National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBY' January 2024



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(SCA24)!

A great year for Singapore supercomputing in 2023!

Thank you for helping us make 2023 a milestone year for supercomputing in Singapore. Here is a round-up of the key highlights for NSCC in 2023 as we look forward to an exciting 2024!

As we reflect upon the achievements and milestones of the past year, NSCC thanks all our users, stakeholders, partners, and friends for their unwavering support. Our continued collaborations, joint initiatives and HPC support have contributed to a stronger HPC community in Singapore and forged new paths toward excellence in high-performance computing. Here's a snapshot of the year in review.

NSCC wishes you all the best for the New Year and have a safe 2024 ahead!

NSCC's Supercomputers



Decommissioning of **ASPIRE 1**

NSCC bade a fond farewell to Singapore's first national petascale supercomputer, the ASPIRE 1. Having served the research community with high-performance much-needed computing (HPC) for 7 years, the ASPIRE 1 was officially decommissioned on 31 August 2023.



ASPIRE 2A DC recognised for innovation and sustainability

NSCC's newest next-generation national supercomputer, the ASPIRE 2A. showcases a green, warm-water cooled system which was awarded the Data Centre Award at the 2023 Singapore **Business Review Technology Excellence** Awards.



Co-organised by supercomputing centres from Australia, Japan, Singapore and Thailand, the SCA23 in Singapore was the largest ever conference since its inception in 2018. Themed "Sustainable Supercomputing for a Greener Future", the event featured 160 speakers and panellists sharing their knowledge and expertise with more than 1,100 registered participants from 35 countries and 315 organisations.



SCA23 Co-Located Events

The International Conference on High-Performance Computing in the Asia-Pacific Region (HPC Asia) and the Conference on Next Generation Arithmetic (CoNGA) were co-located with SCA23.



3rd HPC Centre Leaders Forum

The third HPC Centre Leaders Forum brought together like-minded leaders from HPC Centres in Japan, Australia, Finland, Thailand, the United States, and Poland to discuss common areas of interest, challenges faced as well as ways to leverage strengths and resources and grow HPC talent.



3rd EU-ASEAN-Japan Symposium

Key opinion leaders and principals from EU, ASEAN and Japan provided updates on the most recent HPC-related initiatives and partnerships in the various regions and countries and discussed ways to broaden the level of HPC cooperation.

Working with International Partners

Closer international ties







CSC and NSCC signed an agreement in August 2023 that leverages HPC resource collaboration between the 2 centres, in particular GPUs.

Next generation of HPC Leaders



HPCIC23

HPC 101

HPC101 is a collaboration between NSCC and ITE College West, where participants were co-trained by ITE lecturers and NSCC specialists on basic HPC knowledge and how to access HPC remotely from a virtual platform.

6th Asia Pacific HPC-AI Competition

Hosted by the HPC-AI Advisory Council, NSCC and National Computational Infrastructure (NCI) Australia the annual competition hosts graduate, advanced degree and undergraduate students from across the APAC region to develop their skills and challenge their understanding of HPC and AI technologies to tackle the pressing problems of climate change.

HPCIC23

Co-organised by NSCC, Infocomm Media Development Authority (IMDA) of Singapore and AI Singapore, the annual High Performance Computing Artificial Intelligence Innovation Challenge (HPCIC) seeks powerful solutions that apply to both HPC and AI to tackle key challenges in today's society.

NSCC inked 4 more Molls in 2023 with HPC centres around the world such as Taiwan's National Centre for High-Performance Computing (NCHC). Korea's Korea Institute of Science and (KISTI). Technology Information Thailand's Thai SC and more.

Strengthening Singapore-**Japan HPC partnership**

R-CCS and NSCC signed an amendment and extension of the Memorandum of Understanding (MoU) for Research NSCC Collaboration. currently collaborates with RCCS on a call for projects to use resources on the supercomputer Fugaku which grants the local research community access to Asia's cutting-edge supercomputer.

Singapore-Finland HPC **Resource Collaboration**



NTU student HPC team top virtual category at ISC23's international competition

NSCC provides support for the NTU team in the form of HPC fundamentals, resources and competition task training for the student team, which is one of the top ranked teams in the world.

MoUs with local polytechnics, ITEs and some unis for training programs

Educational institutions, like polytechnics and ITE, and professional associations will have access to supercomputing resources to advance teaching and education, especially in areas like AI and machine learning.







