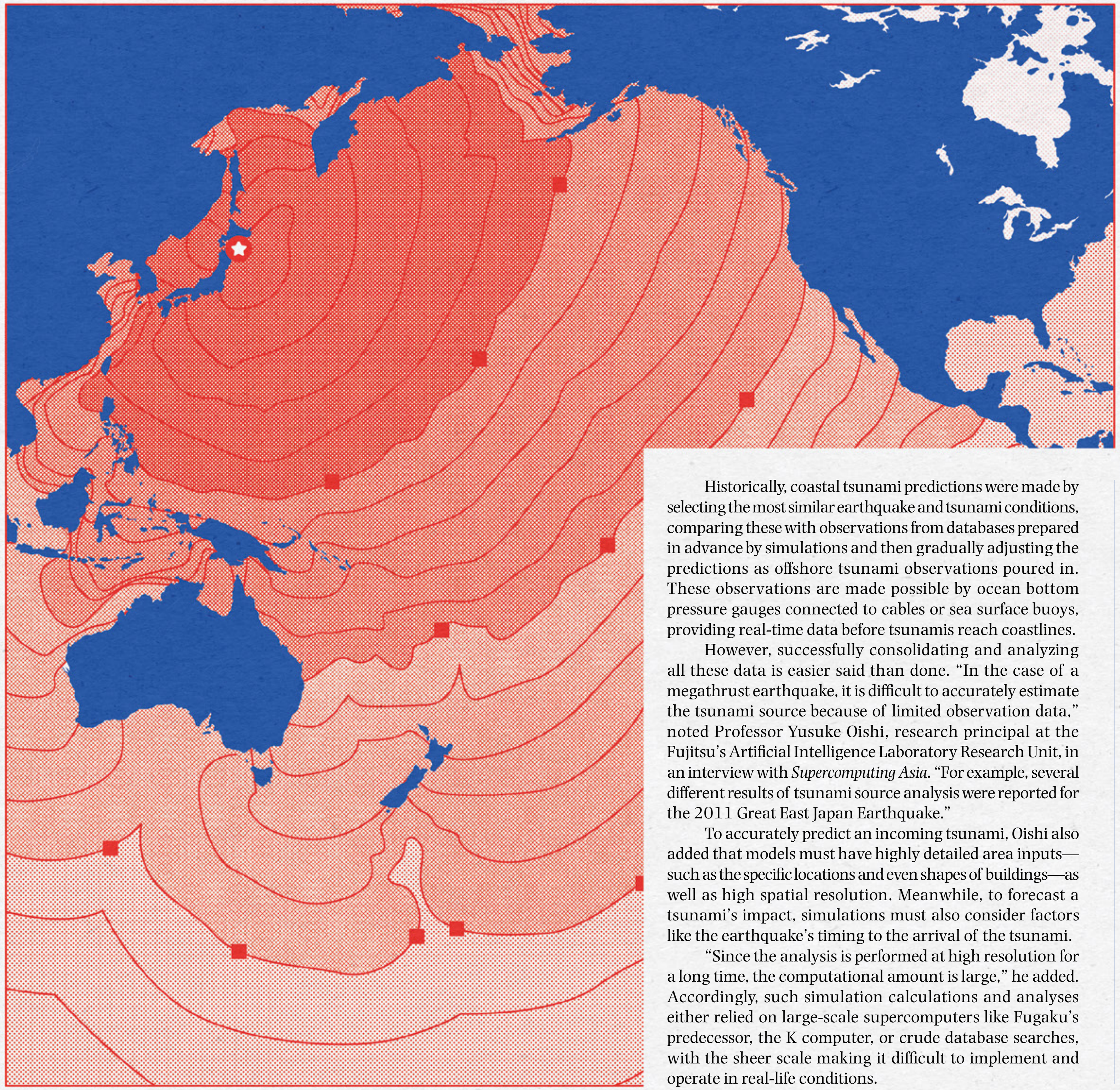
PITFALLS OF PAST PREDICTIONS

Around one minute before the 2011 Great East Japan Earthquake was felt, the nationwide Earthquake Early Warning system—made possible by over 1,000 seismometers scattered across the country—notified millions of the impending quake. Minutes later, at 2:49 PM, the Japan Meteorological Agency (JMA) issued the first tsunami warning.

Despite their timely warnings for the two hazards, JMA critically underestimated the earthquake's magnitude and the tsunami's height. At first, the agency estimated the magnitude at 7.9 and the tsunami to have heights of three to six meters. Given these estimates, certain residents in the Iwate Prefecture opted to remain in place as they felt that the ten-meter seawalls would protect them. It was only 30 minutes after the earthquake that the tsunami height was updated to more accurate estimates of six to ten meters.

Ultimately, the seawalls offered little security against the towering tsunami, with the waves streaming over and partially damaging the walls. By then, most power and communications systems had failed, with the revised information failing to reach most members of the public. True enough, subsequent surveys by the Japanese government showed that nearly half of the population in the affected areas did not receive any information about the tsunami—and up to 70 percent did not receive the revised information on tsunami heights.

> "In the case of a megathrust earthquake, it is difficult to accurately estimate the tsunami source because of limited observation data."
>
> **Professor Yusuke Oishi**
> Research Principal
> Artificial Intelligence Laboratory Research Unit
> Fujitsu



Historically, coastal tsunami predictions were made by selecting the most similar earthquake and tsunami conditions, comparing these with observations from databases prepared in advance by simulations and then gradually adjusting the predictions as offshore tsunami observations poured in. These observations are made possible by ocean bottom pressure gauges connected to cables or sea surface buoys, providing real-time data before tsunamis reach coastlines.

However, successfully consolidating and analyzing all these data is easier said than done. "In the case of a megathrust earthquake, it is difficult to accurately estimate the tsunami source because of limited observation data," noted Professor Yusuke Oishi, research principal at the Fujitsu's Artificial Intelligence Laboratory Research Unit, in an interview with *Supercomputing Asia*. "For example, several different results of tsunami source analysis were reported for the 2011 Great East Japan Earthquake."

To accurately predict an incoming tsunami, Oishi also added that models must have highly detailed area inputs—such as the specific locations and even shapes of buildings—as well as high spatial resolution. Meanwhile, to forecast a tsunami's impact, simulations must also consider factors like the earthquake's timing to the arrival of the tsunami.

