National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

September 2021

In this Issue…

CORPORATE NEWS

Supercomputing Frontiers Asia 2022 (SCFA22) Call for Papers

Abstract and paper submissions are now open!

SupercomputingAsia 2022 (SCA22), the annual international conference that encompasses an umbrella of notable supercomputing events with the key objective of promoting a vibrant and relevant HPC ecosystem in Asia, will return from ***1 – 3 March 2022***. Co-organised by HPC centres from Australia, Japan and Singapore, the SCA22 will be held as a hybrid conference at Suntec Singapore Convention & Exhibition Centre and Online.

The technical papers portion of SCA, Supercomputing Frontiers Asia 2022 (SCFA22), will be held in conjunction with the conference as a key co-located event. The SCFA session aims to provide a platform for thought leaders

Interested to have your research published in NSCC'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 **e-news@nscc.sg** and we'll be in touch with you!

from both academia and industry to present their research as well as discuss visionary ideas, global trends and the latest innovations impacting the world of supercomputing.

The SCFA22 consists of four tracks:

APPLICATION, ALGORITHMS & LIBRARIES

ARCHITECTURE, NETWORK/COMMUNICATIONS & MANAGEMENT

PROGRAMMING & SYSTEM SOFTWARE

DATA, STORAGE & VISUALISATION

Topics of interest include, but are not limited to:

Application, Algorithms & Libraries

- Bioinformatics and computational biology
- Climate, weather and earth sciences
- Materials science and chemistry
- Scalable numerical methods
- Fault-tolerant algorithms
- Energy-efficient algorithms
- Domain-specific, language, libraries or frameworks
- Sustainable software development

Architecture, Network/ Communications & Management

- Novel memory architecture
- Embedded and reconfigurable architectures
- Scalable system architectures
- Energy-efficient architectures
- Interconnect technologies
- Fault tolerant networks
- Architecture for converged HPC/Big Data
- Administration, monitoring and maintenance tools

Programming & System Software

- Compiler analysis and optimisation
- Runtime systems
- Parallel programming languages
- Tools for parallel programme development
- Resource and job management
- HPC system software/operating systems
- Energy-efficient middleware

Data, Storage & Visualisation

- Scalable structured storage
- Next-generation storage systems
- Data intensive computing
- Visualisation tools for Big Data
- Middleware for Big Data management
- Reliability and fault tolerance in storage
- Big Data application studies

Technical Papers Co-chairs

Dr. Michael Sullivan
Department Director, Material Science and Chemistry
Institute of High Performance Computing, A*STAR, Singapore

Dr. Dhabaleswar K. (DK) Panda
Professor and Distinguished Scholar, Computer Science and Engineering
The Ohio State University (OSU), United States of America

Abstract Submissions Due: 22 October 2021

Paper Submissions Due: 19 November 2021

Notice of Acceptance: 10 January 2022

SUBMIT HERE

The conference proceedings will be published in Springer Nature's Lecture Notes in Computer Science (LNCS).

For more information about SCFA22, please visit https://easychair.org/cfp/SCFA22 or contact the SCFA22 Technical Paper Co-chairs or email papers@sc-asia.org for any questions/clarifications.

Back to main content list

Submit your HPC resource requirements!

Looking to augment and supercharge your research work with high performance computing? From now till 30 Sep 2021, apply for supercomputing resources on NSCC's ASPIRE 1 and AI System. NSCC's January 2022 Cycle Call For Research Projects is now open for submissions.

NSCC is pleased to announce the next Call for Projects Proposal for the January 2022 cycle. Interested applicants from stakeholder organisations i.e. A*STAR, NTU, NUS, SUTD, NEA, TCOMS will be able to apply for resources on ASPIRE 1 and AI System.

Since July 2017, NSCC officially started allocating resources on a per-project basis for users who require resources beyond the personal quota of 50 GB storage and 100,000 CPU core hours for NSCC's ASPIRE 1 supercomputer.

Also available for use is the AI@NSCC Platform. This platform is deployed in support of AI Singapore (AISG), a national programme set up to drive AI adoption, research and innovation in Singapore. The system consisting of six DGX-1 nodes are meant for projects that focus on AI research with the particular novelty on scale and/or throughput breakthrough.

