

NEWSBYTES

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CORPORATE NEWS

SupercomputingAsia 2021 (SCA21) returns from 2 to 4 March 2021 as a fully virtual conference

Themed "Supercomputing in the New Norm - Adapting to COVID-19 and beyond", the three-day virtual event will showcase the role that supercomputers and HPC have in a much more digitalised, post-pandemic society.



Co-organised by HPC centres from Singapore, Japan and Australia, SCA21 is an annual conference that encompasses an umbrella of notable supercomputing and allied events with the key objective of promoting a vibrant and relevant HPC ecosystem in Asia. SCA21 will be held as a virtual conference from 2 to 4 March 2021.

The SupercomputingAsia (SCA) conference incorporates a number of important supercomputing and allied events that together aim to promote a vibrant and shared high performance computing (HPC) ecosystem, for both the public and private sectors, in Asia.

The conference will be graced by Guest of Honour Dr Vivian Balakrishnan, Minister for Foreign Affairs and Minister-in-charge of the Smart Nation Initiative Singapore, who will be giving the Opening Speech as well as HE Jun Yamazaki, Ambassador of Japan to Singapore and Japan's Council for Science, Technology and Innovation, who will be giving the Opening Keynote during SCA21's Opening Ceremony on 2 March, 2pm-3pm.

Some of the SCA21 highlights include session tracks related to HPC-AI developments, Quantum Computing and Networking, HPC-enabled Climate Research, HPC in Education, international HPC collaborations, and the inaugural HPC Centre Leaders Forum. The tracks are also supplemented by Industry talks highlighting the latest HPC technology innovations and developments, and industry workshops.



SCA21 Supercomputing 2021
Gathering the **Best of HPC** in Asia
Supercomputing in the New Norm
Adapting to COVID-19 and beyond

SCA21 PROGRAMME HIGHLIGHTS

| 2 March 2021 | 3 March 2021 | 4 March 2021 |
|---|---|---|
| <p>SCA21 OPENING CEREMONY</p> <ul style="list-style-type: none">Opening Speech by Guest of Honour Dr Vivian Balakrishnan, Minister for Foreign Affairs and Minister-in-charge of the Smart Nation Initiative, SingaporeOpening Keynote on 'Japan's Endeavour to Realise Society 5.0' by HE Jun Yamazaki, Ambassador of Japan to Singapore and Japan's Council for Science, Technology and Innovation (CSTI) <p>HPC CENTRE LEADERS' FORUM - NAVIGATING HPC IN THE NEW NORM</p> <p>Like-minded leaders and organisations from Asia, Australia and Europe will discuss common areas of interest such as shared best practices, leveraging strengths and resources, and growing HPC talent, and challenges like HPC upgrade funding and HPC resource optimisation, amongst many others.</p> <p>HPC-AI FOR COVID NEW NORMAL</p> <p>Learn how Singapore's A*STAR IHPC demonstrates computational model-ing expertise using HPC and artificial intelligence (AI) to promote safe reopening of economic activities and distancing measures.</p> <p>APAC HPC-AI COMPETITION AWARDS CEREMONY</p> <p>This session will introduce HPCAIAC; present the winning solutions from the 2020 APAC HPC-AI Competition; and be the platform to launch the 2021 APAC HPC-AI Competition.</p> <p>HPC-AI IN HEALTH AND BIOMEDICAL SCIENCES</p> <p>Hear from invited speakers about the latest in HPC-related R&D, in particular COVID-19 related research.</p> | <p>PLENARY SESSIONS</p> <ul style="list-style-type: none">by Prof Satoshi Matsuoka, Director, RIKEN Center for Computational Scienceby Dr Larry Smarr, Distinguished Professor Emeritus, University of California San Diegoby Prof Sean Smith, Director of the Australian National Computational Infrastructure (NCI), Conjointly Professor of Computational Nanomaterials Science and Technology, Australian National Universityby SCA21 Platinum Sponsors <p>ASIA PACIFIC RESEARCH PLATFORM (APRP)</p> <p>The third APRP track at SCA21 will be co-chaired by Mr Yves Poppe, Consultant, NSCC Singapore, and Jeonghoon Moon, Senior Researcher, KISTI Korea, and will feature an update of the APRP activities.</p> <p>INDUSTRY TRACK SESSIONS</p> <p>by SCA21 sponsors</p> | <p>HPC IN EDUCATION / WHAT IS HPC AND WHERE DO I START?</p> <p>Have you ever wondered what HPC is capable of? If you are a student who is interested in how supercomputers are helping to change the world we live in, come and join our panel of speakers who will talk about their favourite HPC topic and give you insights on what it takes to be an HPC expert.</p> <p>EU-ASEAN-JAPAN SYMPOSIUM</p> <p>Stakeholders within the ASEAN HPC working group, EU HPC initiatives, and in Japan, including 'Fugaku' the world's top supercomputer, will present updates on these collaborations. This track is a convergence of the current HPC related initiatives and partnerships in EU, ASEAN and Japan.</p> <p>CLIMATE RESEARCH WITH HPC FORUM</p> <p>Learn more about how HPC is being applied in modern day climate research and how it is continually evolving with developments in areas like machine learning and AI.</p> <p>QUANTUM SAFE NETWORKS</p> <p>Hear from researchers and end user experts from the entire quantum networking value chain and learn more about this revolutionary quantum security technology of the future.</p> <p>INDUSTRY TRACK SESSIONS</p> <p>by SCA21 sponsors</p> |