"Since the analysis is performed at high resolution for a long time, the computational amount is large," he added. Accordingly, such simulation calculations and analyses either relied on large-scale supercomputers like Fugaku's predecessor, the K computer, or crude database searches, with the sheer scale making it difficult to implement and operate in real-life conditions.

TWO TECHNOLOGIES, ONE POWERFUL COMBO

Hoping to prevent a replay of the Great East Japan Earthquake, Fujitsu, Tohoku University and the University of Tokyo joined forces to harness artificial intelligence (AI) and high performance computing to take tsunami forecasting to the next level—with their work representing the culmination of a decade's worth of research efforts.

For instance, in a 2015 *Geophysical Research Letters* publication, the Oishi-led team described the development of a parallel version of the TUNAMI-N2 (Tohoku University's Numerical Analysis Model for Investigation of Near-field Tsunamis) model that could be run on 9,469 cores of the K computer. Their five-meter resolution simulation of flooding conditions in Sendai, the largest city in the Tohoku region, on the supercomputer took only 93.2 seconds; the same computations would have taken several days on a workstation.

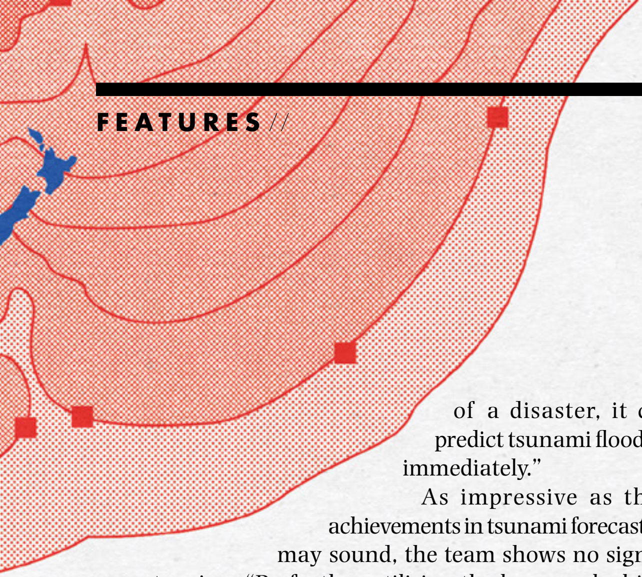
Applying their findings to the 2011 disaster, it took the model five minutes to analyze the tsunami wave source and ten minutes to provide basic flood predictions. As the tsunami took an hour to reach Sendai, having such information publicly available so shortly after the quake could have turned the tide in terms of survival.

Despite this breakthrough in tsunami forecasting, the model's computational demands make it largely inaccessible and impractical should such a scenario happen again. To this end, Oishi and colleagues later proposed leveraging a convolutional neural network (CNN) for end-to-end tsunami flooding forecasting, publishing their findings in *Nature Communications* in early 2021.

To develop the CNN, a form of artificial neural network used in image recognition and processing, the team conducted tsunami simulations for a total of 12,000 scenarios—synthetically generating 10,000 cases for training and then evenly splitting the remaining 2,000 cases between validation and testing. The network's training was performed in the AI Bridging Cloud Infrastructure, a GPU-accelerated, 226-petaFLOPS supercomputer operated by the National Institute of Advanced Industrial Science and Technology in Japan.

Incredibly, the trained CNN took only 0.004 seconds on average to provide a forecast using a single CPU node with 40 cores. Compared to the previous 1.5-minute standard set by the K computer, the team's approach was not only much faster, but also required fewer computational resources.

"AI-based tsunami forecasting makes it possible to predict the state of flooding directly from observed offshore tsunami waveforms, without relying on tsunami source estimation results," noted Oishi. "While the AI requires large amounts of calculation during training, in the event



of a disaster, it can predict tsunami flooding immediately."

As impressive as their achievements in tsunami forecasting may sound, the team shows no sign of stopping. "By further utilizing the large-scale, high-speed performance of Fugaku and training the system with additional tsunami scenarios, Fujitsu aims to realize an AI that can offer predictions for unexpected tsunami and flooding predictions over a wider area," added Oishi.

THE FUTURE OF FORECASTING

True enough, by February 2021, the same team announced that they had successfully leveraged Fugaku to streamline the development of a new AI that can instantaneously predict tsunami flooding even on regular computers. Building upon their earlier study, the researchers used the supercomputer to generate 20,000 possible tsunami scenarios based on high-resolution, three-meter unit simulations.

They then trained the AI on these datasets, allowing the team to build a model that first roughly approximates land flooding based on offshore observations of tsunami waveforms. The algorithm then increases the resolution of estimated flooding conditions and optimizes calculations, enabling the prediction of floods in coastal areas before landfall at high spatial resolutions.

To put their new technology to the test, Oishi and colleagues sought to glimpse into potential tsunami flooding in Tokyo Bay caused by a theoretical quake in the Nankai Trough. Earthquakes of magnitude 8.0 and higher have occurred repeatedly in the trough every 100 to 200 years, with the next one anticipated by the Japanese government to likely happen within the upcoming 30 years.

"A magnitude 9.0 earthquake can be expected in the case of massive earthquake in the Nankai Trough," he said. "Therefore, we built an AI model based on training data with such a magnitude."

Running the simulation on just a desktop computer, the AI generated highly accurate tsunami flood forecasts for the coastal urban areas of Tokyo Bay in a matter of seconds. Their results were comparable to the tsunami model used by the Cabinet Office of Japan, which is known among seismologists as the largest possible earthquake model built, according to Oishi.

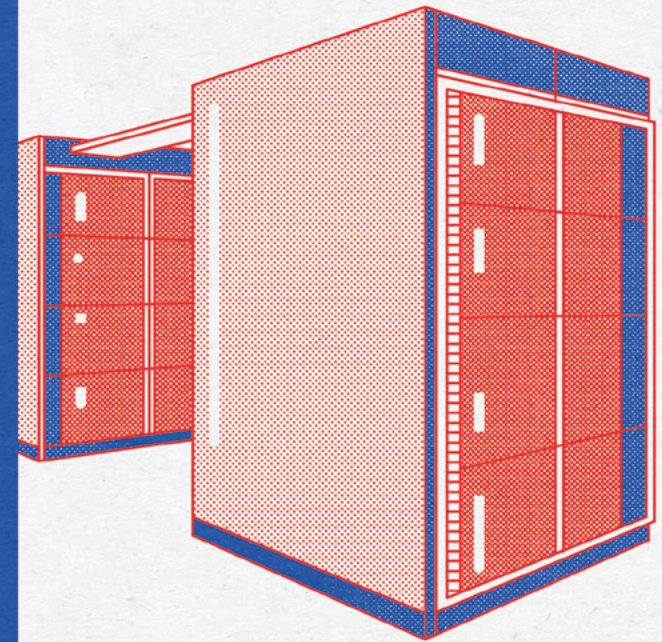
"In AI-based tsunami prediction, properly designed training data is important. In the future, we will further leverage Fugaku's high performance and high speed to generate various tsunami scenarios with the aim of predicting 'unexpected' tsunamis."

