National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

November 2020

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Gathering the Best of HPC in Asia

Supercomputing in the New Norm

Adapting to COVID-19 and beyond

2 – 4 March 2021

SCA conference goes virtual

Upcoming NSCC Webinar Series:

Pandemic-Proofing Society

The role of HPC and HPC-enabled technologies in the new normal, and beyond

19 November 2020

10.00am - 11.15am (UTC+8)

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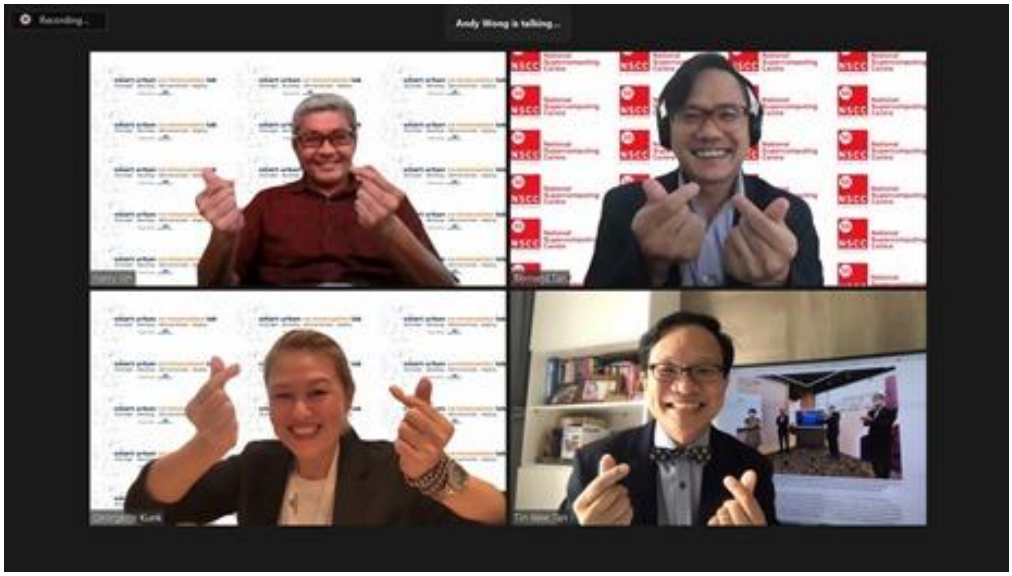
CORPORATE NEWS

NSCC and new Co-Innovation Lab to explore HPC resource collaboration with technology start-ups

Ascendas Innovation Pte Ltd (AIPL) and NSCC signed a Memorandum of Understanding (MoU) to leverage the ecosystem of technology tenants at the newly launched Smart Urban Co-Innovation Lab.

The new Smart Urban Co-Innovation Lab, which is owned by AIPL and managed by AIRmaker, focuses on smart city technologies in areas like Intelligent Estates, Smart Mobility, Digital Wellness and Agritech. With artificial intelligence (AI) and the Internet of Things (IoT) being synonymous with smart city technologies, the potential for HPC to be used as an enabling resource in such an advanced environment is high. Access to HPC resources could also provide the additional edge that new technology start-ups need to make their mark in a highly competitive technology market.

"Many technology companies are now applying AI across different Smart Cities sectors. Having the know-how and the access to HPC resources will accelerate development," said Mr Harry Lim, Chief Technology Officer, AIRmaker.



The MoU was signed by Mr Harry Lim (top left) and Mr Bernard Tan (top right), and witnessed by Ms Georgette Quek, Managing Director for AIRmaker (bottom left) and Associate Professor Tan Tin Wee, Chief Executive for NSCC (bottom right).

