National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

April 2023

In this Issue…

CORPORATE NEWS

NSCC's ASPIRE 2A Data Centre – A tropical supercomputing data centre that is a game-changer in energy efficiency

Specially designed for the tropics, find out how the data centre (DC), which houses Singapore's newest supercomputer, has pioneered innovative efficiency solutions ahead of the curve.

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Thank you!

LET'S BEGIN

FINAL CALL FOR RESEARCH PROJECTS ON ASPIRE 2A

This is the final call for Research Projects on the ASPIRE 2A supercomputer. Interested applicants can apply for resources on ASPIRE 2A and the Köppen system via this call.

Application Period

3 Apr 2023, 1000 hrs – 2 May 2023, 2359 hrs

Resource Allocation Period

1 Jul 2023 –30 Jun 2024

MORE INFO

As a National Research Infrastructure funded by the National Research Foundation, NSCC supports the HPC research needs of the public and private sectors in Singapore. This includes research institutes, institutes of higher learning, government agencies and companies. This amount of computing requires a large amount of energy. With rising costs and environmental mandates, this energy has to be managed efficiently and power needs to be saved wherever possible.

In this context, the NUS-NSCC i4.0 DC – a Tropical Supercomputing Data Center, which houses Singapore's newest supercomputer, won the W.Media Southeast Asia 2022 award for Energy Efficient Innovation. NSCC as a national research HPC infrastructure plays a part in exemplifying best-of-breed infrastructure and pioneering efficiency solutions ahead of the curve of the wider DC industry.

What innovation has NSCC adopted to achieve energy efficiency goals?

The new NSCC DC adopts a number of unique power saving features. It is a specially-designed tropical DC which leverages a hot hall, ambient temperature water-dry cooler system. The 300 sqm, double-height DC is also computer room air conditioner (CRAC)-less- meaning that the main compute server hall does not employ air-conditioning to cool the system, which is unlike most conventional data centers. The system also uses special designed-in-Singapore technologies like the Cool Hall rear-door heat exchange (RDHX) with the patented KoolLogix Thermosiphon gas system, which further helps to increase energy efficiency by better dissipating heat.

What are some of the challenges in constructing 'smart' data centres?

Modern 'smart' DCs are generally equipped with intelligent monitoring / AI-assisted operations, advanced DCIM and leveraging Digital Twin technology with integrated IoT sensors, data analysis with CFD and AI, to facilitate controls and optimize real-time DC operations. Such additional tools and electronics require increased energy resources adding to the already high-power usage of DCs. One of the greatest challenges is being able to tap into more sustainable and carbon-friendlier energy sources such as renewable solar energy supplies. In the absence of abundant renewable energy sources in Singapore, NSCC relies on unique, innovative DC designs to reduce the carbon footprint but is also exploring other alternative solutions. Other exploratory decarbonization initiatives include new concepts like recycling excess cool energy from industrial processes such as LNG or leveraging international partnerships to tap on carbon-friendly infrastructure and energy resources.

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HPC 101 - Developing high-performance computing skillsets

Equip yourself with the basic knowledge of high-performance computing by registering for the Certificate of Competency (CoC) in Introduction to High Performance Computing (HPC).

A collaboration between NSCC and ITE College West, course participants will have the opportunity to be co-trained by ITE lecturers and NSCC specialists on how to access HPC remotely from a virtual platform. Participants will gain the experience of working on thousands of computing nodes that can perform complex programme tasks at high speed, which in turn will accelerate the building of deep learning AI applications.

Training accounts with computing resources will be provided by NSCC. Upon completion of the course, participants will be awarded a CoC in Introduction to HPC from ITE as well as a Certificate of Participation by NSCC Singapore.

At the end of this course, participants will acquire skills and knowledge on:

- Basic building blocks of a supercomputer
- Understanding PBS Job Scheduler
- Use-case & Accessing of HPC
- Environment Setup & File Transfer
- Resource Allocation & Job Submission
- Hands-on AI Project using HPC

Upcoming intake:

21 June 2023, 9am – 5pm

For more information, head over to https://www.ite.edu.sg/courses/course-finder/course/coc-in-introduction-to-high-performance-computing-(hpc).

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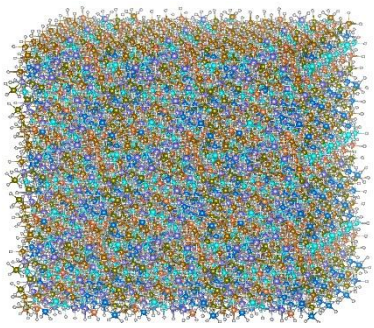
Leveraging machine learning and supercomputers to accelerate new materials development

Researchers from NUS utilise high performance computing resources to accelerate the discovery and development of new materials.



The development of novel functional materials has led to numerous technological breakthroughs and advancements, such as the development of high-performance batteries, flexible electronics, advanced sensors, and quantum computers. As technology continues to evolve, the demand for new and innovative materials with unique properties and functions will only continue to grow. The ability to modify the physical properties of materials and design them with on-demand characteristics is crucial for advancing technology.

The design space for nanomaterials is vast, and traditional trial-and-error methods can be time-consuming and inefficient. For most devices and technologies, the careful design of material properties through methods such as alloying, creating heterostructures or composites, or controlled introduction of defects is necessary. However, the potential configuration space of such design elements can be extremely large, making it impractical to explore each possibility one by one.

