National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

August 2020

CORPORATE NEWS

NTU student team making an impact on the global HPC Student Cluster Competition stage

NTU teams, which are regular competitors in the annual HPC student competition circuit, are ranked 4th in the new HPC-AI Advisory Council Student Cluster Competition Worldwide Leadership List

Adding to the long list of accolades for the Nanyang Technological University (NTU) HPC student team, NTU has now been ranked fourth in HPC-AI Advisory Council's Student Cluster Competition Leadership List in Worldwide.

The Student Cluster Competition Leadership List is a collaborative project by the HPC-AI Advisory Council and Gabriel Consulting Group which ranks student cluster teams based on their achievements and involvement in the global HPC student competitions including the ISC Student Cluster Competition, SC Student Cluster Competition and the regional competitions such as the APAC competition, since 2007.

The NTU HPC student competition team is one of the top ranked teams worldwide according to the HPC-AI Advisory Council.

The NTU team, which is made up of undergraduates from the NTU's School of Computer Science and Engineering, has been taking part in the annual competitions for over five years and has chalked up an impressive collection of silverware. These include the NTU team being crowned the Overall Champion at the international SC17 conference and more recently, clinching the coveted LINPACK Benchmark award at the SC19 conference for the third year in a row. You can read more about their achievements in the past issues of our NewsBytes (December 2019) and NewsBytes (September 2019).

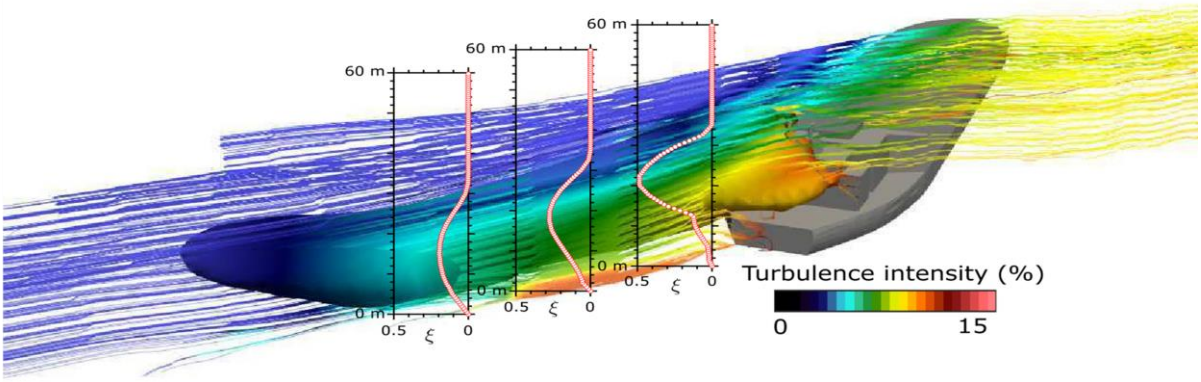
The team will be participating next in the upcoming Student Cluster Competition at SC20, which will be held as a fully virtual event from November 16 through November 20, 2020. With sponsorship from vendor partners, the student teams will be tasked to design and build virtual clusters in the Microsoft Azure cloud, learn scientific applications, apply optimisation techniques for their chosen cloud configurations, and compete in a 72-hour challenge around the world to complete a set of benchmarks and real-world scientific workloads.

Congratulations once again to the NTU student team and we wish them all the best at the upcoming SC20 competition!

Simulating combustion processes in marine engines to reduce carbon footprint

Using supercomputers to study the various aspects of fuel utilisation in shipping helps combat pollution

The drive for enhanced energy efficiency, lower pollution and decarbonisation in the marine sector is increasing in pace and importance worldwide. For Singapore, energy use and pollution from the marine sector has significant impact on this vital economic sector due to the large number of ships plying Singapore's waters and producing harmful emissions that could affect local air quality. Better use of fuels, alternative low-carbon fuels, fewer polluting engines and clean-up systems are of vital importance in mitigating the environmental burden from shipping.



