



National Supercomputing Centre (NSCC) Singapore e-newsletter

NewsBytes

May 2020



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contact@nsc.sg

CORPORATE NEWS

New projects call offers teachers and students supercomputer access for curriculum and education activities

NSCC's [Call for Educational HPC Projects](#) opens up new high performance computing (HPC) opportunities for educationists and students in curriculum, school projects or student competitions.

As a national research infrastructure NSCC provides supercomputing resources to local research institutes, companies and institutes of higher learning (IHLs), which include autonomous universities and polytechnics.

While education-based curriculum and projects have access to wet-lab experiments, unique HPC resources offer educationists and students new capabilities to perform larger dry-lab experiments beyond those available on site or chargeable cloud service resources. HPC support also introduces a new dimension in experiential learning by providing students with new opportunities to explore larger and more complex problems that are beyond typical textbook examples.

The new project call is an opportunity for all IHLs to request for additional HPC resource quotas of up to 1M core-hours and 0.1 TB of storage in addition to existing quotas. To help new users get started on HPC resources, NSCC has developed a pool of user



guides, supporting materials and training workshops on how to access and use NSCC's resources.

The new Educational HPC Projects call is part of NSCC's plans to further open up access to national HPC resources and to create awareness about the benefits of supercomputing power at the education level. "The call provides both students and their educators the opportunity to explore HPC, how it can benefit their teaching and how to nurture HPC talent," said Associate Professor Teo Yong Meng, the new NSCC Director for HPC in Education who leads the call. "Imbuing HPC in education helps prepare and equip our future talent with the necessary HPC skills needed for the future digital economy and for advanced research."

Examples of teaching modules that could benefit from such HPC resources include science and

engineering (eg. in areas such as modelling & simulation), AI, machine learning and big data analytics. Other possible uses of educational HPC resources include supporting lab exercises and projects in teaching modules, project-based modules and competitions like datathons, among others.

Applications will be reviewed by an Educational HPC Projects Selection Committee comprising HPC experts from both academia and industry.

For more information about the call please contact NSCC at projects-admin@nscg.sg or bizdev@nscg.sg for further queries.

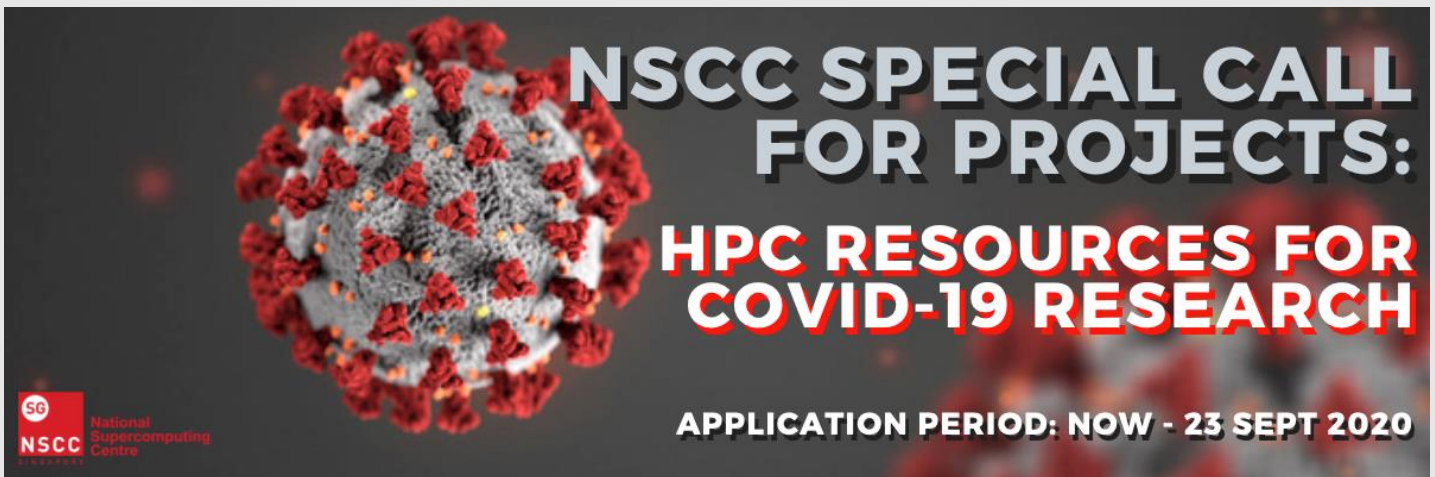
Call for Educational HPC Projects (April 2020)

Application period

4 May 2020 to 30 June 2020

Application portal


<https://help.nscg.sg/nscg-call-for-educational-hpc-project/>



NSCC SPECIAL CALL FOR PROJECTS:

