National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

August 2021

In this Issue…

CORPORATE NEWS

The silver lining in COVID's dark cloud

From cross-border collaborations to advancing accessibility, supercomputers play an important role in helping the world recover from COVID-19.

As COVID-19 spread across the globe in early 2020, flights halted, borders closed and people stayed home. But while the pandemic made national borders painfully apparent, it brought countries together, too. Researchers across the world sequenced and shared the SARS-CoV-2 genome; nations sent masks, testing kits and even their own doctors to the hardest hit regions; and millions of dollars flowed in the name of international aid.

Likewise, the pandemic has drawn the high-performance computing (HPC) community closer together over the past year, as people rose to the occasion and channelled their supercomputing powers for good. Supercomputers not only sequenced millions of viral genomes, but also helped us model how the disease is spread and what measures could possibly counteract it.

Coming online several months early to begin working on such problems was Japan's Fugaku supercomputer, which was originally scheduled to begin operating only in 2021, shared Professor Satoshi Matsuoka, director at the RIKEN Center for Computational Science in Japan. Matsuoka was speaking at the inaugural HPC Center Leaders Forum, an expert panel at the SupercomputingAsia 2021 conference held virtually from March 2–4, 2021.

From screening existing therapeutics for repurposing into COVID-19 drugs, to detailed simulations of droplet aerosols modelling transmission, Fugaku was immediately put through its paces and harnessed to combat COVID-19, Matsuoka said. "You go from very microscopic atomic levels all the way to societal levels in various simulations in trying to provide solutions to the pandemic."

Building on this initial success, there are plans to open up access to Fugaku for international research partnerships, Matsuoka continued. "We have already developed a system that allows for very effective sharing of data across HPC supercomputers. We are testing this to see if we can expand it to Australia, Singapore and other Asian countries," he said. "With this system, [researchers from other countries] will be able to use Fugaku through the cloud. A file can be local to Singapore, with gigabytes of data transferred transparently in an instant."

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 more about the role of HPC collaborations in the new normal.

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: Sheryl Lee, Staff Writer, Asian Scientist Magazine

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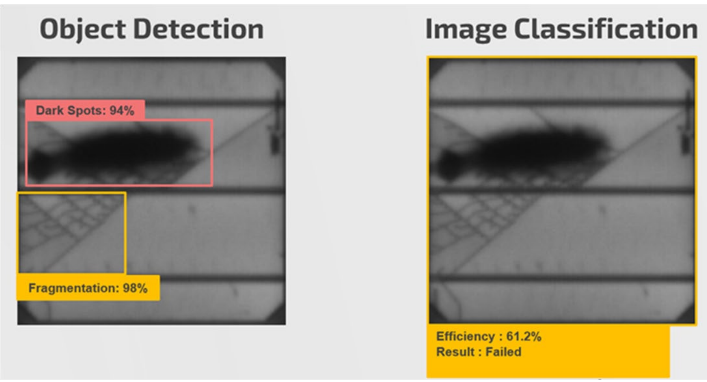
Automating the detection of defects in recycled solar cells

Researchers at NTU are using HPC to automate and more accurately detect visual defects in solar panels in a bid to reduce the workload required for manual inspections.

Amid the growing interest in the renewable energy sector, the solar photovoltaic (PV) industry has witnessed an exponential growth in recent years. As new solar technologies emerge, businesses are challenged to upgrade their solar farms and recycle their existing solar installations.

This is usually done by gauging the life expectancy and equipment effectiveness of existing solar panels by checking for visual defects. However, most inspections are currently performed manually in the industry, which requires significant manpower, time and costs. A team of researchers at Nanyang Technological University's School of Computer Science & Engineering, in conjunction with Etavolt Pte Ltd, are tapping onto NSCC's high performance computing resources to automate the detection of visual defects in solar panels by employing image recognition technologies and object detection models. The team seeks to significantly reduce the resources required and improve the work productivity via the developed technology in this work.



The two main categories of models utilised in the research.
Credit: NTU

Unlike many other machine learning tools, the team is analysing multiple different models and combining their final results, which significantly amplifies the amount of computational resources required. The benefits in doing so are to identify the single best model for the solar industry and also utilise a new novel technique to combine models to improve the accuracy of detection.

