National Supercomputing Centre

# e-Science Activities in Singapore

Prof Tan Tin Wee | Chief Executive, NSCC Singapore

International Symposium on Grids & Clouds (ISGC) 2024 Conference | 27 March 2024

NSCC.SG


# NSCC Introduction

- National Research Infrastructure funded by National Research Foundation (NRF)
- National high performance computing (HPC) resource open to all Singapore researchers from IHLs, Research Institutes and industry
- Set-up in 2015
- HPC is an indispensable resource in key research areas like genomics, climate research, AI, materials science, etc.
- Funded by NRF and administered by A*STAR

# Singapore upgrades HPC Infrastructure

## ❑ Upgrading Infrastructure

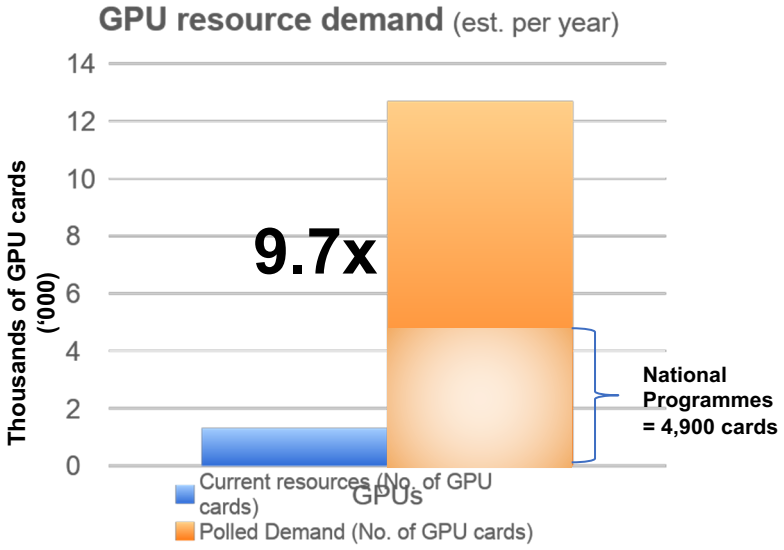
- From ASPIRE 2A to ASPIRE 2A+ and ASPIRE 2B

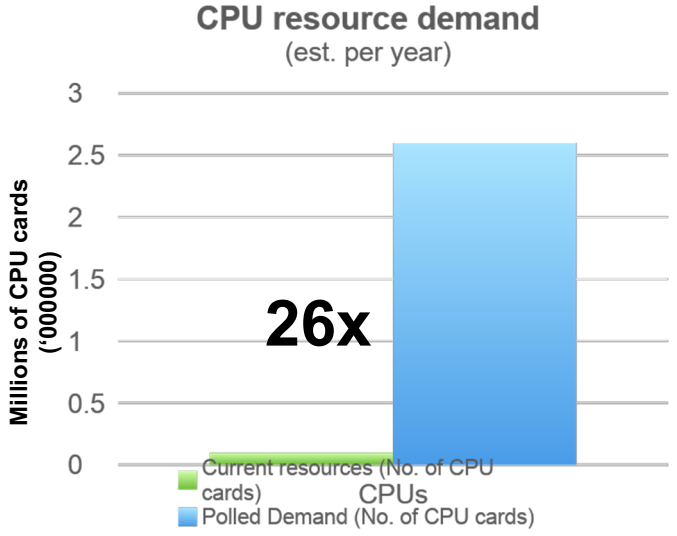
## ❑ Connecting Singapore Research with the World

- Our links and connectivity in partnership with SingAREN

## ❑ Growing Local HPC Community & Int'l Collaboration

- e.g. Installation of CHROMA @SingHealth, Prescience @NUHS



# 1 PFLOP (2016) to 10-20 PFLOPS (2025)

## PREVIOUS – ASPIRE 1


### 1 PFLOPS System
- 1,288 nodes (dual socket,12cores/CPU ES-2690v3)
- 128GB DDR4 RAM/node
- 10 large memory nodes (1x6TB, 4x2TB, 5x1TB)