HPC RESOURCES FOR COVID-19 RESEARCH

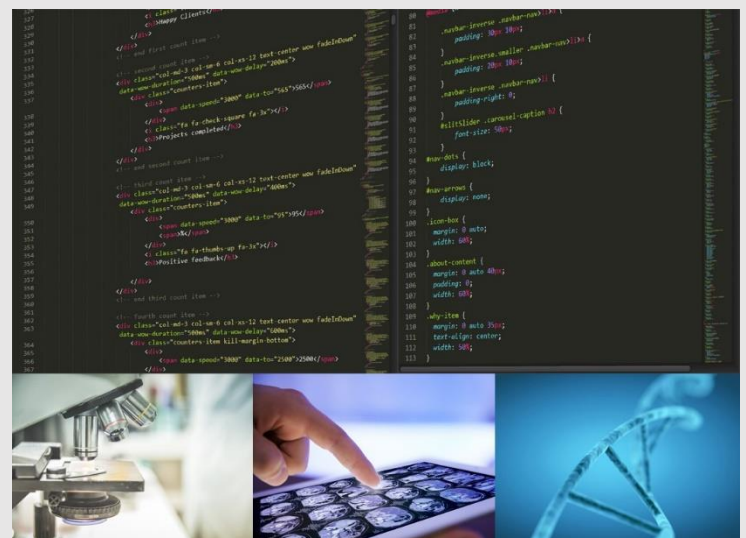
APPLICATION PERIOD: NOW - 23 SEPT 2020

 National Supercomputing Centre

First COVID-19 research projects begin using Singapore's supercomputer

The initial batch of COVID-19 related research projects have been approved for fast-tracked and prioritised supercomputer resources.

Since the launch of the [Special Call for COVID-19](#) projects on 24 March 2020, NSCC has received a number of applications from local research teams of research institutes, universities and private companies for supercomputing resources to aid in their research projects. The applicants come from a variety of organisations including research institutes, universities and private companies.



"It's only been about a month but the initial response to this unique call has been very encouraging," said Dr Kenneth Ban, the NSCC Director for Health & Biomedical Sciences initiatives who chairs the COVID-19 Projects Selection Committee, which comprise Singapore HPC Bioinformatics and Molecular Biology experts. "We will now help to facilitate the journey of these projects so that they can fully optimise and leverage the unique HPC resources that they now have access to so that the COVID-19 research can be advanced as quickly as possible."

The COVID-19 projects cover a variety of research areas including modelling and simulation of the virus, machine learning protein analysis of the virus structure as well as assessing therapeutic targets and diagnostics for COVID-19. These projects will have access to some of the most advanced HPC systems in Singapore such as the ASPIRE1 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.

"Studies point to several proteases playing a vital role in the life cycle of COVID-19 virus. However, prediction of the protein structure based on their sequence has always been a challenging problem," said Dr Cheng Yuan, a Senior Scientist with A*STAR's Institute of High Performance Computing (IHPC) and principal investigator of one of the successful projects which has been given priority HPC resources in the NSCC COVID-19 projects call.

Dr Cheng Yuan added, "We are using AI-assisted methods, machine learning and multiscale simulations, to predict and analyse the structure-function correlations of the virus-associated proteins, taking into consideration possible mutations of the protein. NSCC's powerful computational resources, particularly the GPUs, will be especially helpful for performing the deep learning calculations in our work, which is aimed at developing possible therapeutic mechanisms through targeting of the pathological protein."

"Targeted drug design is crucial in the development of a vaccine for COVID-19 but identifying drug inhibitors using experimental trial and error can be a very time-consuming process," said Dr Shen Lei, Senior Lecturer at the NUS Department of Mechanical Engineering and principal investigator of another research project that has successfully been granted access and priority usage to supercomputing resources.

"Our project uses quantum-mechanics-based high-throughput calculations to quickly and accurately discover small molecules that effectively and efficiently inhibit the virus. This approach may greatly narrow down the scope and duration for drug design," commented Dr Shen Lei. The project leverages NSCC's supercomputer resources to perform molecular reaction simulations and intrinsically complex large-scale quantum calculations which require intensive computations using GPUs and large data storage space.

The Call is open to all local researchers working on COVID-19 related projects, including both existing NSCC users and non-users, from now till September 2020. Interested researchers keen on taking up this unique opportunity should contact NSCC at projects-admin@nscg.sg or bizdev@nscg.sg for further queries.

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

<https://help.nscg.sg/anticovid/>

Applications open from now till September 2020!

New HPC system for climate and environmental research

NSCC's new Köppen system will be a boon for local researchers in the area of climate and environmental monitoring especially with Singapore's focus on addressing climate change, which is one of the biggest challenges the nation faces.

At Singapore's National Day Rally 2019, the Prime Minister outlined climate change as one of the nation's gravest challenges and an area where "Singapore is already feeling the impact".

Rising temperatures and sea levels, evolving weather patterns, flash floods, trans-boundary haze and global warming are currently taking its toll on Singapore's environment and are expected to get worse in the years to come.

As part of the action to mitigate the effects of climate change on Singapore, the government is investing more resources into combating the phenomena. This includes the setting up of the Centre for Climate Research Singapore (CCRS) where meteorologists and scientists work on weather research like models and predictions, and often with the aid of supercomputers.

An addition to the petascale supercomputing resources at NSCC's ASPIRE 1, the newly commissioned Köppen system at NSCC is specifically designed to support HPC research activities in climate and environment research in areas such as advanced modelling and simulation and weather pattern analysis.