The original goal of the work was to find a model that was best suited to the collected data by the solar PV industry. The team has since expanded their work scope and are now combining multiple models through a novel ensemble technique - contextual multi-armed bandits. This allows them to better utilise the different architectures in the different machine learning models to further boost the reliability and reduce bias in the predictions, while also managing conflicting results through a deconflicting process. This method is more intuitive to the user and has resulted in an approximately 8% increase in accuracy and reliability.

"Due to the computational resources required, we utilised HPC in our projects to speed up our analysis by a factor of ~7 times, or equivalently from 1 week to just about 18 hours. Thanks to NSCC's support and resources, we are able to reiterate much faster in our research to analyse and compare multiple machine learning models and techniques which would otherwise not be possible."

Liew You Sheng
Researcher
School of Computer Science & Engineering
Nanyang Technological University

"As the solar industry rapidly expands at an unprecedented rate, vast quantities of data regarding solar panel defects are generated as well. The AI-centric HPC system from NSCC has been invaluable in our research to improve on the efficiency of solar panel defect analysis," said Mr Liew You Sheng, a researcher with the NTU team.

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

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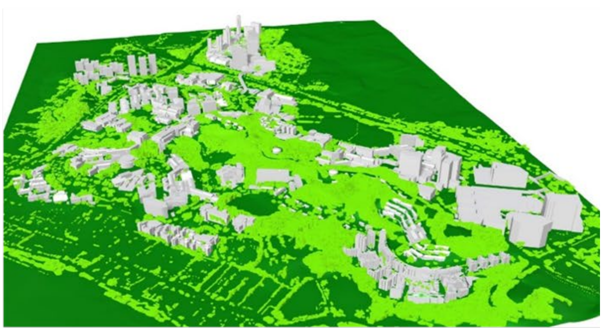
Microclimate modelling research to curb rising temperatures in Singapore

A research team from NUS is tapping on NSCC's supercomputing resources to develop an urban microclimate model for the local Singapore environment at the NUS Kent Ridge campus test-bed environment.

As a densely-populated city-state, Singapore's rapid urban development and growing population poses challenges, especially in trying to provide its residents a healthy, comfortable and liveable environment.

Rising temperature is one of the main environmental concerns. The annual average surface temperature in Singapore has increased from 26.6°C in 1972 to 27.7°C in 2014 (Meteorological Service Singapore (MSS), 2015) and is predicted to rise by 1.4-4.6°C by 2099 in the context of global warming (MSS, 2015). The urban heat island (UHI) effect signifies that a city area is significantly warmer than its surrounding rural areas, which is indeed found to be quite evident. The densely built urban areas, such as central business district (CBD) area, is up to 4°C hotter than green spaces (e.g., parks, forests, catchment areas, etc.) during hot afternoons.

3D model of the site around Kent Ridge campus
Credit: NUS



Kent Ridge campus with vegetation
Credit: NUS

A group of researchers at National University of Singapore's School of Design and Environment are making use of the NUS Kent Ridge campus as a test-bed environment for model calibration and validation to develop an urban microclimate model for the local Singapore environment.

The biggest challenge the team faced was the lack of an integrated, clean and detailed 3D model that is suitable for the requirements of the environmental simulation. The integration of the buildings, structures, tree canopies and terrain require significant computational time to ensure they fit together nicely. In addition, the most common material properties on the surfaces needed to be identified and measured on site. Other issues included getting appropriate boundary conditions from weather stations or Weather Research and Forecasting (WRF) Models for the simulation, and the lack of parallel CPU cores to handle the simulation of very large 3D models.

"Our existing workstations do not have massive amounts of CPU cores that can run the large 3D model in a short span of time. NSCC's supercomputer resources helped by contributing massive parallelization of CPU cores and memory that was needed for a large and detailed 3D model such as the NUS Kent Ridge campus and its immediate surroundings."

