National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

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CORPORATE NEWS

NSCC Steering Committee Chairman Honoured at the 2023 President's Science and Technology Award

The President's Science and Technology Awards (PSTA) is the highest honour conferred upon research scientists and engineers in Singapore whose work has resulted in significant scientific, technological, or economic benefits for the country.

NSCC Chairman Mr Quek Gim Pew (bottom left) with President Tharman Shanmugaratnam, DPM Mr Heng Swee Keat and the other PSTA winners at the Istana.

Interested to have your research published in NSCC's NewsBytes?

We are looking for ***guest writers / contributors*** to be part of our e-newsletters, which are sent out to a subscriber base of more than **7,500** monthly.

If you are interested in contributing content to our NewsBytes, drop us an email at **e-news@nscc.sg** and we'll be in touch with you!

The President's Science and Technology Medal was awarded to NSCC Steering Committee Chairman, Mr Quek Gim Pew, for his outstanding contributions in shaping Singapore's Research, Innovation, and Enterprise (RIE) ecosystem. These include developing local capabilities in science and technology, particularly in space technology, quantum engineering, artificial intelligence, and high-performance computing, and championing STEM-related initiatives to nurture the next-generation of scientists and engineers.

NSCC Chairman Mr Quek Gim Pew (third from left) with the other PSTA winners.

With his extensive experience in R&D management and capability development, Mr Quek continues to contribute to various national RIE programs. Being a consensus builder and a strong believer in collaboration with a strong network, he helps to harness synergy across organisations and across RIE domains to enhance the deliverables and outcomes in these programs. Mr Quek became the Chairman for the NSCC Steering Committee in January 2023 and has since been providing valuable guidance in shaping high performance computing to serve national needs and contribute to the continued growth of Singapore's R&D landscape.

Heartiest congratulations Chairman and thank you for your contributions in fostering innovation and research excellence in Singapore!

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Supercomputing Asia 2024 (SCA2024) is back from 19–22 February 2024!

Themed "Exascale Readiness in AI, HPC, and Quantum", the conference aims to promote a vibrant and shared high-performance computing and artificial intelligence ecosystem, for both the public and private sectors, in Asia.

For the first time in the event's history, SupercomputingAsia (SCA) will be held in Sydney, Australia! Co-organised by leading supercomputing centres of the region including those in Australia, Japan, Singapore, Thailand and Aotearoa New Zealand, SCA is an annual conference that encompasses an umbrella of notable supercomputing and allied events in Asia and beyond with the goal to promote a vibrant and shared high-performance computing (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.

The SCA2024 Conference will be held in Sydney from **19 – 22 February 2024** at the **International Convention Centre Sydney, Australia.**

Who you will hear from at SCA2024 in Sydney, Australia

Professor Rick Stevens is the Associate Laboratory Director of the Computing, Environment and Life Sciences Directorate at Argonne National Laboratory. He is also a Professor of Computer Science at the University of Chicago. At Argonne, he is leading the Laboratory's AI for Science initiative and works on advancing learning experiments with supercompute-scale AI. He is also part of a team that is launching Argonne's first exascale computer.

Professor Dieter Kranzlmüller is the Chairman of the board at the Leibniz Supercomputing Centre (LRZ). He is also a Professor at the Ludwig-Maximilians-Universitaet Munich (LMU). He will be sharing insights on the topic of 'More Compute with Less Energy: How HPC drives Energy Efficiency in Data' during the conference, which will feature the latest developments at LRZ towards more energy efficiency for high performance computing. These technologies can also be utilized in AI infrastructures.

Professor Francisco J. Doblas-Reyes is a ICREA Research Professor and director of the Earth Sciences Department of the Barcelona Supercomputing Centre. His presentation on 'A digital twin for climate adaptation' will illustrate how supercomputing and big data work together with domains from the natural and social sciences to develop a digital twin of the climate system. The digital twin provides interactive unprecedented information to decision makers who need to implement multi-sectoral strategies to adapt to a changing climate.