"NSCC's HPC resources enabled us to construct a large database of materials using high-throughput density functional (DFT) calculations. Additionally, these resources facilitated the training of advanced machine learning models that can accurately predict the physical properties of materials."

Dr Pengru Huang
Senior Research Fellow,
Institute for Functional Intelligent Materials,
National University of Singapore

Therefore, a team of researchers from the National University of Singapore's Institute for Functional Intelligent Materials are tapping onto the computational power of NSCC's resources to carry out high-throughput first-principle calculations, resulting in the generation of a large database of materials. They will then structure the datasets and construct descriptors and representations before applying state-of-the-art machine learning methods to train models that can predict the physical properties of materials based on the input data. This will ultimately allow them to accelerate the discovery and development of new materials with desired properties.

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

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Capping Carbon on Asia's Supercomputers

Thoughtful processor design, optimized programming and strong government support are helping to make high performance computing ecosystems more sustainable.

When Pixar and Disney first shared a glimpse of their 2013 animated film Monsters University, fans quickly noticed one striking detail: the fur covering Sulley, one of the movie's two protagonists, was extremely realistic. Millions upon millions of tiny strands of fur swayed convincingly whenever the gentle giant moved his limbs, and even ruffled under a tight shirt, just as you'd expect them to. The animators' secret? A supercomputer that would've ranked among the world's fastest at the time, automatically redrawing every single strand of fur and letting it catch and reflect light with each frame of movement.

Ordinary desktop machines don't have the processing prowess to carry out this type of animation—in fact, even the higher-end versions would have had trouble with it. But animators revealed that Sulley and other monsters in the film, along with every texture, shading and frame, owe their crisp, vivid existence to high-performance computing (HPC).

Able to handle billions of calculations easily, this is the same type of technology that is being leveraged to predict tsunamis, supercharge healthcare innovation and study the origin of super massive black holes. Combining powerful processors, sophisticated software and other cutting-edge computing technologies, HPC employs thousands of computing nodes working simultaneously to complete extremely complex computing tasks much quicker than a regular computer can.

There's just one problem. With great computing power comes great energy liability. Even as HPC systems are helping solve some of the most pressing problems in society in the decade since Monsters University, they pose another problem: their massive carbon footprint.

To balance computing power and sustainability, supercomputers across Asia are increasingly being designed with more energy-efficient processors and programming. Meanwhile, governments are waking up to the need for more sustainable energy sources and policies as they shape their growing HPC ecosystems.

Head over to https://www.asianscientist.com/2023/04/print/capping-carbon-on-asias-supercomputers/ to read the full article published in the January 2023 issue of NSCC's Supercomputing Asia Magazine to find out how supercomputers across Asia are increasingly being designed with more energy-efficient processors and programming.

This article was first published in the print version of Supercomputing Asia, January 2023.
Credit: Tristan Manalac, Writer, Asian Scientist Magazine

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THE LAST BYTE...
<SHARED CONTENT>

Shared articles and news from the HPC world.

Keeping Singapore firms and workers at the forefront of AI advancements: Temus and AI Singapore sign MOU to accelerate AI innovation and adoption

Temus, a digital transformation services company, announced an inaugural partnership with AI Singapore (AISG) at the signing of a Memorandum of Understanding (MOU) yesterday.

The strategic partnership aims to accelerate AI innovation and adoption among companies in Singapore, contribute to the National AI strategy and reinforce Singapore's position as a global AI hub. Under the MOU, Temus and AISG will collaborate to catalyse digital transformation, promote AI adoption, and develop new AI technologies, solutions, and applications for firms based in Singapore. The partnership will also provide training, resources, and mentorship to nurture local AI talent and support local research projects and initiatives. Read more at AsiaOne here.

Credit: AsiaOne

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LUMI Supercomputer Powers Generative AI Model for Finnish Language

Generative AI is taking the tech world – and the broader world – by storm, but relatively little word has come out of the major supercomputer centers amid the influx of generative models.

Finnish IT center CSC has announced that its massive EuroHPC supercomputer, LUMI, powered a research project that produced the "largest Finnish language model ever". LUMI is still early in its lifespan, having just hit the Top500 list last May, where it placed third (a position it retained this November). The research team was able to complete the model – called TurkuNLP – because they had been granted special access as one of around thirty pilot projects for LUMI's GPU partition. Read more at HPC Wire here.

Credit: LUMI

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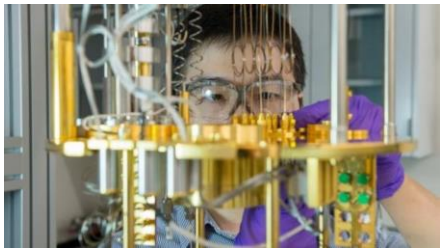
Argonne National Laboratory: Advancing Quantum Information Science

Argonne National Laboratory, part of the U.S. Department of Energy (DOE), has made substantial advances in quantum information science (QIS).

Quantum information science (QIS) investigated the sensing and transmission of information using subatomic particles. It may one day lead to a quantum computer capable of tasks that were previously impossible to execute or a highly secure network for exchanging data. By investigating novel materials, conducting rigorous simulations, and establishing themselves as industry experts, the lab has been working on expanding the boundaries of quantum information science (QIS). Read more at OpenGov here.



Credit: Open Gov

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