National Supercomputing Centre (NSCC) Singapore e-newsletter

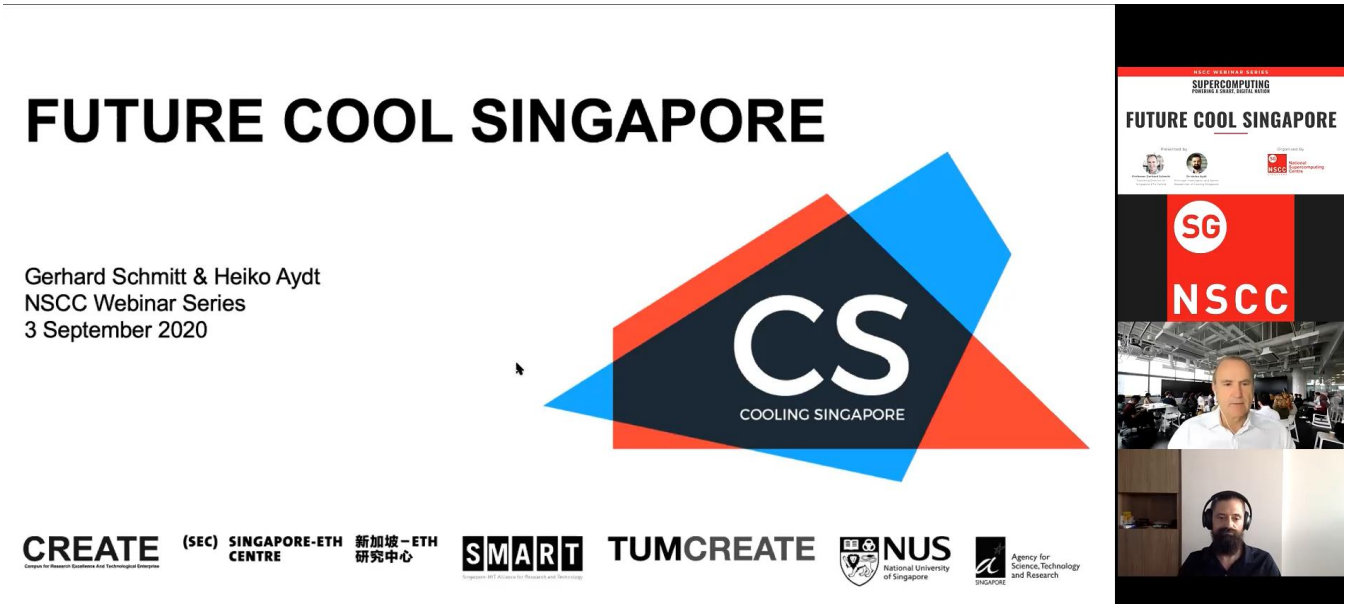
NEWSBYTES

September 2020

CORPORATE NEWS

NSCC's New Webinar Series Kicks Off on a High Note

The first webinar, which is part of the "Supercomputing – Powering a Smart Digital Nation" series, aims to give an introduction to HPC in Singapore using multi-sector case study examples that showcase the benefits of HPC.

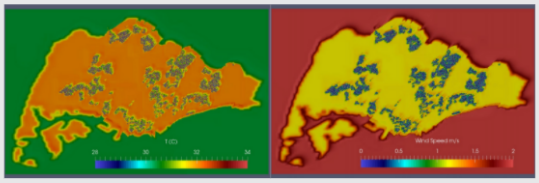


The inaugural session kicked off on 3rd September with an insightful presentation titled '*Future Cool Singapore'* by Professor Gerhard Schmitt and Dr. Heiko Aydt from the Singapore – ETH Centre. The speakers presented the Cooling Singapore initiative - an integrated and holistic approach to address the urban heat challenge for Singapore and other cities around the world as well as the important role HPC has to play in this initiative to help plan for a balanced urban climate system.

An audience of about 120 participants from local and international institutes of higher learning (IHLs), government agencies and industry joined the speakers online.

If you missed the talk and the points discussed, you may access the recorded video of the talk and presentation materials here.

