National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES December 2024



In this issue...



Corporate News	1	A Note from Chief Executive, Dr Terence Hung	2	SupercomputingAsia 2025 (SCA2025)	3	NSCC Singapore's ASPIRE 2A+ Ranks 90 on TOP500 Supercomputers List
	4	Enhancing HPC Capabilities in Singapore – NSCC Singapore's December Workshop Roundup	5	Case Study - Dispersion Analysis for Handling Maritime New Fuels		
Shared News	1	KoolLogix & A*STAR launch GBP £8m cooling lab in SG	2	Google unveils new quantum computer with mind-boggling speed	3	NET4EXA: Advancing European Interconnect for HPC and Al



A Note from Chief Executive, Dr Terence Hung



As 2024 draws to a close, it's an opportune time to reflect on a remarkable year for the National Supercomputing Centre (NSCC) Singapore. It has been an exciting year of challenges but also opportunities for NSCC Singapore as we focus on our role as a national high performance computing (HPC) infrastructure.

This year, we achieved significant milestones that highlight the strength and dedication of our team and Singapore's HPC community.

Together with our HPC community partners, we initiated a restructure of the NSCC Singapore's allocation policies to better streamline, optimise and maximise Singapore's precious national HPC resource. This is to ensure that these resources are best deployed and utilised to support national programmes and research projects that have the potential to create impact for Singapore's society and economy.

We announced our initiatives at NSCC Singapore's inaugural HPC Users Symposium, a new event that will tighten our engagement with our users and collaborators and promote a more vibrant Singapore HPC community. We also co-organised and participated in international events like the SupercomputingAsia 2024 in Sydney, ISC24 in Hamburg and SC24 in Atlanta, where we cemented our partnerships as we continue to leverage the experience and best practices of well-established HPC centres and partners abroad.

Through the hard work of the NSCC Singapore team, we were able to procure, test and commission Singapore's current national supercomputing systems. We launched both the ASPIRE 2A and ASPIRE 2A+ supercomputers with the latter designed to be a quick and much needed addition to meet the rising demand for Singapore's growing AI-centric thrusts. In recognition of NSCC Singapore's role as a critical national infrastructure, the National Research Foundation, Singapore (NRF) announced a S\$270 million grant to further enhance the nation's HPC infrastructure beyond our current systems, build HPC capabilities and research, and promote and develop HPC talent. Furthermore, we signed an MoU with Quantinuum to foster quantum computing collaborations, develop hybrid solutions, and drive innovations in areas such as computational biology, in alignment with Singapore's National Quantum Strategy.

These successes would not have been possible without the dedication of the NSCC Singapore team and support from our key local partners such as the National Research Foundation (NRF), by the Agency of Science, Technology and Research (A*STAR), the National University of Singapore (NUS), the Nanyang Technological University (NTU), the National Environmental Agency (NEA) and many, many more. The insights and cooperation provided by global HPC peers through efforts like the Alliance of Supercomputing Centres (ASC) members continue to play a key role in fostering collaborations and sharing expertise that help strengthen our efforts to drive local advancements in AI, healthcare, climate science, and material science.

Looking ahead to 2025, we are excited to build on this momentum and seize new opportunities for collaboration and growth. On behalf of NSCC Singapore, thank you for your continued support. Wishing you a joyous holiday season and a Happy New Year! Interested to have your research published in NSCC Singapore's NewsBytes?

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 <u>e-news@nscc.sg</u> and we'll be in touch with you!



SupercomputingAsia 2025 (SCA25)



SupercomputingAsia 2025 is back in Singapore! SCA25, an annual international conference bringing together a diverse range of notable supercomputing events, will be held from **10 to 13 March 2025** at the iconic <u>Sands</u> <u>Expo & Convention Centre in Singapore (located at Marina Bay Sands)</u>. This premier event is co-organised by HPC centres from Australia, Japan, Thailand, and Singapore, fostering a vibrant and impactful HPC ecosystem in Asia.

The conference will feature a dynamic program lineup including workshops, tutorials, plenary talks by industry and research leaders, networking opportunities, and an exhibition space showcasing cutting-edge HPC and Quantum technologies and solutions.

Registration and ticket purchase for SCA25 will open soon. Don't miss the chance to be part of this exciting event! Register your interest <u>here</u> to stay updated on the latest developments at SCA2025.

Sneak peek – Some of SCA25's Keynote Speakers



Prof. Jack Dongarra, Professor Emeritus University of Tennessee

Jack Dongarra specialises in numerical algorithms in linear algebra, parallel computing, advanced computer architectures, programming methodology, and tools for parallel computers. He holds appointments at the University of Manchester, Oak Ridge National Laboratory, and the University of Tennessee.