The partners will also work on surfacing 'problem statement' challenges to seek innovative solutions from the ecosystem of companies at the new lab. "We are working closely with AIRmaker to launch the potential problem statements such as green AIoT solutions that could be used in next generation data centres," said Mr Bernard Tan, Director for Strategy, Planning and Engagement at NSCC. "As NSCC develops new national supercomputing infrastructure to meet Singapore's future HPC demands, we are always looking for new out-of-the-box, smarter and greener solutions that can help us better optimise our operations. NSCC is pleased to be a collaborator and part of the vibrant AIoT Innovation Community where innovators, corporations, government agencies, investors, manufacturers and professional service providers interact and co-innovate."

The MoU was signed by Mr Harry Lim and Mr Bernard Tan, and witnessed by Ms Georgette Quek, Managing Director for AIRmaker and Associate Professor Tan Tin Wee, Chief Executive for NSCC.

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William Gropp voted IEEE CS 2022 President

NCSA Director and Chief Scientist William "Bill" Gropp has been voted IEEE Computer Society 2021 president-elect and will serve as president in 2022.

Congratulations to Professor William Gropp! *Apart from being the new IEEE Computer Society president-elect, 'Bill' is also a member of NSCC's Steering Committee, which guides the strategic direction of Singapore's national research infrastructure in supercomputing.*

Credit: University of Illinois at Urbana-Champaign

The president oversees IEEE CS programs and operations and is a nonvoting member of most IEEE CS program boards and committees. The IEEE CS is the world's preeminent organisation for computer science, engineering, and technology. Gropp, who holds the Thomas M. Siebel Chair in the Department of Computer Science at the University of Illinois at Urbana-Champaign, is currently IEEE CS Vice President for Technical and Conference Activities and a Board of Governors member since 2017. Read more at HPC Wire here.

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Stemming mosquito-borne disease outbreaks with the help of supercomputers

Tapping NSCC's supercomputer to support the surveillance and control of vector-borne and environment-related diseases like dengue in Singapore.

In July, the number of dengue cases in Singapore surpassed the entire total number of cases recorded in 2019. While the focus may now be on COVID-19, dengue and other mosquito-borne diseases are a recurring threat in tropical Singapore. The risk of disease outbreaks caused by vector-borne and environment-related pathogens remains high, with notable examples being diseases such as dengue, chikungunya and zika fever.

The Environmental Health Institute (EHI), a public health research laboratory under the National Environment Agency (NEA), conducts research, surveillance and evidence-based risk assessment on infectious diseases of environmental concern in Singapore. The important components of EHI's research programmes include arbovirus surveillance, genetic profiling of vector-borne and environment-related pathogens and associated vectors to understand their spatio-temporal dynamics. Data is also useful for modelling of outbreak risk and data analytics to assess the impact of disease control strategies.

"The improvements in analytical efficiency and throughput provided by NSCC's HPC resources allows timely updates on the genetic profiling of pathogens and related vectors as well as model outputs. These updates provide insights into disease epidemiology that could be useful to assess the outbreak risk and to design appropriate mitigation strategies."

Chanditha Hapuarachchi
Senior Scientist
Environmental Health Institute (EHI), NEA

A team of researchers at EHI are utilising NSCC's supercomputing resources to improve the efficiency and throughput of data analytics required for research and surveillance activities.

A major portion of EHI's analyses is currently focused on generating phylogeography and evolutionary data by using the BEAST software. BEAST requires 100-400 million iterations of MCMC-chain per run, which is time and resource consuming. Therefore, in the NSCC environment, the team has the ability to enhance the speed of analysis by integrating BEAGLE libraries into beast software for effective parallelisation of processes. Using instances of BEAGLE available at NSCC, they are able to improve the speed by 3-5 times relative to BEAST software without parallelisation.

The team is also tapping NSCC's resources for next generation sequencing (NGS) high throughput data analysis by parallelising genome alignment tools and are planning to use NGS pipelines to tap on various NSCC resources such as singularity and conda environments. "With the resources at NSCC, the current project expects to scale up the resolution and efficiency of genetic data analyses that would benefit the evidence-based approaches to maintain high public health standards in Singapore," said Chanditha, the lead of this project.