### Accelerator Nodes
- 128 nodes with Tesla K40 GPUs

### 13PB Storage
- GPFS & Lustre File Systems
- I/O bandwidth up to 500GB/s

### Infiniband Interconnection
- EDR (100Gbps) Fat Tree with full bisectional bandwidth within cluster

**Add-on Systems (ASPIRE 1+)**
- AI.Platform (6 x DGX-1)
- 1,000 cores HTC System
- *Koppen* - 160 TFLOPS Cray XC-50, Climate System

## CURRENT – ASPIRE 2A

**Awarded - 27 April 2021 (ASPIRE 2A)**
- 3.33PF GPU, 2.58PF CPU compute power
- 7x more powerful than current ASPIRE1

## BEYOND

**~10-20 PFLOPS Capacity**

**Note**: **Fl**oating-point **o**perations **p**er **s**econd, or FLOPS, is a measure of compute performance or how quickly and effectively a computer works. P or peta (used in units of measurement) denotes a factor of $10^{15}$. The Top 500 supercomputers today are minimally in the PFLOPS range.

# DEMOCRATISING ACCESS TO RESOURCES

## Some of Our Local and International Partners

## National HPC Support for Local Research

- **Research Projects on ASPIRE 1**
  - Resources provided to date (c.2016-2023):

| | | | |
|---|---|---|---|
| 3.5B | CPU/GPU HOURS PROVIDED | 10,000 | USERS HOSTED |
| | | >1,700 | PROJECTS SUPPORTED |

- **Research Projects on ASPIRE 2A**
  - Resources provided from 2023:

| | | | |
|---|---|---|---|
| 400M | CPU/GPU HOURS PROVIDED | 4,400 | USERS HOSTED |
| | | 500 | PROJECTS SUPPORTED |

National Supercomputing Centre

# DEMOCRATISING ACCESS TO RESOURCES

## Nurturing HPC in education and helping upskill professionals in Singapore

NSCC's new partnership with educational institutes and professional bodies to leverage Singapore's national supercomputer for student education and upskilling of professionals to support future jobs in areas such as HPC, AI, data science and analytics, and advanced simulation and modelling.

Areas of collaboration include:

- ***New HPC curriculum*** development
- ***Training courses*** and workshops
- ***Student competitions*** to nurture interest and build HPC capability