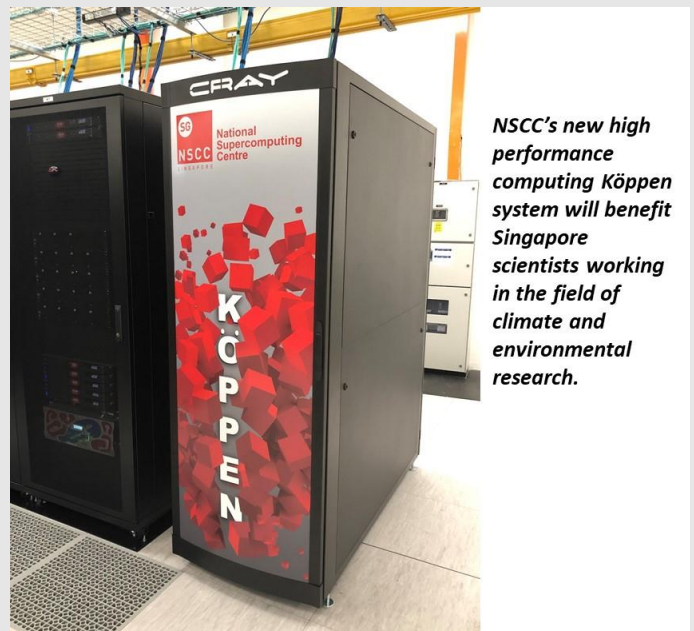
"The Köppen supercomputer system has a performance of over 160 TFLOPS, storage capacity of over 1.2 PB and 52 compute nodes, and is set up as additional capacity and capability in support of

Tech Users Forum

Do you have a question about the supercomputer resources and how you can optimise your research work? Are you having trouble accessing the systems? Do you have a suggestion for new software that you think will benefit the system?

If you are a current NSCC HPC user and have a *byte-ing* question, drop us a note so that we can help you and maybe share your solutions with other users!

Write to us at e-news@nscg.sg.



the climate research community," said Stephen Wong, Technical Director at NSCC.

To find out more about the new Köppen system and how you can benefit from it, please contact bizdev@nscg.sg.

Tips for optimising your work on ASPIRE 1

Are you new to ASPIRE 1? Or are you looking for ways to optimise your HPC work on our supercomputer?

This month's Tips...

Issue 1: My code is not going faster when I run on more CPUs...

Solution for Issue 1: Use a profiling tool to find the bottleneck in your application.

Issue 2: My machine learning code is not using the GPU properly...

Solution for Issue 2: Use the optimised frameworks from NVIDIA.



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

<https://help.nsc.sg>

THE LAST BYTE...

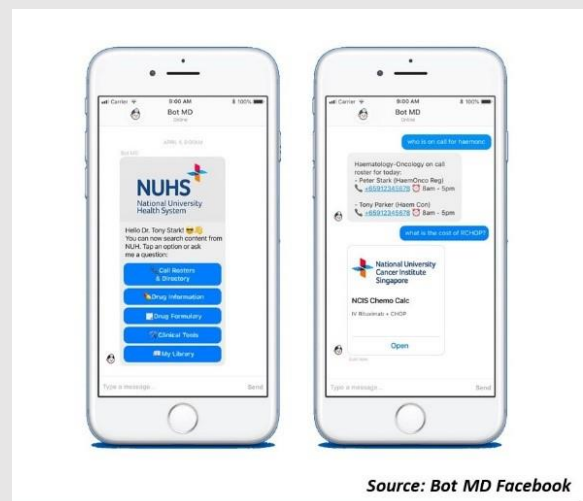
<SHARED CONTENT>

Shared articles and news from the HPC world.

NUHS and Bot MD's COVID-19 info-on-the-go for healthcare workers

New AI assistant gives instant access to COVID-19 information

The National University Health System (NUHS) and Bot MD have launched the NUHS-Bot MD A.I. clinical assistant app to allow frontline medical staff to instantly search hospital specific information including COVID-19 guidelines and operational directives. The initial roll-out to over 500 NUHS doctors, nurses, pharmacists and medical social workers will be expanded to staff across the NUHS healthcare cluster... Read more about the innovation and partnership [here](#).



Source: Bot MD Facebook

IBM and NUS collaboration in quantum computing

New 3-year partnership seeks to train quantum scientists and use quantum computing in real-world problem solving

As part of the collaboration, which is the first in Southeast Asia, NUS researchers will gain access to fifteen of IBM's powerful quantum computing systems via a cloud service. Quantum computers currently have application in areas such as cyber security, medical research and new drug development. The collaboration was made possible through the Quantum Engineering Programme (QEP), which is funded by the National Research Foundation... Read more [here](#).



A mock-up of the IBM Q quantum computer which was showcased at the SupercomputingAsia 2019 (SCA19) conference.

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LET'S BEGIN

THANK YOU!



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Supercomputing in Asia**

National Supercomputing Centre (NSCC) Singapore

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