APPLY NOW

**NSCC is building a new supercomputer which is expected to be commissioned and open to all users in Q2-2022. Please be prepared that you may be required to transition from ASPIRE 1 into the new ASPIRE 2A supercomputer in Q2-2022. Details of the transition will be provided at a later date.*

For more information about the Call for Projects, please visit https://help.nscc.sg/nscc-call-for-project-application/ or contact projects-admin@nscc.sg if you have any queries.

Back to main content list

Supercharge your career with 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 be co-trained by ITE lecturers and NSCC 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.

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 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

Dates:

1 Oct (Fri), 9am – 5pm

20 Dec (Mon), 9am – 5pm

Fees for this course can be paid using SkillsFuture Credits

Scan to register NOW!

tinyurl.com/58cbp9r9

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

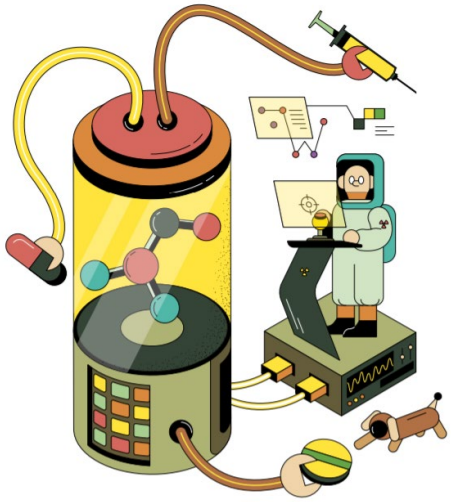
Back to main content list

Accelerating HPC adoption across ASEAN

High performance computing could help the many talented scientists, engineers and businesses in Southeast Asia reach their full potential.

It goes without saying that your morning commute in Hanoi, Vietnam, would be vastly different from what it would be in Houston, Texas. There were over 276 million vehicles on US roads in 2019, a figure that works out to 842 cars per 1,000 people. In contrast, motorbikes dominate the roads in Vietnam, which has just 23 cars per 1,000 people—nearly 37 times less.

Yet when it comes to training autonomous vehicles (AV), the vast majority of data comes from the US and Europe. VinFast, a Vietnamese automotive startup with its sights set on the global market, is hoping to use supercomputers to bridge the difference. “When I came back to Vietnam, I had to relearn how to drive here—the traffic conditions are very different from the US,” said Dr. Hung Bui, an artificial intelligence (AI) researcher formerly with Google DeepMind and Adobe Research, and currently the director of VinAI, the AI research arm of VinFast’s parent company, Vingroup.



"After a while I got the hang of it, but it got me thinking a machine probably will do an even better job—Vietnam's driving conditions provide the ultimate challenge for systems trying to reach Level 5 autonomy," he said, referring to fully autonomous cars that will not even require steering wheels.

Helping VinFast along is the country's most powerful AI supercomputer: VinAI's NVIDIA DGX SuperPOD. Branded as the world's first cloud-native supercomputer, the DGX SuperPOD will be used to retrain VinAI's driving perception system as new data arrives every 24 hours, Hung said.

World-leading AV systems built by private companies in Southeast Asia are just one of the many ways that high performance computing could impact the region. Head over to https://www.nscc.sg/supercomputing-asia-magazine/ to read the full article published in the July 2021 issue of NSCC's Supercomputing Asia Magazine to find out the ways supercomputers are supercharging research and development.

To find out more about the NSCC's HPC resources and how you can tap on them, please contact e-news@nscc.sg.

Visit www.nscc.sg/case-studies to learn more about how supercomputers are helping Singapore.