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

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Tracking down human cancer mutations using supercomputers

Researchers employ NSCC's supercomputer to better understand mutational signatures in human cancers and to explore ways to reduce the risk of cancer.

Mutagenesis is a major cause of cancer. Hence, it is important to deepen the understanding of the roles that specific mutagens play in causing cancer. This increase in understanding offers new opportunities for cancer prevention by reducing exposure to mutagens. Additionally, improvements in in-vitro testing of compounds' mutagenicity and identification of their characteristic mutation signatures will further aid in improving the understanding of the roles mutagens play in cancer risk and epidemiology of cancer.

A research team at the Centre for Computational Biology at Duke-NUS Medical School are utilising NSCC's computational resources to analyse whole-genome sequencing data, generated locally and internationally, in order to study the footprints of mutational processes (so-called mutational signatures) in cancer. Mutational signatures are used as biomarkers for mutagenic exposures in order to study which mutagenic processes contribute to cancer.

The researchers work to identify exogenous mutagenic exposures that contribute to cancer in order to raise public awareness and thereby reduce the number of cancers. The team also studies how mutational processes contribute to cancer formation by identifying specific genes and pathways that are frequently affected by a specific mutational signature, in order to identify molecular targets of tumours showing those mutational signatures.

The team is working to create a platform to directly test mutagenicity in cultured mammalian cell lines to determine extended mutation signatures of known and suspected mutagenic carcinogens using DNA. By leveraging extracted extended mutation signatures from published data sets and in combination with their own library of signatures, the team is also analysing global somatic mutation databases to determine which specific mutagens have contributed to the development of different cancer types.

"NSCC's resources are essential for our work as our group generate a lot of sequencing data, and often re-analyse, in tandem, with many sets of previously published data in order to verify mutational processes reported and also verify our new signatures. Thanks to the resources generously provided by NSCC, our analysis can be completed at a much faster rate; this allows us the capability to gather and analyse even more data and be more thorough in our studies."

Willie Yu
Research Fellow
Centre for Computational Biology,
Duke-NUS Medical School

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

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Mapping the brain's mysteries

Scientists across Asia are harnessing the power of synchrotrons and supercomputers to get a comprehensive understanding of the brain.

Scientists from Singapore, Japan, South Korea and Taiwan are collaborating to produce a first-of-its-kind, ultra-high-resolution 3D comprehensive map of the human brain's neural network. Using synchrotrons—extremely powerful X-ray sources—scientists aim to trace the brain's intricate networks. The project will link the synchrotron facilities in the Asia Pacific region under a collaboration called Synchrotron for Neuroscience—Asia Pacific Strategic Enterprise (SYNAPSE). Each participating facility will work on and image a portion of the same brain.

“Mapping the human brain at a resolution sufficient to chart the connections is a historic mission for science and technology,” said Low Chian-Ming, an Associate Professor at the National University of Singapore and a founding member of the initiative. “SYNAPSE will also generate technological breakthroughs in imaging, computation and artificial intelligence.”

As mapping a human brain will generate a huge amount of data, a high performance computing network will be developed for the project. NSCC, which is a sponsor of the project, will serve as a data hub for the processed 3D mapping data, linking processing facilities like Fugaku at the RIKEN Center for Computational Science, Taiwania at Taiwan’s National Center for High-Performance Computing, and systems at the Daegu Gyeongbuk Institute of Science and Technology, South Korea, via a high-speed 100 Gbps network run by the Singapore Advanced Research and Education Network (SingAREN).

“The images captured by SYNAPSE will form an extensive human brain map,” said Prof. Low. “The map will show how neurons are connected and how they interact to result in cognition and intelligence. Our findings could potentially contribute to effective treatments for increasingly important neurodegenerative pathologies such as Alzheimer’s disease and other forms of dementia.”

Head over to https://www.nscc.sg/supercomputing-asia-magazine/ to read the full piece published in the July issue of NSCC’s Supercomputing Asia Magazine to find out more about how HPC is being harnessed to understand the brain.

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

Visit www.nscc.sg/case-studies to learn more about how supercomputers are helping Singapore.

