National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

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In this Issue…

CORPORATE NEWS

Singapore researchers plug in to world's fastest supercomputer

New collaboration between Japan's RIKEN Center for Computational Science (R-CCS), Research Organisation for Information Science and Technology (RIST) and NSCC allows Singapore scientists to access Japan's Fugaku supercomputer.

A partnership between Singapore's national supercomputing resource, NSCC, and Japan's RIKEN and RIST, allows Singapore-based researchers to directly access the vast supercomputing resources of the world's fastest supercomputer, *Fugaku*. At 442 Petaflops (PFLOPS) of computing power, *Fugaku* is nearly three times more powerful than its nearest competitor and is at the top of the latest November 2020 edition of the global TOP500 supercomputer listing. Singapore researchers will now be able to apply for *Fugaku's* huge computing resources through regular project calls and connect directly via

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SCAsia 2021 Supercomputing
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 (Health & Biomedical)
The role of HPC and HPC-enabled technologies in the new normal, and beyond

14 December 2020
10.00am - 11.15am (UTC+8)

Live Data and Precision Medicine in the Post-Pandemic World

by A/Prof Ngiam Kee Yuan, Group Chief Technology Officer, National University Health System

Real-time Surveillance of Pathogen Evolution and Global Transmission

by Dr Sebastian Mauer-Stroh, Executive Director (Designate), Bioinformatics Institute (BII), A*STAR, Singapore

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dedicated high-speed, high-bandwidth research optical fibre links of up to 100 Gbps. The accessibility to *Fugaku's* computing resources is in addition to Singapore's petascale compute power that local researchers already have available at NSCC.

(Left) Professor Satoshi Matsuoka, Director of the RIKEN Center for Computational Science (R-CCS) and (right) Associate Professor Tan Tin Wee, Chief Executive of the National Supercomputing Centre (NSCC) Singapore signing the Memorandum of Understanding (MoU) to kickstart the partnership between the two centres.

"Singapore researchers will have the honour of being one of the first in Asia to have access to the amazing compute power of *Fugaku*," said Associate Professor Tan Tin Wee, Chief Executive of NSCC.

The broad spectrum of HPC cooperation between the two centres includes joint training, workshops and summer schools; talent exchange and student internship programmes; HPC support for research and talent capability building in areas like high-impact HPC-intensive national research projects and student competitions; and direct high-speed data transfer and storage linkages with both RIKEN and RIST.

NSCC's national supercomputer is already functioning at more than 90% capacity with users from Singapore's research institutes, institute of higher learning (IHLs) and industry leveraging the resources for research, education and industry-based HPC projects. The demand for HPC is expected to increase exponentially in Singapore's drive towards a smart nation. The government announced a S$200 million upgrade of the current supercomputer resources at the SupercomputingAsia 2019 (SCA19) conference in March 2019.

"Singapore's national supercomputing resources are already stretched thin and the HPC upgrades will ensure local researchers and organisations are better enabled, equipped and prepared for a much more digitalised future," added Associate Professor Tan Tin Wee who said that the current 1 PFLOPS system will be enhanced to a 10-15 PFLOPS system over the next few years. "In the meantime, local researchers can be assured of additional seamless, continued access to HPC resources in Singapore and through our partnership with RIKEN and RIST."

"Even before being fully commissioned, *Fugaku* has already made strides in providing solutions for the COVID-19 pandemic by speeding up the identification of potential drug candidates and developing simulations that demonstrate the spread of coronavirus in indoor settings and on trains," said Prof Satoshi Matsuoka, Director of R-CCS and one of the architects of the *Fugaku* supercomputer. "We hope that by sharing such examples and *Fugaku's* resources we can inspire more of our researchers, and colleagues from other countries, to leverage the power of HPC in their own research work. This partnership between the top tier national HPC centres of Japan and Singapore is a significant step in that direction."

Are you interested in using the Fugaku supercomputer for your HPC research?

Singapore researchers who are interested to apply for HPC resources from Japan can do so at https://www.nscc.sg/open-calls-hpc-resources-from-japan/.