Join us at NSCC's next webinar:



Computational Fluid Dynamics (CFD) is becoming popular as a virtual planning tool for urban planners to plan the future development of the urban built environment. However, accounting for the detailed urban physics while keeping the entire modeling process simple for the end-user is a challenging task. In the first part of the talk, Dr. Harish will discuss the complexities of the urban flow physics and the role that high-performance computing can play in reducing the computational bottleneck. Solar energy will power 10% of our countries electricity demand by 2030. The limited land space makes it more challenging to deploy on-shore solar farms. Singapore is looking into floating solar platforms or roof-top solar farms. The second part of his talk will discuss the role of high-performance computing in solar forecasting.

Urban Flow Modeling and Solar Forecasting using High-Performance Computing

by Dr Harish Gopalan, A*STAR's Institute of High Performance Computing (IHPC)

17th September 2020, Thursday

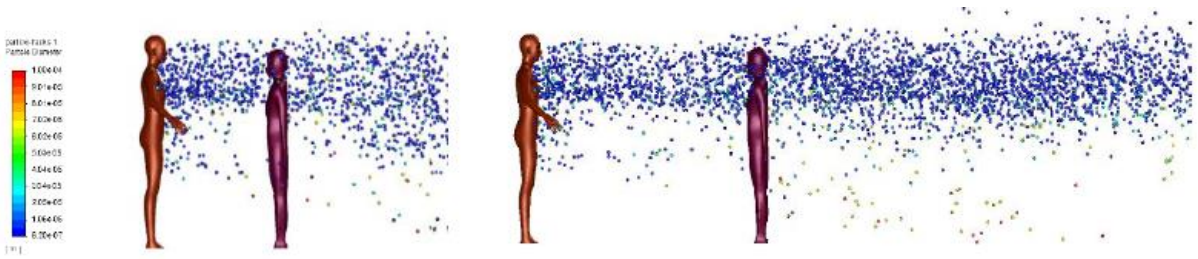
10am – 11am (Singapore time)

Register for the event here or head over to https://www.nscc.sg/hpc-calendar/ for more information about NSCC's Webinar Series and the upcoming activities.

A Cough Goes a Long Way - Understanding the Spread of Airborne Cough Droplets

Studying the dispersion of droplets in environmental transmission using supercomputers is helping researchers better understand what happens when a person coughs, in order to develop potential intervention measures. Such work is crucial in tackling pandemics like COVID-19.

When talking, singing, coughing and sneezing, virus-laden droplets and aerosols are expelled from the mouth of an infected person. The transmission of respiratory droplets or aerosols shows the competing effects between drag, inertia, gravity and evaporation. Each stage in the transmission process is affected by complex flow phenomena, ranging from turbulent jets, flow-induced droplets or aerosols dispersion and sedimentation, to droplet evaporation and deposition. Modelling and simulation based on fundamental thermo-fluid physics is able to provide accurate insight into and visualisation of the droplets or aerosols dynamics and spread process.



Credit: IHPC

A research team at A*STAR's Institute of High Performance Computing (IHPC) has been harnessing the power of NSCC's supercomputer resources to conduct Computational Fluid Dynamics (CFD) extensively to understand and visualise airflow and droplets or aerosol spread due to the effects of various parameters such as wind speed, humidity and temperature.

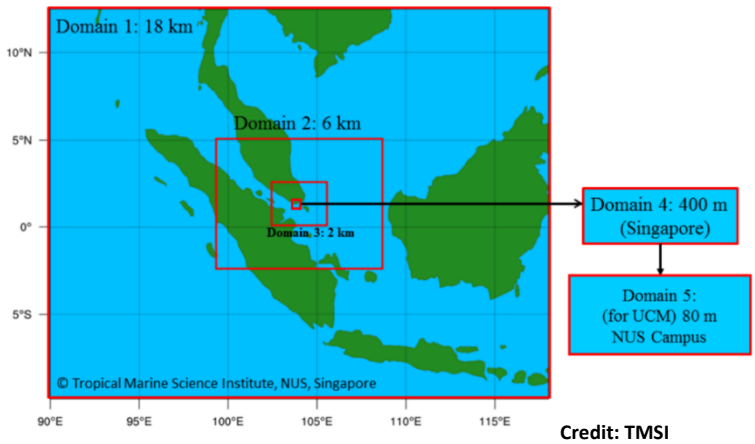
IHPC's Computational Fluid Dynamics (CFD) framework considers key factors including but not limited to expulsion force of fluid volume, droplet or aerosol size distribution, evaporation of water from the particle (temperature and humidity dependent), and viral load in the droplet. The computational framework enables the quantification of droplets falling on human subjects based on air flow due to natural and mechanical ventilation and air-conditioning, and allows risk-based analysis of different configurations. In collaboration with Institute of Materials Research and Engineering (IMRE) who conducts smoke test, the framework coupled with risk-based analysis has also been applied and covered for different settings and scenarios.