In 2019, he received the ACM/SIAM Computational Science and Engineering Prize. In 2020, he received the IEEE-CS Computer Pioneer Award. In 2021, he received the ACM A.M. Turing Award for his pioneering contributions to numerical algorithms and software that have driven decades of extraordinary progress in computing performance and applications. He is a fellow of the AAAS, ACM, IEEE, and SIAM, as well as a foreign member of the British Royal Society, the U.S. National Academy of Sciences, and the U.S. National Academy of Engineering.



Prof. Jingbo Wang, Professor, School of Physics, Maths and Computing, Physics University of Western Australia

Professor Jingbo Wang established and currently leads the Research Centre for Quantum Information, Simulation and Algorithm at the University of Western Australia (UWA). The centre fosters collaboration and entrepreneurship, bringing together academics and industrial partners to develop innovative quantum solutions to tackle otherwise intractable problems and complex phenomena. Wang and her team were among the first to demonstrate the power of quantum walks in extracting local and global information of complex networks, in finding optimal and high-quality solutions to a wide range of combinatorial optimisation problems, in speeding up machine learning and image processing, and in exploring fundamental structures and symmetries in nature. Widely published in prestigious journals like Nature Photonics, Science Advances, and Physical Review Letters, her contributions have significantly advanced quantum computing and laid the foundation for future breakthroughs.

Professor Wang is also a founding director of the Australian Quantum Software Network Limited, director of the UWA-Pawsey Educational Quantum Computing Centre, Chair of the IEEE Quantum on Consumer Technology Technical Committee, chief quantum computing advisor to the WAWEB3 not-for-profit association, a member of College of Experts for the Australian Research Council, among several other notable positions. Professor Wang has played a pivotal role in developing a comprehensive suite of quantum computing lecture courses offered at the undergraduate, masters, and PhD levels. Her leadership significantly contributes to the educational advancement and integration of quantum computing expertise within the academic realm. In addition, Professor Wang serves as the Co-Director of Quantum Girls, an Australian Federal Government-funded project aimed at encouraging more girls and women throughout Australia to explore careers in quantum science, specifically in quantum computing.



Charlie Catlett, Senior Computer Scientist Argonne National Laboratory

Charlie is the founding director of the Urban Center for Computation and Data (UrbanCCD), a joint Argonne-UChicago research centre that brings scientists, artists, architects, technologists, and policymakers together to use computation, data analytics, and embedded systems to understand the dynamics, design, and resilient operation of cities. He is also a visiting artist at the School of the Art Institute of Chicago.

Before joining Argonne in 2000, Charlie served as Chief Technology Officer of the National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign. Beginning at NCSA's founding in 1985, he participated in the development of NSFNET, one of several early national networks that evolved into what we now experience as the Internet. During the exponential growth of the web following the release of NCSA's Mosaic web browser, his team developed and supported NCSA's scalable web server infrastructure.

Key Co-located Event - ACM ASEAN HPC School

We are proud to announce that Singapore will be the host country for the next edition of the prestigious ACM ASEAN School on HPC and AI. Scheduled from 10 to 14 March 2025, the school, hosted by SupercomputingAsia 2025, will provide an immersive learning experience for recent postdocs, PhD students, and exceptional MSc students in computer science and related fields.

The program will be focused on HPC and AI while introducing participants to emerging research areas like Quantum Computing. Over the week, the students will engage in formal lectures, invited talks, and a keynote lecture by Turing laureate Jack Dongarra. Esteemed speakers from leading institutions worldwide, including RIKEN R-CCS, the University of Tokyo, the European Centre for Medium-Range Weather Forecasts, Forschungszentrum Juelich, Agency for Science, Technology, and Research (A*STAR), and the National University of Singapore, will be here in Singapore to contribute to this enriching school program.

Back to Main List

NSCC Singapore's ASPIRE 2A+ Ranks 90 on TOP500 Supercomputers List

The recently launched ASPIRE 2A+ joins the TOP500 list of the world's most powerful supercomputers.



NSCC Singapore's ASPIRE 2A+ ranked number 90 on the 64th edition (November 2024) of the TOP500 list, a widely regarded benchmark that ranks the world's most powerful computer systems based on performance.

ASPIRE 2A+ is a vital national infrastructure for advancing AI research and supporting projects ranging from machine learning models to complex simulations that demand substantial computational power. Its capabilities have attracted considerable interest from research communities in biomedical and health sciences, quantum computing, and sustainable energy. NSCC Singapore's new compute power greatly enhances Singapore's capacity to drive innovation and address global challenges in emerging technologies.