Credit: University of Cambridge

Savvas Gkantonas, a PhD student at the University of Cambridge and a research intern at Cambridge CARES (Centre for Advanced Research and Education in Singapore) is working together with Shrey Trivedi and Prof. E. Mastorakos from the University of Cambridge and Cambridge CARES to tap on NSCC's compute resources to study the various aspects of fuel utilisation in shipping, mainly the flow and combustion inside marine engines and the clean-up of the engine emissions. Using Computational Fluid Dynamics and advanced turbulent reacting flow theory, the team is exploring a wide range of physical phenomena occurring between the nano and the kilometre scale.

The flow and combustion inside marine engines are simulated with high-fidelity Large-Eddy Simulations and detailed chemistry with special focus on the pollutant generation. The simulation tools to be developed will allow the effects of alternative fuels and of fuel additives to be assessed.

"The role of high performance computing in this project is indispensable as our simulations require extensive use of compute nodes with a significant amount of memory and can only be executed via massively-parallel resources. The performance of the supercomputer is also critical for the execution of our codes as it can offer significant benefits in speeding up the research and increasing productivity," said Savvas.

With increasing concern in local air quality in the Port area, the clean-up of the engine emissions is a significant industrial activity for Singapore companies. Tools that can predict the emissions and their dispersion from shipping will facilitate enforcement and allow more informed policy decisions. Detailed simulations of the flow and dispersion of ship plumes in the vicinity of the ship's infrastructure and the port's structures will be made, including unsteady turbulent flow and chemical reactions in the plume. These results will allow low-order physics-based models to be developed for the use by various stakeholders such as ship operators, port authorities, environmental agencies and ship builders.

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

Ecologically engineering Singapore's seawalls to enhance biodiversity

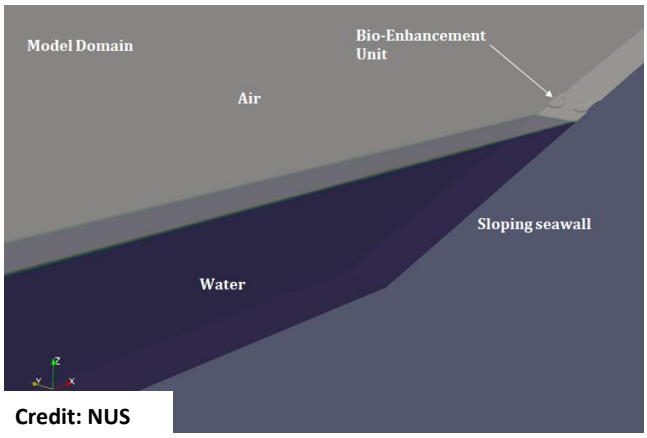
Tapping on NSCC's supercomputing resources to preserve ecosystems and strengthen natural resilience

Due to extensive land reclamation, much of Singapore's original coastal habitats have been destroyed as a result of the construction of coastal defence structures such as seawalls. These coastal infrastructures are generally constructed with the function of protecting coastal areas against tidal flooding, severe waves and storm surges. However, they are usually not designed as surrogates for natural habitats therefore resulting in a loss of ecosystems and natural resilience.

To ecologically engineer the seawalls in order to preserve and enhance the natural biodiversity, Zhao Kuifeng, a research fellow in the Department of Civil and Environmental Engineering at NUS, and his colleagues are leveraging NSCC's high performance computing resources to explore the possibility of designing seawalls ecologically to improve its value as a potential habitat.

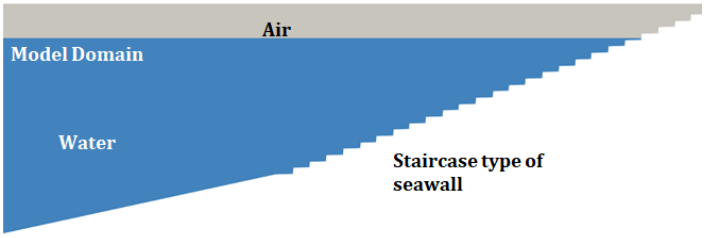
The turbulence and hydrodynamic forces near the seawall plays an important role in controlling the intertidal communities. However the study of wave hydrodynamics on seawalls has been focused on smooth seawalls in literature by numerous scholars and little study has been done on a rough seawall because of its complexity. Therefore, they need to be investigated to ensure that the design of seawalls is suitable.