National collaborations

NUHS-NSCC Supercomputer

In July 2023, NUHS and NSCC launched the Prescience supercomputer, a first in Singapore's healthcare sector. It is deployed to train artificial intelligence models that will boost the delivery of healthcare here.

Singhealth NSCC supercomputer Collaboration

Singhealth and NSCC launched the Computational Health Research and Optimisation for Medical Advancements (CHROMA) supercomputer in September 2023, which aims to accelerate healthcare innovations such as medical technology and digital healthcare solutions.

Our commitment to fostering a robust and vibrant HPC community in Singapore remains steadfast, and we are eager to embark on new ventures and partnerships that will create opportunities for growth, learning, and advancement in the field of high-performance computing. For 2024, NSCC has an exciting line-up of new initiatives and activities that will significantly impact and benefit all our users and the Singapore research community at large. *Look out for exciting news coming out of NSCC in the year ahead!*

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NSCC's HPC Resources Instrumental in the Development of Singapore's 3rd National Climate Change Study (V3)

NSCC's high-performance computational resources were pivotal in streamlining the V3 study's computational demands to produce extensive weather simulations and regional climate modelling that will significantly impact Singapore policy and planning in the years to come.

The Centre for Climate Research Singapore of the National Environmental Agency (NEA) launched the findings of the <u>3rd National Climate Change Study</u> that modelled the next generation of climate projections affecting Singapore and Southeast Asia. The results of the study were unveiled at the symposium, which was opened by Ms Grace Foo, Minister for Sustainability and the Environment, where Minister and Dr Aurel Moise from CCRS highlighted the crucial role that supercomputers and NSCC played in the success of the V3 research.





Minister Grace Foo with the key contributors of the V3 study at the Symposium.

NSCC was critical to the success of the national project by providing the essential national high-performance computing resources that allowed climate researchers to efficiently process vast weather datasets, accelerating the delivery of higher-resolution, complex model simulations that formed the key basis for the recently published V3 results. This enabled in-depth analyses of Singapore's weather patterns and the broader regional climate dynamics.

The V3 model uses historical atmospheric data – such as temperature, rainfall, wind and pressure – to produce climate simulations and projections at high resolution, or distances ranging from 2km to 8km. This is more accurate than the broader resolution of the previous global climate model, which has projections ranging from 75km to 200km. Beyond that, the V3 research team was able to run 1000 years' worth of simulations in just under 3 years and underscored the importance of supercomputing infrastructure in research applications as highlighted in a news feature by the Straits Times.

Read the feature here

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Smart Data for the Smart Government: Highlights from OpenGov Breakfast Insight

On January 18, 2024, the OpenGov Breakfast Insight convened leaders from various sectors, fostering collaboration to delve into the advantages of implementing AI strategies in public administration

Harnessing AI capabilities empowers organizations to manage and leverage extensive data for informed, datadriven decision-making, fostering a more agile government administration. AI-driven advanced analytics, including machine learning and predictive analytics, provide real-time insights for effective data analysis, pattern identification, and trend forecasting. The key lies in promptly identifying areas where integrating AI capabilities will greatly benefit operations.



Leaders from various sectors attending the OpenGov Breakfast Insight.

The exclusive OpenGov Breakfast Insight on 18 January 2024, brought key leaders across industries together to explore the benefits of AI strategies for the public sector. Through interactive sessions, 32 attendees gained valuable insights into the profound impact of AI on smart governance and decision-making.

Associate Professor Tan Tin Wee, Chief Executive at the National Supercomputing Centre (NSCC) Singapore, was a distinguished speaker on the panel, sharing his experience on how AI-enhanced decision-making is key to navigating the future. Embracing AI requires organizations to understand the technology driving extensive data processing. High-performance computing (HPC) resources play a vital role in numerous national projects, with NSCC actively collaborating with various national agencies to meet their specific HPC requirements.



A/Prof Tan (centre) sharing his experience on how AI-enhanced decision-making is key to navigating the future.

A/Prof Tan highlighted NSCC's role in the recent V3 study as an example of such collaborations. With the help of supercomputers, Centre for Climate Research Singapore (CCRS) was able to deliver regional climate models crucial for predicting climate change impacts on Singapore. These models will guide government agencies in anticipatory prevention efforts. The panel then explored the challenges and opportunities in implementing smart data initiatives, emphasizing collaborative efforts to drive innovation and enhance national resilience.

