National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

July 2021

In this Issue…

CORPORATE NEWS

NTU student team clinches second place at the international ISC 2021 Student Cluster Competition

The NSCC-supported NTU student team is consistently one of the top-ranked HPC student teams worldwide. NTU is currently fourth on the HPC-AI Advisory Council's Worldwide Leadership List, which ranks nearly 100 international institutions and the teams that take part in international HPC student cluster competitions.

Co-organised by the HPC-AI Advisory Council and ISC, the 2021 Student Cluster Competition brought together 72 students from 13 teams, and spread across seven locations around the world. The international competition remained as a fully remote one for the second year running thanks to NSCC's ongoing HPC resource support. This year's competition also had the added support from Canada's University of Toronto SciNet Supercomputing Centre.

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We are looking for ***guest writers / contributors*** to be part of our e-newsletters, which are sent out to a subscriber base of more than **7,500** monthly.

If you are interested in contributing content to our NewsBytes, drop us an email at **e-news@nscc.sg** and we'll be in touch with you!

From 24 May to 18 June, the teams competed using the same system configurations at both centres and relied on a combination of skills and knowledge to tackle the complex challenges that were set out in this year's competition. In addition to the standard High Performance LINPACK (HPL), HPC Challenge (HPCC), and High Performance Conjugate Gradient (HPCG) micro-benchmarks, the new HPC applications and coding challenge introduced included Weather Research and Forecasting Model (WRF); classic molecular dynamics with focus on materials modelling (LAMMPS); atomic scale quantum mechanical simulations and density-functional theory (GPAW); and a de novo metagenome short read-assembler (MHM2).

NTU Team Supernova members (from left): GOH Puay Hiang, LI Shenggui, YANG Shenghao, TAN Jia Qing, Aurelio Jethro PRAHARA, DO Xuan Long

The team from China's Tsinghua University emerged this year's winner by topping the LINPACK category and overall competition scores. They were followed closely by Team Supernova from Singapore's Nanyang Technological University. The team from Jinan University, China rounded out the top three teams for this year. Spain's Universitat Politècnica de Catalunya and China's Sun Yat-Sen University won the Fan Favourite and Honourable Mention awards, respectively.

The NTU team comprised students from various undergraduate programmes at the School of Computer Science and Engineering. They were supported by their Advisors NTU A/Prof Francis Lee Bu-Sung and former team captain, Mr Siyuan Liu. The team was also mentored by HPC practitioners from NSCC and industry partners including Dr Jernej Zidar (NSCC), Mr James Chen (AWS), Mr Terry Yin (Nvidia AI Tech Center) and Mr Prannoy Sablok (SingAREN).

"One of the biggest challenges we encountered during the competition was the need for us to work on two separate clusters, each running different Linux distributions and software stacks. Setting up a consistent environment on both clusters so that we could work across them easily took up a significant portion of our competition time," said Mr Yang Shenghao, the team lead for NTU's Team Supernova. Knowing that they were up against some of the best HPC teams in the region, the team prepared for the competition by engaging in weekly training sessions and team meetings before the start of the competition to build up experience with the applications that they were tasked to work on. Their hard work and determination paid off and they took home second place at the ISC 2021 Student Cluster Competition.

"Given the number of prominent teams participating in the competition, we were quite surprised when we learnt about our achievement. Having affirmation that our training and competition strategies were effective, we intend to build on those to strengthen our competitiveness for the next iterations," said Shenghao.

Yang Shenghao
Team leader of
Team Supernova

Congratulations to all the winning teams!

For more details, watch the announcement of the winners at the ceremony of the 10th Annual ISC HPC-AI Advisory Council Student Cluster Competition.

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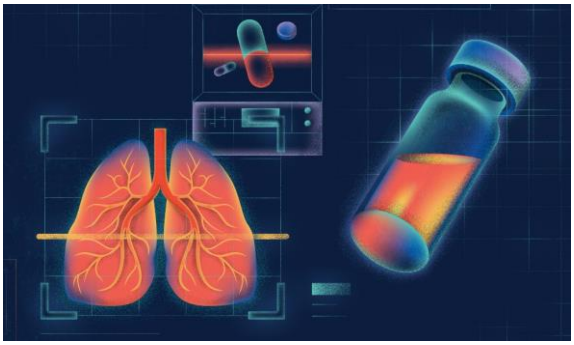
Supercharging healthcare innovation

From bench to bedside, high performance computers are running simulations, crunching big data and suggesting medical treatments to make healthcare more effective and affordable.



