National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

May 2022

In this Issue…

CORPORATE NEWS

5th Annual APAC HPC-AI Student Competition Launched

Jointly organised with NSCC Singapore and the National Computational Infrastructure (NCI) Australia, the 5th iteration of the regional APAC student competition aims to tackle the pressing global problems of human health and sustainability.

Spanning six intensive months, the annual competition hosts graduate, advanced degree and undergraduate students from across the APAC region to develop their skillsets and challenge their understanding of high performance computing (HPC) and AI technologies as well as showcase their mastery of the two disciplines in a spirited international competition. The 2022 APAC HPC-AI Competition will see more than 100 students representing 22 teams from 12 countries and regions in APAC vying for the coveted crown of this year's best team.

This year's competition includes tasks and challenges focusing on three of the hottest research topics and mission critical issues that leverage the power of HPC and AI technologies to further understanding and find solutions for the improvement of human health and sustainability of our planet's resources and environment.

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@nscc.sg** and we'll be in touch with you!

These topics include developing future green energy mechanisms using HPC technology; Analyzing and training satellite data with AI technology for better climate modeling and weather forecasting, and Using deep learning technology to perform DNA Sequence Fast Decoding for enhanced disease prevention and medical care.

HPC-AI Advisory Council, NSCC Singapore and NCI Australia will provide support in the form of HPC and AI fundamental education and competition task training for all participants. Additionally, NSCC Singapore and NCI Australia will provide the CPU and GPU clusters from their HPC centers for all teams to practice their code.

"The human health and environment related tasks of the 2022 competition are especially relevant to the APAC region that hosts some sixty percent of the world's population. The annual HPC-AI Competition is a crucial training ground that nurtures the next generation of HPC and AI professionals, and prepares them to meet such challenges head on," said Associate Professor Tan Tin Wee, Chief Executive of NSCC Singapore. "Our collaboration with the HPC-AI Advisory Council and our close partners from NCI Australia will help accelerate the advancement of HPC and AI skillsets of the region's student communities."

The winning teams will be announced in November 2022 followed by an official award ceremony to celebrate all the competitors at the annual SupercomputingAsia 2023 conference, which will be held in Singapore from 28 February – 2 March 2023.

For more information on the competition please visit www.hpcadvisorycouncil.com.

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NSCC's recent events

20 April 2022

Joint RP Nvidia HPC training workshop by NSCC

Digitalisation has given birth to an avalanche of data - the purposeful use of which can power new innovations in Artificial Intelligence, the Internet of Things, Predictive Analytics, Robotics and more. Crucially, by pairing the multitude of datasets with High-Performance Computing (HPC) technologies, businesses today can scale quickly and derive insights, discoveries and solutions more efficiently than before.

In this 3-hour workshop, jointly conducted by NSCC and Republic Polytechnic, participants experienced how to accelerate their AI tasks and applications using NSCC's supercomputing resources.

29 April 2022

HPC Innovation Challenge for the Environment Briefing Session & DC Tour

The hybrid Briefing Session served as an introduction to the High-Performance Computing Innovation Challenge for the Environment - an NSCC initiative that provides innovators an opportunity to access their resources and build transformational solutions, to address one or more of the following challenge statements for our environment below.

- Enabling a Data-Centric Approach to Manage Our Environment
- Reducing Carbon Footprint
- Planning Our Urban Environment Better
- Building Greater Resilience for Climate Change

Participants who attended the Briefing Session in person had the opportunity to tour Singapore's very first national petascale facility, the ASPIRE 1 Supercomputer as well!

Applications for the High-Performance Computing Innovation Challenge for the Environment are now open!

Head over to https://www.padangecosystem.com/en/page/hpcic-2022-en for more information about the Challenge and to view the recording of the briefing session.

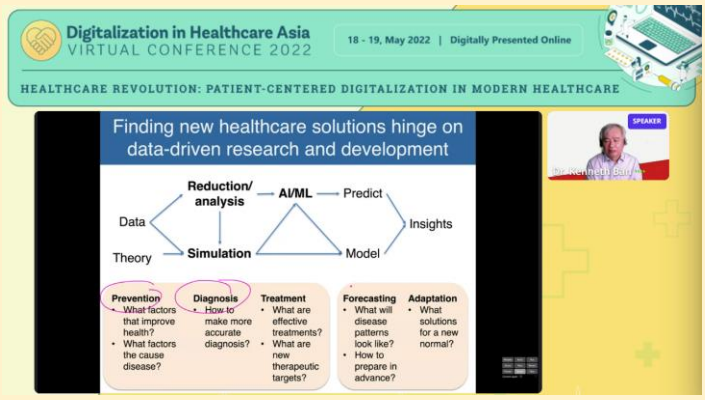
APPLY NOW

19 May 2022

Digitalization x HealthcareAsia 2022 Summit

With digital healthcare becoming more data-driven with the advent of omics technologies and the ability to profile multi-dimensional parameters, analysis of these large and complex datasets can hasten the generation and testing of hypotheses to derive new insights that can improve healthcare outcomes. However, as the size and complexity of data grows, the need for more computational and storage resources has become the bottleneck in analytical pipelines. In recent years, high-performance computing systems are increasingly being used to resolve said bottleneck and accelerate data-intensive pipelines by taking advantage of multiple nodes and high-speed interconnect systems for parallel computing.

