National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

March 2024

In this issue…

CORPORATE NEWS

NSCC Singapore as a resource partner for the Built Environment

NSCC will be a key resource for the Built Environment Accelerate to Market Programme (BEAMP), a multi-agency initiative designed to build a vibrant innovation ecosystem for the Built Environment sector in Singapore.

Organised by the Building and Construction Authority (BCA), JTC Corporation (JTC) and Enterprise Singapore (EnterpriseSG), BEAMP is an initiative set up to bring innovators and companies together to fast-track the innovation process to solve real world industry challenges.

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

BEAMP returns this year to facilitate the adoption of advanced building technologies, enabling greater sustainability, quality, and productivity outcomes in the building and construction sector. NSCC Singapore will be a key resource partner, providing High Performance Computing (HPC) resources to the shortlisted teams to test-bed their innovative solutions. Awarded innovators will gain the opportunity to co-develop, testbed and pilot solutions with leading companies in the Built Environment sector.

Applications for BEAMP's cycle 5 is now open. If you are interested to tap on BEAMP and NSCC's HPC resources, this is your chance to explore test-bedding opportunities with industry players, be mentored by experts, and secure a funded pilot. The early submission deadline for the challenge is 18 April 2024 and the final submission deadline is 10 May 2024. The team is also conducting an information session on the 8 and 9 April 2024.

Find out more

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Showcasing NSCC Singapore's HPC-AI capabilities at the Festival of Innovation

Held on the 26 and 27 March 2024, the Festival of Innovation focuses on digital innovation and technology for the public sector.

NSCC Singapore conducted a HPC-AI panel session titled *"Pushing Gen AI's Boundaries with HPC - Use Cases and Applications of Gen AI Technology"* during the Festival of Innovation. Three key speakers from the HPC and AI community AI Singapore and A*STAR were gathered to talk about the potential of AI technology in Singapore and the crucial role that HPC resources played in the growth of AI research.

Mr. David Ong, Head of Engineering, AI Products at AI Singapore, led the discussions on "LM Data Engineering with NSCC Singapore", followed by a sharing on "Applications of Large Language Model (LLM) - Adapting LLM for NLP Tasks" by Dr. Wu Kui, Senior Scientist at the Institute for Infocomm Research (I2R), ASTAR. Prof. Ivor Tsang, Director of A*STAR Centre for Frontier AI Research (CFAR) gave his insights on "Taming Hallucinations: The Confluence of Generative and Traditional AI".

With over 1000 attendees, mainly from the public sector, the Festival of Innovation aims to inspire, educate and equip the attendees with the tools necessary to render government more efficient, responsive and ultimately more citizen-friendly.

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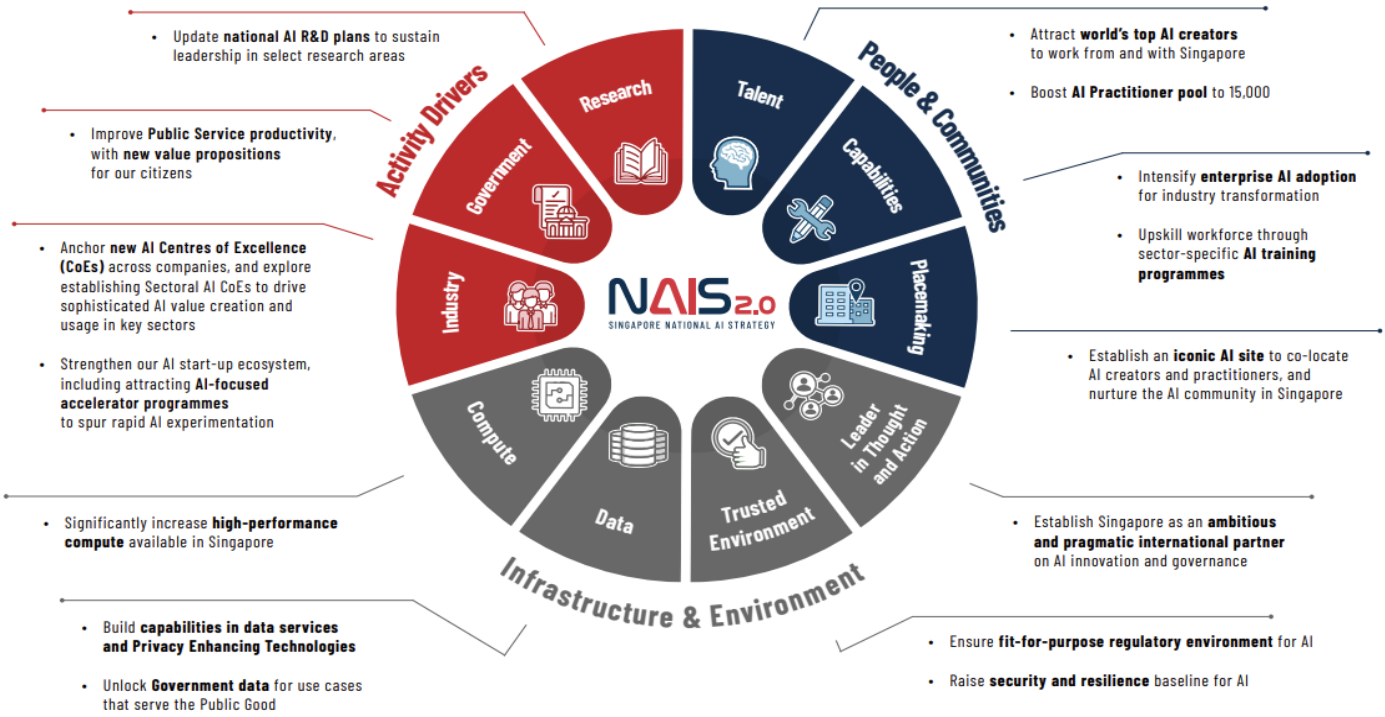
The National Artificial Intelligence Strategy 2.0 (NAIS2.0)

