

NEWSBYTES

July 2023



In this issue



Corporate News

Fostering the next generation of HPC leaders

Taking the guesswork out of leukaemia

Shoba Ranganathan awarded the Outstanding Contributions to the International Society for Computational Biology (ISCB) Award

Tackling antibiotic resistance with HPC

Shared News

SoftServe Partners with NQCH And IMDA to Drive Singapore Quantum Computing Initiatives with Singapore's Inaugural Quantum Bootcamp 2023

SingHealth scaling digital twin project beyond disease outbreak monitoring

Japan's METI to build new supercomputer to help develop AI at home



CORPORATE NEWS

Fostering the next generation of HPC leaders

As the world enters the era of exascale computing, events like the EU-ASEAN HPC School are connecting young scholars across the region with new technologies, experts and each other.



Interested to have your research published in NSCC's NewsBytes?

We are looking for *guest writers / contributors* to be part of our e-newsletters, which are sent out to a subscriber base of more than **7,500** monthly.

If you are interested in contributing content to our NewsBytes, drop us an email at e-news@nsc.sg and we'll be in touch with you!

In 2019, Dr Piyawut Srichaikul traveled 9,673 km from his home city of Bangkok to Barcelona, where he joined researchers from around the world at the Association for Computing Machinery (ACM) Summer School on High Performance Computing (HPC). Co-organized by the Barcelona Supercomputing Center (BSC-CNS), the school featured a full week of lectures and hands-on exercises with some of the biggest names in HPC.

At the event, Srichaikul had an idea. “Instead of flying people to the EU,” Srichaikul asked himself, “What if we could bring a school like this to ASEAN?” Srichaikul is a co-chair of the ASEAN HPC Taskforce and also a senior researcher at the NSTDA Supercomputer Center (ThaiSC), located in Khlong Nueng, north of Bangkok.

It took a few years and the help of the Jakarta-based Enhanced Regional EU-ASEAN Dialogue Instrument (E-READI), but this idea has now become reality: the University of Kasetsart in Bangkok recently hosted the second EU-ASEAN HPC School—the first to be held in person.

The first edition of the event, held in Bangkok in 2021, was fully remote given the health protocols in place at the time. But for the 2022 EU-ASEAN School, a total of 60 students selected from a pool of 300 applications from all 10 ASEAN member states were able to attend the event in person. The School ran from December 5 to 10, 2022, and is one of a growing number of programs and activities in the region encouraging young scholars to learn more about HPC-enabled research.

The EU-ASEAN HPC School founded in 2021 is designed with 2 goals. The first is to create a talent pipeline for the HPC industry and the second, more long-term goal is promoting regional collaboration. According to Dr Fabrizio Gagliardi, Director of the EU-ASEAN HPC School, “The time is now, and the opportunity is here” for young people to explore the different HPC programs available.

NSCC has since organised 2 competitions – 2022 APAC HPC-AI Competition and Inaugural HPC Innovation Challenge for the Environment – to empower young scientists to dive into HPC research. With the opportunities available, the future of ASEAN HPC promises exciting findings in different research areas.

Head over to the [January 2023](#) issue of NSCC’s Supercomputing Asia Magazine to read the full article to find out more about the insights and opportunities in ASEAN HPC!

This article was first published in the print version of Supercomputing Asia, January 2023.

Credit: Marinel Mamac, Writer, Asian Scientist Magazine

[Back to main content list](#)

Shoba Ranganathan awarded the Outstanding Contributions to the International Society for Computational Biology (ISCB) Award

Congratulations to Professor Shoba Ranganathan! The Outstanding Contributions to the International Society for Computational Biology (ISCB) Award was initiated in 2015 to recognize members who have made beneficial and lasting contributions to the Society through their leadership, service, and educational work, or a combination of these three areas. Shoba Ranganathan is a Professor of Bioinformatics at Macquarie University in Sydney, Australia, as well as a consultant to NSCC.



Apart from being the awardee for the ISCB award, Shoba was also selected as **ISCB Fellow in the Class of 2023**. The ISCB Fellows program was created to honor members who have distinguished themselves through outstanding contributions to the fields of computational biology and bioinformatics.

[Back to main content list](#)

Tackling antibiotic resistance with HPC

Researchers from A*STAR BII leverage supercomputing resources to accelerate the process of new antibiotic development.

