National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

ASPIRE2A

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In this issue…

CORPORATE NEWS

Taking a closer look at NSCC Singapore's updated resource allocation policy

Focused on supporting key national R&D programmes and research projects to achieve significant economic outcomes and scientific imperatives for Singapore, the policy will also encourage more prudent and efficient utilisation of precious national High Performance Computing (HPC) resources.

SG NSCC SINGAPORE

NSCC Singapore's Updated HPC Resource Allocation Policy

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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!

With the already running ASPIRE 2A supercomputer and the launch of the additional ASPIRE 2A+ system, an updated Resource Allocation Policy is necessary to better streamline the allocation of the HPC resources available. The updated policy will allow the NSCC Singapore to allocate its HPC resources more effectively as a National Research Infrastructure (NRI).

Here are some key things that you should know about the policy:

NSCC Singapore's resources are part of the NRI

- NSCC Singapore is funded by National Research Foundation in its role as an NRI.
- As an NRI, NSCC Singapore supports key National R&D programmes and research projects in achieving significant economic outcomes and scientific imperatives for Singapore.
- Projects with approved RIE-funding and compute budget will be prioritised.
- A new Strategic Resource Allocation Committee (SRAC) will oversee the resource prioritisation and allocation for the Call for Research Project applications for NSCC Singapore's HPC resources.

Grant proposals must include budget for compute resources

- Budget must be set aside for compute resources (i.e. CPU core hours, GPU card hours and storage) as part of the overall project grants or in applied project funding.
- An approved compute budget is necessary for application for NSCC Singapore's resources but does not guarantee allocation of resources.
- Costing for HPC budgets must be based on cloud service providers (CSP) rates. This is to ensure that projects have enough budget to pursue their HPC-dependent research with CSP resources if application is unsuccessful.
- Successful projects will be allocated HPC resources for the duration of the research project.
- All approved and prioritised projects will be awarded and billed to the host institution's research office managing their respective project grants.
- The updated policy will apply to all new project submissions, effective immediately.

Greater discipline in HPC resource request and utilisation

- All applicants must submit an annual projected utilisation plan to encourage the responsible utilisation of allocated resources.
- A project's track record in the utilisation of allocated HPC resources will be taken into consideration in future applications and allocation of resources.

As we work towards streamlining HPC resources usage, NSCC Singapore is also diversifying the availability of HPC resources for researchers through a variety of sources such as planning for a pipeline of future systems, exploring national HPC cloud options with preferential rates, and leveraging international partnerships with HPC centres, among others.

If you have any questions regarding the new resource allocation policy, please refer to our FAQs or email us at nsccra@nscc.sg.

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Driving Collaboration and Innovation at the HPC Users Symposium 2024

NSCC Singapore's inaugural HPC Users Symposium brought together 178 HPC community members from academia, industry, and government for a day of insightful presentations, engaging discussions, and collaborative exchanges on the future of HPC in Singapore.


Opening speech by Dr Terence Hung, Chief Executive of NSCC Singapore at the HPC Users Symposium 2024.

NSCC Singapore's inaugural HPC Users Symposium, held on 30 August 2024, served as a key platform for HPC users across various fields to present their latest HPC-enabled research, to share innovative ideas, and to discuss the developments of HPC in Singapore. The symposium also provided NSCC Singapore with the opportunity to share the latest resource allocation updates with the research community.

The Symposium featured keynote presentations including "HPC for First Principles Calculations of Catalysts and Materials" by Dr Michael Sullivan, Senior Principal Scientist II at Agency for Science, Technology and Research (A*STAR)'s Institute of High Performance Computing (IHPC), which highlighted how HPC is driving new discoveries in materials science and catalysis. The talk on "GenAI Workloads and Innovation" by Dr Ng Aik Beng, Regional Manager of NVIDIA AI Technology Centre, explored the transformative convergence of HPC and artificial intelligence, showcasing groundbreaking developments in AI-driven computing.