Signing ceremony at SCA23 conference in Singapore, 27 Feb – 2 Mar 2023

Republic Polytechnic

Singapore Polytechnic

Institute of Technical Education

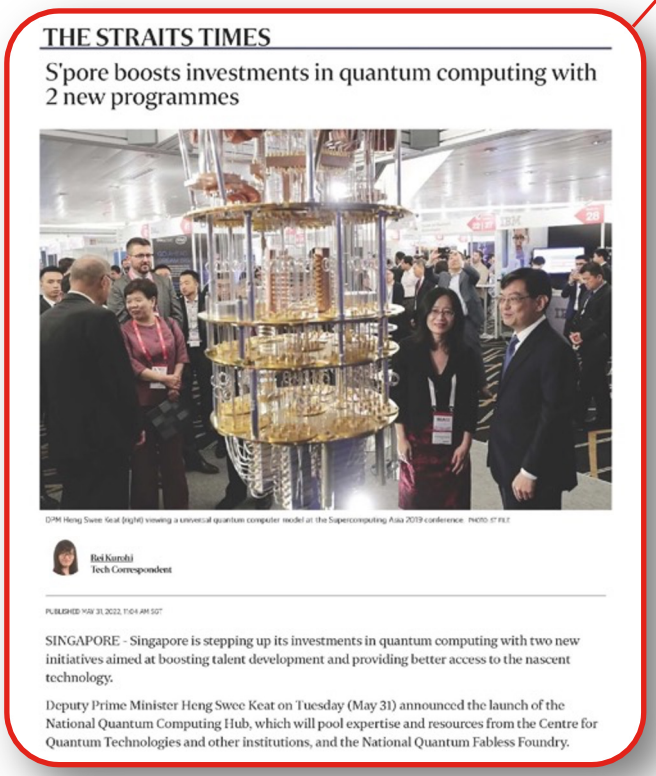
The Institution of Engineers Singapore

Singapore Institute of Technology

AI Singapore

# Growing the Singapore HPC Community

## Singapore HPC and quantum computing



THE STRAITS TIMES

S'pore boosts investments in quantum computing with 2 new programmes

DPM Heng Swee Keat (right) viewing a universal quantum computer model at the Supercomputing Asia 2019 conference. PHOTO: ST FILE

Rei Kurohi
Tech Correspondent

PUBLISHED MAY 31, 2022, 11:04 AM SGT

SINGAPORE - Singapore is stepping up its investments in quantum computing with two new initiatives aimed at boosting talent development and providing better access to the nascent technology.

Deputy Prime Minister Heng Swee Keat on Tuesday (May 31) announced the launch of the National Quantum Computing Hub, which will pool expertise and resources from the Centre for Quantum Technologies and other institutions, and the National Quantum Fabless Foundry.

NATIONAL QUANTUM FABLESS FOUNDRY

NATIONAL QUANTUM-SAFE NETWORK

NATIONAL QUANTUM COMPUTING HUB

The National Quantum Computing Hub (NQCH) is a joint initiative of the NUS ***Centre for Quantum Technologies (CQT)***, A*STAR ***Institute of High Performance Computing (IHPC)*** and ***NSCC***

Centre for Quantum Technologies

Institute of High Performance Computing
IHPC

National Supercomputing Centre

Researchers at **CQT** and **IHPC** will develop quantum computing hardware and middleware.

**NSCC Singapore** will host a ***quantum computing facility*** and ***provide the supercomputing power*** needed to develop and train the algorithms that could eventually be used on quantum computers.

# DEMOCRATISING ACCESS TO RESOURCES

## Support for international data intensive research

**Project Call for Singapore-Japan HPC resources**

- **Call for Fugaku Projects via NSCC – Collaboration with RIST**
  Singapore researchers have unique access to Japan's mighty Fugaku supercomputer since 2021 in a collaboration between NSCC, Research Organization for Information Science and Technology (RIST) and RIKEN Center for Computational Science (R-CCS).

**10** RESEARCH PROJECTS **2,000,000** NODE HOURS


ACCESS TO **FUGAKU**
JAPAN'S TOP SUPERCOMPUTER

**Promoting and facilitating international research data transfers**

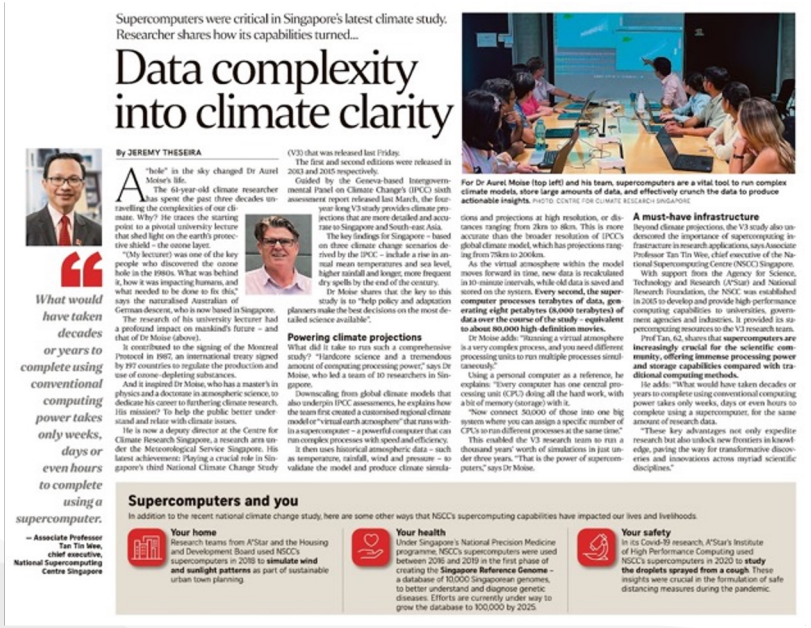
- **New collaboration provides faster access to the Protein Data Bank for Asian / Oceania region researchers**
  San Diego Supercomputing Center (SDSC) and Singapore Advanced Research and Education Network (SingAREN) signed MoU at SCA23 event to facilitate Open Science Data Federation and a cache server of the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB) for regional researchers.


