National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

June 2020

CORPORATE NEWS

Mapping the evolution of the 500 million year-old horseshoe crab

The genomic study of the horseshoe crab, which was done using NSCC's supercomputing resources, can help in the conservation of the horseshoe crab and decipher its remarkably sensitive immune system.

The horseshoe crab has remained relatively unchanged after nearly half a billion years of evolutionary history. New genomic research led by scientists from A*STAR's Institute of Molecular and Cell Biology (IMCB), with help from NUS and Republic Polytechnic researchers, have generated the most contiguous high-quality, chromosome-scale genome assembly for the mangrove horseshoe crab to date. The study was recently published in the journal Nature Communications.

The genomics study is a valuable resource for the conservation of this endangered species and is an important component in providing greater insight about the innate immune system of horseshoe crabs. A protein found in the blood of horseshoe crabs is used in the pharmaceutical and medical industry as an extremely sensitive agent for detecting endotoxin contamination.

Mangrove horseshoe crab.
*Source: A*STAR IMCB*

"An important prerequisite for formulating effective conservation strategies is an understanding of genetic diversity and population structure but at present, there is no information about the population genetics of horseshoe crabs in Singapore," said Professor Byrappa Venkatesh, who is the Research Director that heads the Comparative and Medical Genomics Laboratory at IMCB. Analysis of this highly-contiguous genome has revealed novel information about the evolution of the horseshoe crab including the possibility that there have been three rounds of whole-genome duplication in its lineage.

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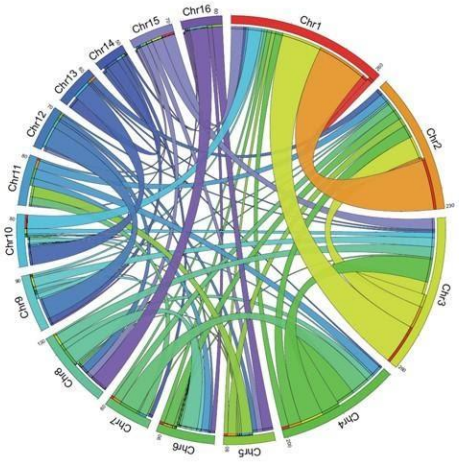
LET'S BEGIN

"Our study has shown that there was a marked decline in the population size of the mangrove horseshoe crab approximately 60,000 years ago coinciding with the onset of the recent ice age which has failed to recover due to the recent increased human activities such as the modification of coastal areas and overexploitation. Some suggestions for managing horseshoe crab stocks are habitat conservation, prohibiting horseshoe crab harvest, and protection of their breeding grounds," added Professor Venkatesh.

Analysis of the mangrove horseshoe crab genome has identified many tandem gene clusters that are specific to its lineage including those that play important roles in the horseshoe crab's innate immunity. For the horseshoe crabs to survive and propagate successfully in a mangrove environment where they are exposed to a variety of pathogens, they have evolved a sophisticated immune system response network for recognising, immobilising and killing of pathogens.



Circos plot showing paralogous segments in the mangrove horseshoe crab genome. The numbers on the chromosomes represent the number of anchor points.
Source: A*STAR IMCB

"The horseshoe crabs' amebocytes are extremely sensitive to bacteria and hence is routinely used as a sensitive agent for detecting bacterial endotoxin," explained Professor Venkatesh. "The expanded immune system gene families identified in our study are likely to be important components of the horseshoe crab's immune response network which helps them mount a rapid and effective immune response to counteract pathogens."

To achieve the chromosome-scale genome assembly study, Professor Venkatesh and his team leveraged NSCC's high performance computing resources. "Our genome project used state-of-the-art 'third-generation sequencing' technology which involves single-molecule real time sequencing (SMRT) that generates reads of 20,000 base pairs (bp) and longer, which are necessary to provide the highest contiguity to the genome," said Professor Venkatesh adding that the horseshoe crab genome is relatively large (approximately 2 Gb) and the team generated SMRT reads amounting to 100 times the size of the genome (200 Gb).