The event, organized by OpenGov in collaboration with NSCC Singapore and NVIDIA, served as a knowledge exchange platform for government agencies, technology experts, and industry leaders.

Read more about the event here

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HPC Centre Leaders Forum will be back in action at Supercomputing Asia 2024 (SCA24)!

Join us in Sydney on 20 February 2024 to hear the latest updates from HPC centres across the world.



HPC Centre Leaders Forum

Happening at Supercomputing Asia 2024 At ICC Sydney On 20 February 2024

Continuing the tradition from the past Supercomputing Asia events, the crowd favorite HPC Centre Leaders Forum will be back for its next edition in SCA24 to bring the latest supercomputer updates from HPC centres around the world. Set on 20 February with a dedicated afternoon track timing, attendees will be able to hear from the centre leaders about the latest technology employed for their national data centres and supercomputers. Topics about energy sustainability, exascale development and quantum interoperability will be discussed by the panel of distinguished leaders.

SCA is an annual conference that encompasses an umbrella of notable supercomputing and allied events in Asia and beyond with the goal to promote a vibrant and shared HPC ecosystem in Asia. This year, ADAC14 Open Symposium and Australasian eResearch Organisations (AeRO) will be co-located with SCA24 at Sydney's International Convention & Exhibition Centre (ICC Sydney).

Some of the SCA24 highlights include session tracks related to the applications of HPC to CFD, astrophysics, material design as well as HPC-AI developments. The conference also features esteemed academic and industry speakers from companies like Lenovo, NVIDIA and Altair Engineering.

For more information and to register for SCA24, please visit <u>https://sca24.sc-asia.org/</u>.

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Singapore Researchers Get Exclusive Access to AMD GPUs from CSC LUMI

NSCC collaborates with Finland's CSC to grant researchers access to their LUMI supercomputer, ranked 5th on the world's Top500 supercomputers.

In the dynamic realm of supercomputing, NSCC understands the challenges that researchers and scientists face – the demanding computations, complex data sets, and the ever-growing need for accelerated results.

In collaboration with Finland's CSC – IT Center for Science, NSCC established a partnership that provides Singapore's research community access to a limited amount of GPU hours (AMD MI250) from the LUMI supercomputer system, which is ranked 5th on the world's Top500 supercomputers as of November 2023.



If you are interested to use the GPU resources from LUMI, provide the following details to us via an email to markengage@nscc.sg:

- 1. A title and brief abstract of your project
- 2. Estimated amount of GPU resources required (in GPU hours)

As the resources are limited, all submitted projects will be assessed on a first come first served basis. CSC LUMI is subject to export control limitations and as such, requires that the Principal Investigators of the interested research projects are not among EU-sanctioned individuals or groups and are not subject to US export control restrictions.

Submit your interest today!

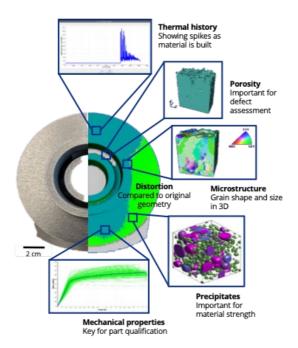
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Using Digital Twin Technology to Optimise the Industrial 3D Printing Process

Researchers from the Institute of High-Performance Computing (IHPC) are utilizing supercomputers to create a high-fidelity digital twin that furnishes users with comprehensive information about manufactured parts.

In industrial 3D printing, quality inconsistencies in the final printed product still pose a bottleneck issue for the broader industry adoption of this technology. Printing quality is influenced by the choice of alloy composition, printer settings, and part orientation during the build. Trial and error is often necessary before successfully printing the parts, thereby limiting the wider adoption of Additive Manufacturing. In order to overcome these challenges and facilitate the industry in harnessing the benefits of 3D printing, the researchers at IHPC have developed a digital twin of the 3D printing process.

Before the development of the Additive Manufacturing Digital Twin (AM-DT), no software was capable of comprehensively show the detailed aspects of a printed component to the user, which includes defects, microstructure, and mechanical properties. Consequently, the industry incurred significant costs in determining optimal process parameters through trial and error with actual test prints.