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

High Resolution Modelling of Weather and Climate over Singapore and Southeast Asia

Using NSCC's supercomputing resources, researchers in Singapore are using complex computer models to look at how climate and weather impact the region.

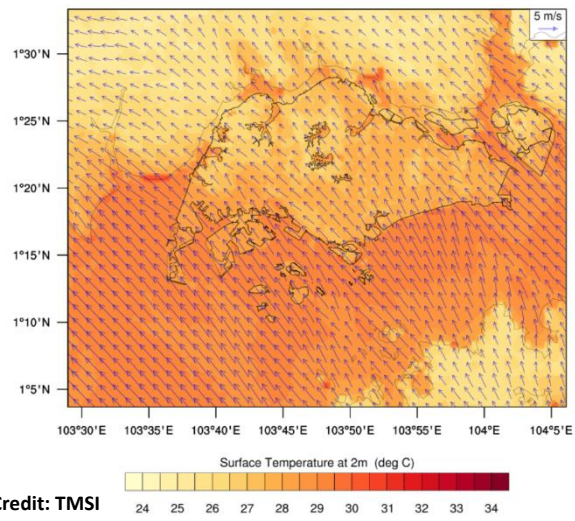
The latest climate projections from the Fifth Assessment Report of the Intergovernmental Panel on Climate Change suggests that global models are still far from reasonable representations of climate features on regional scales, despite improvements in the spatial resolutions of the models and in the understanding of physical processes. This also indicates that downscaling the global models to higher spatial resolutions is still an active area of research in the years to come.



Credit: TMSI

Southeast Asia is a relatively under-studied region when it comes to climate sciences and studying Singapore's climate and its change is challenging given the geographical size of the country. Therefore, supercomputers have become an essential tool for climate change study and weather forecasting due to the large quantity of data required to perform climate simulations.

Dr. Nguyen Ngoc Son, Principal Investigator, and Dr. Sri Raghavan, Head, at the Climate and Water Research cluster, Tropical Marine Science Institute (TMSI) at NUS, have been making use of NSCC's supercomputing resources to model the weather and climate at high resolutions for impact research on urban climates, numerical weather prediction (weather forecasts), haze and climate change, thus bringing tangible benefits to weather and climate research in Singapore.



Credit: TMSI

To provide more accurate local weather forecasts, the team performs weather forecasts, which are complex in dynamics, on NSCC's high performance computer. "With spatial resolutions increasing, faster turn time for the release of timely forecasts is necessary, given these forecasts are issued four times a day. The computations need to be scaled down from global spatial scales to local (city/urban) scales. NSCC's resources are indispensable in terms of both speed of simulations and the facility available to store massive volumes (several GBs) of data," said Dr. Sri.

Dr. Nguyen and Dr. Sri also perform climate integrations on multi-decadal time scales over Southeast Asia and over a Greater Singapore region. These multiple integrations are performed under different climate 'scenarios' to better understand future changes in the climate. "This task requires millions of CPU hours for computation which is impossible to achieve without the help of HPC. At high resolutions, the task is even more challenging. Apart from the needed high speed in model computations, the data storage volumes are in the ranges of several TBs which can only be provided by NSCC's HPC resources," said Dr. Sri.

The Climate and Water Research cluster specialises in high resolution weather and climate modelling. While weather simulations (numerical weather predictions) are undertaken at spatial resolutions of 400 m over the

entire Singapore, the team also perform regional climate simulations over Southeast Asia at about 8-10 km resolutions and microscale simulations at about 80 m spatial resolutions. The applications of these different scales of simulations range from everyday weather forecasts to investigations of regional climate change impacts. More information on these studies are available from:
http://www.tmsi.nus.edu.sg/weather/index.php

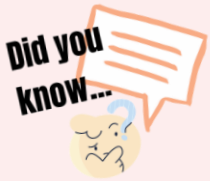
To find out more about the NSCC's HPC resources and how you can tap on them, please contact e-news@nscc.sg.

