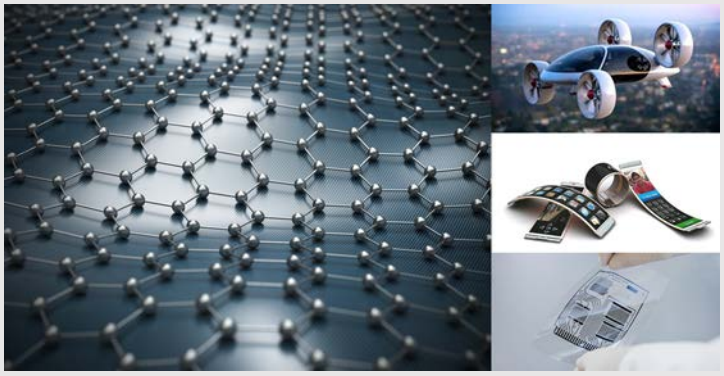
National Supercomputing Centre (NSCC) Singapore e-newsletter

NewsBytes

August 2019

NSCC.SG NSCCSG contact@nscc.sg



Accelerating the discovery of new 2D materials using HPC

Researchers from NUS' CA2DM leverage NSCC's resources to create new next generation materials.

New 2D materials are being discovered every day. At the NUS Centre for Advanced 2D Materials (CA2DM), researchers have been building up a database of 6,000 candidate 2D materials. Such databases are the first step in accelerating the discovery of more 2D materials, by directing experimental efforts to the most promising candidates. "We leverage on tools like AI and machine learning to automate the screening, analyses and simulation of these candidates to faster identify promising materials", says Dr Zhou Jun, one of the researchers at CA2DM who helped put the database together. For the complex task of analysing the thousands of materials on hand, the team turned to the petascale computational power provided by the National Supercomputing Centre (NSCC), Singapore, and its ASPIRE1 supercomputer. The high-throughput capacity computing that NSCC provided allowed the team to speed up their analyses five times faster.

About 2D materials

2D materials, like graphene, are next generation materials that possess unique properties. Graphene, for example, has been proven to be lighter, stronger and tougher than conventional materials like steel and industrial plastics but with added properties like ultra-high electrical conductivity. These materials have huge potential in areas like photovoltaics, electronics, manufacturing, construction and even biomaterials, which could revolutionise sectors such as energy, communications, displays, food, health, transport, defence and the environment.

Reference publications:

- *https://www.nature.com/articles/s41597-019-0097-3*
- *https://www.nature.com/articles/s41586-018-0788-5*

Faster Connectivity between Asia and Europe for Research and Education

World's newest secure 100 Gbps link is set to boost research and education collaboration between Asia Pacific region and Europe with shorter, faster, cheaper connectivity.

The Collaboration Asia Europe-1 (CAE-1), a new 100 gigabit per second (Gbps) link connecting Singapore and London was launched by an international consortium of six research and education (R&E) networks, including AARNet (Australia), GÉANT (Europe), NORDUnet (European Nordics), SingAREN (Singapore), SURF (The Netherlands) and TEIN*CC (Asia-Pacific). The new link is a significant step forward in closing the high-speed connectivity gap between the Asia Pacific region and Europe. The new link is expected to provide additional capacity to meet the rapidly growing bandwidth for transnational education and data-intensive science collaborations.

CAE-1 was officially launched at the TNC19 Conference in Tallinn, Estonia during the signing of the Consortium Agreement - https://www.singaren.net.sg/library/newsroom/20190618_CAE-1_official_launch_TNC19.pdf

**Find out more about how we are helping advance data transfer technologies and networks via the NSCC organised Data Mover Challenge (DMC)!*

'The Race to Exascale'

Are AI and Big Data ready for Exascale? Building an 'unhackable' internet? How is high performance computing transforming the material world?

Read about these and more in the July 2019 issue of Supercomputing Asia magazine.

NSCC hosts ICT leaders from Asia-Oceania

Delegates from the Asian-Oceanian Computing Industry Organization (ASOCIO) meeting visited NSCC on 18 June. The visitors from countries like Singapore, Malaysia, Indonesia, Thailand, Vietnam, Taiwan, South Korea, Japan, Sri Lanka, Nepal and Bhutan represented ICT and academic associations of their home countries.

NSCC @ ISC19, Frankfurt, Germany

Team NSCC was at the annual ISC High Performance conference with over 3,500 researchers and commercial users, and 160 exhibitors. The conference covers the latest technology and products of interest to the high performance computing (HPC) community. NSCC also took the opportunity to renew its collaboration with RIST's High Performance Computing Infrastructure of Japan.

Powering Innovation
Supercomputing in Asia
National Supercomputing Centre (NSCC) Singapore
1 Fusionopolis Way, Connexis South, #17-01 Singapore 138632