National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

June 2021

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CORPORATE NEWS

Another bumper crop for APAC HPC-AI competition!

Some 36 student teams from across 30 universities and educational institutions from across the Asia Pacific (APAC) region have registered for the 4th annual student competition.

Launched at the SupercomputingAsia 2021 Conference (SCA21) in March this year, the fourth edition of the competition encourages APAC university and technical institute teams to showcase their HPC and AI expertise in a friendly yet spirited competition that builds critical skills, professional relationships, competitive spirits and lifelong comraderies. The annual competition is co-organised by the HPC-AI Advisory Council (HPCAIAC) and NSCC.

GROMACS (GROningen MAchine for Chemical Simulations), a popular molecular dynamics simulation tool designed for biochemical molecules like proteins and nucleic acids, will be chosen as the HPC task for the HPC-AI competition. DLRM (Deep Learning Recommendation Model), a neural network-based recommendation tool, will be used for the AI task of the competition to utilise the model parallelism while exploiting data parallelism to scale-out compute from the fully-connected layers. The competition will also continue to include topics related to the global fight against COVID-19. Teams will be tasked with mastering the same complex HPC and AI workloads that are integral to today's major advances.

The student teams will be collaborating and competing remotely, and will have hands-on access to NSCC's advanced supercomputing resources with dedicated cycle time provided by NSCC.

The winning teams will have the opportunity to represent the APAC region at the 2022 ISC Student Cluster Competition. The winning APAC teams will be announced in November this year, followed by an official award ceremony at the SupercomputingAsia 2022 (SCA22) Conference in March 2022.

For more information on the 2021 APAC HPC-AI Competition please visit https://www.hpcadvisorycouncil.com/events/2021/APAC-AI-HPC/teams.php.

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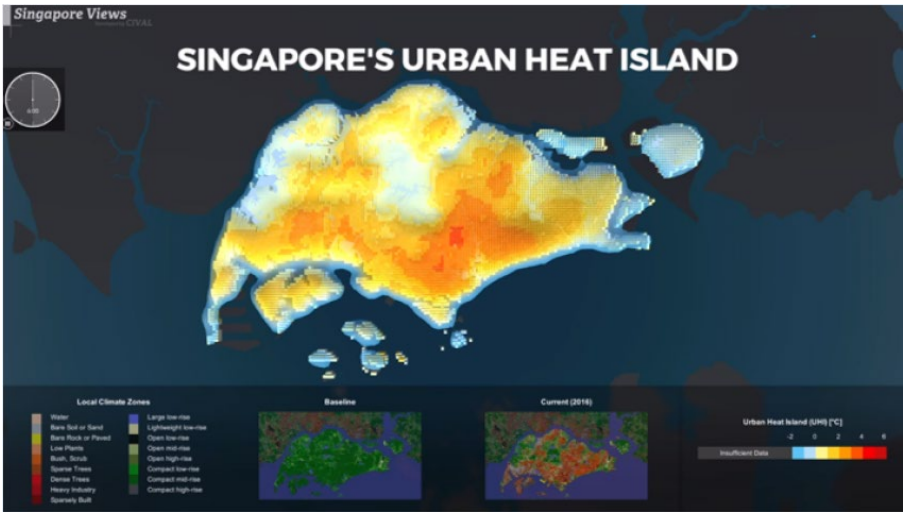
Singapore-ETH Centre (SEC) is tapping on HPC in Cooling Singapore

The SEC joins NSCC's HPC user community as a major stakeholder! Singapore's national supercomputing infrastructure is giving the research centre a boost in its research on urban warming.



Credit: Singapore-ETH Centre

The Singapore-ETH Centre (SEC) has embarked on research to cool Singapore since 2017, and NSCC is now giving it a boost with its HPC resources. In the current phase of the Cooling Singapore project, researchers are building a digital urban climate twin (DUCT). This federation of computational models represent different facets of the city – including weather, vegetation, industry, traffic, and buildings, among others. The tool will allow planners to ask "what-if" questions and provide the relevant information to improve outdoor thermal comfort and reduce the urban heat island effect in Singapore.