The Australian voice of Siri is set to be the SCA2024 emcee

Siri has guided millions of us throughout our day to day lives and now Karen Jacobsen will lead us through the conference as our esteemed emcee. With her distinct voice, Karen/Siri has become a symbol for technology's ability to help our everyday lives, making her a perfect fit for the SCA2024 conference.

REGISTRATION IS OPEN! Register now and secure your spot at this transformative gathering of experts, innovators, and thought leaders. Early bird discounts are available till 30 November 2023. Head over to www.sca24.sc-asia.org/ for more details on the conference.

REGISTER NOW!

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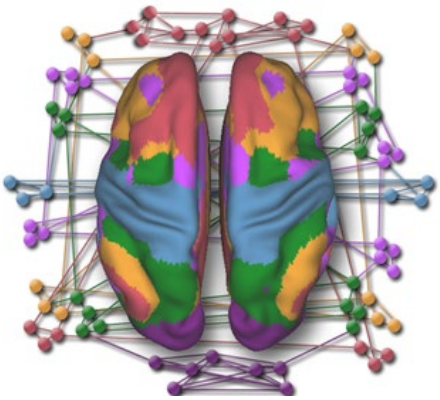
Gaining Deeper Insights into Mental Disorders through Brain Imaging and High-Performance Computing

Researchers from NUS are leveraging supercomputing to develop better strategies for the prevention and treatment to mitigate the impact of mental illness.



The human brain is a marvel of biological complexity, comprising a network of hundreds of billions of neurons. This intricate web of neural interactions orchestrates every facet of human behaviour and cognition, shaping our daily lives in profound ways. However, the prevalence of mental health concerns such as anxiety, depression, and dementia can cast a shadow over these lives, which therefore emphasises the urgency of gaining a deeper understanding of the brain's inner workings.

One promising avenue for progress lies in the exploration of brain biomarkers. To this end, the Computational Brain Imaging Group (CBIG), led by A/Prof Thomas Yeo at the Centre for Sleep & Cognition and the Department of Electrical & Computer Engineering at the National University of Singapore, embarked on a journey to unlock the secrets of the human brain with the aid of supercomputing resources.

The Research

In the last decade, medical imaging technologies, such as magnetic resonance imaging (MRI), have undergone remarkable advancements. These technologies empower researchers to acquire detailed information about both the structure and function of the brain. In parallel, collaborative efforts by researchers worldwide have amassed large-scale population brain-imaging data. This invaluable data resource holds hundreds of thousands of individual brain imaging scans. However, the sheer volume and complexity of the data necessitates the use of powerful computational capabilities and substantial storage capacity.

This is where the supercomputing resources provided by the National Supercomputing Centre (NSCC) Singapore proved indispensable. By utilising NSCC's high-performance computing (HPC) resources, CBIG researchers were equipped to process and analyse the vast troves of brain imaging data. Through such computational investigations, the team was able to uncover biologically relevant biomarkers of mental health, offering a direct link between changes in the brain and psychiatric symptoms. These biomarkers, in turn, fostered a deeper knowledge about the diverse nature of mental illnesses. Furthermore, advanced machine learning algorithms allowed for the development of personalised treatments, offering targeted brain stimulation to individuals suffering from mental disorders.

The Approach

Data Processing: Leveraging NSCC's HPC resources, immense volumes of raw MRI imaging data (often measuring in hundreds of terabytes) were processed. These pre-processed data repositories served as inputs for multiple subsequent investigations.

Machine Learning: Employing complex machine learning and deep learning tools, CBIG developed pipelines to map the structural and functional organisation of the brain. These pipelines enabled the prediction of how changes in brain structure and function relate to various pathologies, providing critical insights into mental health.

Artificial Intelligence (AI): Using AI techniques, specific brain regions can be identified as targets for transcranial magnetic stimulation. The development of such precise targeting methods promises a potential enhancement of treatment responses in patients.