Come join our line-up of exciting Keynotes, Speakers and Partners as we explore the role of supercomputers, and unravel the possibilities for HPC in the 'new normal'. View the latest SCA21 programme here <https://www.sc-asia.org/programme/> and head over to <https://www.sc-asia.org/> for more details on the conference.

REGISTER NOW

Are you a student with a polytechnic, ITE or university?

If so, then you get to register at SCA21 for **FREE!**



Interested to find out more about supercomputers and how supercomputers are helping to change the world we live in?

Come and join our **What is HPC and where do I start?** talk on **4 March** where our panel of speakers will talk about their favourite HPC topic and give you insights on what it takes to be an HPC expert.

A preview of our speakers & topics line up:

- With great supercomputing power comes great responsibilities
by Ms Julie Faure-Lacroix, Science Liaison Agent, Calcul Québec - Université Laval
- HPC powered solutions for a sustainable future
*by Dr Kang Chang Wei, Deputy Department Director (Fluid Dynamics Department), Institute of High Performance Computing, A*STAR*
- Creating chemistry in computer clusters
*by Dr Adrian Matthew Mak, Scientist (Materials Science and Chemistry), Institute of High Performance Computing, A*STAR*
- The roads that led me to HPC
by Dr. Jernej Zidar, Senior HPC Analyst, National Supercomputing Centre (NSCC) Singapore
- The many faces of HPC
by Ms Ann Backhaus, Education & Training Manager, Pawsey Supercomputing Centre
- Chaired by: Dr Freda Lim, Senior Scientist & Innovation Lead, Institute of High Performance Computing, A*STAR

**REGISTER
NOW**



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Using HPC to help conserve Southeast Asia's biodiversity

NSCC's supercomputer is being used to accelerate the analysis of the evolutionary history and biogeography of 'ancient' trapdoor spiders so that they can be used as a model system to look at how geology and climate help shape the biodiversity in the region.

Southeast Asia (SEA) is renowned for its strikingly high biodiversity and endemism, and contains four (Indo-Burma, Sundaland, Wallacea, and the Philippines) of the 34 global biodiversity hotspots due to the region's complex geological and climatic histories. However, these are increasingly under threat leading to huge efforts to conserve its biodiversity.

The conservation of biodiversity in the SEA region cannot be fully understood without considering the region's complex geology and climate. Three major outstanding problems have impeded the understanding of SEA's

diversity patterns – 1) how geological and climatic processes have driven species diversification across SEA is still not well understood; 2) prior studies of SEA biodiversity and biogeography have primarily focused on vertebrates yet few studies have explored diversification and biogeography of invertebrates, ancient lineages, poor dispersers, pre-Pleistocene vicariance, and/or large areas within SEA; 3) elucidating well-supported phylogenies necessary for reconstructing evolutionary and biogeographic histories has been shown to be challenging for a variety of taxa including spiders, even when multiple loci are used.



Using trapdoor spiders as a model system to test how geological and climatic events have shaped SEA biodiversity

“We cannot imagine what we would do without NSCC’s supercomputing resources. Without these resources, we would not be able to perform our analyses of phylogenetic relationships, divergence dating, and biogeographic history reconstruction of these segmented trapdoor spiders. NSCC’s resources enable us to finish the project by speeding up the analyses via parallel processing.”

Li Daiqin

Associate Professor
Department of Biological Sciences
NUS



A team of researchers at the [Department of Biological Sciences, NUS](#), is utilising NSCC’s high performance computing resources (HPC) to investigate the evolutionary history and biogeography of primitively segmented trapdoor spiders by performing phylogenomic and molecular dating analyses based on the genome-scale data comprising over 2,000 ultraconserved element loci. These spiders belong to the family Liphistiidae and are considered as “living fossils” because they are the sole surviving lineage in the suborder Mesothelae, which forms the sister lineage to all other extant spiders such as tarantulas and black widow spiders. Thus, the team aims to use these spiders as a model system to test how geological and climatic events have shaped SEA biodiversity. Additionally, studying this group has the potential to shed light on the deep evolutionary history of spiders and also other eight-legged animals.

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

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High-throughput, data intensive study on male infertility using HPC

A team from Duke-NUS Medical School is using supercomputers to aid in the building of a molecular ‘atlas’ for sperm generation to better understand human male infertility and develop potential new therapies.