Want access to supercomputing power?

If you are interested to come on board as a stakeholder of NSCC or would like to find out more about what it entails, drop us an email at e-news@nscc.sg to find out more!

The SEC was established in 2010 by ETH Zurich (Swiss Federal Institute of Technology Zurich) and Singapore's National Research Foundation (NRF), as part of the NRF's CREATE campus. SEC and its partners – National University of Singapore, Singapore Management University, Singapore-MIT Alliance for Research and Technology, TUMCREATE and Cambridge Centre for Advanced Research and Education – will tap on NSCC's supercomputing resources and data storage facilities to simulate scenarios to tackle the urban heat island effects in the Cooling Singapore project.

Find out how supercomputers and HPC play an important role in modelling the impact of various strategies to mitigate the urban heat island effects in the NSCC-organised 'Future Cool Singapore' webinar video.

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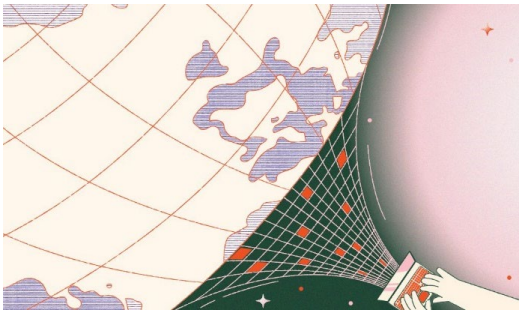
Crunching the numbers of climate change

From short-term weather forecasts to decades-long climate simulations, supercomputers are giving scientists a peek into our planet's future.



When much of the world began to implement lockdowns in March last year, shops shuttered, people stayed home and roads were emptied of traffic. Cities from Bangkok to Delhi collectively inhaled fresher air and basked under bluer skies. While you'd assume near-universal stay-at-home orders would significantly cut carbon emissions—especially those from transport—think again. Though emissions had declined an unprecedented 17 percent by April, scientists note that this marked change is likely only temporary. After all, even as economic activity virtually ground to a halt, greenhouse gases continued to be emitted by everything from household appliances to factories.

Individual behavioural change—whether it's commuting less or recycling more—will only have a small impact without a broader revamp of our energy system and industries. But how do we even quantify the environmental impacts of industrial activity? Or visualise the world as it warms so that we can better deal with it?

To find out, scientists have been collecting data 'snapshots' of our climate, measuring everything from temperature to air pressure and sea levels. Hidden within this deluge of data is a latent prophecy of a world decades from now—a future we can unlock with the help of powerful supercomputers that can rapidly process large amounts of data. Whether they are trying to predict the weather in sunny Singapore or understanding planetary trends, climate researchers need supercomputers to help them understand the sheer scale and complexity of this place we call home.

Head over to https://www.nscc.sg/supercomputing-asia-magazine/ to read the full article published in the January 2021 issue of NSCC's Supercomputing Asia Magazine to find out more about how researchers are modelling our climate change through HPC.

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, January 2021.
Credit: Sheryl Lee, Staff Writer, Asian Scientist Magazine

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Increasing the effectiveness of antibiotics by analysing antibiotic resistance using supercomputers

Researchers from NTU are utilising NSCC's supercomputing resources to understand the permeation of antibiotics in order to design new novel antibiotics.

Antibiotic resistance is a global concern for healthcare and for many economies. It is estimated that by 2050, 10 million people could die every year due to infectious diseases with antimicrobial resistance. Despite the advancements in medicine and microbiology, there are still a lot of questions about the mechanisms of antibiotics and why some antibiotics can permeate, or enter, bacteria cells while others cannot.

