National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

July 2022

In this Issue...

CORPORATE NEWS

A sneak preview of Singapore's latest petascale supercomputer

The new ASPIRE 2A was introduced to some key users and stakeholders in the first of such engagements with Singapore's high-performance computing (HPC) community.

The NSCC Roadshow, in collaboration with CPU component partner AMD, was held on 26 July 2022. The aim of the event was to introduce the ASPIRE 2A to the Singapore research community. This involved a Technical session where the key features, software and applications of the new supercomputer were presented by NSCC's Technical Team as well as a parallel Technical-lite session where invited speakers presented real-world HPC use cases for researchers and the HPC community.

Summary of the event programme:

Keynotes
ASPIRE 2A – Fulfilling the Aspirations of Singaporean Researchers *by Mr Rajesh Chhabra, Regional Sales Manager, HPC & AI – APAC, Hewlett Packard Enterprise* **NSCC Supercomputing Digital Sandbox – Democratising HPC for All** *by Mr Bernard Tan, Director (Strategy, Planning & Engagement), NSCC*

Track 1 – Technical	Track 2 – Technical-Lite
System Architecture Design of the ASPIRE 2A System *by Mr Paul Hiew, Senior System Manager, NSCC* **NUS-NSCC i4.0 Data Centre – A Tropical Supercomputing DC** *by Mr Vincent Lim, Senior Facilities Manager, NSCC* **Useful System Reports and Information Available to the User in ASPIRE 2A** *by Mr Ng Kheng Ghee, System Engineer, NSCC* **HPC Software Environment in ASPIRE 2A** *by Mr Chung Shin Yee, Senior HPC Analyst, NSCC* **Kubernetes Platform in ASPIRE2A System** *by Mr Teguh Satria, Assistant System Manager, NSCC* **Applications: Spack and Gromacs Performance** *by Mr Jernej Zidar, Senior HPC Application Analyst, NSCC* ***SingAREN: High Speed Network to Serve the Research and Education Community*** *by A/Prof Francis Lee, Associate Professor,* *School of Computer Science and Engineering,* *Nanyang Technological University*	**HPC Possibilities in the Urban Setting** *by Mr Eugene Seah, Managing Director (Smart City Solutions), Surbana Jurong* **3D Urban Tree Modelling for Environmental Studies** *by Dr Like Gobeawan, Computer Scientist,* *A*STAR Institute of High Performance Computing* **AMD Environmental Sustainability & Roadmap** *by Mr John Hampton, Senior Director, WW Customer Field Support, Advanced Micro Devices, Inc.* ***DCWiz: Transforming Data Center Operations and Management (O&M) with AI*** *by Prof Wen Yonggang, Professor and President's Chair, Computer Science and Engineering,* *Nanyang Technological University* ***Efficient at Scale Performance Using NVIDIA Accelerated Solutions for HPC and AI*** *by Dr. Gabriel Noaje, Principal Solutions Architect,* *NVIDIA APAC South*

The **A**dvanced **S**upercomputer for **P**etascale **I**nnovation, **R**esearch and **E**nterprise, or ASPIRE 2A, will be an upgrade of Singapore's first petascale machine, the ASPIRE 1, which was commissioned back in 2016. The ASPIRE 2A is now undergoing trials and is slated to be ready for Singapore research community by the end of the year.

If you want to learn more about the ASPIRE 2A supercomputer and would be interested to attend future Roadshows, please write in to e-news@nscc.sg.

Coming soon – NSCC's new Supercomputing Digital Sandbox (SDS)

The SDS tool is designed to make the experience of using HPC resources much easier and simpler for researchers who may not possess in-depth HPC knowledge.

A new feature of the upcoming ASPIRE 2A supercomputer is the Supercomputing Digital Sandbox, which is a platform that caters to basic or new HPC users to create a better user experience. The aim is to allow scientists to testbed their research projects and to give them the opportunity to learn how best to make optimal use of the supercomputer resources.
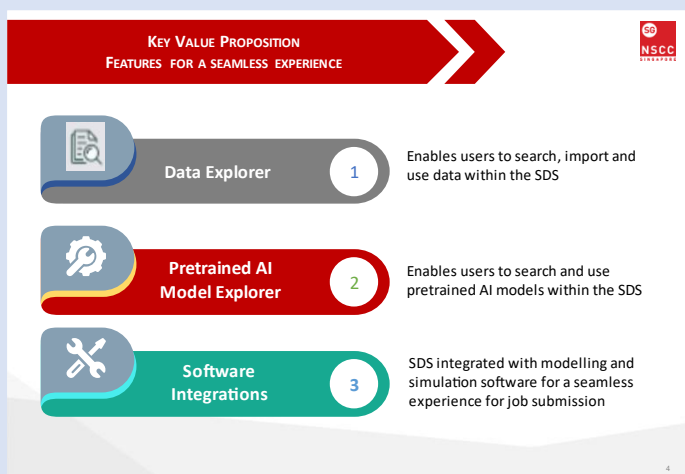
The SDS supports R&D, proof-of-concept development and training across various research domains through its user-friendly features and integrated HPC resource. The SDS will be available to all users in the public sector, institutes if higher learning (IHLs), research organisations and industries.

If you are interested in learning more about NSCC's Supercomputing Digital Sandbox (SDS) or would like to sign-up to use it, please contact e-news@nscc.sg.

Research projects that have benefitted from NSCC's supercomputing resources

Featured here are recent highlights of research publications and projects that have leveraged the Singapore's national high-performance computing resources.