"RIST has been collaborating with NSCC by exchanging information on promotion of shared use of supercomputers since 2016. Project calls for supercomputer *Fugaku* have started this year, and NSCC and RIST have been exploring cooperation on supercomputer *Fugaku*. I believe that the new establishment of the partnership between NSCC and RIKEN will promote the collaboration between Singapore and Japan and we can work together to produce amazing outcomes on *Fugaku*," said Dr Hideyuki Takatsu, Managing Director of RIST.

A MoU was endorsed on 16th September 2020 between R-CCS and NSCC, and complements an existing MoU with RIST. The collaboration with RIKEN covers access and data sharing to *Fugaku* while RIST will work with NSCC on promoting HPC research utilisation by cooperating on HPC project research calls and shared supercomputing use.

***Fugaku* – on top of the world**

The supercomputer *Fugaku* boosted its Linpack score to 442 petaflops, up from its debut listing at 415 petaflops six months ago, thanks to the addition of 6,912 nodes, bringing it to its full implementation of 158,976 nodes (each of which has one 48-core A64FX CPU).

The Fujitsu Arm-based system also increased its performance on the new mixed precision HPL-AI benchmark to 2.0 exaflops, up from 1.4 exaflops six months ago. On HPCG, it scored 16.00 petaflops, up from 13.40 previously, posted the highest score by far on the Graph 500 ranking and maintained its standing in the upper echelon of the Green500 energy-efficiency rankings, holding onto tenth position with 14.78 gigaflops-per-watt.

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Winners of the 2020 Asia-Pacific HPC-AI competition announced

Thirty teams across the Asia Pacific (APAC) region participated in the six-month competition that trains student teams to practice and produce solutions using HPC and AI platforms.

The HPC-AI Advisory Council in collaboration with NSCC have announced the university team winners of the 2020 APAC high performance computing (HPC) and artificial intelligence (AI) competition.

The '*TinpoC*' team from the National Cheng Kung University (NCKU), Taiwan returned to the winner's circle with another first place victory while the team from the National Tsing Hua University (NTHU), Taiwan secured second place. Both teams will be advancing to the ISC-HPCAIAC Student Cluster Competition in June 2021. Third place went to the team from China's Southern University of Science and Technology (SUSTech).

Special merit awards were also presented to 2 teams from Nanyang Technological University (NTU) and team 'Valkyrie' from National Cheng Kung University (NCKU), Taiwan.

Over 150 graduate and undergraduate students balanced the added demands of the six-month competition amidst the pandemic with their regular class and course loads. Competing across APAC, teams tackled HPC challenges in natural language processing and climate simulation and two novel bioscience and open innovation challenges with the potential to positively contribute to global research efforts to end the COVID-19 crisis.

Teamwork, determination and mentorship support – A recipe for success

"Time was very tight for us as we just competed in the international ISC20 student competition in June and the new semester started in August," said Ms Zhang Shengjing, the team lead for NTU's Team 2. "There wasn't much time for team members to take a break and we needed to balance the competition and study of the new semester." In the end, their dedication and perseverance earned them a Merit Award at the 2020 APAC HPC-AI Competition. Shengjing attributed the Merit Award to the hard work put in by every member of the team as well as to the valuable support provided by their mentor, Associate Professor Francis Lee from NTU's School of Computer Science and Engineering, and former NTU competitors.

"We learned a lot from the competition and had a lot of fun participating in it but there is still much more room for improvement," said Shengjing about the competition. "Learning from our mistakes is as important as winning the Merit Award." The team is already planning for the next edition of the student competitions and is looking to recruit more students who are interested in HPC. "We organised biweekly training sessions for interested students last semester and will continue to do so in the next semester."

Zhang Shengjing
Team Leader of NTU-2

"Our collective futures greatly depend on nurturing every student's potential, especially in times of adversity such as these. The commitment and resilience demonstrated by this year's competing teams reminds us all that we need to meet challenges head on and be flexible in adapting to the new normal," said Associate Professor Tan Tin Wee, Chief Executive at NSCC. "We congratulate this year's winners and all the 2020 student competitors for going above and beyond to deliver truly inspiring work and solutions despite having to cope with one of the most disruptive times in history."