Professor Yusuke Oishi
Research Principal
Artificial Intelligence Laboratory Research Unit
Fujitsu

"By generating training data of 20,000 cases using Fugaku, we also predicted tsunamis three times the height of the Cabinet Office's model," he added.

As the model can be run on conventional computers, practical, real-time flood prediction systems are now within reach even in locales that lack access to powerful supercomputers not just in Japan, but also potentially in other disaster-prone countries. Such an approach will hopefully allow disaster management teams to make better data-driven mitigation and evacuation measures in the future—minimizing the loss of life and preventing a replay of the Great East Japan Earthquake.

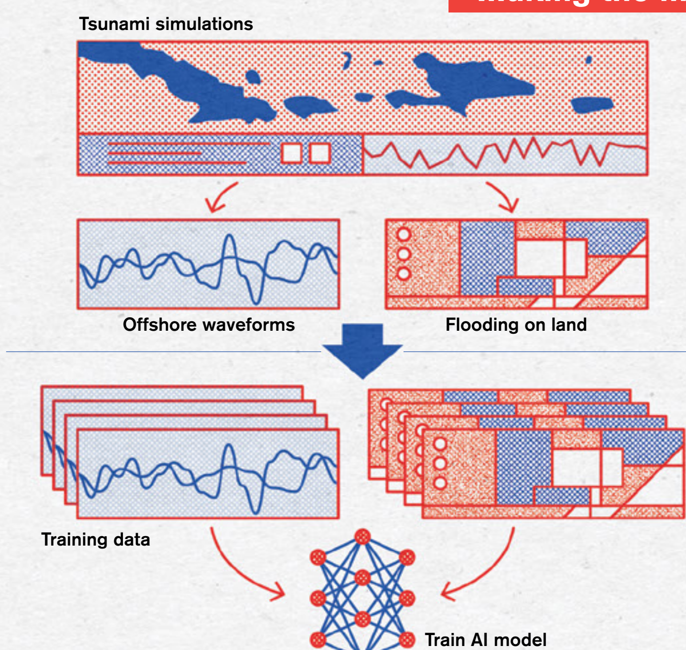
"In AI-based tsunami prediction, properly designed training data is important. In the future, we will further leverage Fugaku's high performance and high speed to generate various tsunami scenarios with the aim of predicting 'unexpected' tsunamis," concluded Oishi. S



Keeping an AI on disasters

The Fugaku-trained AI model not only delivers real-time tsunami flood predictions, but can also be deployed on your run-of-the-mill desktop computer. Here's how it works.

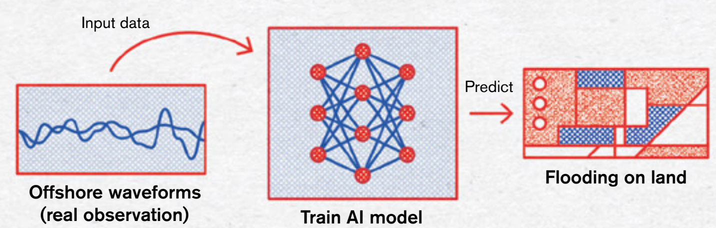
Making the model



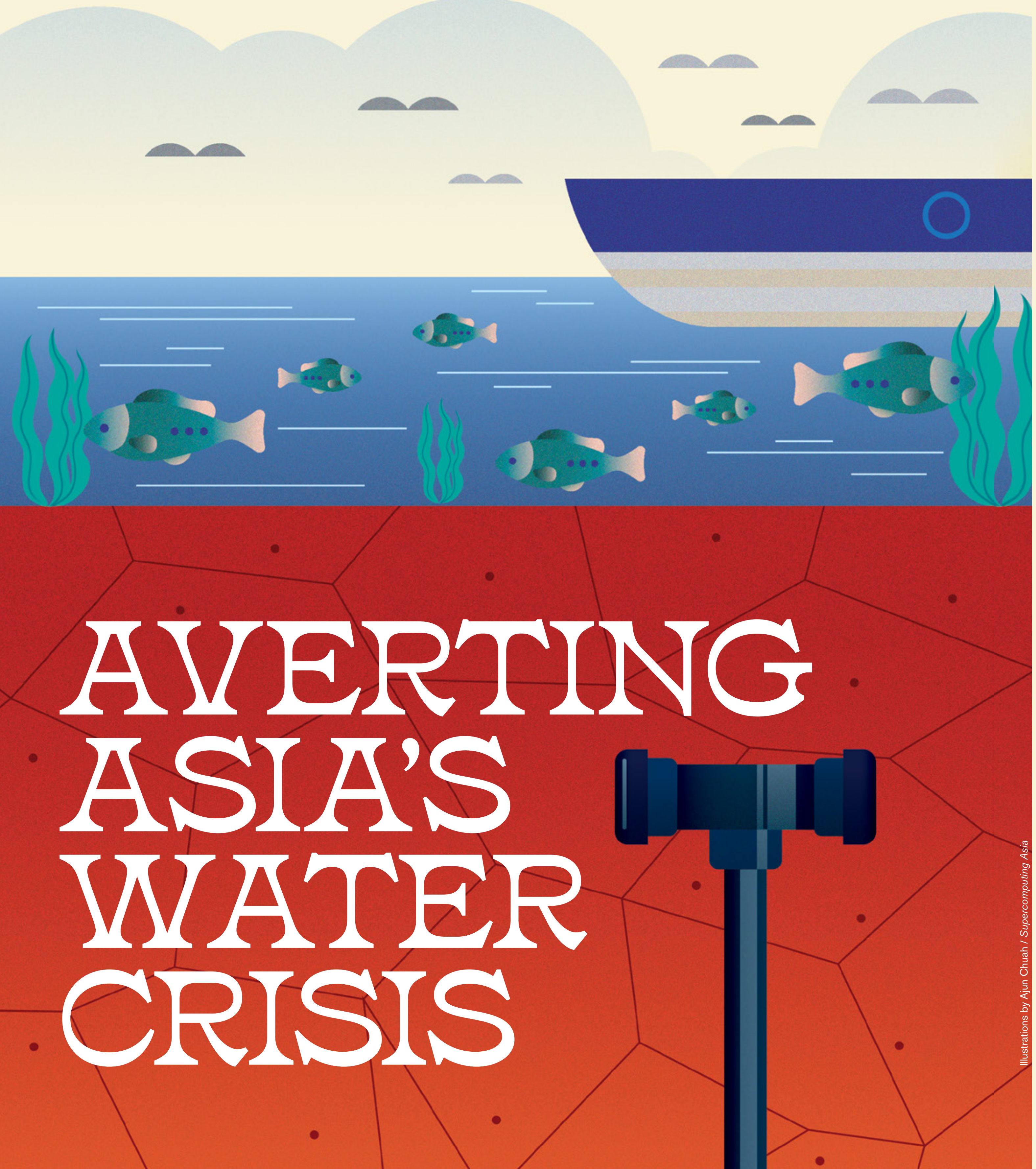
1 Generation of training data:
High-resolution tsunami simulations for 20,000 possible scenarios were generated on Fugaku.