Wong Nyuk Hien
Principle Investigator
School of Design and Environment
National University of Singapore

Through the use of NSCC's high performance computing resources, the team was able to carry out their research with the aim to develop a multiscale microclimate model for simulating the UHI effect (mesoscale phenomenon) and local hotspots (microscale) on the neighbourhood scale. The team is also integrating the urban microclimate model to the 3D model of the NUS campus, i.e., Virtual NUS, for enhancing the simulation and visualisation and using the NUS Kent Ridge Campus to validate the developed model.

The results of the project would ultimately serve to predict the impact of the current urban microclimate as well as future scenarios where physical and boundary condition alterations are made to the current condition.

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

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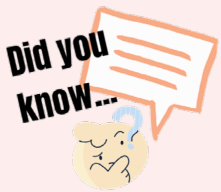
TECHNICAL NEWS

Do more with PBS Pro on ASPIRE 1

Part 2.



It is possible to run several tasks inside a single PBS Pro job file.

Have you ever wondered if it is possible to run several tasks inside a single PBS Pro job file? For example, prepare the required input files, run the parallel part of the job and do some processing at the end? Of course, it can. What you, the user, needs to take care of is the syntax of the commands you are trying to execute and make sure all the required modules are loaded and the PATH variables are set correctly.

You should also remember that you have the full set of Bash commands at your disposal, so you can use a `while` or `for` loop, check whether your simulation completed successfully using an `if` statement.

In the example below, the user is trying to do a multi-step preparation of his biomolecular system before running the scientifically-relevant production runs. In step 1, the relevant module is loaded, and step 2 runs the first step of the multi-step preparation. This can be easily extended with a `for` loop that goes across all the relevant input files as long as the total walltime does not exceed 24 hours. The command `gmx grompp` will use a single CPU core and will take just a few seconds to execute so very little CPU time is lost. While the example is using Gromacs, it can be readily adapted to suit other applications as well.

Example with the PBS section removed:

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

# set input that will be used a basename for all outputs
input=my_initial_input_file
base="$input"

# 2. Prepare input and run first simulation
export GMX_MAXCONSTRWARN=-1
gmx grompp      -f ./input/step6.0_minimization.mdp \
                -o step6.0_minimization.tpr \
                -c "$base" -p "$base" -r "$base" -n "$base" \
                -maxwarn 1
mpirun  -genv KMP_AFFINITY=compact,verbose mdrun_mpi -v -deffn step6.0_minimization
unset GMX_MAXCONSTRWARN

# 3. Run more tasks
```

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

https://help.nscc.sg

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THE LAST BYTE...

<SHARED CONTENT>

Shared articles and news from the HPC world.

Singapore's Quantum Engineering Programme teams up with AWS to boost quantum technologies

The National University of Singapore (NUS) has signed a Memorandum of Understanding (MoU) with Amazon Web Services (AWS) for a collaboration to boost the development of quantum communication and computing technologies, and explore potential industry applications of quantum capabilities.

The collaboration is led by the Quantum Engineering Programme (QEP), a national initiative launched in 2018 by the National Research Foundation, Singapore (NRF), which aims to leverage quantum technologies to solve real-world problems. The programme is hosted by NUS. Under the MoU, AWS will support QEP in the development of quantum computing research and projects, and connect to the National Quantum-Safe Network for quantum communications. Read more at HPC Wire here.

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Scientists are worried by how fast the climate crisis has amplified extreme weather

Until recently, climate change had been talked about as a future threat. Its frontlines were portrayed as remote places like the Arctic, where polar bears are running out of sea ice to hunt from. Sea level rise and extreme drought was a problem for the developing world.

But in the past month, it's been the developed world on the frontline. In the past four weeks, floods in Germany engulfed streets and swallowed homes that had stood for more than a century in the quiet village of Schuld. A Canadian town of just 250 -- known more for its cool, mountain air -- burned to the ground in a wildfire that followed unprecedented heat. Read more at CNN here.

Credit: CNN

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Supercomputers are becoming another cloud service. Here's what it means

Designing for the usual cloud workloads isn't the same as designing for high performance computing.

These days supercomputers aren't necessarily esoteric, specialised hardware; they're made up of high-end servers that are densely interconnected and managed by software that deploys high performance computing (HPC) workloads across that hardware. Those servers can be in a data centre – but they could also be in the cloud as well. Read more at ZD Net here.

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