TECHNICAL NEWS

Everyone Loves a Cheat Sheet

It's the cherry on top!

CONDA



Conda is an open source package management system and environment management system that runs on Windows, macOS and Linux. Conda quickly installs, runs and updates packages and their dependencies. Conda easily creates, saves, loads and switches between environments on your local computer. It was created for Python programs, but it can package and distribute software for any language.

Conda Basic	
conda info	Display information about current conda install.
conda update conda	Update conda to the current version
conda install PACKAGENAME Example: conda install python conda install python=2.6.17	Install a package included in Anaconda Install python, conda will install the latest version Install python, conda will install the specific version
conda update PACKAGENAME	Update any installed program

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

https://help.nscc.sg

Managing Environments	
conda create –n nScc python=3.5	Create a new environment named nScc, install python=3.5
source activate nScc	Activate the new environment to use it
conda env list	List the Conda environments. Active environment is shown with *
conda create --clone nScc –n CcR	Make exact copy of an environment
conda list	List all packages and versions installed in active environment
conda list –revisions	List the history of each change to the current environment
conda install –revision 21	Restore environment to rev=21
conda list –explicit > condalist.txt	Save environment to a text file
conda env remove –n cCrs	Delete an environment and everything in it
source deactivate	Deactivate the current environment
conda env create -f condalist.txt or conda env create -f conda_env.yml	Create environment from a text file Or Create environment from a YAML file
conda env export > conda_env.yml	Save environment to a YAML file
conda create -p /app/python-environment/ccrs/ccrs-clone --clone /app/python-environment/ccrs/ccrs	Clone the location instead to a new location

THE LAST BYTE...

<SHARED CONTENT>

Shared articles and news from the HPC world.

A Supercomputer Analysed Covid-19 — and an Interesting New Theory Has Emerged

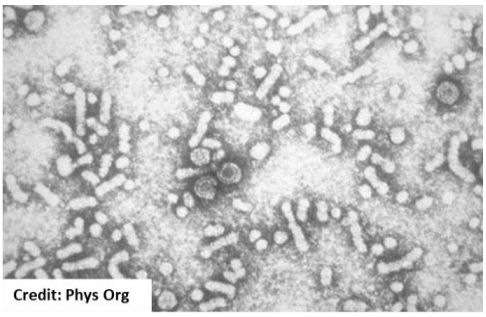
A closer look at the Bradykinin hypothesis.

Credit: Elemental

Earlier this summer, the Summit supercomputer at Oak Ridge National Lab in Tennessee set about crunching data on more than 40,000 genes from 17,000 genetic samples in an effort to better understand Covid-19. Summit is the second-fastest computer in the world, but the process — which involved analysing 2.5 billion genetic combinations — still took more than a week. Read more at Elemental here.

Researchers Use Supercomputer to Gain Insights into Hepatitis B

Researchers at the University of Delaware have gained new understanding of the virus that causes hepatitis B and the "spiky ball" that encloses the virus's genetic blueprint.



Credit: Phys Org

The research, which has been published online, ahead of print, by the American Chemical Association journal ACS Chemical Biology, provides insights into how the capsid — a protein shell that protects the blueprint and also drives the delivery of it to infect a host cell — assembles itself. Read more at Phys Org here.

Supercomputers Just Hosted the Most Detailed Tornado and Earthquake Simulations Ever

Even with the pandemic raging, natural disasters are having a busy 2020.

Credit: HPC Wire

Tornadoes ravaged Nashville a few months ago; the chances of a new “big one” have dramatically risen in California’s fault zones; and meteorologists are anticipating a stronger-than-usual hurricane season for the U.S. More than ever, understanding and anticipating these events is crucial – and now, two teams of researchers have announced that they have used supercomputers to run the higher-resolution-ever simulations of tornadoes and earthquakes. Read more at HPC Wire here.