2 Training of AI model:
The simulated data is then used to train the AI model, allowing it to predict land flooding based on offshore tsunami waveform observations.

Putting the platform into practice



3 Real-time prediction:
When an earthquake strikes, the AI model installed on a desktop computer can predict tsunami flooding within seconds.



AVERTING ASIA'S WATER CRISIS

Illustrations by Ajun Chuah / *Supercomputing Asia*

Through high-speed, high-resolution exascale computing, researchers and citizen scientists are tackling water stress across Asia by discovering better ways to treat water and monitor its flow.

By **Erinne Ong**

For many communities around the world, rivers and seas are their lifelines. To meet nutritional needs, fisherfolk haul in marine catches, while farmers need constantly flowing water to irrigate their agricultural lands. For sanitation, drinking and livelihood security, access to clean water is arguably the most vital resource. Asia, however, is facing a snowballing water crisis.

More than half of the global population resides in Asia, with urban population growth expected to rise by a staggering 60 percent by 2025. Yet the region has less freshwater, at just under 4,000 cubic meters allocated to each person per year, than every other continent on the planet, barring Antarctica. By 2030, the demand for freshwater will far surpass supply by 40 percent if interventions are not put in place.

The effects of such a daunting water gap are already tangible today. Take India, for example, where over 90 million lack access to safe water and nearly 230 million lack access to improved sanitation, such as proper sewage systems and private toilets. As many households continue to depend on untreated surface or groundwater, the health and economic toll is on the upswing—21 percent of India's communicable disease cases are linked to water stress.

Indonesia faces a similar situation with groundwater dependence, as less than half of the population had access to piped water in the 1990s, playing a role in the Jakarta's sinking landmass today. While targets sought to improve coverage to 98 percent by 2017, the real figure stood at just under 60 percent.

As climate change and water shortage collide, communities may become increasingly burdened by frequent disasters, worsening health and a planet sinking in untreated waters. Urgently, scientists and innovators are looking towards the pinnacle of high performance computing (HPC)—exascale computing—to turn the tide in Asia and the globe's water crisis.

SCALING UP SUPERCOMPUTING POWER

The fastest machines on the planet can solve a whopping quadrillion (10^{15}) calculations per second, earning them the right to be called petascale systems. With such computational power, they are already speeding through complex problems and detecting patterns from tons of data that no human could ever manually scour through in their lifetime.

But across Asia, researchers and industry leaders are now making strides towards the elusive exascale, capable of a quintillion (10^{18}) operations each second or one exaFLOPS. Winning the 2021 Gordon Bell Prize for HPC, the Chinese team behind the Next Generation Sunway supercomputer recently showcased their machine could reach speeds of up to 4.4 exaFLOPS, rivaling the power of Google's Sycamore quantum computer.

Scientists at Tsinghua University in China have also developed new memory management technology to bump up Sunway's capabilities in artificial intelligence (AI) algorithms, which learn from input data and improve over time. Their innovation transformed variably sized data sets and filed them in Sunway's memory slots, improving access to data without disrupting the machine's main memory.

Not only can exascale computers solve typical AI problems faster, but they would importantly enable more realistic simulations of processes, from the natural environment to synthetic industries. These would open the floodgates for HPC's potential to advance scientific discovery and develop impact-driven applications, such as by generating more exact maps of the Earth's water bodies, climate patterns and any disruptions to them.

With higher computing speed comes greater resolution—referring to seeing systems and patterns in finer detail—and therefore more accurate simulations and predictions. For example, simulations could zoom in to storms in specific cities, looking into microclimates that depend on local situations like the presence of valleys, amount of forest coverage and other structures.