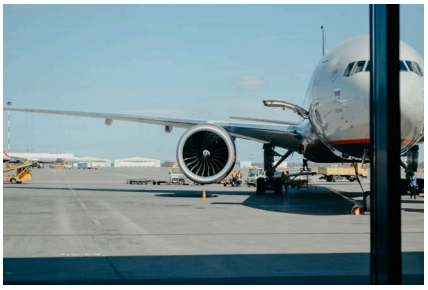
This article was first published in the print version of Supercomputing Asia, July 2021.
Credit: Tim Hornyak, Writer, Asian Scientist Magazine

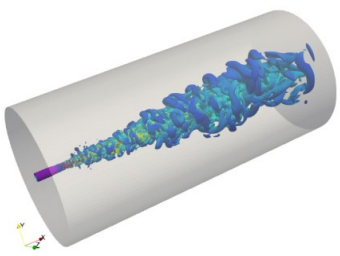
Back to main content list

A quieter way to fly - Reducing jet engine noise through HPC research

Researchers from NUS are harnessing the power of supercomputing to understand the mechanism of noise generated by jet engines to reduce the impact of noise emission on the environment and human health.

The noise generated by modern aircraft has been a long-standing noise-pollution problem since the first commercial jet-engine-powered aircraft entered in the early 1950's. The elevated acoustic noise levels from aviation in flight has serious adverse impact on the health and well-being of people who live or work near airports. These health problems include, but are not limited to, hearing impairment, sleep disturbance, increased stress levels and the increased risk of hypertension and heart disease, which affect all age groups, especially children.





Computational domain and vortex structures of jet superimposed with velocity distribution
Credit: NUS

A typical turbofan civilian aircraft during take-off can generate an overall sound pressure level (OASPL) of approximately 100 dB, measured about 100ft away from the runway centre line. Much of the noise emission from jet-engine-powered aircraft originate from the airframe and engines. The noise produced from jet exhaust is by far the major source of noise pollution especially for low bypass ratio engines.

To reduce its impact on the environment and health, it is essential to understand the mechanism of noise generation, which can be challenging due to the complex physics of turbulent flow and its interaction with the

acoustic field. A team of researchers at NUS' Temasek Laboratories are utilising NSCC's supercomputing resources in an attempt to employ the computational aeroacoustics (CAA) method with high-fidelity numerical simulations to accurately resolve the jet flow and predict its noise emissions. The research hopes to improve the understanding of the underlying physical process of noise generation and radiation.

"For the noise prediction by CAA with high-fidelity fluid simulations, the smaller magnitude of acoustic pressure and the greater acoustic timescales require higher numerical schemes, finer mesh of computational domain and a larger number of time steps. The nature of the problems inevitably need huge amounts of computational resources. With the support of petascale CPU supercomputing resources and ample develop r tools from NSCC, the code development is facilitated and the simulation of jet noise is significantly accelerated and completed in just a few months. The small magnitude of acoustic pressure is well captured and the radiation of noise sources from the jet is predicted in the far-field. The advanced storage system of HPC from NSCC also allows longer storage of the heavy datasets and provides significant support for the post-processing."

Shan Ruiqin
Research Scientist
Temasek Laboratories
National University of Singapore

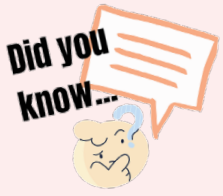
To find out more about how NSCC's HPC resources can help you, please contact e-news@nscc.sg.

Back to main content list

TECHNICAL NEWS

Do more with PBS Pro on ASPIRE 1

Part 3.



It is possible to submit a job running in 24-hour chunks and resume from where it last ended.

While it would be great, if one could run his jobs on a supercomputer indefinitely, this is seldom possible because every supercomputer imposes a maximum period (i.e., walltime) a particular job can run. On NSCC's ASPIRE1, this limit is set to 24 hours. Any job trying to run for even a second longer will be terminated by the PBS Pro scheduler. While it might be ever so slightly annoying, it also allows other users to make use of the computing resources.

Is it possible to submit a job so it would run in 24-hour chunks and resume where it was last ended? Yes, it is possible but you should bear in mind this feature critically on the application you are trying to run. Most popular molecular dynamics applications such as Gromacs, CHARMM, NAMD support this feature out of the box, whereas in quantum chemical codes like VASP, NWchem, Qchem, ... this feature is less common and its availability depends on the computational method employed.

To submit a job so it runs in 24-chunks we will use a Gromacs example that you can readily modify for other supported applications. We will achieve this by preparing a single PBS job input file and adding a second job as a dependency of the first one.