ASPIRE 2A+ consists of NVIDIA DGX SuperPOD with NVIDIA H100 systems with a theoretical system peak performance of 21.73 petaflops.

The system features:

- A DGX SuperPOD with 40 DGX H100 systems, containing a total of 320 NVIDIA H100 GPUs
- 400 Gb/s NVIDIA InfiniBand (Networking)
- 2TB (System Memory) per system
- 27.5 PB (Home Storage), 2.5 PB (Scratch Storage)

ASPIRE 2A+'s first set of users includes multiple groundbreaking applications, including national AI projects, health sciences and quantum simulations.

Find out more about the <u>ASPIRE 2A+</u> and our <u>ASPIRE 2A</u> system at <u>www.nscc.sg</u>.

Back to Main List

Enhancing HPC Capabilities in Singapore – NSCC Singapore's December Workshop Roundup

NSCC Singapore organised an introductory workshop for ASPIRE 2A and welcomed the 10th intake of Certificate of Competency (CoC) in Introduction to HPC participants.



Attendees of the introductory workshop for ASPIRE 2A (left) and participants from the 10th intake of CoC in Introduction to HPC (right).

Held on 11 December 2024, NSCC Singapore organised an introductory workshop for ASPIRE 2A to provide participants with a comprehensive overview of NSCC Singapore and essential concepts of HPC.

The agenda included an introduction to key components such as the PBS Pro scheduler, compilers, libraries, developer tools, and accelerators, as well as guidance on basic operations like user enrolment, logging into NSCC login nodes, file transfers, and creating job submission scripts. Participants also learned to load environment modules, compile simple programs, and create scripts for MPI job submissions, concluding with a Q&A session for further clarification.

The 10th intake of CoC in Introduction to HPC was conducted on 12 December 2024, attracting participants from industry, Institutes of Higher Learning (IHLs), and the Advanced Remanufacturing and Technology Centre (ARTC). Co-organised by Institute of Technical Education (ITE) lecturers and NSCC Singapore specialists, this SkillsFuture-approved course, an initiative that drives lifelong learning, equipped participants with

foundational HPC knowledge and provided hands-on experience in remotely accessing HPC systems via a virtual platform. Participants were given the opportunity to leverage thousands of computing nodes to execute complex program tasks at high speeds, a critical skill for advancing deep learning AI applications.

NSCC Singapore regularly holds training and engagement workshops for users and the HPC community in Singapore. Be sure to check our <u>Events</u> page for updates on upcoming user workshops!

Case Study - Dispersion Analysis for Handling Maritime New Fuels

Researchers in Singapore aims to accelerate the adoption of alternative fuels to reduce the environmental impact of maritime operations.

Introduction

The A*STAR Centre for Maritime Digitalisation (C4MD), led by A*STAR Institute of High Performance Computing (IHPC) is positioned as a pivotal research and development node in supporting Singapore's decarbonisation efforts in the maritime sector. A key strategic focus is on accelerating adoption of alternative fuels, such as methanol and ammonia to reduce the environmental impact of maritime operations. However, these new fuels present unique challenges due to their chemical properties, including flammability and toxicity. Multi-fidelity digital models – combining computational fluid dynamics (CFD) and fast surrogate modelling – were developed and used for leakage risk assessment to address these challenges. The research is in close collaboration with the Maritime and Port Authority (MPA) of Singapore.

Bunkering Vessel



Container Vessel

Heatmap of methanol spread: Contours of exposure time to flammable plumes during an accidental release scenario during ship-to-ship bunkering.



Heatmap of ammonia AEGL3 footprint on deck and jetty from an accidental release scenario during shore-toship bunkering taking into account uncertain wind condition

The Research

Adopting low-carbon fuels in the maritime sector requires precise risk assessment for storage, transportation and bunkering. Supported by the supercomputing resources of NSCC Singapore, the team has deployed

advanced multi-fidelity digital models on ASPIRE2A for predictions of gas plume dispersion from potential leakage scenarios during methanol and ammonia bunkering operations.

These models take into account important factors like wind speed, direction, vessels, surrounding blockage structures, and complex interactions to provide a more realistic picture of how toxic and/or flammable clouds might spread from accidental releases. The resulting safety footprint from any hazardous scenario is determined from sampling through a wide parametric space of environmental conditions by executing high-fidelity simulation model on HPC resource at NSC Singapore. This approach helps capture effects of the uncertain real-world environments on risk assessment; thus addressing the unique safety challenges posed by methanol and ammonia and pave the way for safer maritime practices.

The Technology

The multi-fidelity digital models combined two advanced computational approaches—Computational Fluid Dynamics (CFD) and Fast Surrogate Modelling.