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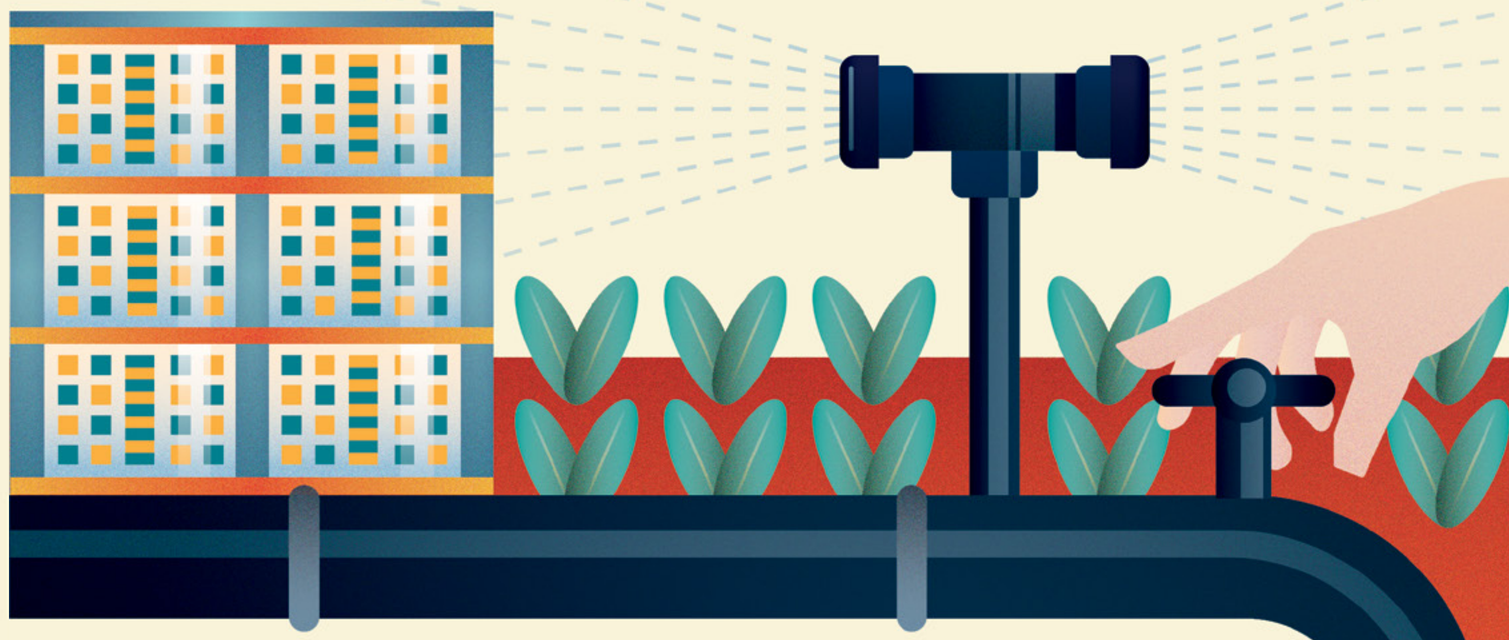


INTO THE EYE OF THE STORM

Climate change and catastrophic events are inherently intertwined with the water crisis, with 74 percent of all natural disasters between 2001 and 2018 being related to water. With altered climate patterns, the normal water cycle is also shifting, causing droughts and water shortages in some areas and heavier flash floods in others.

To build up disaster resilience, Aleph, the 1.43-petaFLOPS supercomputer at South Korea's Pusan National University, simulated historical climate patterns and atmosphere-ocean interactions over regions and countries. These interactions are key to how storms intensify or weaken over time, enabling the model to predict landfalling tropical cyclones and their destructive potential.

Given the tantalizing volume of climate data available, the simulations ran for 13 months—not an easy feat on any level. But the power of exascale computing could potentially accelerate the process and reduce calculation errors.

Meanwhile, in the heart of Japan, the world's top supercomputer, Fugaku, has a peak speed surpassing one exaFLOPS at the single precision or 32-bit level. But based on the LINPACK benchmark measured at double precision or 64 bits, Fugaku has yet to break the exascale barrier, with a score of 442 petaFLOPS.

In early 2021, researchers from the University of Tohoku, University of Tokyo and Fujitsu Laboratories leveraged Fugaku's power to run 20,000 tsunami flooding scenarios. By running these simulations to train a deep learning model, they optimized the model's calculation performance to predict tsunami size and flooding effects in near real-time.

These models aren't limited to flowing water, either. Much of the planet's water is packaged as ice, such as the glaciers in the Himalayan mountain range. Besides rainfall, glacial melt and snow melt contribute to High-mountain Asia's water flows, which not only change with seasons but also differ according to the western or eastern side of the mountains. With more data and exascale-powered modeling, researchers can paint a more accurate picture of the local water cycle.

By better anticipating natural hazards, climate change-aggravated disruptions and fluctuating water sources, scientists and societal leaders together can devise mechanisms to limit the damage and ensure a sustainable water supply even when disasters strike.

Moreover, such monitoring efforts could aid agricultural planning. Rather than lose valuable resources to floods or droughts, farmers can adjust crop rotations to changing water patterns and gather their harvest in time.

BEYOND A GRAIN OF SALT

Besides mapping how water flows through both natural and human-made systems, exascale computing could transform water treatment and desalination, or the removal of salt from water. As 96 percent of the world's water resources are saline, humans have ingeniously built filters and treatment plants to turn unusable water into a safe supply. However, desalination as it stands may not yet be the silver bullet to the water crisis.

Purifying water comes at a stark cost: the faster the desalination, the higher the power required to push water through the filter or heat it up to separate liquid from salt. Because of this inevitable trade-off, pushing up the power output to accelerate desalination rate might solve one sustainability issue only to cause another planetary problem.

To resolve this dilemma, scientists are looking to make better membranes, but doing so is proving to be tricky business. For one, the exact dynamics of this trade-off relationship can vary depending on the initial water supply's salt content and the extent of salt removal needed—after all, clean water for sanitary purposes is much different from potable water.