Permeation of antibiotics through the Gram-negative bacterial cell envelope is a complex process, where the outer membrane of cells serves as an effective barrier. It is not well understood why some drugs are able to penetrate the outer membrane whilst others cannot. A team of researchers at NTU's School of Physical and Mathematical Sciences are tapping onto NSCC's supercomputing resources to address the problem of the permeation of antibiotics through the outer membrane of *Escherichia coli*, using all-atom molecular dynamics

"We are extremely fortunate to have access to NSCC's resources, which provides us with the ability to work on this cutting-edge scientific project. We would not be able to perform our atomistic MD simulations, on the scale of microseconds, along with comprehensive analysis without the critical GPU and CPU resources that NSCC provided to us."

Yong Ee Hou
Assistant Professor
School of Physical and Mathematical Sciences
Nanyang Technological University
Singapore

(MD) simulations. The team is investigating the permeation mechanism of several clinically significant antibiotics to understand which antibiotics can penetrate the bacteria's outer membrane better than others.

From a pharmaceutical perspective, this methodology using HPC provides a high-throughput screening of candidate compounds that could help accelerate the design of novel antibiotics. This approach may open up new avenues in the virtual screening of antibiotics in current drug design pipelines.

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

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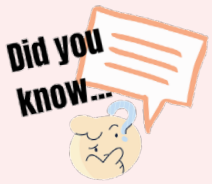
TECHNICAL NEWS

How to stay connected after your connection is terminated?

Keeping the terminal sessions running even when disconnected.



When the internet connection is poor, it is often a challenge to connect to a remote system like ASPIRE 1. The connection would be unstable and suddenly drop, preventing you - the user - from doing any meaningful work. tmux, the terminal multiplexer, helps alleviate this problem.

a) Before using tmux on ASPIRE1, you have to load appropriate module: module load tmux.

b) You start tmux by typing either `tmux`, or `tmux -s my_gmx_session`. The string "-s my_gmx_session" names the session "my_gmx_session".

c) From this point onwards, you can type the commands, submit jobs, ... as you would normally do. Now, if the connection to ASPIRE1 drops, you can easily pick up from where you left off by connecting back to ASPIRE1 and typing `tmux attach -t my_gmx_session`.

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

https://help.nscc.sg

d) Useful key combinations within tmux:
CTRL+b c - Create a new shell window.
CTRL+b n - Go to the next shell window.
CTRL+b p - Go to the previous shell window.
CTRL+b d - Detach from the tmux client.
CTRL+d - Exit current shell window.
The tmux session terminates after exiting all the shell windows.

e) Useful tmux commands:
tmux ls - List all tmux sessions.
tmux attach - Attach the most recently used tmux session.
tmux attach -t my_gmx_session - Reconnect the tmux session called "my_gmx_session".

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THE LAST BYTE...

<SHARED CONTENT>

Shared articles and news from the HPC world.

Watch a supercomputer simulation of a star forming

As scientists continue to investigate humanity's cosmic origins, they deploy more and more supercomputer simulations.

A team of researchers at the European Space Agency, for example, wants to build a digital twin of Earth to better understand our planet's history. Now, another team of scientists is developing an initiative to study star formation in the digital realm. And, amazingly, they call the endeavor STARFORGE. Read more at Nerdist here.

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Credit: Mike Grudić

Pushing HPC beyond traditional boundary

In support of the AI/ML adoption into HPC folds, there needs to be a strategy with agility in mind when deciding any future scientific computing development.

AI adoption in our digital economy has been increasing rapidly over the past few years. Starting from the re-emergence of Deep Learning application in the ImageNet challenge, the resulting key technologies and techniques have been embedded in and influenced many aspects of research. Read more at NUS IT here.

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Credit: NUS IT

Going to the moon via the cloud

High-performance cloud computing has allowed start-ups to develop prototypes and run simulations — including one to the moon — that were previously done on supercomputers.

Firefly Aerospace, a start-up based in the suburbs of Austin, Texas, is building a rocket to fly to the moon. This is an example of how the ubiquitous availability of high-performance computing through the internet has unleashed a global wave of creativity. The "cloud," that fuzzy euphemism for networks of massive computer farms that anyone can access with a laptop and a credit card, has put even the wildest dreams within reach of people with enough know-how. Read more at The New York Times here.

Credit: The New York Times

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