NEWSBYTES

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REACHING OUR USERS

In this Issue…

CORPORATE NEWS

Winners for the 10th Lee Kuan Yew Global Business Plan Competition (LKYGBPC) announced

Finalists from various leading universities in Asia, Europe and the United States of America vied for various awards including the NSCC Supercomputing Resource Prize.

Organised by Singapore Management University's (SMU) Institute of Innovation and Entrepreneurship (IIE), the Lee Kuan Yew Global Business Plan Competition (LKYGBPC) invited young innovators, entrepreneurs, scientists, researchers, engineers, or designers to come up with innovative ideas that would help cities, businesses, and communities adapt and thrive during and after the COVID-19 pandemic.

The competition offers a unique forum on how to re-imagine cities as smart, prosperous and resilient societies for the next generation of urban innovators and entrepreneurs. 850 entries from 650 universities across 60 countries were submitted to this year's competition.

NSCC contributed supercomputing resources as one of the competition prizes. Five teams walked away with the NSCC Supercomputing Resource Prize – a 2-month Gold Package subscription of supercomputing resources worth a total of $64,000.

Congratulations to the winning teams - Iterative Scopes, MyrLabs, Polybee, Wootzano and Zhen Robotics!

Since the onset of COVID-19, a research team at A*STAR's Institute of High Performance Computing has been studying the dispersion of droplets in environmental transmission and has developed a simulation which more accurately models the spread of droplets when a person with COVID-19 coughs in Singapore's tropical environment, in order to develop potential intervention measures.

Watch the interview video here to find out more about their research, the challenges they faced, and how NSCC's supercomputing resources have aided in their research study.
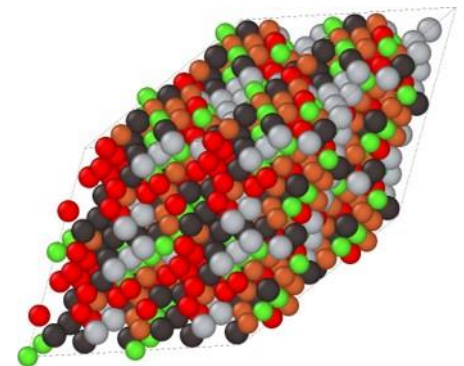
Head over to https://www.nscc.sg/case-studies/ for more case studies of how supercomputers are helping Singapore and follow NSCC's LinkedIn and Facebook page to be kept updated on all things HPC.

Speeding up the process of materials discovery and development using HPC

NSCC's supercomputer helps perform high-throughput computations to accelerate the process of alloy development and to make it more cost effective.

Traditional pathways in the development of new alloys often occur through several empirical observations and optimising the composition and fabrication methodology. Such conventional methods may take up to 20 years of work before the alloy is ready for deployment.

A team of researchers at the Institute of High Performance Computing (IHPC), A*STAR are leveraging NSCC's supercomputing resources to perform high-throughput computations and experiments coupled with machine learning techniques. This helps accelerate the process of alloy development to just 3 years in the case of fabricating a novel high entropy alloy (HEA).

An example of a HEA showing the large amount of compositional disorder

"The ASPIRE 1 supercomputer has been invaluable to us for investigating the massive HEA composition parameter space using first-principles simulations. We also have plans to use NSCC's supercomputer for generating a large set of mechanical data through molecular dynamics simulations as the project moves ahead."

Zachary Aitken
Scientist II
Institute of High Performance
Computing (IHPC), A*STAR

To achieve this, IHPC is leveraging various domain expertise that covers first-principles simulations, molecular dynamics, and computational thermodynamics to generate a database that is used to train the machine learning model. Such a database holds a huge amount of data and requires large-scale, high-performance computing resources to analyse.

By using NSCC's resources, the team has been able to generate more than 1 million data

points that have been used to train machine learning models that predict the microstructural phase of an HEA for a given composition.

