National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

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In this Issue…

CORPORATE NEWS

WE WOULD LIKE TO HEAR FROM YOU!

Do you have a minute to spare to give us some feedback on our newsletter? As a valued subscriber, we are continuously looking for ways to improve our newsletter to provide relevant and suitable content for you. Click on the link below to begin!

Thank you!

LET'S BEGIN

More to come for Singapore's national supercomputing in 2022

The light at the end of the tunnel...

The pandemic has changed the way we live, play and work. But our world has also become more connected than ever and with accelerated digitalisation, one thing is certain - high performance computing (HPC) will play a BIGGER role in smart nation research and advancements. NSCC has been working hard during the pandemic to lay the groundwork and develop Singapore's next generation HPC. The new system will pave the way for new HPC resources to support and supersize Singapore's research! Here's a look back at some of the highlights for NSCC this year and as we look forward to an exciting 2022 ahead!

COMING SOON! Upgraded National Supercomputing Resources

The tender for the development of the next generation national supercomputer system plus upgrades to the national storage and research network infrastructure was awarded to Hewlett Packard Enterprise (HPE). The new system is expected to provide up to 10 Petaflops (10 PFLOPS) of computing capacity and is eight times more powerful than the current supercomputer.

New Supercomputer Powers Singapore's Healthcare Research

NUHS and NSCC sign agreement to build and site a petascale national supercomputer at NUHS that will serve Singapore's medical and healthcare research needs by middle of next year.

Nurturing HPC Talent

Certificate of Competency for Introduction to HPC

ITE and NSCC collaborate to launch new training course to equip participants with basic HPC knowledge.

The 10th Annual ISC 2021 Student Cluster Competition & 4th Annual APAC HPC-AI competitions

went virtual for the second time running through NSCC's ongoing HPC resource support.

New International Links Benefit Singapore Researchers

Finland - Singapore MOU on HPC collaboration

NSCC, Singapore Advanced Research & Education Network (SingAREN), the Quantum Engineering Programme of the National University of Singapore (NUS) and Finland's CSC-IT Centre for Sciences ink partnership to accelerate cross-border collaborations in network linkages, green DC tech and quantum encryption research.

Plugged in to world's fastest supercomputer

First-of-its-kind agreement between NSCC, R-CCS and RIST enables Singapore researchers to have regularly access to world's No.1 supercomputer, Japan's Fugaku.

Doing Our Part For Decabornisation - Green Supercomputing

New Green Data Centre concept to make use of LNG chilled water discharge

SLNG, NSCC, NUS and Surbana Jurong ink partnership to collaboratively explore the development of a Proof-of-Value (POV) for a Green Modular Data Centre System, which would be the first-of-its-kind in Singapore.

Sustainable Data Centre with a smaller carbon footprint

New purpose-built data centre at NUS Innovation 4.0 to house Singapore's newest Supercomputer fitted with energy saving features and is awarded Platinum Green Mark.

HPC Community Grows - New NSCC Stakeholders

Singapore-ETH Centre (SEC)

SEC will tap on NSCC's supercomputing resources and data storage facilities to simulate scenarios to tackle the urban heat island effects in the Cooling Singapore project.

Precision Health Research Singapore (PRECISE)

PRECISE's National Precision Medicine Programme will tap on NSCC's HPC resources and data storage capabilities to enable the team to deploy state-of-the-art genome analytics algorithms at an industrial scale to uncover the genetic variants of each individual.

Supercomputing & Quantum Computing

CQT, A*STAR's IHPC and NSCC collaborate to advance the quantum computing ecosystem in Singapore through research, training and development of applications for quantum computing.

SCA Goes Fully Digital

SupercomputingAsia (SCA) 2021 Conference, jointly organized by HPC centres from Singapore, Japan and Australia went fully virtual for the first time ever.

As we enter into a new year, we would like to thank all of you - our users, stakeholders, partners and friends for your continued support. We look forward to working closely with you in 2022 to build a stronger HPC community in Singapore.

NSCC wishes you all the best for the New Year and have a safe 2022 ahead!

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SupercomputingAsia 2022 (SCA22) returns from 1 – 3 March 2022 as a hybrid conference

Themed "Towards Supercomputing for All", the annual conference reflects the growing accessibility and ubiquity of high-performance computing (HPC) resources.

Co-organised by supercomputing centres from Australia, Japan, Singapore and Thailand, SCA22 encompasses an umbrella of notable supercomputing and allied events with the key objective of promoting a vibrant and relevant HPC ecosystem in Asia. The conference programme covers a wide range of topics including the latest supercomputing trends, AI and quantum computing in areas like healthcare, weather & climate change, green data centres and quantum-enabled encryption, among many others. SCA22 will also host several international collaborative tracks such as the HPC Centre Leaders Forum, EU-ASEAN-Japan Symposium and the Asia Pacific Research Platform.

The SCA22 conference will be officially launched by **Guest-of-Honour Dr Janil Puthucheary**, Senior Minister of State, Ministry of Communications and Information & Ministry of Health, Minister-in-charge of GovTech Singapore, who will be giving the opening address.

