National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

July 2020

CORPORATE NEWS

NSCC helps ISC2020 HPC-AI Advisory Council Student Cluster Competition go fully online

First ever virtual version of the annual ISC conference competition used NSCC's supercomputing resources to allow 14 international teams affected by COVID-19 travel restrictions to take part in the competition.

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Thank you!

LET'S BEGIN

Co-organised by the HPC-AI Advisory Council and ISC, the 2020 Student Cluster Competition (SCC) was the first in the competition's history to be run as a fully online challenge. The digital 2020 competition was enabled by NSCC resources which allowed the teams to remotely configure, code and benchmark a series of HPC and AI applications on the Singapore centre's supercomputer.

Held from June 1 to June 24 and concluding with an award ceremony that took place live during the ISC 2020 Digital conference, the SCC joined the global fight against COVID-19. This year's competition was expanded to include applications that addressed education and applied learning towards accelerating bioscience research and discovery. The aim was to train the next generation of scientists and programmers to aid in solving future real-world challenges such as viral outbreaks or pandemics.

The 14 international student teams were challenged to demonstrate their HPC and AI skills by running *TinkerHP*, a massively parallel molecular dynamics package for multiscale simulations of complex systems, currently being used by the bioscience research community. Students were also tasked to demonstrate mastery of several other complex challenges, from climate change analysis using *Elmer/ICE* to running molecular dynamics and cosmology simulations using *GROMACS* and *ChaNGa*.

The teams from the University of Science and Technology of China (USTC) clinched this year's top spot, with South Africa's Centre for High Performance Computing (CHPC) and China's Tsinghua University placing second and third place, respectively. The *Fan Favorite* award went to the Universitat Politecnica de Catalunya, Spain while Singapore's six-member Nanyang Technological University (NTU) team clinched the *Honourable Mention* award.

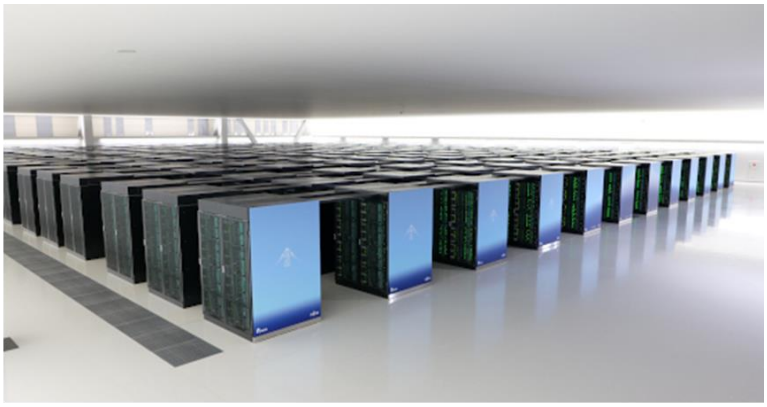
Congratulations to all the winning teams!

Watch the opening ceremony of the 9th Annual ISC HPC-AI Advisory Council Student Cluster Competition here.

New Fugaku supercomputer claims top spot in Top500 supercomputer list

Japan's Fugaku emerged as the new world's fastest supercomputer, clocking in at 415.5 petaflops and 2.8x more powerful than the second-placed system.

Coming in first place in the TOP500 list of the world's most powerful supercomputers is Japan's *Fugaku*, a machine installed at the RIKEN Center for Computational Science (R-CCS) in Kobe, Japan. The last time that Japan took the top spot was in June 2011 when Fugaku's predecessor, the *K computer*, debuted in first place.



Supercomputer Fugaku.
Source: RIKEN

Powered by Fujitsu's 48-core A64FX system-on-chip, this is the first time a computer based on ARM processors has topped the list. *Fugaku*, named after Japan's famed Mount Fuji, turned in a High Performance Linpack (HPL) result of 415.5 petaflops, far outperforming the now second-place Summit system, an IBM-built supercomputer that delivered 148.8 petaflops on HPL. On HPCG, it scored 13,400 teraflops using 138,240 nodes, and on HPL-AI it gained a score of 1.421 exaflops—the first time a computer has even earned an exascale rating on any list - using 126,720 nodes. *Fugaku* also topped the ranking on various workload tests including Graph 500, HPL-AI, and HPCG, an impressive feat as no former supercomputer has ever achieved this. The prototype for *Fugaku* was also awarded the top spot on the Green 500 list for being the most energy efficient supercomputer on the Top500 list at the international supercomputing conference, SC19, in Denver, Colorado, in November 2019.

Fugaku is intended for a wide range of applications that will address social and scientific issues such as drug discovery, personalised and preventive medicine, weather and climate forecasting, clean energy development, and exploring the fundamental laws and evolution of the universe. It is currently being used experimentally for research on COVID-19, including the diagnostics, therapeutics, and simulations of the spread of the virus. The new supercomputer is scheduled to begin operation in April 2021.