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

High performance computing for studying and preserving marine ecosystems

The Reef Ecology Lab at NUS leverages NSCC's supercomputing capabilities for marine genomic analyses to better understand and design solutions for marine conservation in Singapore.

Singapore is known as a shipping hub for maritime trade around the world. However, Singapore is also home to a diverse marine ecosystem which stretches along Singapore's coastline with over 700 species of fish and 200 species of corals recorded. Local impacts and global climate change have placed coastal habitats around the world under great stress, creating urgent need for targeted conservation solutions.

A snapshot of the rich biodiversity hidden under Singapore's seawaters

"The power of genomics cannot be overstated. With vast quantities of data being generated at an unprecedented pace, there is a pressing need for computing capabilities to keep up with advancing sequencing technologies. NSCC's computing cluster has been invaluable in our quest to unravel the mysteries of the sea around Singapore, and to guide our efforts towards conserving marine ecosystems and their functions for future generations."

Randolph Quek
Graduate Student
Department of Biological Sciences
National University of Singapore

With the advent of next-generation DNA sequencing, a team of researchers at the Reef Ecology Lab at NUS are looking into genomic analyses of hard corals in Singapore, using molecular techniques and cutting-edge bioinformatics. The team is tapping onto NSCC's high performance computing resources to employ advanced genomic and sequencing technologies to characterise the biodiversity and adaptive capacity of marine ecosystems. The application of high-throughput sequencing is central to a wide range of marine genomic research—from characterising microorganisms and their functions to tracking megafauna such as sharks and dolphins by sequencing their DNA from environmental samples, or "eDNA".

Genomic analyses also provide the necessary tools to test species' responses to local and global stressors and, more fundamentally, reconstruct species histories and their responses in the past. These analyses yield precise projections about the habitats of the future and valuable insights for devising strategies to improve their outcomes.

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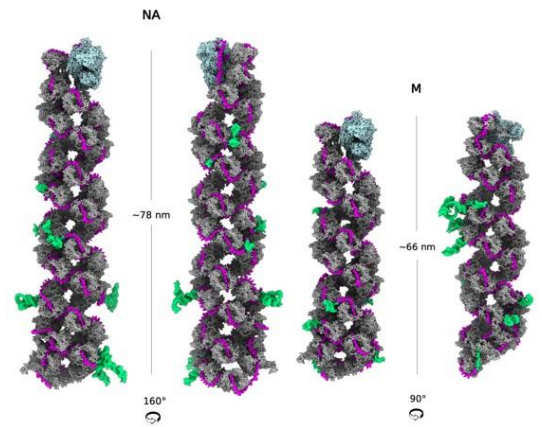
Studying the mutation mechanisms of the flu virus to develop better vaccines

Utilising high performance computing to understand the life cycle of Influenza A Virus to aid in the development and commercial production of vaccines.

Influenza A Virus (IAV) is a perennial public health threat that causes both seasonal epidemics and, less frequently, global pandemics. Statistics from the World Health Organisation (WHO) show that between three to five million severe IAV infections annually result in considerable economic losses, and more poignantly, nearly half a million deaths, particularly among the elderly, immunocompromised patients, and children.

The IAV genome consists of RNA and is divided into eight segments. All eight segments need to be packaged into a viral particle to form an infectious virus. However, the segmented genome allows for a process of re-assortment whereby segments are exchanged between infectious human strains and between human IAVs and animal IAVs, resulting in new virus strains of which there is no prior human immunity. Such strains may give rise to pandemic influenza.

A research team at A*STAR's Bioinformatics Institute (BII) is making use of numerical simulations based on experimental data to understand the behaviour of the genomic segments and the role particular RNA structures play. The team is leveraging NSCC's

Model of Influenza A genome segment

supercomputing resources to conduct coarse-grained and atomistic simulations of IAV segments that reveal the dynamics of these structures which will allow them to understand how these segments are interacting with one another during viral encapsidation.