The winning teams will present their solutions and accomplishments at the annual SupercomputingAsia 2021 (SCA21) conference, which will be held virtually from 2 to 4 March 2021.

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Reducing the risk of fires with the help of supercomputers

Unlocking the interactive physics in two-phase chemically reacting flows with NSCC's high-performance computing resources to mitigate fires in buildings and enclosed spaces.

Fire risk in urban buildings and tunnels are a big concern for modern cities like Singapore. Therefore, it is important to have a comprehensive understanding about fire dynamics in these structures and their interaction with the local ventilation, toxic gas emission, heat radiation and smoke movement in order to reduce the risk of fires in urban areas.

Two-phase chemically reacting flows are widely used in the field of engineering such as in the analsyis of propulsion systems, power generation, industrial hazard prevention and nanomaterial flame synthesis. Studies include dispersed droplets or particles in a continuous gas phase field, where elementary chemical reactions proceed. However, comprehensive interactions occur between these two phases which renders it difficult to accurately articulate how the dispersed droplets behave and influence the reacting flow dynamics.

A research team in NUS is tapping on high performance computing to unveil the underlying interactive mechanisms behind the chemically reacting flows based on high-fidelity numerical simulations and advanced data analysis methods. The team is utilising NSCC's computational resources to work on a wide range of fundamental studies associated with two-phase reacting flows such as liquid fuel spray flames, hydrocarbon/hydrogen detonation and explosion inhibition with water mists, high-efficiency detonation-based energy conversion technology, and combustion synthesis of nanomaterials.

"The advanced computing environment and CPU resources in ASPIRE 1 from NSCC provide significant support for our research activities. With them, we can accurately simulate the droplet phase and gas phase in a temporally and spatially evolving event, through tracking a huge amount of Lagrangian particles and discretising the gas phase field with ultra-fine resolutions," said Assistant Professor Zhang Huangwei, Department of Mechanical Engineering, NUS.

"Unlocking the interactive physics in two-phase chemically reacting flows necessitates highly-resolved flows, accurately tracked droplets, detailed chemical reactions, high-fidelity numerical algorithms and data mining techniques, and excellent computational power. NSCC offers us the computational power that we rely on to explore the unknown and tell scientifically reliable stories to our international colleagues and to everyone."

Zhang Huangwei
Assistant Professor
Department of Mechanical Engineering,
NUS

The research outputs provide the general scientific solutions for the relevant areas of low-emission and high-efficiency fuel and combustion, novel nanomaterial synthesis or manufacturing method, industrial safety, and urban resilience. High-fidelity data from NSCC is then mined with advanced analysis method such as chemical explosive mode analysis to identify the dominance of chemical species and/or elementary reactions and therefore pinpoint the interactions between the two-phases. The scientific computing or mathematical analysis libraries, such as GSL, also offer versatile solutions for the researchers in the team to carry out data post-process and theoretical analysis.

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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Developing new diabetes screening and monitoring methods using HPC

Researchers employ NSCC's supercomputer and high performance computing (HPC) to monitor glucose levels in diabetes patients and to explore ways to reduce the risk of diabetes.

Diabetes mellitus is one of the most common and severe threats to human health. Currently, most patients rely on the finger-stick method to measure blood glucose levels. However, this method is painful, invasive and inconvenient. Such drawbacks have resulted in low patient compliance and often leads to poor results in glucose controls.

In contrast, monitoring glucose levels in human body liquids (such as saliva and tears) using fluorescent chemo-sensors that have a high affinity for glucose have the inherent advantage of being non-invasive and simple to use.

The availability of high-performance fluorophores and fluorescent probes is key to accelerating the evolution and adoption of these medical diagnostics as well as other advanced imaging technologies, such as super-resolution fluorescence microscopy. The deployment of these techniques will, in turn, expedite the development of biotechnologies, from fundamental research to clinical applications. Yet, the quantitative

design of these fluorophores and probes continues to be a challenging task as dye chemistry is still largely based on trial-and-error.