Fertility problems are on the rise globally, potentially affecting 1 in 6 couples with nearly half of them having an underlying male factor. To understand this, a team of researchers at the Laboratory of Reproductive Biology and Stem Cells at [Duke-NUS OBGYN ACP](#) have created a molecular ‘atlas’ for sperm generation using high-throughput single-cell gene expression profiling technology. The team uses single-cell sequencing techniques to generate multiple types of data such as scRNA-Seq and scATAC-Seq using testis tissue samples from different species like monkeys, humans and mice to understand the developmental trajectory of spermatogenesis.



As the data produced from these experiments are high-dimensional and require high-throughput computational power to process and analyse, the team is tapping onto NSCC’s supercomputing resources to aid them in their handling and analysis of such data. For example, one single-cell experiment can generate a

few hundred million reads from 20 – 50 thousand cells, which requires computational time ranging from 10hrs to a few days depending on the data and the scaling up of memory requirements as data sizes increase.

“Single-cell RNA sequencing is able to capture gene expression information from thousands if not millions of single cells. The handling and analysis of such data requires HPC resources. Expression data will also be integrated with other high-dimensional data, e.g. spatial and genomic information, all of which requires computational throughput and complex data analysis. This is where HPC resources come into their own and make these things possible.”

Mahesh Sangrithi

Assistant Professor
Laboratory of Reproductive Biology
and Stem Cells
Duke-NUS OBGYN ACP



Findings from the research will yield greater insight into the transcriptional and epigenetic landscape of germ cells and somatic cells in the testis of infants, juveniles and adults and will help characterise the cell types and identify gene expression and epigenetic markers for each cell type. This research will add new knowledge to the understanding of human male infertility, and will contribute towards the development of improved tests or potential therapies. The findings of this study have been published in the journal, [Developmental Cell](#).

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

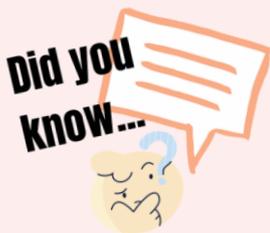
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TECHNICAL NEWS

Tips to avoid contention

What’s the best practice?



When many files in the same directory are to be opened, it creates contention.



Avoid having a large number of files in a single directory.

Opening a file keeps a lock on the parent directory. When many files in the same directory are to be opened, it creates contention. A better practice is to split a large number of files (in the thousands or more) into multiple subdirectories to minimise contention.

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

<https://help.nscg.sg>

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Shared articles and news from the HPC world.

Simulating cities under pandemic conditions to make predictions about future outbreaks

An international team of researchers has used modelling techniques borrowed from chemistry applications to create a new kind of city simulator.

In their paper published in the journal Proceedings of the Royal Society A, the group describes using their models to create simulations of COVID-19 spread for two real-world cities: Birmingham England and Bogota Columbia. One of the more frightening aspects of the current global pandemic is the knowledge that it could be a lot worse—it could have been a disease that killed everyone it infected. So scientists have been hard at work trying to develop tools to more effectively handle the next pandemic. Read more at Phys Org [here](#).



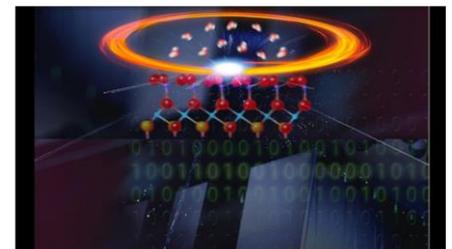
Credit: Phys Org

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Do simulations represent the real world at the atomic scale?

Computer simulations hold tremendous promise to accelerate the molecular engineering of green energy technologies.

However, the predictive power of these simulations depends on having a means to confirm that they do indeed describe the real world. Such confirmation is no simple task. Many assumptions enter the setup of these simulations. To address this challenge, a team of scientists at the U.S. Department of Energy's (DOE) Argonne National Laboratory, the University of Chicago and the University of California, Davis, developed a groundbreaking validation protocol for simulations of the atomic structure of the interface between a solid (a metal oxide) and liquid water. Read more at Science Magazine [here](#).



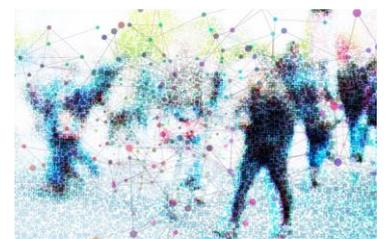
Credit: Science Magazine

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AI holds the key to even better AI

For all the talk about how artificial intelligence technology is transforming entire industries, the reality is that most businesses struggle to obtain real value from AI.

A major factor behind these struggles is the high algorithmic complexity of deep learning models. If human-developed algorithms inevitably run up against barriers of cost, time, manpower, and business fit, how can the AI industry break those barriers? The answer lies in algorithms that are designed by algorithms – a phenomenon that has been confined to academia to date but which will open up groundbreaking applications across industries when it is commercialised in the coming years. Read more at Venture Beat [here](#).



Credit: Venture Beat

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