"Ten years after the initial concept was proposed, and six years after the official start of the project, *Fugaku* is now near completion. *Fugaku* was developed based on the idea of achieving high performance on a variety of applications of great public interest, such as the achievement of Society 5.0, and we are very happy that it has shown itself to be outstanding on all the major supercomputer benchmarks. In addition to its use as a supercomputer, I hope that the leading-edge IT developed for it will contribute to major advances on difficult social challenges such as COVID-19," said Professor Satoshi Matsuoka, Director of RIKEN R-CCS. Professor

Matsuoka is also a member of NSCC's Steering Committee and a recipient of the '*Asia HPC Leadership Award*' at NSCC-organised SupercomputingAsia 2019 (SCA19) conference, which was held in Singapore.

Making better streamlines - Stability analysis and numerical simulations of complex flows

Leveraging NSCC's supercomputing resources to unravel the underlying physics in complex flows.

The study of flow instability determines how an undisturbed flow transitions to turbulence, a topic which is very important for both industry application and academic research. For example, delayed transition to turbulence will reduce skin drag on airplane wings. This significantly decreases energy consumption, which is essential for aerodynamic efficiency and performance. Similarly, a minute amount of added polymers in a certain solution can lead to a remarkable skin drag reduction of up to 80%. These phenomena are actively being investigated by a research team led by Mengqi Zhang, Principal Investigator from the Department of Mechanical Engineering, National University of Singapore (NUS).

In studying the flow instability and its subsequent development, the team carries out advanced stability analyses and conducts high-fidelity direct numerical simulations. The linear stability theory is particularly useful in approximating and elucidating the dynamics of dominant flow structures in transition to turbulence, which is essentially a non-linear problem. The full and exact solution requires a case-by-case computational solving of the *Navier-Stokes* equation, the governing law for all fluid motions.

"Due to the complexity of transitional and turbulent flows, advanced and highly accurate Computational Fluid Dynamics (CFD) simulations are indispensable and important for our project since it allows problems to be tackled within realistic time scales and provides the details that are hard to obtain in experimental investigations," said Wenjun Yuan, a senior research fellow in Mengqi's research team.

In order to cover the research fields on flow instability phenomena within non-Newtonian fluids and electrohydrodynamics, and also machine-learning based techniques for flow control problems, Mengqi and team tap on NSCC's high performance computing resources. "With high-speed supercomputers (HPC), better solutions can be achieved and are often required to solve the largest and most complex problems. NSCC's HPC resources made the simulations efficient and fast as the team relied on distributed memory parallelism, shared memory parallelism, vectorization and memory access optimisations," said Wenjun.

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

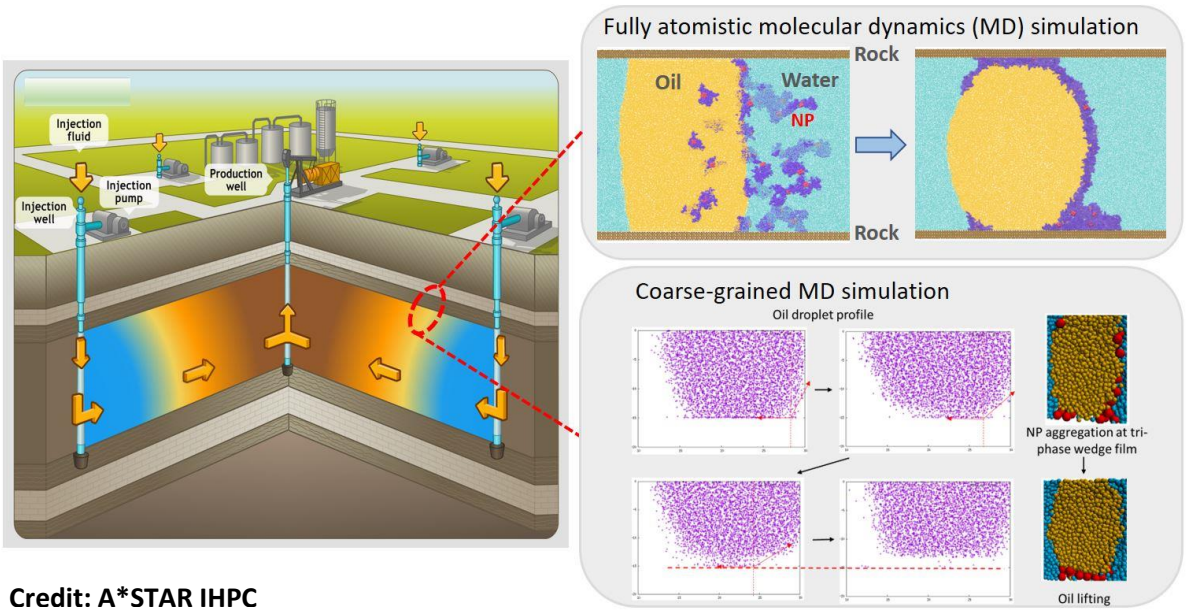
Enhancing oil recovery techniques for the oil and gas industry

Developing advanced functional polymer particles for enhanced flow assurance through the use of NSCC's supercomputing resources.