SDSC-SingAREN MOU


Data Mover Challenge 2023

- **Data Mover Challenge (DMC) 2023**
  The DMC a biennial competition that bring together experts from industry and academia in a bid to test their software and solutions for transferring huge amounts of research data. Winners of the DMC 2023 was invited to share their solutions at the SCA24 conference.
  https://www.nscc.sg/data-mover-challenge-2023

# Singapore's 3rd National Climate Change Study (V3)

Supercomputers were critical in Singapore's latest climate study. Researcher shares how its capabilities turned...

## Data complexity into climate clarity

By JEREMY THESEIRA

A "hole" in the sky changed Dr Aurel Moise's life.

The 61-year-old climate researcher has spent the past three decades unravelling the complexities of our climate. Why? He traces the starting point to a pivotal university lecture that shed light on the earth's protective shield – the ozone layer.

"(My lecturer) was one of the key people who discovered the ozone hole in the 1980s. What was behind it, how it was impacting humans, and what needed to be done to fix this," says the naturalised Australian of German descent, who is now based in Singapore.

The research of his university lecturer had a profound impact on mankind's future – and that of Dr Moise (above).

It contributed to the signing of the Montreal Protocol in 1987, an international treaty signed by 197 countries to regulate the production and use of ozone-depleting substances.

And it inspired Dr Moise, who has a master's in physics and a doctorate in atmospheric science, to dedicate his career to furthering climate research. His mission? To help the public better understand and relate with climate issues.

He is now a deputy director at the Centre for Climate Research Singapore, a research arm under the Meteorological Service Singapore. His latest achievement: Playing a crucial role in Singapore's third National Climate Change Study (V3) that was released last Friday.

The first and second editions were released in 2013 and 2015 respectively.

Guided by the Geneva-based Intergovernmental Panel on Climate Change's (IPCC) sixth assessment report released last March, the four-year long V3 study provides climate projections that are more detailed and accurate for Singapore and South-east Asia.

The key findings for Singapore – based on three climate change scenarios derived by the IPCC – include a rise in annual mean temperatures and sea level, higher rainfall and longer, more frequent dry spells by the end of the century.

Dr Moise shares that the key to this study is to "help policy and adaptation planners make the best decisions on the most detailed science available".

### Powering climate projections

What did it take to run such a comprehensive study? "Hardcore science and a tremendous amount of computing processing power," says Dr Moise, who led a team of 10 researchers in Singapore.

Downscaling from global climate models that also underpin IPCC assessments, he explains how the team first created a customised regional climate model or "virtual earth atmosphere" that runs within a supercomputer – a powerful computer that can run complex processes with speed and efficiency.

It then uses historical atmospheric data – such as temperature, rainfall, wind and pressure – to validate the model and produce climate simulations and projections at high resolution, or distances ranging from 2km to 4km. This is more accurate than the broader resolution of IPCC's global climate model, which has projections ranging from 25km to 200km.