Antimicrobial resistance (AMR) is a global healthcare issue, which has resulted in 1.27 million deaths in 2019 and is expected to cause 10 million deaths by 2050. The excessive use of antibiotics is often cited as the major contributing factor for the evolution of bacterial resistance. Traditional antibiotics often fail in the treatment of multi-drug resistant (MDR) bacterial infections as they interfere with biosynthetic pathways that can easily be circumvented by the bacteria through mutation.



Membrane-active antimicrobials such as synthetic mimics of antimicrobial peptides (SMAMPs), is a potential solution to this problem as these molecules interfere with membrane function, an essential component of bacterial survival. However, the development of SMAMPs is largely by trial and error and little is known about how the membrane should be designed to target molecules due to the lack of molecular principles and poor understanding of the action mechanism.

A research team at [A*STAR Bioinformatics Institute \(BII\)](#) is tapping on NSCC's supercomputing resources to employ a multi-disciplinary approach that involves in silico simulations and experimental validations to accelerate the development of membrane targeting antimicrobials. For example, based on the atomistic insights obtained from in silico simulations, the team has developed a pharmacophore model for the design of new antimicrobials targeting the bacterial membrane (Figure 1), which greatly accelerated the development of new antibiotics. One of the in silico designed compound displayed excellent antimicrobial activity and has been patented for further development.

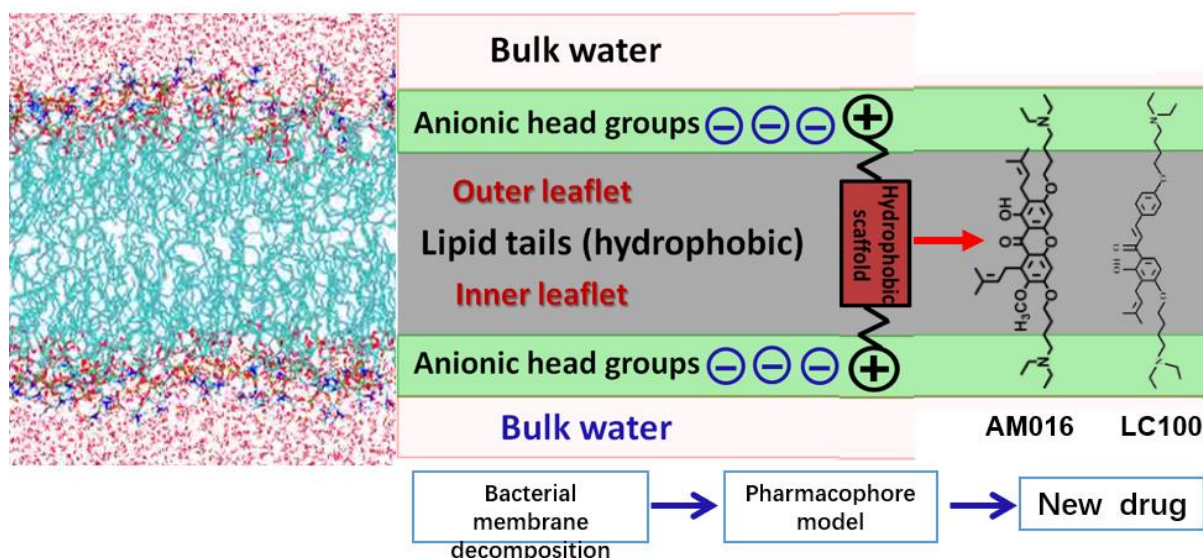


Figure 1. A pharmacophore model for rational design of membrane targeting antimicrobials

“NSCC’s supercomputing cluster is an indispensable resource for us to carry out large scale molecular dynamics simulations, which not only deepens our understanding of the action mechanism, but also provides useful guidelines for the design of new antimicrobials.”

Dr Li Jianguo
Senior Research Scientist
Bioinformatics Institute,
A*STAR



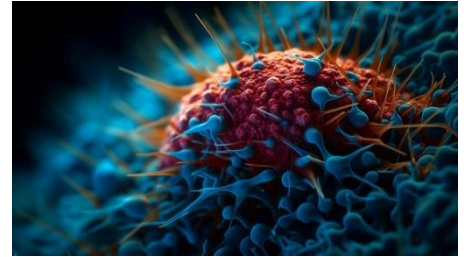
New analogues will be designed based on the atomistic insights from the simulations. The translation of in silico insights to practical antibiotic development will greatly accelerate the drug discovery process, providing cost saving measures, as well as the basis for a continued developmental process to meet new challenges presented by pathogens.