The Fluorescence Research Group from Singapore University of Technology and Design (SUTD) has been tapping onto NSCC's supercomputing resources to establish quantitative prediction models for the development of spontaneously blinking fluorophores for super-resolution imaging applications, as well as many other fluorescent probes with improved signal-to-noise ratios for various bio sensing applications (such as detecting cellular viscosity and biomolecules). The group worked towards these goals via extensive quantum chemical calculations and analysing the correlations between computational and experimental results (Figure 1).

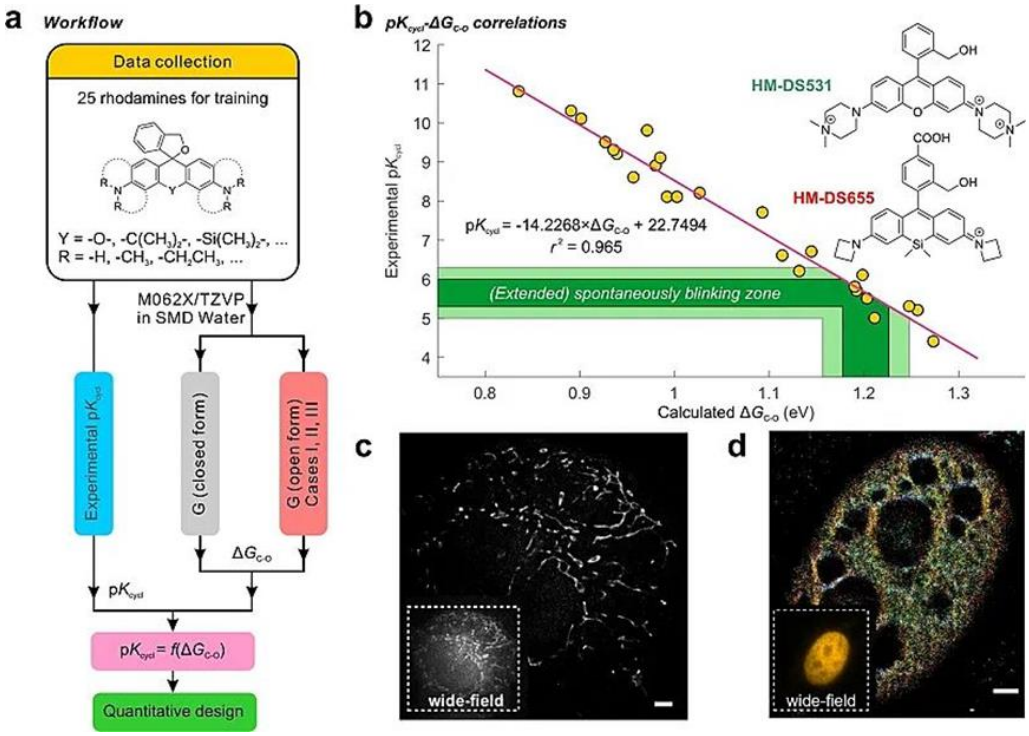

Figure 1. (a) The workflow of a quantitative design method for developing spontaneously blinking dyes based on quantum chemical calculations. (b) The correlation between calculated Gibbs free energy ($\Delta G_{C\text{-}O}$) and experimental parameters (pK_{cycl}), which enables the precise molecular design of spontaneously blinking dyes, such as **HM-DS531** and **HM-DS655**. (c) & (d) Bioimaging of mitochondria and nucleus of biological cells based on spontaneously blinking dyes.

"Our research involves benchmark studies on quantum chemistry methods, the understanding of experimental data using these computational methods, and quantitative molecular engineering of organic dyes based on a deep understanding of their structure-property relationships. Therefore, the HPC resources provided by NSCC are essential to our research as each of these steps requires high-throughput calculations and data analysis. We make use of Python and MatLab codes to manage a wide range of calculations, collect results, and analyse data that are generated at NSCC."

Liu Xiaogang
Assistant Professor
Department of Science, Mathematics & Technology, SUTD

The work contributes to the transformation of dye chemistry from trial-and-error to molecular engineering, by establishing detailed molecular design principles for the creation of various dyes with tailored properties. The team has demonstrated a quantitative chemical product design method by a cohesive integration of quantum chemical calculations and experimental validations. This methodology is expected to inspire the effective creation of abundant high-performance fluorophores.