Some of the SCA22 highlights include session tracks related to Supercomputing Frontiers Asia (SCFA), Inclusivity and Diversity, Accelerating HPC Upskilling without Borders, HPC-AI developments, Quantum Computing and Networking, HPC-enabled Climate Research and international HPC collaborations. The tracks are also supplemented by Industry talks highlighting the latest HPC technology innovations and developments, and industry workshops.

Conference on Next Generation Arithmetic (CoNGA), the leading conference on emerging technologies for computer arithmetic, will be held in conjunction with SCA22. Gain the latest news and updates on the developments of breakthroughs with next generation data formats and their corresponding hardware, tools, applications and services and exchange ideas on what next generation arithmetic should be.

Come join our line-up of exciting Keynotes, Speakers and Partners as we explore the role of supercomputers, and unravel the possibilities for HPC. Register now at https://sca2022.sg/registration or head over to https://www.sc-asia.org/ for more details on the conference.

REGISTER NOW

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Curbing the spread of Dengue

Researchers at A*STAR are tapping HPC resources to gain a deeper understanding of the dengue virus in order to design improved therapeutic strategies.

Dengue virus (DENV) is a member of the flavivirus genus and infects hundreds of millions of people worldwide each year. A Flavivirus is like an onion; the outermost layer is made up of "envelope proteins" embedded in a lipid membrane, while the inner core contains capsid proteins in complex with an RNA genome.

Experimental structures of viruses correspond to single "snapshots" at a given physiological condition but do not always reflect their dynamic nature or important conformational changes related to binding of antibodies or drugs. For example, consecutive infections by different serotypes of DENV can lead to "antibody dependent enhancement" (ADE) in which antibodies from the first infection bind to the infecting virus particle but do not neutralize it – this can result in a severe case of dengue.

At present, there are no approved drugs or highly effective and safe vaccines for DENV. Therefore, a team of researchers from Peter J. Bond group at the Bioinformatics Institute (BII) at A*STAR, in collaboration with multiple experimental groups in Singapore, are leveraging on NSCC's supercomputing resources to get a detailed understanding of the structural and dynamical properties of DENV.

"Our work relies on access to powerful computational resources and NSCC is a key provider. Since we are describing the motions of entire viruses, our simulation system sizes can typically reach ~5 million particles or more. Our simulations are propagated via Newton's laws of motion in very small-time steps, and so to reach timescales of viral dynamics that are biologically meaningful, our calculations must be performed hundreds of millions times. This is computationally very expensive and cannot be run on a single desktop machine. Therefore, we are grateful for the resources provided by NSCC."

Jan K. Marzinek
Senior Post Doctoral Research Fellow
Multiscale Simulation, Modelling and Design (MSMD) Group
Bioinformatics Institute (BII), A*STAR

The team recently explored the molecular details of ADE and proposed a new mechanism by combining computational methods with experimental snapshots. The team used a "virtual microscope" approach based on molecular dynamics simulations, in order to relate static snapshots of virus-antibody complexes to their dynamics. They particularly focused on the DENV envelope proteins since these are crucial for the virus to attach to the host cell during infection and are also recognized by antibodies during a host immune response.

Through probing virus dynamics at the molecular level, an improved understanding of the mechanisms of disease and antibody binding can be achieved and the team hopes to ultimately work towards improved therapeutic strategies.

To find out more about how NSCC's HPC resources can help you, please contact e-news@nscc.sg.

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THE LAST BYTE...

<SHARED CONTENT>

Shared articles and news from the HPC world.

Singapore lifts data center moratorium - but sets conditions

Minister for Trade and Industry says the country will be "more selective" in future.

Singapore appears to have lifted its moratorium on new data center projects, according to a statement by the Trade and Industry Minister this week - but new data centers will have to meet certain conditions. Data centers contribute to Singapore's growth, but must be sustainable, said Minister Gan Kim Yong, in a written answer to Parliament on Tuesday, Jan 11. The country has paused new data center development since 2019, but this will now resume, though the government will impose measures to make them more efficient, he said. Read more at Data Centre Dynamics here.

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Quantum computing is coming. Now is the right time to start getting ready

CIOs must start exploring potential use cases now or risk being left behind in the quantum race. They also need to be wary of technical and ethical concerns.

From supporting a continuing shift to the cloud to embracing data-led services, CIOs already have a jam-packed digital transformation agenda for 2022 – and now the evidence suggests they need to make room for another line item: quantum computing. CIOs who start investigating quantum will find a fast-growing area. Read more at ZD Net here.

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Edge to Exascale: A Trend to Watch in 2022

Edge computing is an approach in which the data is processed and analyzed at the point of origin – the place where the data is generated.

Credit: HPC Wire

This is done to make data more accessible to end-point devices, or users, and to reduce the response time for data requests. HPC-class computing and networking technologies are critical to many edge use cases, and the intersection of HPC and 'edge' promises to be a hot topic in 2022. In this Q&A, Hyperion Research Senior Adviser Steve Conway describes the characteristics of edge computing and its relationship with HPC, including the edge-to-exascale paradigm. Read more at HPC Wire here.

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Powering Innovation
Supercomputing in Asia

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