Smart Nation Singapore released its NAIS2.0 in 2023, directing the nation towards a clear path of Artificial Intelligence (AI) adoption in public and private sectors.

Guided by the vision "AI for the Public Good, for Singapore and the World", NAIS 2.0 seeks to attain the twin goals of excellence and empowerment. The key thrust is to uplift individuals, businesses, and communities to use AI with confidence, discernment, and trust. These efforts will direct AI towards addressing the needs and challenges of our time, such as in areas of global importance like population health and climate change. The NAIS2.0 highlighted 10 enablers to achieve this vision through 3 systems.



Credit: Smart Nation Singapore and Ministry of Communications and Information

To support high-value AI activities, NSCC Singapore stands ready to provide reliable and localized access to HPC resources. The national HPC resource will empower national research programmes with enhanced computational power, enabling them to efficiently process vast amounts of data and testbed their innovations.

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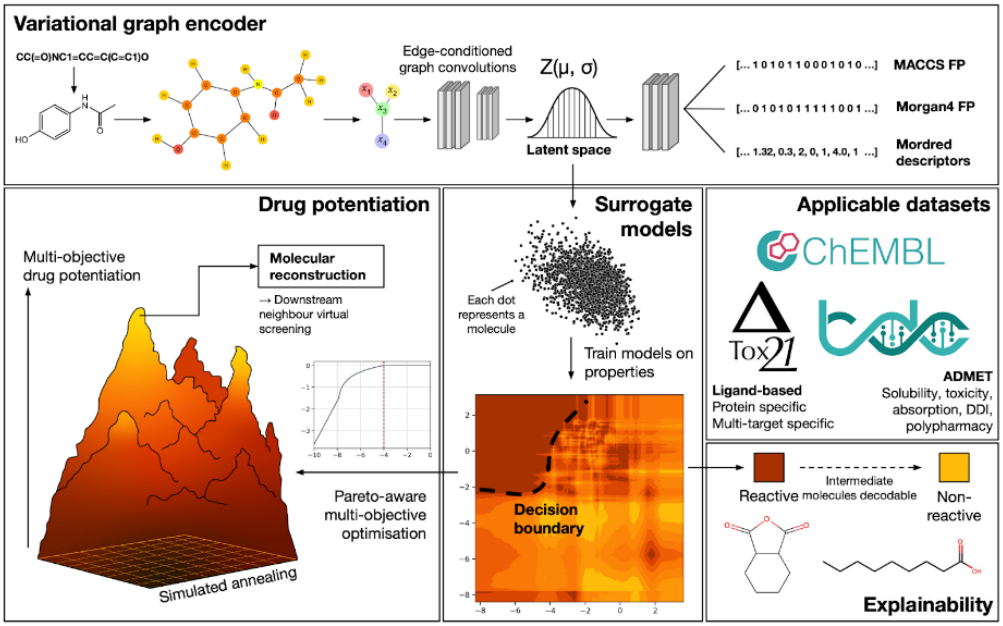
Advancing drug discovery research using NSCC HPC resources

Researchers from Nanyang Technological University (NTU) are applying variational graph encoders as an effective generalist algorithm in computer-aided drug design (CADD)



Selecting ideal drug molecules from a chemical space of over 10^{63} molecules is extremely challenging, compounded by high failure rates in clinical research, which make the time and the financial costs of drug development daunting. Although CADD has significantly reduced these costs, there are still many issues to be resolved in practical research.