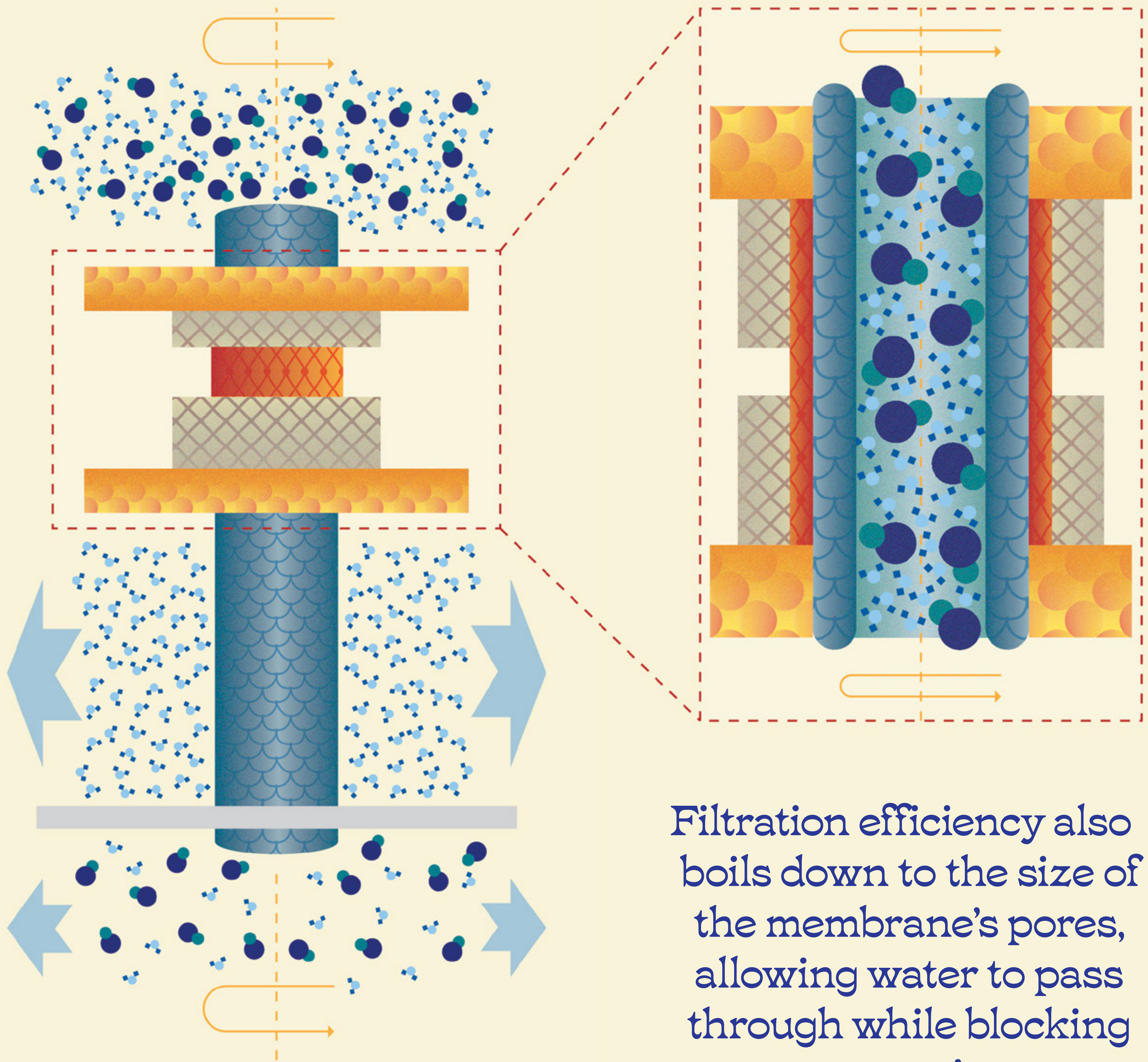
Filtration efficiency also boils down to the size of the membrane's pores, allowing water to pass through while blocking out contaminants. However, another trade-off exists between the membrane's salt rejection capacity against the speed and volume of water flowing through the filtering system.

Against this backdrop, researchers have been devising AI models to dissect material properties, identifying the best ways to design more efficient membranes. While AI has already revolutionized scientists' exploration of the chemical space—the set of all possible compounds we might ever encounter—only a tiny fraction of that space's infinite depths have been discovered.

With the dawn of exascale computing, however, such expansive modeling could accelerate materials discovery as well as analyze how structure and orientation influence the properties of existing membrane materials. In turn, this could yield more accurate insights into the characteristics that drive membrane filtration capacity.

Scientists from Japan, for example, ran virtual experiments to predict the properties of carbon nanotube materials, which could be used to devise filters with extremely tiny pores for enhanced water permeability. Within an hour, they completed over 1,700 virtual simulations via their deep learning framework, a type of AI that imitates the human brain by using multiple layers of networks to extract insights from raw data.

Exascale-powered AI could also equip innovators with an enhanced ability to simulate different scenarios at high speeds. By allowing precise manipulation of membrane parameters and accurate predictions of the results, these computing solutions could bypass the need for the typical time-consuming and wasteful trial-and-error processes during development.



Filtration efficiency also boils down to the size of the membrane's pores, allowing water to pass through while blocking out contaminants.

What was once a tedious ordeal of running experiments involving miniscule materials like nanosized filters could now be left to the supercomputer to figure out in a matter of minutes.

CASTING A WIDER DATA NET

Excitingly, breaking the exascale barrier doesn't solely rest on the shoulders of scientists. On the contrary, exascale can be achieved by the global public, as seen during the COVID-19 pandemic. Over a million citizen scientists—including thousands from Asian nations like Japan, Singapore and the Philippines—contributed a part of their computer resources to a shared platform called Folding@home. Collectively, they created the world's largest supercomputer, simulating the proteins found on the COVID-19-causing virus named SARS-CoV-2.

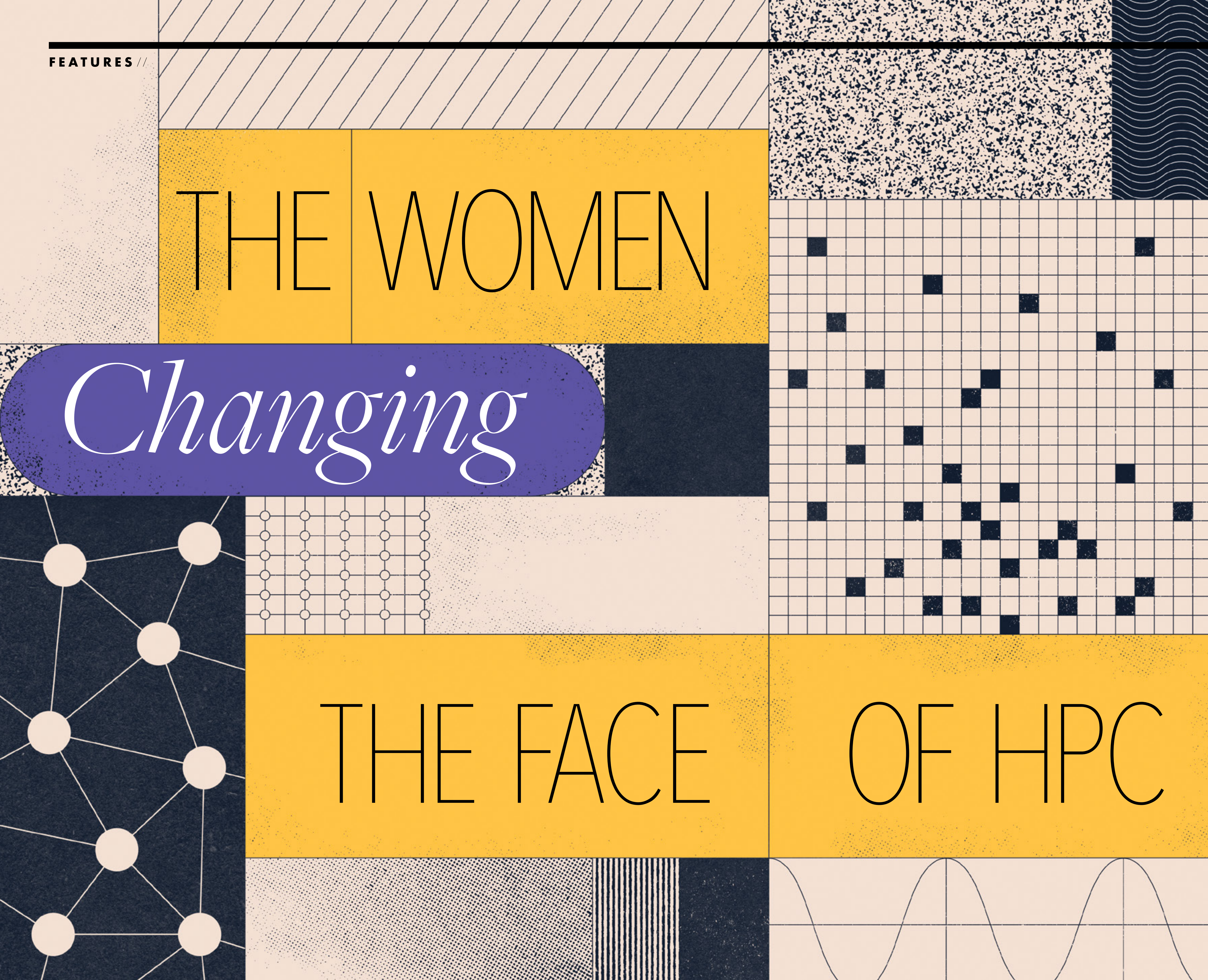
These protein dynamics captured the full range of conformations that molecules can adopt and how they change structure, lending unprecedented insight into their functions. However, as these simulations require significant computational resources, Folding@home distributes the task into smaller chunks that citizen scientists' personal computers can perform.