In the PBS job, we define the resources required and specify the job to be resumed (or restarted) from a checkpoint file. For Gromacs this is achieved by specifying the '-cpi' switch as indicated below:

```
# 1. Load the necessary modules and setup the environment
module load gromacs/2018.2/gcc493/impi

# set input that will be used as basename for all outputs
input=my_initial_input_file
output="$input"

# 1. Run it.
mpirun mdrun_mpi -v -deffnm "$input" \
                 -pin on -cpi -maxh 23.9

# 2. Process trajectory - optional but useful because it enables checks for the simulation progress
echo 0 | gmx trjconv      -f "$output".trr \
                          -o "$output".xtc \
                          -s "$output".tpr \
                          -pbc whole
```

For more information and FAQs on ASPIRE 1, please visit:

https://help.nscc.sg

If you submit this job it should start and end just before the 24-hour limit because of the switch `-maxh 23.9` specified in the mpirun line. To have it continue, you first have to take note of the Job ID of the first job by issuing a `qstat` command and look for a long number that ends in .wlm01.

You will add the next job (or iteration) as job dependency by using the same PBS input like this:

qsub -W depend=afterok:<JOB_ID> myjobscript.pbs

If you then issue a `qstat` command, you will see your first job is (most likely) running, whereas the second one is waiting for the first one to complete without errors. For really long jobs that need a week to complete, one could just issue the above command seven times, replacing the <JOB_ID> with the ID of the previous job. You can also replace the `afterok` with `afternotok`, if you want to use a different PBS input in case the first job ends with an error.

For more information, click here (under section 3.5 Job Dependencies).

Back to main content list

THE LAST BYTE...

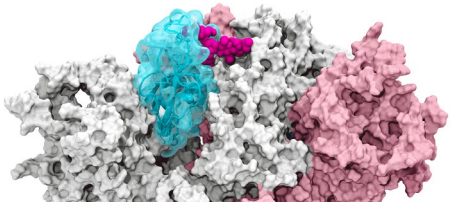
<SHARED CONTENT>

Shared articles and news from the HPC world.

Using supercomputing, researchers discover hidden SARS-CoV-2 'Gate' that opens to allow COVID infection

Since the early days of the COVID pandemic, scientists have aggressively pursued the secrets of the mechanisms that allow severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) to enter and infect healthy human cells.

Early in the pandemic, University of California San Diego's Rommie Amaro, a computational biophysical chemist, helped develop a detailed visualisation of the SARS-CoV-2 spike protein that efficiently latches onto our cell receptors. Now, Amaro and her research colleagues from UC San Diego, University of Pittsburgh, University of Texas at Austin, Columbia University and University of Wisconsin-Milwaukee have discovered how glycans—molecules that make up a sugary residue around the edges of the spike protein—act as infection gateways. Read more at HPC Wire here.



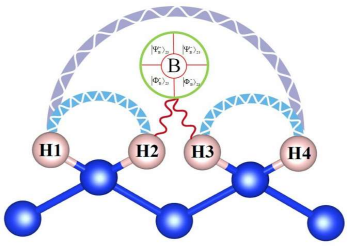
Credit: Terra Sztain, Surl-Hee Ahn, Lorenzo Casalino (Amaro Lab, UC San Diego)

Back to main content list

The best of both worlds: Combining classical and quantum systems to meet supercomputing demands

Quantum entanglement is one of the most fundamental and intriguing phenomena in nature.

Recent research on entanglement has proven to be a valuable resource for quantum communication and information processing. Now, scientists from Japan have discovered a stable quantum entangled state of two protons on a silicon surface, opening doors to an organic union of classical and quantum computing platforms and potentially strengthening the future of quantum technology. Read more at Phys Org here.



Credit: Phys Org

Back to main content list

Breakthrough: Quantum computers will soon fit in your phone

Quantum Brilliance has developed a diamond-based quantum computer that can run at room temperature and be miniaturised.

A quantum computer small enough to sit on your desk — or be embedded in a satellite, car or even a mobile phone — is no longer a pipe dream. The first such machines are actually starting to be delivered to early customers, thanks to advances in qubits created using synthetic diamonds. Read more at Sifted here.

Credit: Sifted

Back to main content list