"The only way we could assemble the genome was by using the large number of high-performance nodes of the NSCC as conventional computational systems are incapable of assembling such a large amount of long reads. This allowed us to assemble the genome in a reasonable period and attempt several combinations of parameters to generate alternate assemblies that enabled us to obtain the best possible final genome assembly."

For more information about the study, please refer to the paper entitled, "Chromosome-level assembly of the horseshoe crab genome provides insights into its genome evolution"

IHLs across Singapore apply for Educational HPC resources

The number of applications from local universities and polytechnics to use HPC resources in curriculum and education training have been extremely encouraging.

The NSCC Call for Educational HPC Projects opens up supercomputing resources for education-related activities.

Close to forty education-related projects from institutes of higher learning (IHLs) have submitted requests to date for high performance computing (HPC) resources since the launch of NSCC's Call for Educational HPC Projects in early May 2020. The new project call gives educators and students from universities and polytechnics the opportunity to access supercomputing resources for curriculum activities, school projects or student competitions. HPC offers a new dimension in experiential learning and allows educators and students the chance to explore larger and more complex problems that are beyond typical textbook examples.

"The encouraging response from IHLs for educational HPC resource use is a clear indication of the value and benefit that educators and students see in using HPC in training and education," said Associate Professor Teo Yong Meng, the new NSCC Director for HPC in Education.

Teams from a majority of the local polytechnics and universities across Singapore have applied for access to use HPC resources in their educational activities. Faculties such as mechanical engineering, aerospace engineering, computer science, materials science, infocomm technologies as well as electrical and electronic engineering are proposing to use HPC in education activities for a wide range of fields including artificial intelligence (AI), modelling & simulation, cybersecurity and big data.

Call for Educational HPC Projects

Application period

4 May 2020 to 30 June 2020

Application portal

https://help.nscc.sg/nscc-call-for-educational-hpc-project/

The applicants will be notified respectively about the status and success of their applications.

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

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30 student teams sign up for 3rd APAC HPC-AI competition

The 2020 competition, jointly organised by the HPC-AI Advisory Council and NSCC, has added applications that address education and applied learning in bioscience research, and uses real-world scenarios such as the COVID-19 pandemic.

The thirty student teams from across the Asia Pacific region participating in the 2020 APAC HPC-AI Competition include teams from Australia, Bangladesh, Bhutan, China, Hong Kong, India, Malaysia, Singapore, Sri Lanka, Taiwan and Thailand. The competition, which is open to university and technical institute teams from across the entire APAC region, includes both creating missions and addressing challenges around AI development and testing, and high-performance computing workloads.

For the first time, the teams will be taking part in the competition via online due to the COVID-19 pandemic and the cancellation of the ISC2020 conference, the event where the competition was to be held. The student teams will use the supercomputing platforms at NSCC to remotely configure, code and benchmark the competition applications.

The final results of the competition are expected to be announced later in the year at the Supercomputing Conference 2020 (SC20) in November at Atlanta, Georgia, USA. The winner of the competition will then be invited to the award ceremony which will take place at the SupercomputingAsia 2021 (SCA21) conference in March in Singapore.

For more information, please refer to the article about the 2020 APAC HPC-AI Competition.

TECHNICAL NEWS

Supercomputing resources for advanced AI research work

NSCC's AI Platform is designed to support large, advanced and complex AI workloads.

The NSCC Artificial Intelligence (AI) system consists of six NVIDIA DGX-1 servers which are integrated with the ASPIRE 1 supercomputer system. It was set up as an AI Platform to facilitate capability development in HPC and AI-Deep Learning as well as to be an enabler for the AI community in Singapore such as AI Singapore, the HPC community and industry users. The DGX-1 nodes are suited to large, batch AI workloads such as those used in training complex models with large datasets.