The Impact

CBIG's research is a significant step towards the collective aspiration of exploring new frontiers in understanding mental disorders. The derived knowledge will pave the way for improved prevention and treatment strategies,

mitigating the impact of mental illness on society and families and ultimately providing a brighter future for those impacted by these conditions.

"This ambitious interdisciplinary effort between the Centre for Sleep & Cognition and the Department of Electrical & Computer Engineering at the National University of Singapore, united computer engineers, data scientists, and neuroscientists in their dedicated quest to unravel the intricacies of the human brain and its link to mental health. With the backing of NSCC's HPC resources, CBIG researchers are driven and well-equipped to unravel the mysteries of the human brain."

Dr. Sina Mansour L.
Postdoctoral researcher
Computational Brain Imaging Group,
Centre for Sleep & Cognition
National University of Singapore

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

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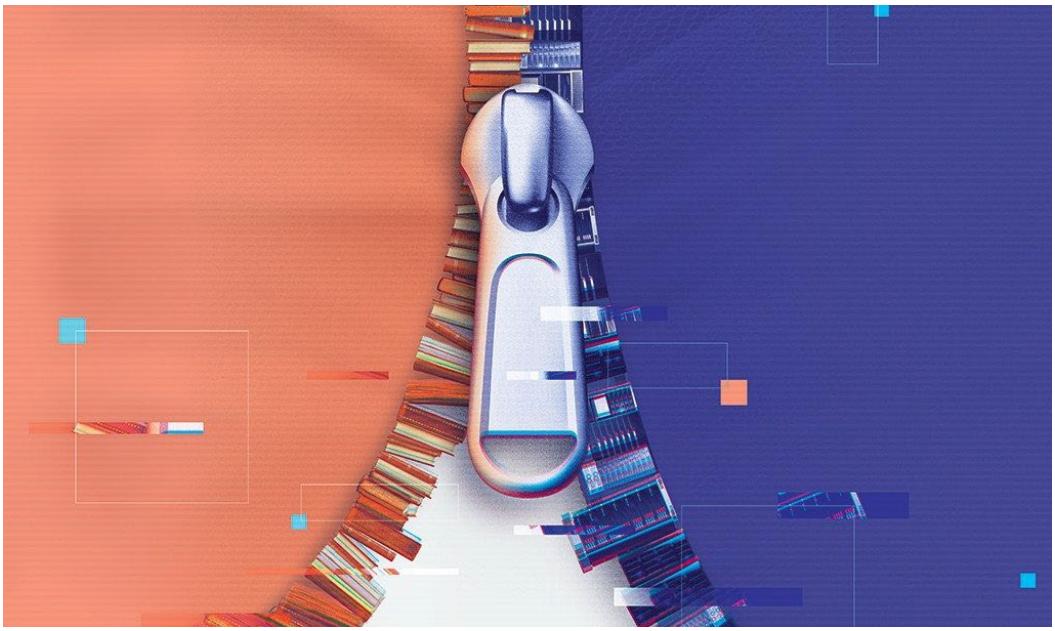
Closing the Gap Between HPC Tech and Education

The relationship between HPC technologies and its literacy is inextricably intertwined—each relying on the other to advance the field and unlock its full potential.



The last few decades of human history represent a tiny fraction of our time on Earth. However, the technological breakthroughs within this short period have transformed the human experience, from space probes venturing beyond our solar system in search of the universe's origin to the countless artificial intelligence (AI) innovations that enable more accurate medical diagnoses, new communication methods and efficient renewable energy systems.

But this breakneck speed of technological growth and implementation comes at a cost. Many are left behind when technology races ahead of society's ability to adapt to the new changes. This lag in learning poses a

challenge for policymaking and labor markets, and also perpetuates pre-existing inequalities, particularly in developing nations.

High-performance computing (HPC) is especially susceptible to this challenge. While its lightning-fast capabilities have empowered us to solve a myriad of scientific conundrums, maintaining this momentum is critical for the next generation of HPC scientists, experts and the public to keep HPC literacy on pace with its rapidly evolving landscape.

