National Supercomputing Centre (NSCC) Singapore e-newsletter

# NEWSBYTES

**March 2021** 









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## SupercomputingAsia 2021 (SCA21) wraps up successful first virtual conference and exhibition

Themed "Supercomputing in the New Norm - Adapting to COVID-19 and beyond", the threeday virtual event featured more than 100 speakers and panellists from research and industry who shared their knowledge and expertise.



Co-organised by HPC centres from Singapore, Japan and Australia, SCA21 concluded recently after three days of insightful conference sessions and exhibitions on the latest HPC technology innovations and developments. Support from SCA's partners, speakers, sponsors and participants resulted in more than 1000 registrants from across 30 countries and as many different organisations participating in the SCA conference series' first fully virtual event. The SCA21 conference was also a watershed one with many firsts, including an inaugural HPC Centre Leaders Forum and the first EU-ASEAN-Japan Symposium.

"...the crisis has underscored the importance of international cooperation in the fight against the virus around the world."



**Dr Vivian Balakrishnan**, Minister for Foreign Affairs and Minister-incharge of the Smart Nation Initiative, Singapore



"The growing size and diversity of the audience, the quality of speakers, and the sustained support of our many sponsors and partners reflects the spirit of sharing that this conference exemplifies."

Mr Peter Ho, Chairman, NSCC Steering Committee

"It's really an honour to be co-hosting it (SCA21) because it's a conference that has been growing in various respects over the past several years..."



**Prof Satoshi Matsuoka**, Director, RIKEN Center for Computational Science

#### Launch of the inaugural HPC Centre Leaders Forum





The leaders of supercomputing centres from the APAC region and Europe gathered to discuss the opportunities and challenges that each faced in designing and operating HPC centres, and shared best practices for running HPC centres of the future. The HPC centres from Japan, Australia, Singapore, Thailand and Finland were chosen to kick-off the inaugural forum because of the significant HPC developments in their respective centres and countries. These centres include Finland's CSC, which manages the development of Europe's most powerful pre-exascale supercomputer, the soon-to-be operational LUMI, and Japan's RIKEN-CCS, which developed Fugaku, currently the world's Number One ranked supercomputer according to the TOP500 supercomputer list.

"It's a privilege to support the HPC Leaders' Forum and share insights from national HPC centres from across the region as they set the foundation for post-COVID operations. Our shared experiences during a global pandemic support increased strategic regional cooperation. The Leaders' Forum will strengthen bilateral and multilateral partnerships in HPC and the high-impact research supported by our national centres" said Mr Mark Stickells, Executive Director of Australia's Pawsey Supercomputing Centre and the Moderator of the inaugural Forum.

#### First EU-ASEAN-Japan Symposium







Key opinion leaders from the EU, ASEAN and from Japan also came together at SCA21 to discuss how to promote greater cooperation by synergising their various HPC initiatives and collaborations. Capability building, talent development and HPC skill capacity building for the ASEAN HPC community were some of the areas discussed. These initiatives included programmes like the Enhanced Regional EU-ASEAN Dialogue Instrument (E-READI) and the organisation of a virtual HPC school by Thailand.

#### **Virtual Exhibition Hall**



SCA21 attendees had the opportunity to visit 20 exhibition booths at the virtual exhibition hall where they had the chance to chat live with SCA21 sponsors, download brochures and find out more about what the exhibitors had to offer.

A big **THANK YOU** to all our sponsors, speakers, participants, supporters and co-organisers for making the SCA21 virtual conference a success!

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



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# MOU between HPC centres from Finland and Singapore explores new network links, better data transfer security and green data centres

The Memorandum of Understanding (MOU) between Singapore entities and Finland's CSC-IT Centre for Science is a new partnership that will explore collaboration in key HPC areas as well as cooperation activities that promote and encourage HPC capability and talent development for both countries.



An MOU signed between National Supercomputing Centre (NSCC) Singapore, Singapore Advanced Research & Education Network (SingAREN) and the Quantum Engineering Programme of the National University of Singapore (NUS), and Finland's CSC-IT Centre for Science reflects the ongoing collaborative spirit in the HPC community. The MOU took centre stage at the Opening Ceremony of the SCA21 virtual conference when it was announced by Dr Vivian Balakrishnan, Minister for Foreign Affairs and Minister-in-Charge of the Smart Nation Initiative.