Currently, many models specialize in predicting a single property of a chemical compound, such as solubility. Existing CADD techniques focus on discovering and optimizing small molecule drugs, but predictions and optimizations of pharmacological and toxicological properties remain unsatisfactory.

Therefore, researchers from NTU have embarked on this work to find a single model capable of predicting multiple properties simultaneously. The model will be able to expedite the drug discovery process.

<u>The Research</u>

Molecules and compounds used in our daily drugs vary in shapes and sizes. Currently, there are an estimated 10^{63} unique compounds that have the potential to be used as pharmaceutical drugs. However, these molecules are discrete in nature and cannot be easily represented mathematically.

In this research, the researchers employed a variational graph encoder to convert individual molecules into a continuous numerical space. Consequently, each molecule can now be represented using 64 numbers.

Using these 64 numbers, they demonstrated the capability to predict various compound properties, including absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiles.

This research specifically showcased that building smaller models based on these 64 numbers generated competent models that were comparable to or on par with state-of-the-art approaches, hence it was tagged as a "generalist" model. Additionally, the researchers discovered that the 64 numbers output from the model can be directly explored using other AI methods, enabling the effective specification of desired drug properties and automatic exploration for molecules that meet the criteria through the use of AI.

The Technology

Molecule clustering from the ZINC database: Approximately 690 million molecules sourced from the ZINC database were split on their tranches and used for downstream training of the variational graph encoder.

Latent space surrogate model: Training of a specific machine learning model to predict the binding affinity of small molecules to a specific protein.

HPC resources: The project was allocated 500,000 CPU and 500,000 GPU hours from NSCC Singapore. These resources facilitated large-scale virtual screening, computational tasks and scoring of the test targets.

The Impact

Increased Speed: The surrogate models developed by the researchers using latent space information, not only excel in predicting properties like ADMET but also notably accelerate virtual screening in ligand-based drug design.

Increased Accuracy: Employing the surrogate support vector machine model alongside five scoring functions, the researchers predicted compound affinity for five target proteins. The results demonstrated comparable accuracy in ranking ability to specialized scoring functions, while reducing computational time by 1-2 orders of magnitude. This significantly minimizes the computational resources required to process the evaluations.

Prospects: The NTU team will be working towards applying this innovative methodology to conduct virtual screenings across extensive datasets within the molecule library.

"We utilized NSCC Singapore's HPC resources to train a series of surrogate models for predicting various properties on the latent space extracted by graph convolutional variational encoders. This approach significantly reduces time consumption while predicting multiple properties, providing a feasible solution to enhance CADD techniques."