By constructing maps out of milliseconds of simulation data, researchers could then examine SARS-CoV-2 protein dynamics in much greater detail, highlighting the conformations relevant to viral replication inside human cells and identifying potential targets for novel therapies.

Whether running climate models or simulating filter materials, a citizen science-empowered exascale project could similarly make waves in addressing the water crisis. As more people become involved in addressing this pressing issue, the available data sources would expand and diversify, potentially showing highly localized data for each individual context. By tapping into the lesser studied areas across Asia, exascale computing can sift through these copious amounts of data, extracting novel insights with greater accuracy and speed.

With more data and the technological resources to process it efficiently, Asia's communities may soon witness a new wave of solutions for treating water, improving sanitation systems and preventing diseases and disasters in the face of population growth and changing climate patterns.

THE WOMEN *Changing* THE FACE OF HPC



Against all odds, women are taking the world of high performance computing by storm. Find out how two stellar researchers are advancing commercial computing and driving collaboration in the region.

By **Jill Arul**

Augusta Ada Byron, more commonly known as Ada, Countess of Lovelace, was a mathematician widely lauded as the first computer programmer. Despite naysayers doubting her contribution to Charles Babbage's Analytical Engine machine, today, her name and legacy stand out as a shining celebration of women in science, technology, engineering and mathematics (STEM).

Despite computing being significantly male-dominated, women pioneers have made their mark in the history of the field. An all-woman team programmed ENIAC, the first large-scale electronic machine that sparked the computer age, with Admiral Grace Hopper inventing the first high-level computer language.

As recently as 2017, however, women have represented only ten percent of all high performance computing paper authors. While there is not yet an abundance of women in HPC, their contributions have been impactful and far-reaching. *Supercomputing Asia* spoke to two female researchers who have made a name for themselves in the sector, not solely as women in computing, but as distinguished specialists in their fields.

Illustrations by Lam Oi Keat / *Supercomputing Asia*

DR. FREDA LIM

Computing everyday chemistry

A computational chemist by training, Dr. Freda Lim of Singapore's Agency for Science, Technology and Research (A*STAR) seeks to understand the interactions of consumer care formulations, like pain relief patches or skin care products, on consumers. Her research leads to effective solutions that go beyond the lab bench and onto the bathroom shelf.

As a young student pursuing her undergraduate degree, Lim was not fully convinced of her future in computing. Uninspired by what she perceived to be mundane, repetitive and unguided work at the time, Lim had all but made up her mind to never pursue a career in computational chemistry.

It wasn't until her graduate studies, influenced by the patience and intelligence of her supervisor, that she discovered the joy of building, refining and testing modeled electrons, atoms and molecules within a system—the core of computational chemistry.

Today, Lim conducts research in the area of consumer care products while playing a leading role in A*STAR's Institute of High Performance Computing (IHPC) as senior scientist, innovation lead and deputy department director. Her many hats culminate in advancing HPC in the consumer care industry and ultimately formulating the products we use in our bathrooms every day.

"My first 'real' computational chemistry project in graduate school involved semiconductor materials while my second was trying to find catalytic materials for carbon monoxide oxidation at IHPC," explained Lim. "Though both topics intrigued me, nothing fascinated me more than looking into the chemistry and interactions behind consumer care products because these are what we come into intimate contact with every day."

Harnessing the power of HPC, Lim and her team study the interactions between polymers and other ingredients like nanoparticles, surfactants or even other polymers. By using molecular dynamics simulations, Lim is also able to understand how these different formulations interact with soft material like hair and skin—contributing to the development of effective and safe products for people to use.

As a mentor to young researchers and a speaker at conferences like SupercomputingAsia and in the Skin Research Society Singapore webinars, Lim plays an active role in advancing Singapore and Asia's HPC landscape.

"The Asian presence in the field of HPC has been growing consistently over the last decade with with Japan's K computer and Fugaku, and China's Tianhe systems," she said. "My hope for the coming years is for the power of HPC to be democratized and accessible to students in more parts of Asia, so that we can benefit from a healthy and continuous pool of talent that can be trained for careers in HPC."

DR. CHRISTINE OUYANG

A team sport

In addition to being boosted by accessible education and mentorship, the world of HPC is also spurred by collaboration between academia, industry and government entities as they work to address global challenges like climate change and public health.

A strong proponent of this type of collaboration, and one of the changemakers leading the effort, Dr. Christine Ouyang holds several titles at IBM as a distinguished engineer, master inventor and IBM systems CTO lead. Equally passionate about education in HPC, part of Ouyang's work has revolved around the IBM Global University Programs designed to build relationships with academic institutions.