"The MOU and the other collaborative sessions at SCA21 are a reflection of the resolve by the HPC community to continue cooperation as a tool in fighting global challenges like the current pandemic, and to better prepare us to face the challenges to come," said Associate Professor Tan Tin Wee, the Chairperson of the SCA21 Steering Committee, and the Chief Executive of NSCC. "For Singapore, the new collaboration between CSC and

the Singapore entities is significant as it could help future-proof Singapore's HPC resources by creating new research links and connectivity to Europe, develop better ways to protect the transfer of data over long distances, and helps us explore new ways to create more efficient and greener data centres."

Among other things, the collaboration will explore a new high-speed, high-bandwidth research fibre optic link between Finland and Singapore as well as more secure ways of protecting data transfer by using quantum technology. NSCC and CSC are also studying Finnish green data centre models which have the potential to significantly lower data centre power consumption costs – the largest cost component in most data centres - by leveraging climate and renewable energy sources.

For more information about the MOU, please refer to the SCA21 Media Release.

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## Pawsey Supercomputing Centre unveils new supercomputer 'Setonix'

Named after Western Australia's icon and global tourist attraction, the quokka, the HPE Cray EX supercomputer will be 30 times more powerful than Pawsey's existing systems, Magnus and Galaxy.

The world's friendliest animal will lend its name to Australia's fastest new research supercomputer, with the Pawsey Centre confirming its new system will be named Setonix – the scientific name for the quokka. The system has been designed to give Australian researchers an edge in emerging research fields such as artificial intelligence and machine learning and will be used to help accelerate research projects such as the Square Kilometre Array, which will be the world's largest telescope and have a section based in WA.



"The quokka is an iconic Western Australian animal that has helped promote our State to the world, just as our work at Pawsey helps raise the profile of Western Australian and Australian researchers on the world stage," said Mr Mark Stickells, Executive Director of Pawsey Supercomputing Centre. "We also have a close connection with Rottnest Island, with our systems used to model ocean surface currents and sea temperature around the island — important work for oceanographers as well as for events such as the Rottnest Island Swim. Selecting Setonix as the name for our new supercomputer recognises our pride in being a national supercomputing facility located in WA, and the work we do in enabling science and accelerating discovery."

The existing supercomputers at the Pawsey Centre, Magnus and Galaxy together have 1.83 petaFLOPS of raw compute power while Setonix will deliver 50 petaFLOPS of power. Setonix marks a step change in Pawsey's supercomputing firepower, which currently supports the work of more than 1600 researchers from its Kensington facility. From discovering new galaxies to developing improved diagnostic tests for coronaviruses, Pawsey's high-performance facilities are already being used to solve some of the most important research questions in the world.

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## Using HPC to better understand psychiatric disorders

Researchers from A\*STAR leverage NSCC's supercomputer to stratify illness and subtypes in psychiatric disorders in order to facilitate better diagnosis and monitoring.

Mental health is an integral and essential part of health. The World Health Organisation constitution states that "Health is a state of complete physical, mental and social well-being and not merely the absence of disease or infirmity." Institute of Mental Health of Singapore asserts that "There is no health without mental health" to illustrate the importance of mental health and the lifetime prevalence of mental illness in the Singapore,

where 12% of the resident population, or 1 in 8, are affected by one type of mental disorder or another (Singapore Mental Health Study 2010).

Schizophrenia, one of the more serious mental disorders, in which people interpret reality abnormally, is a broadly defined disorder with patients suffering from a range of clinical symptoms. Psychiatric disorders like Schizophrenia, Bipolar disorder, Major Depressive disorder are a multifaceted set of disorders with overlapping symptoms, long duration of illness preceded by long prodromal phase, exerting immense emotional burden on individuals and caretakers.



Current clinical diagnosis is based on subjective patient examination due to a lack of quantitative biomarkers for differential diagnosis, and stratification of illness course or patient response. Identifying neuroimaging-based biomarkers underlying these psychiatric conditions can complement extant measures and aid in understanding these disorders better. Recent advances in magnetic resonance imaging (MRI) have opened the doors to better visualisation of the detailed structural, functional, and biochemical changes in the brain of individuals with schizophrenia to allow comparison with the brain of healthy subjects.