- **"Accurate somatic variant detection using weakly supervised deep learning"**
  Krishnamachari, K., Lu, D., Swift-Scott, A. et al. Nat Commun 13, 4248 (2022). https://doi.org/10.1038/s41467-022-31765-8

- **"Effect of exchange-correlation functionals on the estimation of migration barriers in battery materials"**
  Devi, R., Singh, B., Canepa, P. et al. npj Comput Mater 8, 160 (2022). https://doi.org/10.1038/s41524-022-00837-0

- **"Bioinspired stretchable molecular composites of 2D-layered materials and tandem repeat proteins"**
  Mert Vural, Tarek Mazeed, Dong Li, Oguzhan Colak, Reginald F. Hamilton, Huajian Gao and Melik C. Demirel PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES, Vol. 119, No. 31, August 2, 2022. https://doi.org/10.1073/pnas.2120021119

- **"A first-principles-based high fidelity, high throughput approach for the design of high entropy alloys"**
  Sorkin, V., Yu, Z.G., Chen, S. et al. Sci Rep 12, 11894 (2022). https://doi.org/10.1038/s41598-022-16082-w

Visitors from the French Defense Innovation Agency

The French delegation from the Defense Innovation Agency at NSCC's data centre

On 20 July 2022, NSCC hosted Dr. Emmanuel Chiva, Director of the Defense Innovation Agency, and the French delegation from the Defence Innovation Agency during their visit to Singapore as part of the France-Singapore bilateral cooperation in research, technology and defence innovation. The delegation was joined by His Excellency Marc Abensour, French Ambassador to Singapore.

The Defense Innovation Agency federates the French Ministry's innovation initiatives by ensuring the coordination and coherence of all innovation initiatives. While pursuing work on technological innovation over the long term, the Agency is the sensor of opportunity innovations for the benefit of all end users, whatever their field: operations management, equipment, support, operation, administration.

During their visit, they learned about NSCC's latest developments and services and were brought on a tour of the ASPIRE 1 data centre.

Supercomputers help scientists better understand peanut allergies
Researchers from A*STAR leverage high-performance computing (HPC) resources to develop advanced structural model and simulations of the interactions between antigens and allergens.

Food allergies are a common health problem worldwide. It is estimated that nearly 5% of young children may be affected by allergies in Singapore. In particular, allergy to peanuts is a growing top trigger of severe allergy in children.

The mechanism that triggers a peanut allergy involves biological components and their interactions. These components include the human antibody IgE, peanut allergens, and IgE's partner receptors on mast cells. Disrupting these interactions could intervene with severe allergic immune responses.

A team of researchers from A*STAR's Bioinformatics Institute (BII) are conducting in-depth studies on these IgE interactions at a molecular level by combining computational modelling and experimental validation. The

team aims to find out how changes to the IgE structure can affect peanut allergies and the potential for the results to be used for therapeutic purposes and allergy intervention. The molecular complex of interest includes IgE, the antigen (peanut allergen, e.g. Ara h1) and the FcεRIα (IgE receptor). Since most available crystals and current nuclear magnetic resonance (NMR) data of these structures are mostly truncated forms and submodules, the team's objective is to characterise the conformational changes that the IgE undergoes upon binding to the FcεRIα and the peanut allergen separately, and together.

"The project aims to develop a holistic understanding on the structural model of the whole peanut allergen-IgE-receptor complex," said Dr Chinh Tran-To Su, the Principal Investigator (PI) for the project. "This is done via the combination of advanced structural modelling and the latest cross-linking Mass Spec (XL-MS) technology."

The project team hopes that the holistic analysis of IgE interactions would benefit future allergen-specific IgE studies and the engineering of therapeutic by enhancing the understanding of the role of IgE in allergy pathogenesis.

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

"The advanced modelling and simulations as well as the full-atom molecular dynamics were performed on NSCC's ASPIRE 1 supercomputer. The HPC resources greatly facilitated the simulation of the dynamics of the large systems, which are composed of the IgE and the IgE-allergen-receptor complexes. The team is currently using GROMACS at this stage of the project.

Chinh Tran-To Su
Research Scientist
Algorithms and Models of Protein
Machinery (AMPM) Group,
Bioinformatics Institute (BII),

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Shared articles and news from the HPC world.

S'pore's third national climate change study to be completed in Sept 2023

Singapore's third national climate change study, which will provide localised and high-resolution climate projections till 2100, will be completed in September next year.

The study will provide South-east Asia's most advanced climate projections, zeroing in on every square of land or sea spanning 8km. The model will divide Singapore and the rest of the region's land and sea into grid cells of 8km by 8km, and each cell's changes in temperature, humidity, wind speed, rainfall amount and sea level rise will be projected till 2100. The Centre for Climate Research Singapore (CCRS) has been working with the National Supercomputing Centre to scale down global climate models to produce the 8km resolution forecasts. Read more at The Straits Times here.

ORNL Debuts Cumulus-2 Cluster for Climate Data

The Oak Ridge National Laboratory (ORNL) launched the Cumulus-2, an HPC cluster serving the DOE's Atmospheric Radiation Management (ARM) user facility.

Cumulus-2, built by Dell, consists of 32 total chassis. 28 of those are equipped with four nodes each, with each of those nodes containing dual AMD Epyc "Milan" 7713 CPUs and 256GB of memory. Four additional chassis contain four high-memory nodes each, which contain 512GB of memory rather than 256GB. (ORNL didn't have a flops estimate on-hand, but we estimate it around 524 theoretical peak teraflops of computing power.) Cumulus-2 is networked with Nvidia's InfiniBand HDR200 and connected to a 7PB filesystem.The ORNL team started conceptualizing the system in early 2020. Read more at HPC Wire here.

Credit: Carlos Jones/ORNL

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