National Supercomputing Centre (NSCC) Singapore e-newsletter

January 2023

# NEWSBYTES



hardcore science

## In this Issue...



Corporate News	More to come for Singapore's national supercomputing in 2023	Register now for SupercomputingAsia 2023 (SCA23)!	Developing nanomedicines through the use of supercomputers
Shared News	Japan's Riken plans quantum link to supercomputer Fugaku	The world is heading for a 'quantum divide': here's why it	LUMI supercomputer puts GPU partition through its paces with



## More to come for Singapore's national supercomputing in 2023

matters

Here's a look back at some of the highlights for NSCC in 2022 and as we look forward to an exciting 2023 ahead!











#### ASPIRE 2A - Singapore's latest petascale supercomputer

#### Call for Early Use of ASPIRE 2A

The call opens the ASPIRE 2A to all NSCC, SingHealth and NVIDIA collaborated interested applicants for the early use of the system in preparation for the official hardware and software tools to support system launch. This will allow users to be healthcare and medical research at better prepared to use the system more Singapore's largest public healthcare effectively.

#### Another Green Data Centre Award

NSCC Singapore has been conferred a W.Media Southeast Asia Cloud and Datacenter (DC) Award 2022 in the Energy Efficient Innovation category for the new "NUS-NSCC i4.0 DC - A Tropical Supercomputing DC". The i4.0 DC had already been conferred a Building & Construction Authority (BCA) Platinum Green Mark Award for Data Centres last vear.

#### SupercomputingAsia (SCA) Goes Hybrid

SCA22 Conference, jointly organized by HPC centres from Singapore, Japan and Australia went hybrid for the first time ever, bringing the HPC community back together.

#### Launch of annual SCA Awards

The SCA Awards recognises and celebrates those who have contributed significantly in one way or another to HPC, or those who have been instrumental in the development of the HPC ecosystem.

#### New Public-Private Partnership to Support Advanced Healthcare Research

to develop a research ecosystem of cluster. These include a new supercomputer and access to advanced software, training and HPC-enabled pretrained AI models to significantly accelerate large-scale and complex healthcare research.

#### Growing the next generation of HPC leaders

#### Inaugural HPC Innovation Challenge for the Environment

Organised by NSCC and supported by GeoWorks, SGTech and SGInnovate, the HPC Innovation Challenge (HPCIC) aims to enable local organisations and students to innovate using HPC and apply HPC to address different areas for our environment.

#### The 11th Annual ISC 2022 Student Cluster Competition & 5th Annual APAC HPC-AI competitions

NSCC provides support in the form of HPC and AI fundamental education and competition task training for all participants as well as providing its HPC resources for.

#### New International Links Benefit New Collaborations to Develop Singapore Researchers

#### Australia - Singapore MOU on HPC Capabilities collaboration

Infrastructure (NCI) Australia ink Bio-Informatics, and user training, and data sharing for bioinformatics. both organisations over the next three years.

#### Plugged in to one of the world's fastest Singapore's supercomputers

supercomputer.

## **HPC-enabled Bioinformatics**

NSCC, Asia-Pacific Bioinformatics Network NSCC and National Computational (APBioNET) and Association for Medical and Singapore (AMBIS) partnership to deepen their joint activities collaborated to explore joint activities aimed into areas that will further improve at developing and promoting the use of technology, software development, staff high-performance computing in the field of

#### Supercomputing & Quantum Computing

Quantum Engineering Programme (QEP) launched three national Five Singapore research projects approved platforms to grow the country's capabilities to use HPC resources on Japan's Fugaku in quantum computing, quantum-safe system in the first-of-its-kind agreement communication and the manufacturing of between NSCC, R-CCS and RIST which quantum devices. NSCC is a key partner in enables Singapore researchers to have Singapore's new National Quantum regular access to the Fugaku Computing Hub and will host a quantum computing facility and provide the supercomputing power needed to develop and train the algorithms that could eventually be used on quantum computers







We would like to take the opportunity to thank all of you - our users, stakeholders, partners and friends - for your continued support. We look forward to working closely with you in 2023 to build a stronger HPC community in Singapore.

### NSCC wishes you all the best for the New Year and have a safe 2023 ahead!

Back to main content list

## Register now for SupercomputingAsia 2023 (SCA23)!

Join us at SCA23 for 4 days of insightful keynotes and talks by local and international industry leaders and experts across topics such as sustainability, green supercomputing, AI & machine learning and quantum computing.



Co-organised by HPC centres from Australia (NCI and Pawsey), Japan (RIKEN-CCS), Singapore (NSCC) and Thailand (ThaiSC), SCA is an annual conference that encompasses an umbrella of notable supercomputing and allied events in Asia and beyond with the goal to promote a vibrant and shared HPC ecosystem in Asia. The International Conference on High Performance Computing in the Asia-Pacific Region (HPC Asia) and Conference on Next Generation Arithmetic (CoNGA) will be co-located with SCA23.

Some of the SCA23 highlights include session tracks related to Inclusivity and Diversity, HPC-AI developments, Quantum Computing and Networking as well as several international collaborative tracks such as the HPC Centre Leaders Forum and the Asia Pacific Research Platform. The tracks are also supplemented by Industry talks highlighting the latest HPC technology innovations and developments, and industry workshops.