The team is investigating the fluid mechanics aspect of the ecologically designed seawalls by adopting both experimental and computational fluid dynamics (CFD) simulations to look at the effects of waves on the seawall. Various types of seawall designs and roughness configurations were examined to study how they affect wave run up, reflection and absorption.



Credit: NUS

A screenshot showing part of a 3D model – bio-enhancement units installed on a sloping seawall



A part of a simplified 2D model domain that has a de-novo design – staircase type of seawall

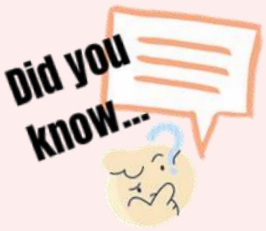
"The complex geometry and 3D simulations requires huge amounts of computer resources for computation therefore we are grateful that with the supercomputing resources provided by NSCC, we can speed up the calculation and achieve satisfying results," said Kuifeng.

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

Waiting time too long?

Ever wondered how long you'll have to wait until it's your turn?



Users are able to see how busy the queue is by using the "gstat" command.

**Do note that the "gstat" command is a stripped down readonly cached version of qstat for all user jobs.*

Below is a sample output of gstat command. The command does not need any arguments to be specified.

```
[fsg1@nscc03 ~]$ gstat
Wed Jul  8 17:18:01 SGT 2020
Node States:

free : 78
job-busy : 1217
job-exclusive : 0
offline : 4

********************************************************************************

Wed Jul  8 17:18:01 SGT 2020

                                  Req'd  Req'd   Elap
Job ID               Queue        SessID  NDS  TSK  Memory   Time  S Time
-------------------------------------------------------------------------------
165634.wlm01         medium       --    1        24         40gb       23:58 Q --
229101.wlm01         medium       --    1        24         96gb       24:00 H --
```

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

https://help.nscc.sg

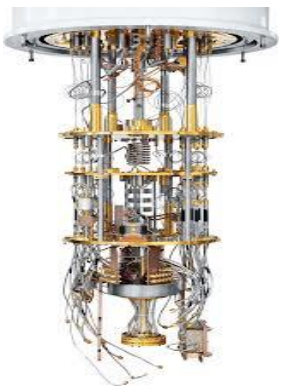
THE LAST BYTE...

<SHARED CONTENT>

Shared articles and news from the HPC world.

EDBI invests in quantum computing startup Rigetti's US$79m Series C round

California-based quantum computing startup Rigetti Computing raised US$79 million in a Series C funding round to advance its efforts in making quantum computing commercially viable



Credit: Rigetti

EDBI, the corporate investment arm of Singapore's Economic Development Board, also participated in the round, along with Franklin Templeton, Alumni Ventures Group, DCVC, Morpheus Ventures and Northgate Capital. The company builds and delivers integrated quantum systems over the cloud, and develops software solutions optimised for hybrid quantum-classical computing. Read more at The Business Times here.

Pawsey Announces PACER Program to Prepare Australian Researchers for the New Era of Supercomputing

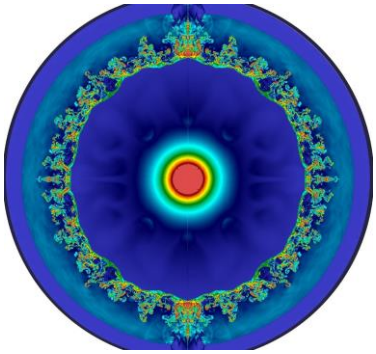
The Pawsey Supercomputing Centre for Extreme scale Readiness (PACER) program is coming soon to advance Australian computational researchers

Credit: Pawsey Supercomputing Centre

In 2018 the Australian Government awarded $70 million to upgrade Pawsey's supercomputing infrastructure, on top of the $80 million granted in 2009 to establish a petascale supercomputing facility. The Pawsey upgrade, as a major part of the national High-Performance Computing (HPC) infrastructure, is ensuring Australia continues to enable computationally and data-intensive research. Read more at HPC Wire here.

Supercomputer simulation shows a supernova 300 Days after it explodes

The answers to many questions in astronomy are hidden behind the veil of deep time



Credit: Universe Today

One of those questions is around the role that supernovae played in the early Universe. It was the job of early supernovae to forge the heavier elements that were not forged in the Big Bang. How did that process play out? How did those early stellar explosions play out? Read more at Universe Today here.