"Numerical simulations allow us to observe the interactions within and between segments accurately on an atomic level which is not accessible experimentally. The overall dynamics we observe in our simulations are consistent with data obtained by experiments which allows us to have confidence in the quality of our models."

Dr Roland G. Huber
Assistant Principal Investigator
Bioinformatics Institute (BII),
A*STAR

This is important for the development and commercial production of vaccines where antigenic segments are combined with segments optimised for growth under laboratory conditions to maximise yield. Moreover, re-assortment of viral genome segments is a key mechanism by which pandemic viruses cross species and hence understanding the molecular basis for this process will support efforts at early detection of dangerous mutations.

The team is now using the data derived from the simulations to parametrise ultra-coarse-grained models. This technique will allow them to observe genome assembly from the segments in real time and test computationally which parts of the genome drive virus packaging and re-assortment.
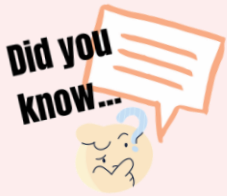
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TECHNICAL NEWS

Data manipulation with AWK
For increased productivity!

Let's say you have a file, 123.xyz containing the following array:

```
$ cat 123.xyz
1 apple1 111 orange1
2 apple2 222 orange2
3 apple3 333 orange3
4 apple4 444 orange4
5 apple5 555 orange5
```

Using the first row as an example, you can rearrange the first three elements and remove the last element resulting in the following row:

```
111 1 apple1
```

AWK can be used to do the proposed data manipulation shown above on 123.xyz and save the resulting output to another file, 321.xyz; all in one line.

```
$ awk '{print $3 " " $1 " " $2} ' 123.xyz > 321.xyz
$ cat 321.xyz
111 1 apple1
222 2 apple2
333 3 apple3
444 4 apple4
555 5 apple5
```

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.

World's first market-ready diamond-based quantum accelerator coming to Pawsey Supercomputing Centre

Quantum Brilliance, a venture-backed Australian quantum computing startup from The Australian National University, will install the world's first diamond quantum accelerator at the Pawsey Supercomputing Centre.

With the installation, Pawsey will become one of the first supercomputing centres globally to host a universal quantum computer onsite. Pawsey and Quantum Brilliance will join forces with other Australian industry leaders and researchers as part of Pawsey's Quantum Pioneer Program to develop cutting-

edge quantum applications in machine learning, logistics, defence, aerospace, quantum finance and quantum research. Read more at HPC Wire here.

Innovators in Japan are developing new technologies to counter coronavirus

As the global coronavirus pandemic continues, the world is searching for new measures that will minimise the risk of infection while allowing essential institutions such as hospitals, government, and schools to continue to function.

In any public health plan for public spaces, two issues that must be addressed are countermeasures against viruses in the air and viruses on surfaces that are touched by many different people. Solutions are needed as we face this "new normal" and several innovators have stepped forward with some new ideas. Read more at London Daily here.
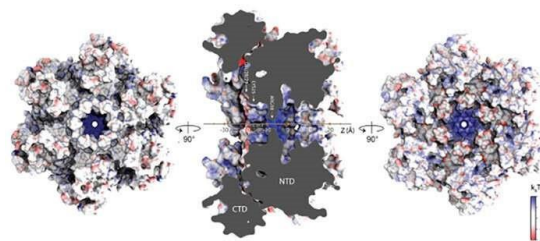

Credit: London Daily

Getting to the core of HIV replication

Viruses lurk in the gray area between the living and the nonliving, according to scientists. Like living things, they replicate but they don't do it on their own. The HIV-1 virus, like all viruses, needs to hijack a host cell through infection in order to make copies of itself.

Supercomputer simulations supported by the National Science Foundation-funded Extreme Science and Engineering Discovery Environment (XSEDE) have helped uncover the mechanism for how the HIV-1 virus imports into its core the nucleotides it needs to fuel DNA synthesis, a key step in its replication. Read more at Phys Org here.

Credit: Phys Org