As the virtual atmosphere within the model moves forward in time, new data is recalculated in 10-minute intervals, while old data is saved and stored on the system. **Every second, the supercomputer processes terabytes of data, generating eight petabytes (8,000 terabytes) of data over the course of the study – equivalent to about 80,000 high-definition movies.**

Dr Moise adds: "Running a virtual atmosphere is a very complex process, and you need different processing units to run multiple processes simultaneously."

Using a personal computer as a reference, he explains: "Every computer has one central processing unit (CPU) doing all the hard work, with a bit of memory (storage) with it.

"Now connect 50,000 of those into one big system where you can assign a specific number of CPUs to run different processes at the same time."

This enabled the V3 research team to run a thousand years' worth of simulations in just under three years. "That is the power of supercomputers," says Dr Moise.



For Dr Aurel Moise (top left) and his team, supercomputers are a vital tool to run complex climate models, store large amounts of data, and effectively crunch the data to produce actionable insights. PHOTO: CENTRE FOR CLIMATE RESEARCH SINGAPORE

### A must-have infrastructure

Beyond climate projections, the V3 study also underscored the importance of supercomputing infrastructure in research applications, says Associate Professor Tan Tin Wee, chief executive of the National Supercomputing Centre (NSCC) Singapore.

With support from the Agency for Science, Technology and Research (A*Star) and National Research Foundation, the NSCC was established in 2015 to develop and provide high-performance computing capabilities to universities, government agencies and industries. It provided its supercomputing resources to the V3 research team.

Prof Tan, 62, shares that **supercomputers are increasingly crucial for the scientific community, offering immense processing power and storage capabilities compared with traditional computing methods.**

He adds: "What would have taken decades or years to complete using conventional computing power takes only weeks, days or even hours to complete using a supercomputer, for the same amount of research data.

"These key advantages not only expedite research but also unlock new frontiers in knowledge, paving the way for transformative discoveries and innovations across myriad scientific disciplines."



*What would have taken decades or years to complete using conventional computing power takes only weeks, days or even hours to complete using a supercomputer.*

– Associate Professor Tan Tin Wee, chief executive, National Supercomputing Centre Singapore