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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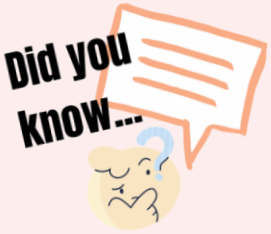
TECHNICAL NEWS

Working faster with a long file list in Linux

Have a long list within a large folder to work with? Fret not!



You can list recently updated files without going through the long list in a large folder.

Use "ls -lt --color | head" command to list recently updated files without going through the long list in a large folder. This is very handy to check out any new or updated output files.

Use "ls -lS --color | head" command to list files sorted by the file size from largest to smallest. It's very useful when there is a need to clean up for more space without going through a long list of files.

To make the two commands handy, we can create aliases with the following commands.

```
$ alias lsh='ls -lt --color | head'
$ alias lss='ls -lS --color | head'
```

To have these "lsh" and "lss" commands available by default, we can add the two aliases above into ~/.bashrc file.

The two commands will be available after you issue the "source ~/.bashrc" command.
Alternatively, they will be available by default from your next login.

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

https://help.nscc.sg

THE LAST BYTE...

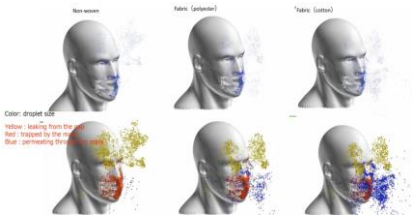
<SHARED CONTENT>

Shared articles and news from the HPC world.

It's Fugaku vs. COVID-19: How the world's top supercomputer is shaping our new normal

Fugaku is currently the most powerful publicly ranked supercomputer in the world – but we weren't supposed to have it yet.

The supercomputer, situated at Japan's Riken scientific research institute, was scheduled to come online in 2021. When the pandemic struck, Riken decided to launch Fugaku almost a year ahead of schedule. Since then, Riken and Fugaku have found a particular niche in the crowded COVID-19 research landscape, conducting a swath of intensive simulations focused on how viral droplets proliferate through masks, face shields, train cars and more – and in the process, drawing a very direct line between supercomputing and the general public. Read more at HPC Wire here.



Credit: RIKEN

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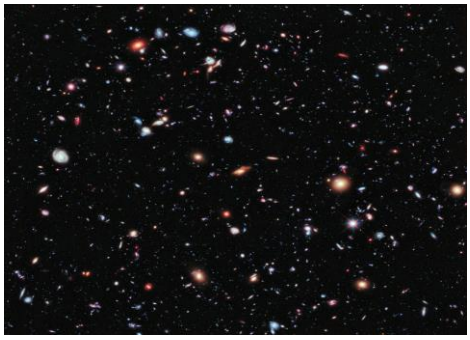
An extreme simulation of the universe's first stars

For astronomers, astrophysicists, and cosmologists, the ability to spot the first stars that formed in our Universe has always been just beyond reach.

On the one hand, there are the limits of our current telescopes and observatories, which can only see so far. On the other, up until about 1 billion years after the Big Bang, the Universe was experiencing what cosmologists refer to as the "Dark Ages" when the Universe was filled with gas clouds that obscured visible and infrared light. Luckily, a team of researchers from Georgia Tech's Center for Relativistic Astrophysics recently conducted simulations that show what the formation of the first stars looked like. Read more at Universe Today here.



Credit: Universe Today

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Astonishing blue whirl flame structure revealed with supercomputers

Texas Advanced Computing Center's Stampede2 supercomputer simulates 3D structure of vortex breakdown with combustion.

Lightning struck a bourbon warehouse, setting fire to a cache of 800,000 gallons of liquor in the Bardstown countryside of Kentucky in 2003. Some of it spilled into a nearby creek, spawning a massive fire tornado, or "bourbonado," as reported locally. Aerial video of it inspired scientists to investigate fire whirls, tornados of fire, as something promising for oil spill remediation because the alcohol burned with relatively little soot. Their fire whirl investigations in the lab led them to find something that astonished them. The chaotic and dangerous fire whirl transformed into a tame and clean burning flame they call a "blue whirl." Read more at SciTech Daily here.

Credit: SciTech Daily

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