Around 60% of oil deposits remain unrecovered in oil reservoirs even after traditional prime and secondary oil recovery methods. To increase oil extraction efficiency, various chemicals can be injected into oil reservoirs as an enhanced oil recovery (EOR) technique to further recover bypassed and residual oil trapped in the reservoir.

Among these chemicals, polymeric nanofluids, a combination of nanoparticles and polymers in water, have excellent potential for EOR applications. However, the designing of the most effective combination of nanoparticles (NPs) and polymers involves a large number of parameters. Screening the parameters using conventional experimentation is expensive and inefficient. The high temperature and salinity conditions of oil reservoirs are also inaccessible to experimental studies.

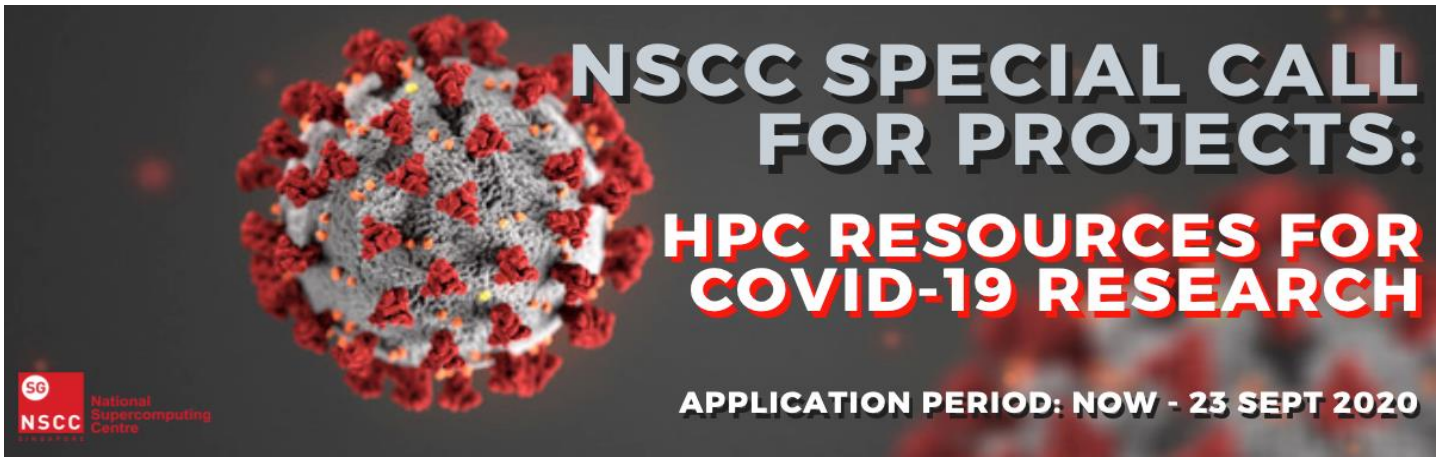
Researchers from A*STAR's Institute of High Performance Computing (IHPC) are using NSCC's supercomputing resources to run multi-scale molecular simulations to understand oil removal mechanisms and screen through the large number of design parameters so as to provide useful guidelines for experiments.



Credit: A*STAR IHPC

"Our simulations on atomistic scales probe the behaviour of complex multi-component systems, which utilise NSCC's large number of high-performance CPU nodes and large data storage space. In addition, our mesoscopic simulations require intensive calculations with NSCC's GPUs," said Zheng Jianwei, Deputy Department Director and Senior Scientist at A*STAR's IHPC.

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



NSCC's COVID-19 Special Call for Projects still ongoing

Application window remains open for local COVID-19 related research projects who wish to get special fast-tracked access to supercomputing resources at NSCC to speed up research on the virus.

Open till 23 September 2020, local scientists who require supercomputing resources for COVID-19 research are welcome to apply for the call. Successful applications will benefit from a fast-tracked approval process, a priority queue for access to supercomputing resources and access to some of the most advanced high performance computing (HPC) systems available in Singapore. These include the ASPIRE 1 petascale supercomputer with 1,288 nodes of CPU and 128 accelerator nodes with NVIDIA K40 GPUs; an AI System with six state-of-the-art 8-GPU NVIDIA DGX-1 with V100 cards; and 13PB of high performance storage.