### **KEYNOTE SPEAKERS LINE UP**



Prof Satoshi Matsuoka Director RIKEN Center for Computational Science (R-CCS), Japan



Dr Benoît Dinechin Chief Technology Officer Kalray, France



Prof Michelle Spencer Deputy Director, Centre for Digital Innovation STEM RMIT University, Australia



Mr Mark Stickells Executive Director Pawsey Supercomputing Centre, Australia



Prof Amanda Barnard Senior Professor, Deputy Director, and Computational Science Lead The Australian National University, Australia



Prof Torsten Hoefler Professor of Computer Science ETH Zurich, Switzerland

Come join our line-up of exciting Keynotes, Speakers and Partners as we explore the role of supercomputers, and unravel the possibilities for HPC. Register now at https://www.sc-asia.org/registration-fee-structure/ or head over to https://www.sc-asia.org/ for more details on the conference.

**REGISTER NOW** 

Back to main content list

#### Designing safer nanomaterials and medicines with the of aid supercomputers

### Researchers from Nanyang Technological University leverage high-performance computing resources to better understand the interactions between nanomaterials and biological systems.

The field of nanotechnology is rapidly advancing and has the potential to revolutionise a wide range of industries, from medicine to electronics to energy. Nanomaterials, in particular, are utilised in the development of nanomedicines. Therefore, it is crucial to understand the interactions between nanomaterials and biological systems, such as cellular membranes, by carrying out systematic investigations on the pathological responses and molecular mechanisms in order to safely design, apply, and regulate novel engineered nanomaterials, in particular, 2D nanomaterials.

To date, most of the available data has been accumulated from studies on graphene-based materials. The results from these studies have shown that material geometries such as size and shape influence 2D materials' interaction with cell membranes, and that sharp edges from



"Tree with Forbidden Fruits in a Nanoworld": A simulation which illustrates how hBN nanosheets can induce water channels across lipid bilayer, leading to damage of the cell membrane. Credit: Qian Xuliang

graphene sheets can spontaneously penetrate cell membrane, leading to lipid extraction and membrane damage.

However, little is known about the biological interaction mechanisms of emerging 2D materials such as hexagonal boron nitride (hBN), a material which has great potential for application as substrates for electronic and optoelectronic devices, and as building blocks for engineered nanocomposites. What happens to a cell membrane upon the penetration of 2D materials with different sizes and shapes? How does hBN nanosheets interact with cell membranes? What is the driving force and the underlying mechanisms of such interactions.

"The NSCC HPC resources in the project played a key role in our research by speeding up our large-scale MD simulations & analysis, as well as helping us in visualizing the cell-nanomaterials interaction."

Dr Qian Xuliang Research Fellow School of Mechanical and Aerospace Engineering (MAE) Nanyang Technological University



To address these questions, a team of researchers from Nanyang Technological University (NTU)'s School of Mechanical and Aerospace Engineering (MAE), alongside Professor Gao Huajian, a Distinguished University Professor NTU, at are tapping onto NSCC's supercomputing resources to gain а deeper understanding of the interaction mechanisms between nanomaterials and biological systems. By grouping different 2D nanomaterials into regulatory and risk categories, the team hopes to develop safe design strategies for the use of these materials in various applications and ultimately, generate substantial knowledge that will help guide the safe development and use of 2D nanomaterials in the future.

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

Back to main content list



Shared content>
Shared articles and news from the HPC world.

## Japan's Riken plans quantum link to supercomputer Fugaku Institute aims to launch hybrid computing in 2025, helping boost competitiveness

Japan's Riken research institute aims to bring quantum computing technology into real-world use by around 2025 through integration with the Fugaku supercomputer, a move that could help Japanese companies compete better in cutting-edge drugs, materials and other fields. Riken will establish a communications link between a quantum computer and Fugaku, the world's second-fastest supercomputer, to overcome this weakness. Read more at Nikkei Asia here.



Back to main content list

**The world is heading for a 'quantum divide': here's why it matters** *The impact of quantum technology will be far-reaching, in fields ranging from cybersecurity to drug development.*  Currently, 17 countries have invested in a national program of quantum technology research and development, while more than 150 have not. Leaders in quantum technology must commit to inclusivity in quantum education, in order to close the divide. Read more at World Economic Forum here.

Credit: Getty Images/iStockphoto

## LUMI supercomputer puts GPU partition through its paces with hardcore science

### Simulates the Sun's atmosphere, peers deep into Earth's interior, and can probably run Crysis

Finland's LUMI supercomputer has hit a new milestone, successfully completing the pilot phase of its GPU partition that extends the processing power of the system. LUMI is the fastest supercomputer in Europe and the third fastest globally, according to the Top500 list published in November 2022. It was inaugurated in June last year, but the system's GPU partition had not fully been installed at the time. Read more at The Register here.



Back to main content list

Back to main content list

Credit: LUMI



Powering Innovation Supercomputing in Asia National Supercomputing Centre (NSCC) Singapore 1 Fusionopolis Way, Connexis South, #17-01 Singapore 138632