- **High-fidelity Model:** CFD simulates fluid movement to predict gas dispersion in a wellresolved geometrical surrounding with highly uncertain environmental conditions, capturing complex interactions that could impact dispersion patterns and consequences.
- **Fast Surrogate Modelling:** Enabling rapid assessments of plume dispersion by using model reduction technique built from high-fidelity CFD database. The model allows for quick probabilistic estimation of safety zones and emergency responses.
- **HPC resources used:** The project was allocated 2 million CPU hours on NSCC Singapore's supercomputing resources

Benefits of HPC

- Dedicated computational power: Supported large parametric study with complex simulations, enabling faster and more accurate predictions.
- Enhanced model performance for realistic simulations: Enabled the creation of advanced, reliable consequence analysis tailored to complex scenarios, uncertain variables. Ensured that risk assessments accurately capture real-world complexities and challenges.
- Optimised efficiency: Significantly reduced CFD computation time to hours, making it feasible to effectively assess a broad range of potential scenarios towards meeting practical demand from operation and planning.

The Impact

This advanced risk assessment capability is one of the planning tools that supported the Maritime and Port Authority (MPA) of Singapore and team to conduct the following world's first bunkering trials in Singapore:

- First Methanol Ship-to-Container Ship (STS) Bunkering Operation in the Port of Singapore (July 2023).
- World's First Bulk Liquefied Hydrogen Carrier, Suiso Frontier, to the Port of Singapore (September 2023).
- First Use of Ammonia, in combination with diesel, as a Marine Fuel in a Dual-Fuelled Ammonia-Powered Vessel, the Fortescue Green Pioneer in the Port of Singapore (March 2024).
- First Successful Simultaneous Methanol Bunkering for Container Vessels and Cargo Operation (SIMOPS) at Tuas Port (May 2024).

The success supports Singapore's position as a global bunkering hub committed to grow the multi-fuel bunkering capabilities to support the maritime fuel transition. The insights gained from these trials will improve future operations, helping to set safety standards for international maritime practices. With these steps, the Port of Singapore is prepared for commercial methanol bunkering, and similar approaches are being applied to other new fuels like ammonia.

"HPC resources were essential to our research, enabling us to perform complex, large-scale simulations and develop highly accurate risk assessments for alternative fuels like methanol and ammonia. The research will help guide our approach for future pilots and trials of new marine fuels. With NSCC Singapore's supercomputing capabilities, we incorporated intricate environmental variables, ensuring the precision needed to support Singapore's decarbonisation goals safely and effectively."

> Vinh-Tan Nguyen Senior Principal Scientist, Flud Dynamics (FD) Agency of Science, Technology and Research (A*STAR), Institute of High Performance Computing (IHPC)





Shared articles and news from the HPC world.

KoolLogix & A*STAR launch GBP £8m cooling lab in SG

KoolLogix and A*STAR have launched a USD \$8 million Joint Lab in Singapore focused on developing energy-efficient cooling solutions for AI and GPU-driven data centres.

The new joint facility will concentrate on innovative cooling technologies, promoting decarbonisation within the industry. This collaboration aims to enhance KoolLogix's cooling capabilities by incorporating A*STAR's research in predictive maintenance, intelligent control systems, AI, IoT technologies, and digital twin solutions. The focus is on developing adaptive cooling systems that meet rising demands while reducing energy use, costs, and environmental impact. Read more



Credit: ITBrief Asia

Back to Main List

Google unveils new quantum computer with mind-boggling speed

The Willow chip does in minutes what it would take leading supercomputers 10 septillion years to complete.



Credit: The Straits Times

Google said its computer using the new Willow quantum chip beat the Frontier supercomputer in running a benchmark algorithm, doing in minutes what would take the Frontier 10,000,000,000,000,000,000,000 years – far longer than the age of the universe.

That is exponentially faster than Google's stated performance in 2019, when it said it could solve a 10,000-year task in minutes. Read more

NET4EXA: Advancing European Interconnect for HPC and AI

Supported by EuroHPC JU funding, the NET4EXA research and innovation project aims to develop innovative interconnect technologies

NET4EXA builds upon the research carried out in the EuroHPC JU-funded RED-SEA project, which focused on optimising interconnect scalability and performance.

The project aims to enhance these technologies to deliver greater efficiency, capacity, and adaptability for future supercomputing needs. To demonstrate these innovations, the project will deploy a pilot system, ready for integration into exascale and post-exascale infrastructures. <u>Read more</u>



Credit: HPCwire

Back to Main List



Powering Innovation Supercomputing in Asia National Supercomputing Centre (NSCC) Singapore 1 Fusionopolis Way, Connexis South, #17-01 Singapore 138632