As the COVID-19 pandemic rages across the globe, medical professionals, scientists and public health officials are in a race against time to curb the spread of the novel coronavirus.

While we may need them now, the development of new diagnostic tools, vaccines and therapeutics remains complex and may take longer than we can wait for. This is where supercomputers, well known for their ability to rapidly process large amounts of data, can help to accelerate the process. After all, the top 500 supercomputers in the world can perform more than 1 quadrillion— that's 1 with 15 trailing zeros—operations per second on average.

Beyond tackling the immediate challenges of infectious diseases, supercomputers can also be applied to other aspects of healthcare. From laboratory based medical research to clinical practice, here's how supercomputers are augmenting human abilities and helping medical professionals deliver personalised care.

Supercomputers that simulate how complex biological molecules behave have emerged as a useful tool in responding to the COVID-19 pandemic. Armed with a peak performance of 1.3 petaFLOPS, the MDGRAPE-4A supercomputer at Japan's RIKEN completed a simulation of the protease protein involved in the replication of the SARS-CoV-2 virus on March 17, 2020. More than being just a static image, the simulation showed how the 2,416 atoms making up the protease protein move and wobble around in solution, allowing scientists to screen for potential antiviral compounds that can block it. Such a trial-and-error process could be performed virtually as well, with supercomputers iterating through a much wider range of compounds than what is physically possible. Although not specifically applied to COVID-19 research, a software framework developed at the National Supercomputer Center in Guangzhou, China, trawled through ten million molecules in a trial run, taking just 22.31 hours using the Tianhe-2 supercomputer, which boasts a peak performance of close to 34 petaFLOPS.

Head over to https://www.nscc.sg/supercomputing-asia-magazine/ to read the full article published in the July 2020 issue of NSCC's Supercomputing Asia Magazine to find out the ways supercomputers are shaping the future of healthcare.

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: Li Lidao, Writer, Asian Scientist Magazine

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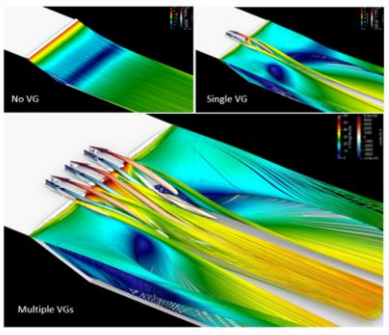
HPC powers aerodynamic improvements to turbine blades

Researchers at NTU are tapping HPC resources to investigate methods to improve turbine blade aerodynamics that could lead to energy and fuel savings.



Credit: NTU

Flow separation is a common occurrence in many engineering problems, especially in industries like the aerospace and automotive sectors. The separation of a laminar or turbulent boundary layer can severely lower the efficiency of a turbine blade, for example.

To address this, a team of researchers from Nanyang Technological University's School of Mechanical and Aerospace Engineering are leveraging NSCC's high performance computing resources to investigate the use of

vortex generators (VGs) to mitigate flow separation across a sharp-edge ramp. Using numerical simulations, the team qualitatively evaluates and compares flow characteristics with and without VGs to determine the resulting performance enhancements.

"The simulations are computationally intensive and through NSCC's support, we are able to speed up the analysis and undertake simulations with more refined discretisation for increased accuracy."

Ng Bing Feng
Assistant Professor
School of Mechanical and Aerospace Engineering
Nanyang Technological University

The team's fundamental research on flow separation and recirculation as well as on flow control strategies based on bio-inspired vortex generators, provides deep insights to performance enhancement and optimisation. The research findings help to uncover design parameters and optimal configurations for direct implementation so that improvements in energy / fuel savings can be achieved.

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

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When is water not just water?

NSCC's supercomputing resource is helping researchers gain a better understanding of the true nature of water, and its properties.