The Research

The IHPC researchers used the supercomputers at NSCC to develop a digital twin of the 3D printing process. This involved employing advanced physics-based models that accurately simulate the printing

outcome by processing information about the printer type, materials used and printing conditions. The virtual manufacturing product provides users with full information about the quality of the printed part, encompassing details such as thermal history, microstructure, defects, mechanical properties, residual stress, and part distortion.

The Technology

Digital Twin - Advanced computational modelling and virtual simulations were conducted to minimize the amount of experimental work required to derive a perfect physical product. Massive computational power was required to achieve a very high resolution in the calculation of the 3D-printed parts.

Batch processing - The queuing system facilitated the execution of numerous individual calculations employed for code development, testing, and validation. The researchers executed over a hundred jobs, each demanding 256 CPU cores and approximately 200 GB of scratch disk.

The Impact

The research outcome, AM-DT, has been developed into a complete software that can be directly deployed to industry. Currently, several companies have already benefited from calculations by AM-DT of their parts and specific manufacturing processes. With AM-DT, companies can digitally design their parts before initiating an actual print, determine the optimal process parameters, and pre-assess the expected microstructure and mechanical properties. Users can explore workflows fully digitally rather than relying on experimental methods, resulting in significant time and cost savings.

For instance, in collaboration with Proterial (formerly known as Hitachi Metals), the research team has developed an integrated simulation platform for Laser Powder-Bed Fusion (LPBF). A noteworthy advancement in the platform is its ability to predict the performance of sophisticated metal powders during the printing process.

"Supercomputing resources have proven invaluable to our research, enabling the team to run many calculations to validate each component of our AM-DT against the experimental results. Running the AM-DT on the supercomputer allows the calculation of 3D printed parts, yielding very high-resolution simulations."

Dr Guglielmo Vastola

Co-Principal Investigator & Project Manager

Principal Scientist I, A*STAR's IHPC



Prof. Zhang Yong-Wei Principal Investigator

Distinguished Scientist, A*STAR's IHPC



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

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Shared articles and news from the HPC world.

QuEra Computing and Pawsey Unite to Boost Global Quantum Computing and Supercomputing Innovation with up to 256 Qubit Machines

The partnership aimed at driving advancements in quantum technology and enhancing the capabilities of both organizations.

QuEra Computing, a neutral-atom quantum computing company, and Pawsey Supercomputing Research Centre have announced a partnership to advance quantum technology. They are jointly developing quantum emulation software for Pawsey's Setonix supercomputer. QuEra will also provide Pawsey with access to its neutral-atom-based quantum computers, hosted in Boston. QuEra's Aquila-class quantum computers are 256-qubit devices with a unique analog quantum processing mode. Read more <u>here</u>.



Credit: Quantum Zeitgeist

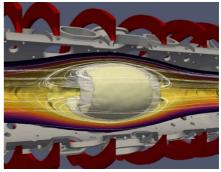
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Hot Fusion: Exascale Computing Drives Earthly Efforts to Produce the Energy That Powers the Sun

There are plans to build the world's first prototype hydrogen-boron fusion power plant, in the early 2030s.

Nuclear fusion processes similar to the sun's have the potential to transform energy production on Earth. With Da Vinci, TAE Technologies's seventh-generation test machine, the company seeks to fuel a renaissance in world energy production. Viable fusion energy could generate affordable, abundant carbon-free energy for everyone with no meltdown risk and far fewer environmental impacts and harmful byproducts than fission or fossil fuels. Read more <u>here</u>.

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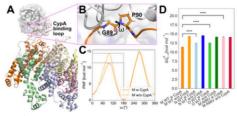


Credit: HPC Wire

Jülich's JUWELS Supercomputer Reveals Key Insights into HIV-1's Evasion of Human Immune Defense

Recent research by Prof. Dr. Holger Gohlke and Prof. Dr. Carsten Münk uncovered a new understanding of how HIV-1 M adapts to human cells.

The study identifies a potential vulnerability in HIV-1, offering hope for new drugs. By suppressing the binding of cyclophilin A to the virus, researchers may develop drugs to combat HIV-1. For this, computationally intense umbrella sampling molecular dynamics simulations of HIV-capsid protein/cyclophilin A complexes were performed on the JUWELS Booster module, exploiting the excellent performance of the AMBER molecular simulation code on GPUs. Read more at <u>here</u>.



Credit: HPC Wire

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