With recent achievements in exascale computing, many challenges and questions are emerging: What educational strategies are necessary to bridge the ever-expanding gap between progress in HPC technology and our understanding thereof? How can we ensure HPC literacy becomes a priority in our educational systems? And, finally, why is bridging this gap so crucial?

Discover how the collective efforts of the HPC community are slowly bridging the gap between HPC technology and education.

Head over to the July 2023 issue of NSCC's Supercomputing Asia Magazine to read the full article.

This article was first published in the print version of Supercomputing Asia, July 2023.
Credit: Mitchell Lim, Writer, Asian Scientist Magazine

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THE LAST BYTE...
<SHARED CONTENT>

Shared articles and news from the HPC world.

EuroHPC Amplifies European Research and Industry with JUPITER's Exascale Potential

JUPITER is set to achieve a significant milestone for European High Performance Computing (HPC) as the first European system capable of one exaflop, or one billion calculations per second.

This next-generation supercomputer marks a notable advancement in European technology and its unprecedented computing capacity will have a substantial impact on scientific progress across Europe. JUPITER's computing power will support the development of high-precision models of complex systems and artificial intelligence (AI) applications in science and industry alike. Applications will include training large language models in AI, simulations for developing functional materials, creating digital twins of the human heart or brain for medical purposes, and high-resolution simulations of climate that encompass the entire Earth system. Read more at HPC Wire here.

Credit: JSC

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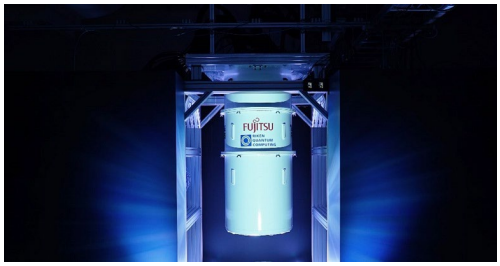
Fujitsu and Riken Develop Superconducting Quantum Computer at the RIKEN RQC-Fujitsu Collaboration Center, Paving the Way for Platform for Hybrid Quantum Computing

Platform leverages new 64 qubit superconducting quantum computer to accelerate R&D for quantum chemistry calculations and quantum financial algorithms.

Fujitsu and RIKEN announced the successful development of a new 64 qubit superconducting quantum computer at the RIKEN RQC-Fujitsu Collaboration Center. Accompanying this announcement, Fujitsu and RIKEN further revealed the launch of a platform for hybrid quantum computing, which combines the computing power of the newly developed 64 qubit superconducting quantum computer with one of the world's largest 40 qubit quantum computer simulators developed by Fujitsu. Read more at Fujitsu's website here.



Credit: Fujitsu

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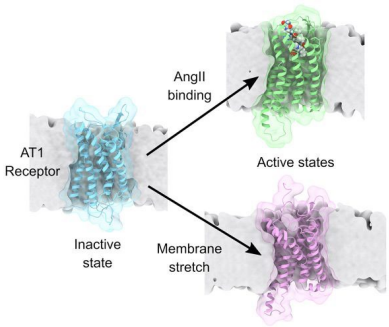
Computer Simulations Reveal New Information About Key Protein's Role in Treatment of Heart, Kidney and Other Diseases

Researchers from Oregon State University and the University of Vermont used Expanse at the San Diego Supercomputer Center (SDSC) at UC San Diego and Anton 2 at the Pittsburgh Supercomputing Center (PSC) to show the effect of physical stimuli on the structural properties of the Angiotensin II Type 1 (AT1) receptor.

If you think of the human body as consisting of a team of organs that plays against a defense of diseases, then the AT1 receptor is a key player — especially when it comes to attacks on the heart and kidneys. The AT1 receptor is heavily studied within the context of activation/inactivation by drugs, but the team's newly run simulations have revealed that the protein can also be directly activated by mechanical forces through stimuli such as external pressure or shear acting on the surface of the cells. These findings have been published in Nature Communications. Read more at HPC Wire here.



Credit: Juan Vanegas, Oregon State University.

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