Attendees at the Poster presentation during lunch.
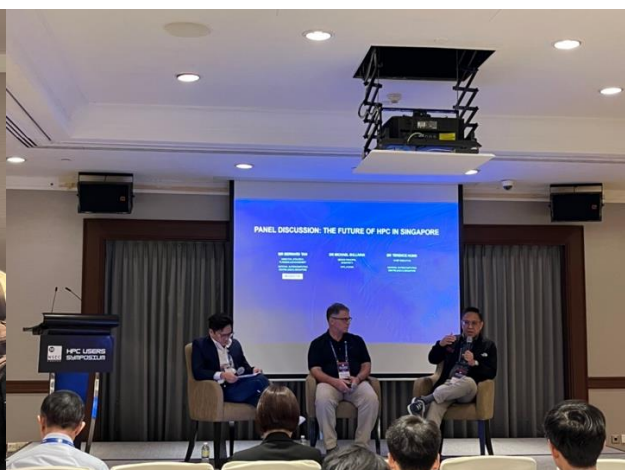
Panel discussion on the future of HPC in Singapore.

The symposium featured presentations from 13 key users, who showcased their research work in diverse fields, emphasizing the critical role of HPC in accelerating their research and the benefit their work brings to the Singapore society. See below for the list of presentations delivered during the symposium.

| Presentation Topic	Presented by
ASPIRE 2A for Excited State Physics: Toward a Sustainable and Smart Nation	Quek Su Ying, National University of Singapore (NUS)
Rainfall Nowcasting in Tropical Southeast Asia with Deep Generative Models	Niu Zhixiao, NUS
HPC & Environmental Sustainability	Kang Chang Wei, IHPC
Qibo: An Open-Source Hybrid Quantum Operating System	Yang Liwei, IHPC
Singapore's Journey in Developing Multimodal Generative AI Model: Merlion AI	Dr Sun Shuo, Institute for Infocomm Research (I^2R)
Waterfall: Framework for Robust and Scalable Text Watermarking	Niu Xinyuan, NUS
HPC in Decarbonization R&D: Hydrogen & Ammonia for Power	Zhang Huangwei, NUS
NUS Computational Coastal Lab: Fluid-Structure Interaction, Energy Harvesting, and Sediment Transport	Hu Zhengyu, NUS
Using HPC to Accelerate Antibiotic Development	Li Jianguo, Bioinformatics Institute (BII)
The Impact of HPC on Research Work at the Tropical Marine Science Institute (TMSI)	Nguyen Ngoc Son, NUS
High-Performance Computing for Density Functional Theory Calculations in Computational Materials Science	Nong Wei, Nanyang Technology University (NTU)
High-Throughput Computations for Design of Light-Weight High-Entropy Alloy	Zach Aitken, IHPC
Developing Sustainable Plastic Materials by Multiscale Simulations	Zheng Jianwei, IHPC

During the event, there was also a poster showcase of 19 research projects to highlight the importance and impact of HPC in research and beyond.

The symposium wrapped up with a panel discussion on 'The Future of HPC in Singapore' which explored the strategic directions, challenges, and opportunities for advancing HPC in Singapore, with a particular focus on sustainability, AI integration, and hybrid computing.

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Say hello to NSCC Singapore's new and refreshed website

NSCC Singapore's new website was launched earlier this month.
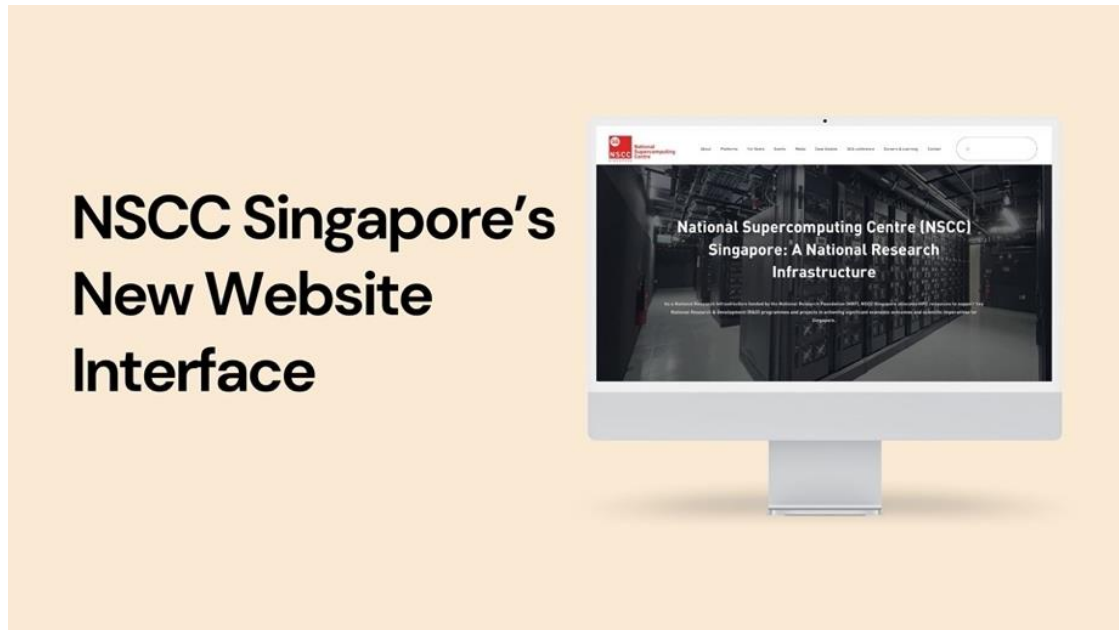
The sitemap has been reworked to make it easier for everyone to find the information that they need. Here's what to look out for.