"We have provided technologies including hardware and software, course materials, IBM PhD fellowships, faculty awards and other academic awards to support research and skills development," Ouyang shared.

Launched over six decades ago, the partnerships forged with schools around the world, from Switzerland to Pakistan, have helped grow the talent pool for private enterprises and government agencies, accelerate innovation from research to market and drive economic development with startups in the region.

In fact, from 2012 to 2013, IBM established 13 Collaborative Innovation Centers (CICs) to advance emerging tech fields like big data, advanced analytics and cloud computing. One such partnership Ouyang worked on continues to bear fruit at the National University of Singapore (NUS). With the launch of this CIC, IBM provided NUS with analytics and artificial intelligence (AI) software, computing hardware as well as industrial use cases from clients and mentors for students. These are all resources that are put to good use in nurturing HPC talent in Singapore.

With 21 years at IBM under her belt, Ouyang has witnessed first-hand what each stakeholder can bring to developing new technologies for advanced computing. She believes that when resources are combined, what emerges is not only beneficial for all parties but often exceeds the results that any one organization could have achieved alone.

"Each stakeholder brings something unique to a problem," she explained. "Academia will provide curious minds eager to work on a problem with a professional network to help them grow. Government agencies typically offer funded challenges that drive academia. Technology providers offer resources like funding and access to consulting. Finally, industry can bring real-world challenges and its subject matter expertise."

With the HPC market continuing its steady rise and expected to reach nearly US$56 billion by 2028, it's no wonder that schools and organizations all over the world are looking to encourage more women to join the field. A 2020 study by AnitaB.org—a non-profit that builds upon the work of Anita Borg, a pioneer in the HPC industry, to recruit and advance women in technology—found that overall representation of women in tech has been increasing steadily and was up 2.9 percent since 2018.

As we continue to understand the trends, highlight the trailblazers and encourage aspiring young computer scientists, researchers like Dr. Freda Lim and Dr. Christine Ouyang represent powerful examples of the success that can be achieved in the HPC space—no matter your gender.

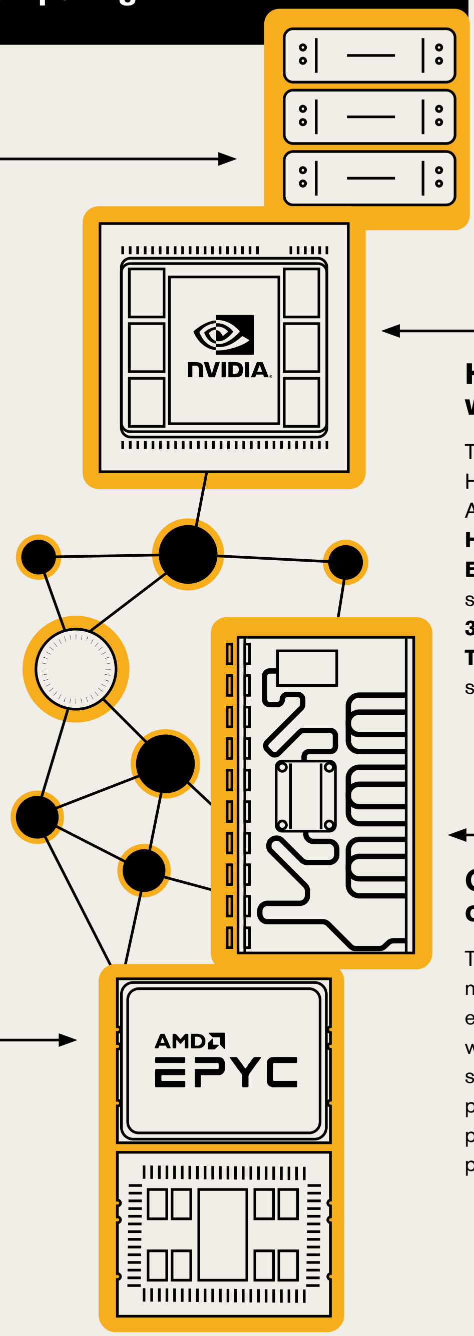
Super Snapshot

SUPERCOMPUTER SPOTLIGHT: ASPIRE 2A TO ARRIVE IN 2022

A sneak peek inside Singapore's next step in supercomputing

As the saying goes, out with the old and in with the new. After five years of operation, the Advanced Supercomputer for Petascale Innovation Research and Enterprise (ASPIRE 1), Singapore's first national petascale supercomputer, will gain a crucial boost thanks to a S$40 million hardware upgrade.

The aptly-named ASPIRE 2A, set to be operational in early 2022, will be eight times more powerful than the present iteration and could soon be one of the world's top 20 most powerful supercomputers. Take a glimpse into the next frontier of the city-state's supercomputing ambitions.



Stepping up storage

With 10 petabytes of storage and over 300 Gbps of reading and writing performance speeds, ASPIRE 2A could land among the upper echelons of the TOP500.

Hitting two birds with one stone

To optimize and accelerate HPC and AI applications, ASPIRE 2A will use the **HPE Cray Programming Environment** integrated software suite along with **352 NVIDIA® A100 Tensor Core GPUs** for such workloads.

Expanding network infrastructure

The **SingAREN-Lightwave Internet Exchange (SLIX)** from the Singapore Advanced Research and Education Network (SingAREN) will provide greater connection between users and supercomputing resources with multiple 100 Gbps links.

Clearing data congestion

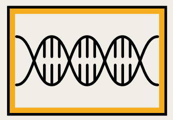
The **HPE Slingshot** network will enable the execution of data-intensive workloads by supporting link speeds of 200 Gbps and providing over 1.2 billion packets per second per port.

Upgrading computing capacity

ASPIRE 2A's improved capabilities will be powered by over 100,000 **3rd Gen AMD EPYC™ processors** containing up to 64 cores, 128 lanes of PCIe® Gen4 connectivity and 4 TB of memory.

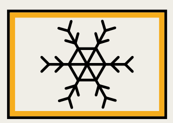
Upcoming Applications Of ASPIRE 2A

Deciphering 100,000 Singaporean genomes

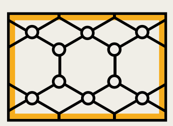


Designing digital twins of products and cities

Powering efforts to cool Singapore



Accelerating novel materials development

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