Associate Professor Mu Yu Guang
School of Biological Sciences, NTU

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

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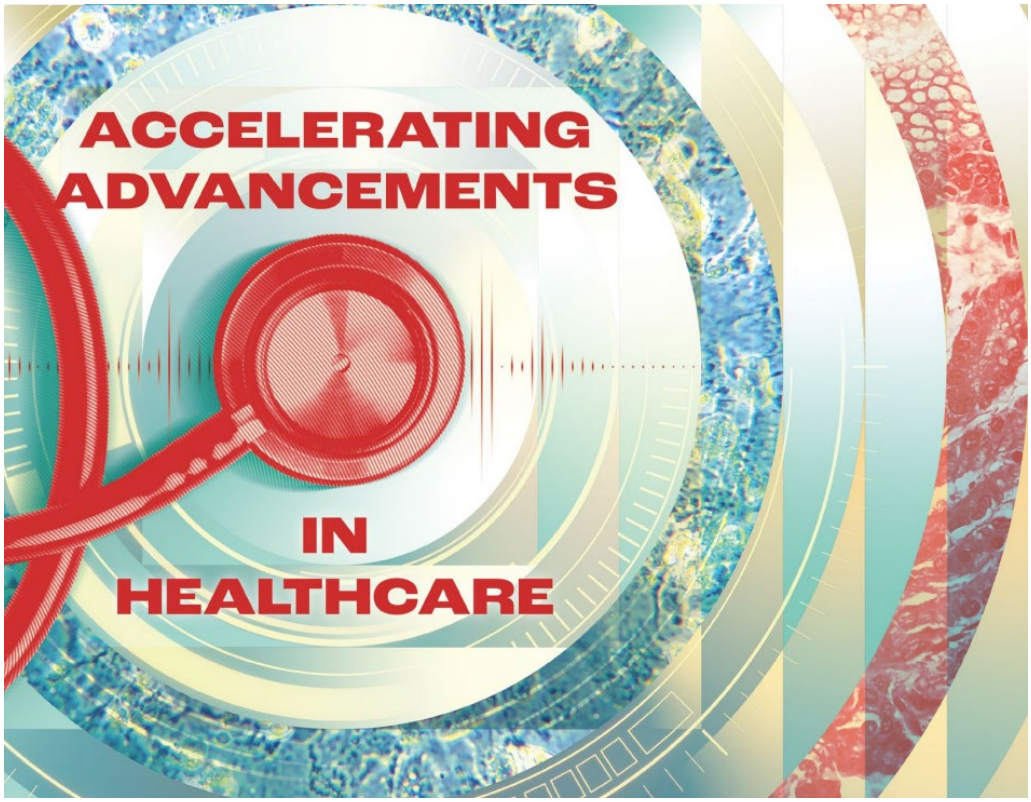
Accelerating Advancements in Healthcare

From disease diagnostics to drug development, healthcare applications are poised to receive a major boost from the combined power of AI and supercomputing.



For seasoned scientists, it often takes one look at an experimental cohort, whether through microscopic images or a series of electrical waves, to pick apart alterations from the norm. In the clinic, physicians can quickly combine information from a battery of tests to spot signs of disease and deliver an accurate diagnosis.

Their uncanny ability to distinguish healthy from sick can be attributed to years of practice, training, and extensive experience with analyzing biological samples. Inspired by the human mind's capacity for learning, artificial intelligence (AI) models are first trained on existing datasets so that they can recognize patterns and apply the same rules to new samples. This opens avenues for various healthcare applications, like detecting diseases early or making predictions about responses to treatment.

As straightforward as the process may sound, the training phase is typically a gargantuan task, especially considering the variability between individuals and their possible symptoms. HPC could be the key to unlocking this bottleneck, offering massive computing power that enables the processing of multitudes of clinical data in a short time span.

By synergizing HPC and AI resources, scientists and physicians can hope to make sense of complex biological phenomena more rapidly and accurately.

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THE LAST BYTE...

<SHARED CONTENT>

Shared articles and news from the HPC world.

NVIDIA Powers Japan's ABCI-Q Supercomputer for Quantum Research

NVIDIA announced that Japan's new ABCI-Q supercomputer — designed to advance the nation's quantum computing initiative.

The high-performance, scalable system is integrated with NVIDIA CUDA-Q, an open-source hybrid quantum computing platform with powerful simulation tools and capabilities to program hybrid quantum-classical systems. The supercomputer is powered by more than 2,000 NVIDIA H100 Tensor Core GPUs in 500+ nodes interconnected by NVIDIA Quantum-2 InfiniBand, the world's only fully offloadable, in-network computing platform.

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Credit: HPC Wire

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Jülich Supercomputing Centre Acquires New 5-Qubit Quantum System from IQM to Advance Research

The Jülich Supercomputing Centre (JSC) has purchased a 5-qubit quantum system from the German–Finnish manufacturer IQM Quantum Computers.

The IQM Spark quantum computer is scheduled to go into operation in July 2024 as part of Jülich's JUNIQ quantum computing infrastructure and will be connected to JSC's classical supercomputers. This gives researchers the opportunity to investigate how calculations on classical supercomputers can be accelerated by quantum computers.

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Credit: HPC Wire

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SDSC and University of Utah Pioneer $6M National Data Platform (NDP) for Equitable Scientific Research

A service ecosystem to make the access and use of scientific data open and equitable across a broad range of communities, including traditionally underrepresented researchers.

Led by SDSC and Utah's Scientific Computing and Imaging Institute (SCI), and in partnership with the EarthScope Consortium, the $6 million NDP pilot is funded by the U.S. National Science Foundation. The pilot will serve as a federated and extensible data and service ecosystem to foster innovation, discoveries and collaboration through the equitable access and use of science data and leveraging existing national cyberinfrastructure capabilities.

Credit: HPC Wire

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