About us

This section offers insights into NSCC Singapore as a company. Discover our goals, origin, and strategic partnerships, as well as the dedicated team behind the national HPC resources.

Platforms

This section offers a concise overview of the supercomputers managed by the NSCC Singapore team. Key specifications for each platform give insights into their capabilities.

For Users

This section is dedicated to NSCC Singapore's users, providing direct access to a catalogue of support resources, key information on project calls, and resource allocation policy. In addition, the user help site (https://help.nscc.sg/) has a refreshed interface that provides users with more specific, system-based assistance.

Events

Our Events page features enhanced classification functionality for a more engaging experience. Upcoming and ongoing events are highlighted with registration options and add-to-calendar features.

Media

This section houses the content hub, press room, and featured reads. The Content Hub serves as a central media resource page where you can find the monthly e-Newsbytes, Supercomputing Asia Magazine, and videos, categorised for your convenience. The 'Press Room' contains past media releases and news about NSCC Singapore while 'Featured Reads' covers informative stories to keep up with the latest trends in HPC.

Case Studies

Find out about our users and the research that they perform using our supercomputers here. This section is aligned with the key pillars of research in Singapore, with articles organized and tagged according to specific areas of interest, making it easier for you to find relevant content.

SCA Conference

This page introduces the Supercomputing Asia (SCA) conference co-organized by Singapore. SCA is a major platform for networking, knowledge exchange, and exploring the latest advancements in HPC, AI, and quantum technologies. The annual event that unites the supercomputing community across the region is set to return to Singapore next year, from 10 to 13 March 2025.

Careers & Learning

This section showcases available positions at NSCC Singapore, encouraging talents to pursue careers in HPC. Additionally, we feature courses and resources for individuals who are interested in pursuing an HPC career or enhancing their professional growth.

Contact

This section provides all the essential information you need to reach out to the NSCC Singapore team and directions to where we are located.

Experience our new website here!

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Bridging Singapore's HPC Community Across Research, Industry and the Public Sector

Co-organized by the Singapore University of Technology and Design (SUTD), NUS, NTU, A*STAR, and NSCC Singapore, the User Group highlights the growing synergy between academia and industry in driving the future of HPC in Singapore.

Full- house attendance at Singapore HPC User Group Event 2024, hosted by SUTD.

The Singapore HPC User Group Event 2024, held at SUTD, brought together around 75 researchers, HPC professionals, and industry leaders from across the region for an afternoon of technical knowledge sharing and collaboration.

The opening address was delivered by Associate Professor Liu Xiaogang, Director of the SUTD Honours and Research Programme (SHARP). In his speech, A/Prof Liu emphasized the importance of collaboration between academic institutions and industry partners in advancing HPC capabilities.

This was followed by a research presentation by Dr Michael Sullivan, Senior Principal Scientist at IHPC, A*STAR, presented benchmark results of Quantum Espresso on ASPIRE 2A. He compared the performance of various HPC machines and compilers, offering valuable insights into optimizing computational efficiency for complex simulations. Shen Tianruo, a PhD student at SUTD, shared his work on fluorescence and first principles calculations. He highlighted how HPC is being used to study fluorescent materials, contributing to advancements in materials science.