To find out more about how NSCC’s HPC resources can help you, please contact e-news@nscg.sg.

Taking the guesswork out of leukaemia

The Malaysia-Singapore Study Group is harnessing high performance computing to further improve the overall treatment outcome for children, adolescents and young adults with Acute Lymphoblastic Leukemia.

Acute Lymphoblastic Leukemia (ALL) is the most common cancer in children. ALL is caused by a constellation of recurrent genomic alterations. Although recurrent, there are many genetic drivers thus making it challenging to diagnose clinically. Additionally, standard laboratory tests are only informative in 60% of patients.



Recent whole genome approach allows unparalleled and unbiased look into these genetic drivers of leukaemia. To harness this approach, the Malaysia-Singapore (Ma-Spore) Study Group is tapping on NSCC's high performance computing resources to develop a diagnostic workflow based on whole transcriptome sequencing. Using NSCC's server clusters, the team constructed an analysis pipeline with 400 historical samples from Asian ancestry. Cobbled with the US and Guatemala dataset, results have shown that ancestry genetics influence the genetic drivers and outcome of ALL in children.

"Identifying the genomic lesions using next generation sequencing data is computationally intensive and requires large amounts of storage. Thanks to the computing and storage facilities of NSCC, we were able to study the data of large sets of patients at the same time, uncovering the unique genomic landscape of childhood leukaemia in Asia."

*Dr Li Zhenhua, Senior Research Fellow,
Department of Paediatrics, National University
of Singapore*

Over the past 20 years, the Malaysia-Singapore (Ma-Spore) Study Group, under the leadership of A/Prof Allen Yeoh at the National University of Singapore, has succeeded in improving the survival outcome of ALL from ~75% to ~90% and remarkably this achievement is made with majority of patients receiving less chemotherapy. The key to this remarkable success is deep knowledge of the genetic driver of each patient's leukaemia.

The team's workflow is currently used in Ma-Spore ALL 2020 study for patient diagnosis. This workflow is used for adult leukaemia in Singapore and Johor as well demonstrating its practical application in real-world scenarios. The group has found the genetic drivers in over 90% of the patients, which allows deep and comprehensive diagnosis for ALL in Malaysia and Singapore.

To find out more about how NSCC's HPC resources can help you, please contact e-news@nscg.sg.

[Back to main content list](#)

**B THE LAST
BYTE...**

<SHARED CONTENT>

Shared articles and news from the HPC world.

SoftServe Partners with NQCH And IMDA to Drive Singapore Quantum Computing Initiatives with Singapore's Inaugural Quantum Bootcamp 2023

Bootcamp-style educational program fosters a new generation of quantum computing experts and innovations.

SoftServe, an IT consulting company offering software development and digital services, in partnership with the National Quantum Computing Hub (NQCH) and the Infocomm Media Development Authority (IMDA) announced the successful launch of Singapore's inaugural Quantum Bootcamp, a transformative educational program for students pursuing careers in quantum computing. Read more at Yahoo! [here](#).



Credit: Pixabay

[Back to main content list](#)

SingHealth scaling digital twin project beyond disease outbreak monitoring

Digital twins are now being applied for resource optimisation and healthcare facilities planning.

Over the past years, the public healthcare group noted the potential of the 3-Dimensional Disease Outbreak Surveillance System (3D-DOSS) test projects for real-life applications. The upcoming 4D-DOSS will not only apply digital twins – a living digital replica or 'twin' of a space or system – for near real-time monitoring, analysis, prediction and simulation of disease outbreaks; the technology will also be used for other use applications across SingHealth institutions by integrating it with data source systems, such as clinical data and bed management systems. Read more at Healthcare IT News [here](#).



Credit: Getty Images

[Back to main content list](#)

Japan's METI to build new supercomputer to help develop AI at home

Research arm will enhance country's top computing ability as early as next year

The Ministry of Economy, Trade and Industry (METI) will introduce a new cutting-edge supercomputer through its affiliated laboratory to support the development of generative artificial intelligence (AI) in Japan. The National Institute of Advanced Industrial Science and Technology (AIST) will develop a supercomputer with a computing capability roughly 2.5 times greater than its existing machine as early as 2024. Read more at Nikkei Asia [here](#).



Credit: Nikkei

[Back to main content list](#)



Powering Innovation
Supercomputing in Asia

National Supercomputing Centre (NSCC) Singapore

1 Fusionopolis Way, Connexis South, #17-01 Singapore 138632