Although it is one of the most common elements, there is an ongoing scientific debate on the structure of water as well as the underlying liquid-liquid phase transitions. Water is simultaneously the most common liquid on earth and the weirdest, judging from the variety of its anomalous properties. For example, water reaches its maximum density at 4 degrees Celsius whereas other simple liquids just expand on heating. The "weird" nature of water may be explained if it is seen as a mixture of two different structures. However, the exact "mixture" of water is still a topic of discussion and not fully elucidated.

"The project requires us to perform simulations on large water cells therefore NSCC's supercomputer resources are essential. Additionally, many undergraduate students get to be involved in the project as they get free access to NSCC's cluster."

Zhuang Bilin
Assistant Professor
Science (Chemistry)
Yale-NUS

A team of researchers at Yale-NUS College are tapping NSCC's supercomputer to analyse in greater detail the structures of the "mixtures" that make up water. The goal is to gain a better understanding of the microscopic structure of water to shed light on the many physical and chemical processes in the aqueous environment.

The group has recently developed a new theory that water is a mixture of two states of water molecules. The team used NSCC's supercomputer to perform complex simulations of the interaction between water molecules. The project will continue to explore the implications of the classification, including the degree of hyperuniformity of the two states and the thermodynamic implications.

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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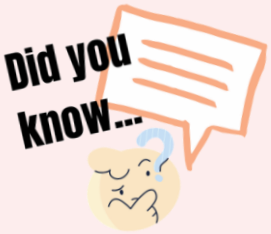
TECHNICAL NEWS

Do more with PBS Pro on ASPIRE 1

Part 1.



Jobs submitted to PBS Pro on ASPIRE 1 seldom start immediately, especially if one requires many compute nodes. This in turn means the user has to periodically login and check the status of his job, which is suboptimal. Fortunately, PBS Pro can let the user know when his job starts, ends or is terminated without any coding.

This can be achieved by adding just two lines to the job's PBS file:
#PBS -m abe
#PBS -M my_preferred@email.address

The first line specifies the mail options and, in this case, will send an email if the job aborts (a), begins (b) or ends (e). The second line specifies one or more email addresses to use.

Reference
https://help.nscc.sg/wp-content/uploads/Getting-Started-ASPIRE-1-v1.08-final.pdf

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.

Singapore developing its own 'crystal ball' for better climate projections

The effects of planetary warming are clear. Global temperatures and sea levels are rising, certain extreme weather events could intensify, and rainfall patterns could become more erratic.

But at a finer resolution, many questions remain about how these changes would manifest in Singapore and South-east Asia. For instance, how fast would sea levels rise around the city-state, and how high could the waters go? If rainfall patterns change, would the country experience more droughts or flash floods? These are questions that scientists at the Centre for Climate Research Singapore (CCRS) – a division under the National Environment Agency's Meteorological Service Singapore – are looking into. CCRS is working with the National Supercomputing Centre to downscale these models to produce grid cells spanning from about 2km to 8km. Read more at The Straits Times here.

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Japan's Fugaku retains title as World's Fastest Supercomputer for 3 consecutive terms

The supercomputer Fugaku, jointly developed by RIKEN and Fujitsu, has successfully retained the top spot for three consecutive terms on all four of the major high-performance computer rankings.

This includes the TOP500 list as well as the HPCG, a performance ranking for computing methods often used for real-world applications, HPL-AI, which ranks supercomputers based on their performance on single- and half-precision computing typically used in artificial intelligence applications, and the Graph 500 ranking, which ranks systems based on graph analytic performance, an important element in data-intensive workloads. Read more at HPC Wire here.

Credit: HPC Wire

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World first operating system breakthrough puts quantum computing on a chip

The first quantum operating system is now available on a chip thanks to Cambridge-based quantum specialist Riverlane's work with New York and London-based digital quantum company Seeqc.

The sensational breakthrough is equivalent to the moment during the 1960s in traditional computing when computers shrunk from being room-sized to being sat on top of a desk. Now, for the first time, a scalable quantum computer has been demonstrated featuring a quantum operating system running on a unique, chip-scale integrated quantum computing architecture. Read more at Cambridge Independent Press here.

Credit: Cambridge Independent

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