In this summit, Dr Kenneth Ban, Programme Director from NSCC shared how NSCC works in partnership with stakeholders in the biomedical and healthcare sector to advance data-intensive analytical pipelines for digital healthcare. Catch the recording of Dr Ban's presentation here.



Head over to www.nscc.sg/events and follow NSCC's LinkedIn and Facebook channels to be kept up to date on all of NSCC's upcoming events and activities.

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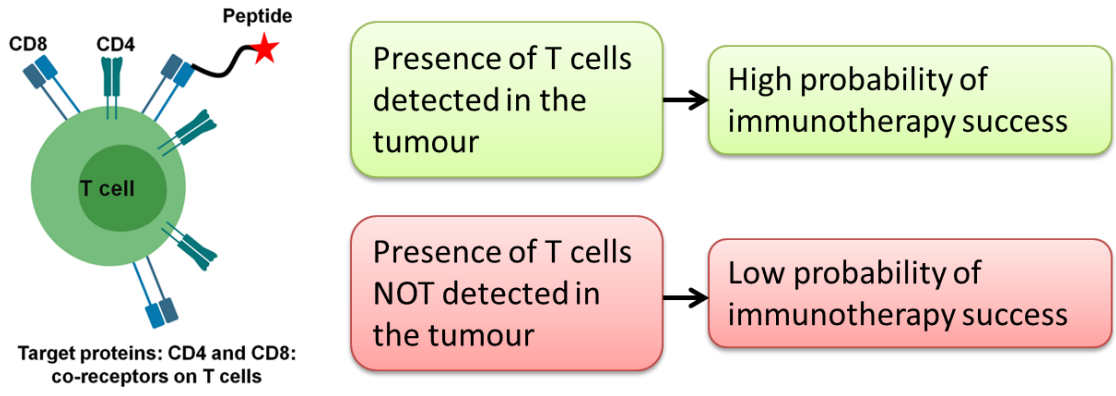
Supercomputers accelerate research to develop more effective cancer immunotherapy

A*STAR researchers leverage supercomputing to predict immunotherapy outcomes in order to better select treatments best suited for patients.

Immunotherapy is a breakthrough cancer treatment that relies on activating the immune system to treat cancer and has been quickly developing over the past decade. However, the success rate remains low (about 20% to 30%) and predicting immunotherapy outcomes has been challenging.

The presence of infiltrating immune cells, such as cytotoxic T cells, in the tumour microenvironment has been linked to improved immunotherapy success. The goal of the CITI (Cancer ImmunoTherapy Imaging) Programme, led by a research team at the Duke-NUS Medical School, is to develop novel peptide-based imaging probes which will bind to proteins on the T cell surface. Such imaging probes, when tagged with a radioisotope can be combined with PET imaging to non-invasively detect the presence of T cells in the tumour. This can aid physicians in predicting immunotherapy outcomes and selecting the appropriate treatments that will best suit patients.



Credit: CITI Programme

A team of researchers from A*STAR's Bioinformatics Institute (BII) is collaborating with the CITI Programme to design and refine lead peptides. Several peptides have been identified so far and are in various stages of in vitro validation and in vivo testing.

"The peptide designing process is complicated as neither the peptide sequence nor the binding site is known. Hence, several potential candidates need to be screened in parallel. NSCC's supercomputing resources allowed us to run multiple simulations simultaneously and reduce screening time by many folds."

Shruti Vijay Khare
Senior Post-Doctoral Research Fellow
A*STAR BII

"Our project involves designing peptide candidates using known binders of target proteins and structural database mining where the identified candidates are screened in silico using molecular dynamics (MD) simulations," explained Dr Shruti Vijay Khare, a Senior Post-Doctoral Research Fellow at A*STAR's BII. "The supercomputer resources offered by NSCC are crucial for parallel screening of several peptide candidates as multiple simulations can be run simultaneously. This allows high throughput screening and speeds up the design process." The ASPIRE1 supercomputer cluster was used to perform MD simulations using GPUs.

The eventual goal for the research team is to translate the research on these radiopharmaceutical imaging probes into viable applications for clinical settings and for the commercial market.

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

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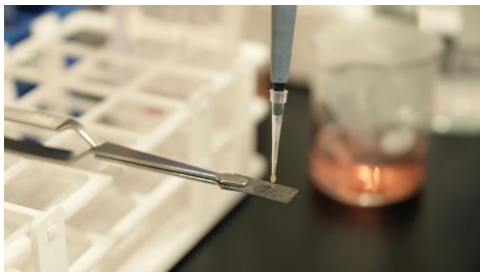
Research on 'greener' fertiliser production using HPC-powered simulations

Researchers at NTU are tapping HPC resources to derive a process for highly selective urea production in order to reduce carbon emissions.



