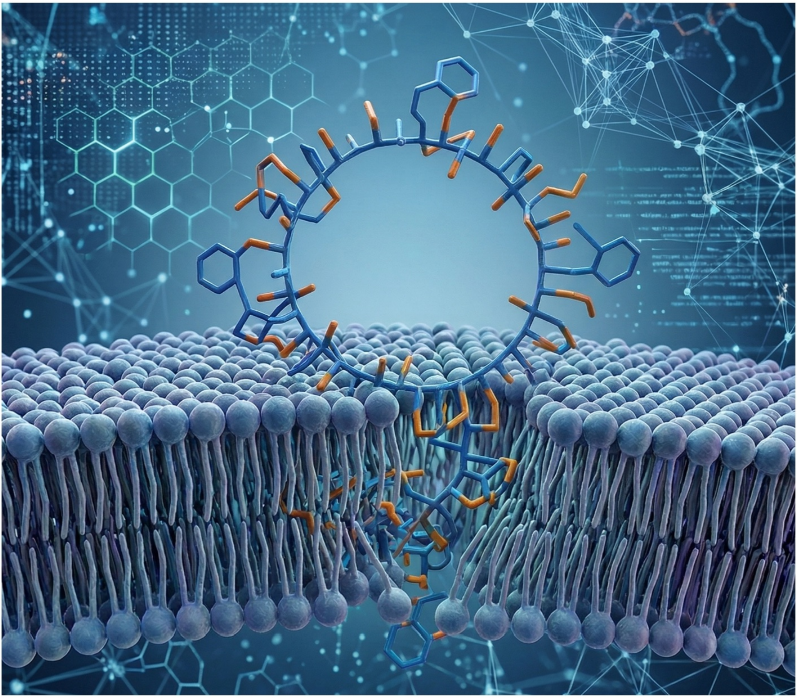
A MONTHLY E-NEWSLETTER BY NSCC SINGAPORE

NEWSBYTES

ASPIRE 2A
NETWORKING

CORPORATE NEWS

A snapshot of NSCC Singapore's key updates and ongoing collaborations



📌 **Featured Read of the Month!**

From Structure to Cell Permeability: Advancing Peptide Drug Discovery with AI

Cyclic peptides are a class of molecules composed of amino acids linked in a ring-shaped structure. This unique configuration enhances their structural stability and enables them to target intracellular protein–protein interactions — a class of targets often considered “undruggable” using conventional small-molecule drugs. These interactions play a critical role in treating cancer and other diseases but are difficult to access due to their size and structural complexity.

However, a key challenge lies in their ability to cross cell membranes efficiently. To do so, cyclic peptides must exhibit a “chameleon-like” behaviour — dynamically changing their conformation to shield polar atoms when moving into membrane environments. Capturing this behaviour requires large-scale molecular dynamics (MD) simulations and advanced AI models that go beyond simple 2D molecular representations.

Powered by NSCC Singapore’s ASPIRE 2A+ supercomputer, researchers from the Agency for Science, Technology and Research (A*STAR)’s Bioinformatics Institute (BII) created CycPeptMPDB-4D, a large-scale dataset detailing the movements and behaviours of over 5,000 cyclic peptides in water and membrane-like environments. The team also developed the Local Update Function Network (LUFnet), an AI model that enhances simulation efficiency by enabling larger time integration steps while preserving physical accuracy.

Read more

National
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Charting the Road Ahead: A Message from Our Chief Executive

2026 marks a defining milestone for NSCC Singapore, as we celebrate our 10th anniversary alongside the launch of our next national supercomputer — strengthening Singapore's capabilities in AI-driven discovery, large-scale simulation and emerging hybrid computing workloads.

Building on this momentum, 2025 saw steady progress across our priorities of Enhancing HPC Capacity & Diversity, Talent & User Enablement, and Operational Excellence, as we expanded both infrastructure capabilities and engagement with the research community.

Beyond infrastructure, NSCC Singapore is also laying the groundwork for the next phase of our evolution — deepening our role as a strategic enabler of advanced computing through algorithm development and co-design, specialised advisory services, and expanded training pathways to help researchers fully harness next-generation systems.

Read the full message from NSCC Singapore Chief Executive

Helping Researchers Optimise their Supercomputing Workloads — HPC Resource Planning Workshop at NTU

Ahead of NSCC Singapore's upcoming 7th Call for Projects (launching 1 April 2026), a two-part engagement session was held at Nanyang Technological University (NTU) Singapore to equip researchers with practical strategies for effective HPC utilisation and resource planning.

Read more

Built for Scale, Enabling Researchers: March 2026 ASPIRE 2A and ASPIRE 2A+ Introductory Workshops

NSCC Singapore's supercomputing systems enable researchers to tackle computational workloads at a scale far beyond what conventional computing resources can support. However, the massive computational power is only half the equation—it is as important for users to know how to effectively harness these resources to drive real-world breakthroughs.

Read more

THE LAST BYTE

Shared reads and cool finds from the HPC world

PM Wong outlines plan to keep S'pore a global innovation hub; growth areas include quantum tech

A new training academy will be set up to systematically equip more than 150,000 public officers with digital, data, design and artificial intelligence skills, it was announced on Monday (Mar 2). Called the Institute of Digital Government (IDG), it is scheduled to launch in the third quarter of this year. Speaking in parliament, Minister of State for Digital Development and Information Jasmin Lau said the goal for the broader public service is to ensure no officer feels "powerless in a digital world".

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Image credit: CNA

HPCWire People to Watch 2026

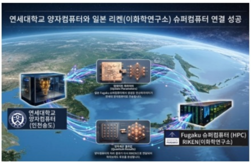
PEOPLE
HPCwire
TO WATCH
2026

The 24th year of HPCwire‘s People to Watch Program recognizes HPC professionals who play leading roles in driving innovation within their particular fields, making significant contributions to society as a whole. Over the course of the program, HPCwire has recognized over 275 HPC luminaries who have gone on to achieve extraordinary things.

Read more

Image credit: HPCWire

Yonsei, RIKEN and IBM to Use Quantum Computing to Probe Causes of Rare Diseases


연세대학교 양자컴퓨터와 일본 리켄(이화학연구소) 슈퍼컴퓨터 연결 성공
(Update Parameters)
연세대학교 양자컴퓨터 (인천송도)
Fugaku 슈퍼컴퓨터 (HPC) RIKEN(이화학연구소)
(Quantum Results)

Yonsei University, Japan’s RIKEN and IBM will connect Japan’s Fugaku supercomputer with Yonsei’s IBM Quantum System One to analyze the causes of rare diseases. According to IBM Korea, the project aims to uncover the mechanism of Leigh syndrome, a rare condition and one of the causes of neonatal mortality. The disorder prevents mitochondria in newborns from producing energy, often leading to death within a year.

Read more

Image credit: IBM Korea

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