The Call is open to all local researchers working on COVID-19 related projects, including both existing NSCC users and non-users. Interested researchers keen on taking up this unique opportunity should contact NSCC at projects-admin@nscc.sg or bizdev@nscc.sg for further queries.

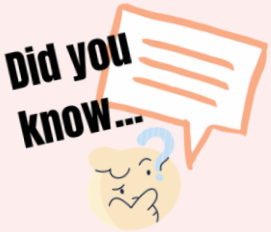
For more information about the NSCC COVID-19 Special Call for Projects, please visit:

https://help.nscc.sg/nscc-special-call-for-projects-hpc-resources-for-covid-19-research/

TECHNICAL NEWS

Never enough - Storage capacity too small?

Frustrated with the fixed home storage capacity given?



All users get 100TB of temporary scratch space in /scratch filesystem.
The scratch disk may be used for storing of trajectory files and temporary data.

**Do note that inactive files will be purged every 30 days.*

To check the quota allocation and usage of home, scratch and projects, use "myquota" command.

```
[ddnuser@nscc01 ~]$ myquota

================================================================
|File System            Usage (GB)        Limit (GB)  |
|ddnuser                  0.49              50.00     |
|/scratch                 110.07            95367.43  |
================================================================
```

Below are the supported options for myquota command:

```
Usage:
myquota
myqouta <user ID>
myqouta -[u][[U]<user ID>
myquota -[p][P] <project ID>
```

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

https://help.nscc.sg

THE LAST BYTE...

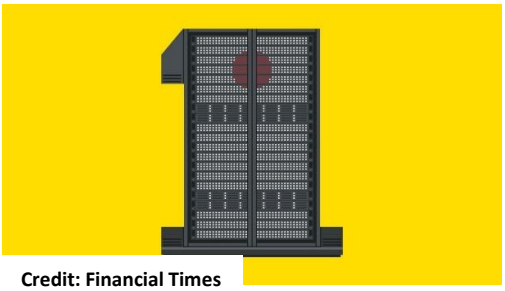
<SHARED CONTENT>

Shared articles and news from the HPC world.

The 416 quadrillion reasons why Japan's supercomputer is number 1

The great processing might of Fugaku will be focused on parsing earthquakes, weather patterns and coughs.

For a good part of last week, the unrivalled highlight of Japanese television — looped on news programmes — was a short computer simulation of a salaryman sitting at his desk and coughing. The reason this simulation is so compelling — and why Japan is so enchanted with it — is how it was produced: on a $1bn-plus made-in-Japan machine called *Fugaku*, whose brisk operating speed of 416 quadrillion calculations per second officially makes it the world's fastest supercomputer… *Read more at Financial Times here.*

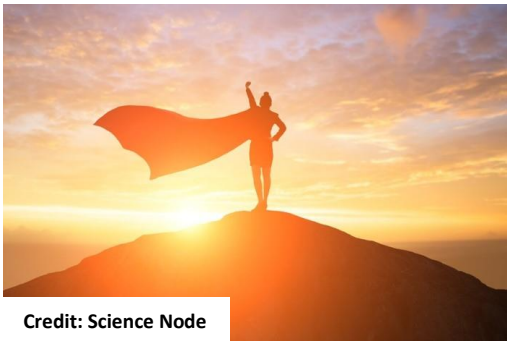


Credit: Financial Times

The 5 fastest supercomputers in the world

Countries around the world strive to reach the peak of computing power--but there can be only one.

Peak performance within supercomputing is a constantly moving target. The field is a continual battle to be the best. Those who achieve the top rank may only hang on to it for a fleeting moment. Let's take a look at the fastest computers as defined by computer ranking project TOP500 — and at what these machines are used for... *Read more at Science Node here.*

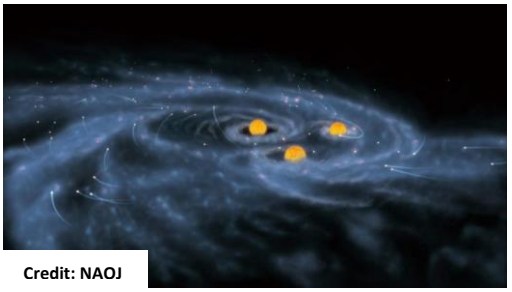


Credit: Science Node

New origin of supermassive black holes revealed by supercomputer simulation

Computer simulations conducted by astrophysicists at Tohoku University in Japan, have revealed a new theory for the origin of supermassive black holes.

In this theory, the precursors of supermassive black holes grow by swallowing up not only interstellar gas, but also smaller stars as well. This helps to explain the large number of supermassive black holes observed today… *Read more about the story at SciTechDaily here.*



Credit: NAOJ

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