### Supercomputers and you

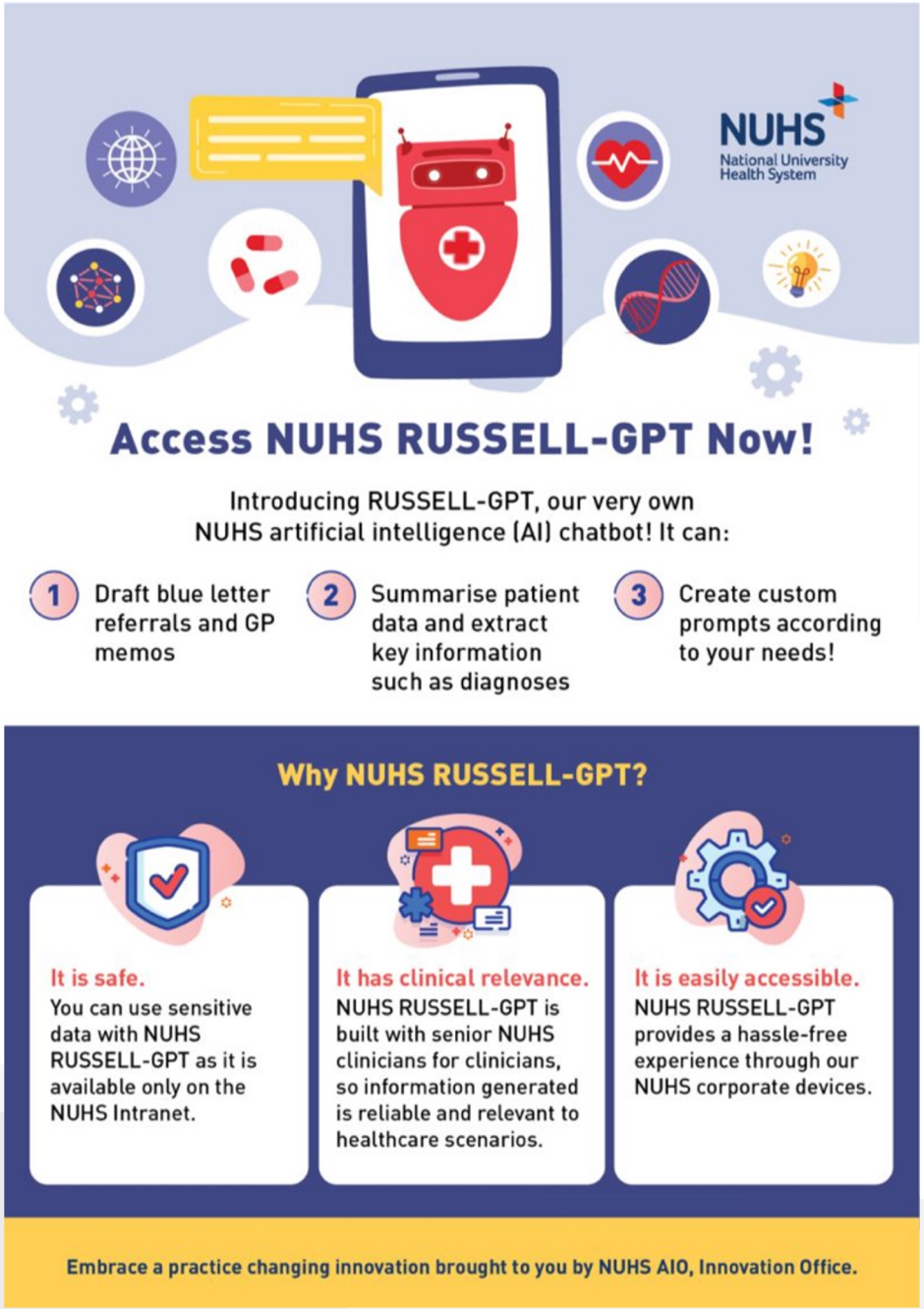
In addition to the recent national climate change study, here are some other ways that NSCC's supercomputing capabilities have impacted our lives and livelihoods.

**Your home**
Research teams from A*Star and the Housing and Development Board used NSCC's supercomputers in 2018 to **simulate wind and sunlight patterns** as part of sustainable urban town planning.

**Your health**
Under Singapore's National Precision Medicine programme, NSCC's supercomputers were used between 2016 and 2019 in the first phase of creating the **Singapore Reference Genome** – a database of 10,000 Singaporean genomes, to better understand and diagnose genetic diseases. Efforts are currently under way to grow the database to 100,000 by 2025.

**Your safety**
In its Covid-19 research, A*Star's Institute of High Performance Computing used NSCC's supercomputers in 2020 to **study the droplets sprayed from a cough.** These insights were crucial in the formulation of safe distancing measures during the pandemic.

- NSCC supercomputer was vital in providing the compute power needed to resolve and complete the climate simulations and models for V3
- HPC power allowed high resolution simulations, more accurate climate forecast models
- Allowed researchers to perform a total of ~2000 model years of dynamical downscaling simulations covering almost entire SEA at 8 km resolution and
- V3's climate change forecasts are set to impact ministry and agency planning and policy for the future in building environmental sustainability and resilience




# NUHS RUSSELL-GPT

NUHS artificial intelligence (AI) chatbot

## Impact

- ❏ Synthesizes precise local medical knowledge
- ❏ Reduces administrative work of doctors and nurses

## How NSCC HPC made RUSSELL-GPT possible

The supercomputing resources provided by NSCC allowed NUHS medical researchers to use local medical big data to train AI models using multiple NVIDIA DGX A100 compute nodes that can accommodate the large sizes of LLMs, which was previously not possible with single graphical processing unit (GPU) systems.