Credit: Nanyang Technological University

Urea (CO(NH2)2) provides low-cost nitrogen and is a vital component in the fertiliser that is used in growing the crops that provide food for the world's population. Urea is mainly synthesised using ammonia (NH3) with carbon dioxide (CO2).

The Haber–Bosch approach is still the current process that dominates the industrial production of NH3, of which approximately 80% is consumed to lay the foundation for urea synthesis. This process involves energy-intensive reactions operating under harsh conditions (100–200 bar and 400–500 °C), and accounts for more than 2% of global energy consumption. With the global drive towards reducing the dependence on fossil fuels and lowering environmental pollution, tremendous efforts have been diverted to the development of innovative routes that enable the synthesis of NH3 under milder conditions.

Joint research teams from the Nanyang Technological University (NTU) are working on a process for highly selective urea production using indium hydroxide ($In(OH)_3$) through the electrochemical coupling of NO_3− with CO_2. With this catalyst, the {100} facets favour the direct C–N coupling by means of the reaction between $*NO_2$ and $*CO_2$ intermediates. $In(OH)_3$ with single {100} facets ($In(OH)_3$-S) could potentially produce an average urea yield of 533.1 μg h−1 mgcat.−1 at −0.6 V versus the conventional reversible hydrogen electrode (RHE) process, as well as the ultra-high FE process of 53.4%, with nitrogen selectivity (Nurea-selectivity) of 82.9% and carbon selectivity (Curea-selectivity) of ~100%.

"Simulating complex systems with developed programmes on NSCC is way faster compared to running them on personal PCs or workstations. NSCC has helped and is continually helping our team to achieve hundred-folds of reduction in calculation time."

Li Shuzhou
Associate Professor
Nanyang Technological University (NTU)

"The team was able to leverage on NSCC's high-performance computing (HPC) resources to perform the advanced, compute-intensive simulations that were a crucial part of the research project," said Associate Professor Li Shuzhou, a long-time user of NSCC resources and overseer of the simulation work in this collaboration. "The supercomputing resource support highly accelerated our simulations and made it possible to publish this work in time."

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

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THE LAST BYTE...

<SHARED CONTENT>

Shared articles and news from the HPC world.

Fujitsu and RIKEN start joint research on next-generation IT drug discovery technology using the supercomputer Fugaku and simulation integrated AI

The joint project aims to accelerate DX (digital transformation) in drug discovery, explore promising new areas in this process, and dramatically reduce development period and costs for new drug development.

The joint research project will leverage high performance computing technologies and the supercomputer Fugaku to accelerate simulation integrated AI that combines Fujitsu's DeepTwin AI technology, which accurately acquires quantitative features from complex data by unsupervised learning, with molecular dynamics simulation using RIKEN's AI drug discovery simulation technology. It is expected that this approach makes it possible to improve the accuracy and speed of molecular simulation and establish innovative technologies that can predict changes in the structure of target proteins over a wide range. Read more at Fujitsu here.

Credit: RIKEN

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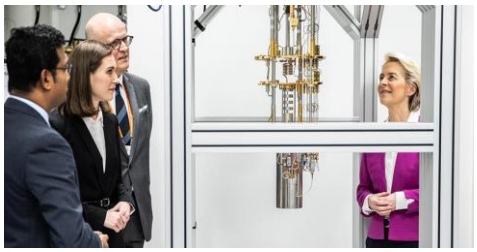
The Ecosystem: Finland punches above its weight in quantum

Finland's quantum ecosystem is attracting foreign start-ups and looking to build on a cooperation agreement with the US government.

Finns joke that their advantage in quantum computing is that the cold you need to run the processors comes for free. But make no mistake, the quantum ecosystem in Finland is heating up. Helmi, a five-qubit computer inaugurated last November in Espoo, will this month connect to the LUMI supercomputer in Kajaani, making blended computing projects possible. And in April, the country inked a cooperation statement with the US for quantum information science and technology, the first such agreement with a country in mainland Europe. Read more at Science Business here.



Credit: Laura Kotila/Prime Minister's Office

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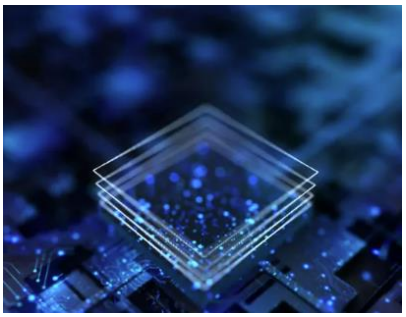
20 Years On: The Evolution of HPC

High performance computing (HPC) is at the core of every research institution and engineering business globally. However, it's only in the last decade that it's gathered momentum to where it is today and revolutionized the way we can solve the world's most complex conundrums.

If we are to look at the evolution of HPC, it was very much in its embryonic stage around 20 years ago and was just starting to find its feet. A relatively small resource that a handful of users would utilize for a particular field of research. It was also very manual. The components were not specifically designed for the tasks they were being used for. Things like GPUs for accelerated computing and high-performance interconnects based on open standards, like InfiniBand, just did not exist at the time. There has been incredible transformation over the past few years, so let's go back to where it all started. Read more at Technology Networks here.



Credit: Technology Networks

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