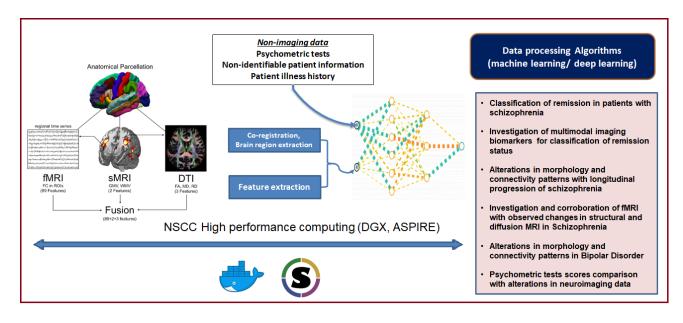
"There was a huge reduction in preprocessing time due to the parallelisation of tasks on NSCC resources (DGX and ASPIRE) that allowed us to process a substantial number of data sets in a week instead of months on a local workstation."

Bhanu Prakash K.N.
Group Leader,
Signal & Image Processing,
Singapore Bioimaging Consortium



Advances in machine learning have enabled investigation in this direction. A team of researchers at A\*STAR's Laboratory of Molecular Imaging are tapping onto NSCC's supercomputing resources to stratify illness and subtypes in psychiatric disorders using diverse multi-modal data (structural, functional, diffusion and psychometric scores) to derive quantitative imaging biomarkers that facilitate better diagnosis and monitoring of illness and subtypes.

The team has built neuroimage processing dockers/singularity images and are now able to work with large datasets requiring huge computational memory at higher throughput. Using machine learning models and neuroimaging data, they are able to accurately stratify the healthy controls, Schizophrenic patients, and bipolar disorder subjects. Work is in progress to understand the correlation and causation with known Psychometric scores.



To find out more about the NSCC's HPC resources and how you can tap on them, please contact enews@nscc.sg.



### The importance of using the right command(s) for your needs

For better efficiency!





The ls -l command displays information such as ownership, permission, and size of all files and directories.



#### **Lustre File System Tips**

Accessing certain file properties recursively in large directories using commands like `ls -l`, `find`, `locate` and `du` can degrade the file system performance for every user. To avoid this situation, we advise against the use of these commands in a large directory or simply specify the full path of the target file. When querying a large directory, we suggest the users to use the command `lfs find` instead of `find`.

List all files in a given directory:

\$ Ifs find ~/scratch

#### More examples here:

https://www.nics.tennessee.edu/computing-resources/file-systems/lustre-troubleshooting

For more information and FAQs on ASPIRE 1, please visit:

https://help.nscc.sg

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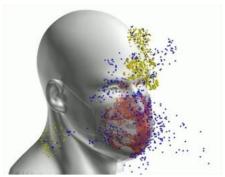
<SHARED CONTENT>

Shared articles and news from the HPC world.

## Double-masking benefits are limited, Japan supercomputer finds

Wearing two masks offers limited benefits in preventing the spread of droplets that could carry the coronavirus compared to one well-fitted disposable mask, according to a Japanese study that modelled the dispersal of droplets on a supercomputer.

The U.S. Centers for Disease Control and Prevention recommended double masking in February, saying Americans should wear a cloth mask over a disposable mask, the latest change to its recommendations on face coverings. But a similar benefit can be had with just one correctly-fitted mask, according to the research carried out in Japan by the Riken research institute and Kobe University using Fugaku, the world's fastest supercomputer co-developed with Fujitsu Ltd. Read more at Bloomberg here.



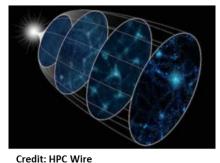
Credit: Riken/Toyohashi University of Technology/Tokyo Institute of Technology

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### Supercomputer turns back cosmic clock

Astronomers have tested a method for reconstructing the state of the early Universe by applying it to 4000 simulated universes using the ATERUI II supercomputer at the National Astronomical Observatory of Japan (NAOJ).

Just after the Universe came into existence 13.8 billion years ago, it suddenly increased more than a trillion, trillion times in size, in less than a trillionth of a trillionth of a microsecond; but no one knows how or why. This sudden "inflation," is one of the most important mysteries in modern astronomy. Read more at HPC Wire here.

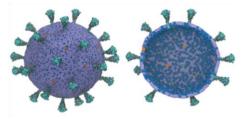


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First complete coronavirus model

A multiscale model of the complete SARS-CoV-2 virion has been developed for the first time using supercomputers.

The COVID-19 virus holds some mysteries. Scientists remain in the dark on aspects of how it fuses and enters the host cell, how it assembles itself, and how it buds off the host cell. Computational modelling combined with experimental data provides insights into these behaviors. But modelling over meaningful timescales of the pandemic-causing SARS-CoV-2 virus has so far been limited to just its pieces like the spike protein, a target for the current round of vaccines. Read more at Science Node here.



**Credit: Science Node** 

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