Source: SingHealth

Source: Straits Times

# CHROMA @SingHealth

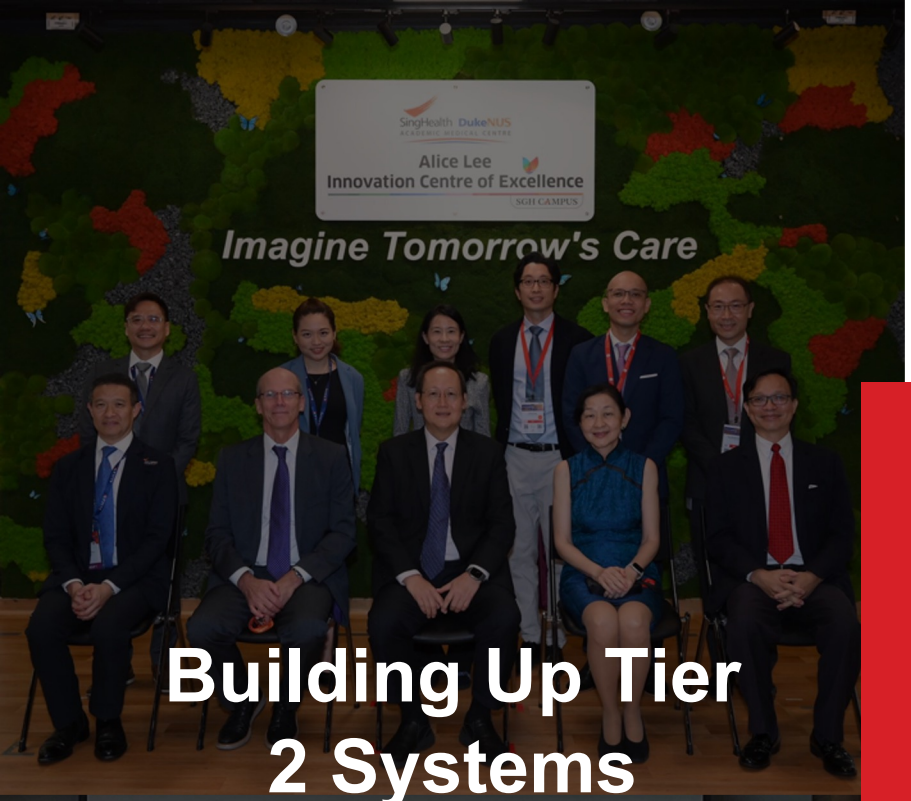
HPC Resources for the Singhealth Community

## Impact

- ❑ Provide HPC resources to SingHealth
- ❑ Facilitate research activities
- ❑ Enables training of AI models for large-scale, complex research, risk of disease predictions and personalised medicine.

## Capabilities of CHROMA

- ❑ Strong Compute Power of **1,024** CPU Cores (AMD EPYC Processors)
- ❑ Fast GPU-Accelerated Computing using NVIDIA DGX-A100, **320GB** GPU RAM
- ❑ High throughput, low latency via InfiniBand, up to **200Gb/s**
- ❑ Fast storage of up to **3,000,000 IOPS**




# Building Up Tier 2 Systems


- HPC is critical in biomedical research and a growing resource in healthcare
- NSCC collaborated with NUHS and SingHealth to install two edge supercomputer systems
- **CHROMA @ SingHealth** enables the training of AI models and algorithms for large-scale complex research, risk of disease predictions and personalised medicine.
- **Prescience @ NUHS** enables the NUHS RUSSELL-GPT that boosts the productivity of healthcare professionals and aids clinicians in their work as well as SMILE AI which involves smart monitoring and intelligent learning aimed at enhancing oral healthcare.

National Supercomputing Centre

# Thank You

Email: contact@nscc.sg

NSCC.SG