The DGX-1 features eight Tesla V100 GPU accelerators connected through NVLink, the NVIDIA high-performance GPU interconnect, in a hybrid cube-mesh network, dual socket Intel Xeon CPUs and four 100 Gbps InfiniBand network interface cards. The DGX-1 system software and libraries are also tuned for scaling deep learning on its network of Tesla V100 GPUs to provide a flexible and scalable platform for the application of deep learning.

To find out more about the NSCC's HPC resources that support work in AI and how you can tap on them, please contact bizdev@nscc.sg.

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@nscc.sg.

The NSCC AI Platform is designed to support large, advanced and complex AI workloads.

ASPIRE 1 cybersecurity and you

A number of HPC centres in Europe were recently affected by cybersecurity attacks which resulted in the shutdown of some HPC centres.

Cybersecurity incidents had been reported at HPC centres in Germany, Switzerland and Spain with crypto mining identified as a possible reason for the attack. The reports indicated that the hacking by one or more parties was facilitated via stolen user SSH credentials. Users of some of the affected systems had lost their access or had their passwords and SSH credentials reset.

The incident highlights the crucial role that users play in securing such valuable HPC systems and resources. Regardless of the fixed cybersecurity measures that are put in place to safeguard HPC systems, all it takes is a single compromised user access credential for attackers to exploit the breach and to bring down the system. The security of any system is only as strong as the weakest link in the chain.

As such, NSCC requires all users to stop sharing passwords, SSH keys or accounts. Users who continue to do so are in breach of NSCC's Acceptable Use Policy. Users have also been asked to change their passwords and SSH keys as a precaution.

Additionally, NSCC has heightened security protocols and is conducting account identity verification checks. The team is also exploring potential multi-factor authentication (MFA) access methods to strengthen the security of the system.

Here's what you can do to strengthen cybersecurity:

- **Do not share your account** – Keep your account to yourself and do not share your account with your project members or collaborators. Shared credentials are hard to account for and may cause a domino effect when a security breach occurs.
- **Use a strong password** – Passwords should be made up of a combination of alphabets, numbers and special characters.
- **Protect your SSH private key** – Install a password for your SSH key. Even if your key file gets stolen without your knowledge, the password will still be able to secure the private key.
- **Multi-factor authentication (MFA)** - Whenever available, use MFA to strengthen the security of your account.

THE LAST BYTE...

<SHARED CONTENT>

Shared articles and news from the HPC world.

Digital twins for sustainable cities

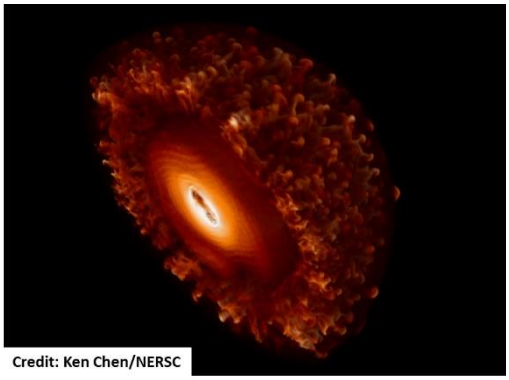
Hyper-realistic 3D models promote improved city planning.

By Eric Gedenk

Data-driven modelling and visualisation offer new ways to understand how cities function. The example of the 'digital twin' for the city of Herrenberg provides valuable information for city planners. Future AI applications and version could include factors like migration, gentrification and economic resilience into the model… Read more about digital twins at Science Node here.

World's first 3D supercomputer simulations of superluminous supernovae

Because no one can actually see a supernova up close, researchers rely on supercomputer simulations to give them insights into the physics that ignites and drives the event.



Credit: Ken Chen/NERSC

For the first time ever, an international team of astrophysicists simulated the three-dimensional (3D) physics of superluminous supernovae - which are about a hundred times more luminous than typical supernovae… Read more about the story at SciTechDaily here.