This article was first published in the print version of Supercomputing Asia, July 2020.
Credit: Tim Hornyak, Writer, Asian Scientist Magazine

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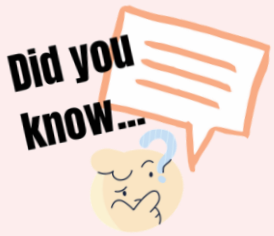
TECHNICAL NEWS

Tips on /scratch filesystem

What you should avoid on the /scratch filesystem.



It is not efficient to access small files on the /scratch filesystem.

Files that are only a few kilobytes do not give good performance in scratch.

Accessing small files on the /scratch filesystem is not efficient. When possible, keep them on a /home filesystem or copy them from /scratch to /tmp on each node at the beginning of the job, and then access them from /tmp.

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

https://help.nscc.sg

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THE LAST BYTE...

<SHARED CONTENT>

Shared articles and news from the HPC world.

HPE to build 50 petaflops Pawsey supercomputer for AU$48m

HPE has been awarded an AU$48m (US$34m) contract to build a 50 petaflops supercomputer for the Pawsey Supercomputing Centre.

The HPE Cray EX system will be Australia's most powerful supercomputer, when it fully launches in Q2 2022. Before then, two racks will be brought online by Q3 2021. The supercomputer will feature 200,000 upcoming AMD Epyc CPU cores and more than 750 Instinct GPUs. The system will replace Pawsey's existing Magnus and Galaxy computers. Read more at Data Center Dynamics here.

Credit: Data Center Dynamics

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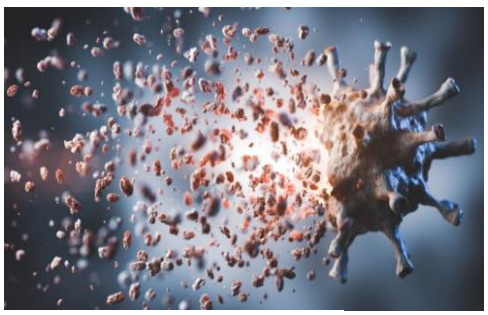
Supercomputer research leads to human trial of potential COVID-19 therapeutic raloxifene

Six months of patient trials with the ostensible COVID-19 therapeutic remdesivir have cast serious doubt on its ability to even reduce the severity of COVID-19, let alone reliably reduce patient mortality.

This has left medical professionals once again without a proven COVID-19 therapeutic as the pandemic shows signs of reaching unprecedented spikes in Europe and North America. As the world confronts the possibility of a dark winter, a supercomputer-powered pharmaceutical research coalition based in Italy is producing a glimmer of light: a repurposed drug called raloxifene, identified by supercomputing research, that will now be entering clinical trials to test its efficacy as a therapeutic for COVID-19. Read more at HPC Wire here.



Credit: HPC Wire

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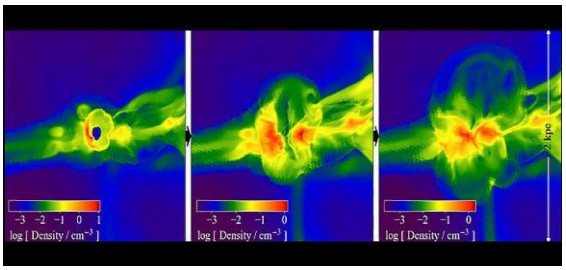
Supercomputers dig into first star fossils

No one has yet found the first stars.

They’re hypothesized to have formed about 100 million years after the Big Bang out of universal darkness from the primordial gases of hydrogen, helium, and trace light metals. These gases cooled, collapsed, and ignited into stars up to 1,000 times more massive than our sun. The bigger the star, the faster they burn out. The first stars probably only lived a few million years, a drop in the bucket of the age of the universe, at about 13.8 billion years. They're unlikely to ever be observed, lost to the mists of time. Read more at Phys Org here.



Credit: Phys Org

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