The event also provided a platform for industry experts to share their perspectives on the future of HPC and AI with sharing from Paul Skaria, Solution Architect Leader at AMD, Chin-Fah HEOH, Senior Solutions Architect at DDN, Manjunath Doddam, Senior Technical Specialist in HPC at Altair and Andy Warner, Senior Distinguished Technologist and Chief Systems Engineer at HPE.

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Workshop with RIKEN Center for Computational Science (R-CCS) on Operational Excellence in Supercomputing

R-CCS and NSCC Singapore recently concluded a successful joint workshop focused on advancing operational excellence in supercomputing.

Professor Satoshi Matsuoka leading the discussion for the joint workshop between R-CCS and NSCC Singapore.

With the participation of 18 HPC experts from Japan and Singapore, NSCC Singapore and the R-CCS conducted a two-day workshop on 21 and 22 August 2024 that served as a strategic platform for enhancing collaboration, sharing best practices, and driving forward innovative solutions in HPC operations.

Beyond the insightful discussions on current operations, the workshop aimed to address critical topics such as the selection of next-generation HPC systems. Both R-CCS and NSCC Singapore reviewed and refined their respective future infrastructure plans. Attendees also explored technical requirements, security frameworks, and the integration of AI and quantum computing technologies, setting the stage for future advancements. The joint workshop underscored the commitment of both organizations to achieving operational excellence and set the groundwork for future joint initiatives in supercomputing.

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Supercharge your HPC Skills with a Certificate of Competency (CoC) by NSCC Singapore and ITE College West

Jointly run by NSCC Singapore and ITE College West, this SkillsFuture CoC course equips participants with the basic knowledge of HPC.

Participants will be co-trained by ITE lecturers and NSCC Singapore specialists on how to access HPC remotely from a virtual platform to experience working on thousands of computing nodes to perform complex program tasks at high speed, which in turn will accelerate the building of deep learning AI applications.

In this course, participants will acquire skills and knowledge on:

- Basic building blocks of a supercomputer
- Understanding PBS Scheduler
- Environment setup and file transfer
- Resource allocation and Job Submission
- Use case and accessing of HPC
- Hands-on AI project using HPC

Training accounts with computing resources will be provided by NSCC Singapore. Upon completion of the course, participants will be awarded a certificate of competency in Introduction to HPC as well as a certificate of participation by NSCC Singapore.

The next intake for the course is on 25 September 2024. Fees for this course can be paid using SkillsFuture credits.

For more information, visit the [CoC website](#).

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Shared articles and news from the HPC world.

IBM, NUS to set up new AI research and innovation centre in Singapore

The proposed centre, a collaboration between IBM and the NUS, aims to accelerate scientific research here by tapping the American tech giant's full-stack AI infrastructure.

Minister for Digital Development and Information Josephine Teo announced the new centre at the IBM Think 2024. This will mark the first time IBM's full-stack AI infrastructure system – the entire spectrum of software and technology required to build, test and deploy an application – is installed on a university campus in the Asia-Pacific region.

Read more

Credit: Straits Times

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RIKEN Introduces Virtual Fugaku to Expand Supercomputing Ecosystem and Innovation

R-CCS has launched the "Virtual Fugaku" project to establish the Fugaku supercomputer as a key piece of social infrastructure and to accelerate the resolution of various social issues.

The "Virtual Fugaku" allows users to access a highly optimized software suite designed for Fugaku on cloud services and non-Fugaku computers. This makes it easier for a wider audience to utilize Fugaku's research capabilities and advanced computing platforms, potentially driving further scientific, technological, and industrial advancements

Read more

Credit: R-CCS RIKEN

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EU Launches Project for Cryogenic Quantum Computing Technologies

The ARCTIC project ("Advanced Research on Cryogenic Technologies for Innovative Computing") brings together 36 partners from 11 countries, coming from industry, academia and leading RTO

ARCTIC intends to establish a complete and comprehensive European supply chain for cryogenic photonics, microelectronics, and, in general, cryo-microsystems around the emerging quantum computing industry and different cryo-enabled ICT applications.
Read more

Credit: HPC Wire

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