National Supercomputing Centre (NSCC) Singapore e-newsletter

NEWSBYTES

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ASPIRE2A

In this issue…

CORPORATE NEWS

Congratulations to Professor Torsten Hoefler on winning the 2024 Max Planck-Humboldt Medal

Prof Hoefler is the Head of the Scalable Parallel Computing Laboratory at the Department of Computer Science, ETH Zurich, Switzerland.

Our heartiest congratulations to Prof Hoefler, NSCC Singapore's Steering Committee member, for being awarded the 2024 Max Planck-Humboldt Medal for his work in increasing the efficiency of algorithms, particularly for applications in high performance computing and artificial intelligence. This is only the second time a computer scientist has received this award.

Max Planck-Humboldt Research Award and Max Planck-Humboldt Medal are the most prestigious German awards presented to internationally outstanding mid-career scientists. Organised jointly by the Max Planck Society and the Alexander von Humboldt Foundation, the award is funded by the German Federal Ministry of Education and Research, the award focuses on individuals who stand out for their promising future potential and innovative research projects across all scientific fields.

This year, the Max Planck Society and the Alexander von Humboldt Foundation are honouring outstanding achievements in the use of algorithms in mathematics, microscopy and climate research. Prof Hoefler's work to improve scientific simulations benefits many research fields such as quantum simulations and global climate predictions.

Congratulations again Prof Hoefler and we look forward to his continued support and contributions to HPC in Singapore.

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NSCC Singapore, IHPC and CSC Finland Foster Deeper Ties in HPC and Research

NSCC Singapore and CSC Finland have been strong HPC centre collaborators since 2020.

NSCC Singapore together with the Agency for Science, Technology and Research's (A*STAR) Institute of High Performance Computing (IHPC) hosted a delegation from CSC Finland on 17 September 2024 in Singapore for talks to strengthen cooperation on a number of areas including HPC-quantum, AI, future systems strategies and plans, green computing and digital twins research.

Led by Dr Kimmo Koski, Managing Director of CSC Finland, the delegation of Mr Damien Lecarpentier, Director of International Collaborations and Partnerships and Dr Mari Walls, Director of Research Organization Collaboration and Academic Partnerships participated in the trilateral meeting aimed at deepening centre-to-centre cooperation, HPC-related research activities, and HPC-Quantum integration efforts.

The close ties between NSCC Singapore and CSC have been fostered through numerous engagements and initiatives, including touch points in the Alliance of Supercomputing Centres (ASC) network and facilitating access to LUMI's GPU resources for Singaporean researchers.

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Thank you!

LET'S BEGIN

Trilateral meeting between CSC Finland, NSCC Singapore and A*STAR's IHPC

In the evening, representatives from government, research institutions, and companies within Singapore's HPC ecosystem, as well as Finland, attended a seminar event hosted by the Finland Embassy in Singapore. Themed "Advanced Computing and AI Infrastructures Supporting Research and Innovation in a Changing Global, Environmental and Socio-Economic Context", the seminar aimed to encourage closer collaboration between the Singaporean and Finnish HPC and research communities.

Dr Terence Hung introducing the key strategies of NSCC Singapore.

Panel session on the critical role of advanced computing in research, the economy, and society.

The seminar included introduction and updates from CSC and NSCC Singapore as well as a Keynote by Professor Tuuli Toivonen from the University of Helsinki, focusing on the role of advanced computing infrastructures in sustainable urban development and a human-geographic approach to sustainable use of space. The event concluded with a panel session on the critical role of advanced computing in research, the economy, and society.

CSC Finland hosts LUMI, the fastest supercomputer in Europe, ranked fifth globally and renowned as one of the greenest supercomputers in the world. NSCC Singapore have much to learn from them and look forward to future collaborations and the continued exchange of knowledge and expertise.

September Workshops Roundup

NSCC Singapore organised two workshops in September to engage the HPC community in Singapore.

The workshops, attended by 56 users, were designed for participants with varying levels of HPC experience to learn more about using the ASPIRE 2A system.

Attendees of the ASPIRE 2A Introductory Workshop

The introductory workshop for ASPIRE 2A provided new users with information on the overall setup of the ASPIRE 2A system. With a hands-on session, participants experienced the system onboarding process and learned how to submit job requests to the system.

Advanced users at the ASPIRE 2A Optimisation Techniques Workshop

For more experienced users. NSCC Singapore organised the ASPIRE 2A Advanced Workshop Optimisation Techniques which provided a high-level overview of key concepts for enhancing the

performance of compute-intensive applications. The workshop covered information on the underlying hardware, system software, and available performance optimisation techniques, with practical demonstrations through hand-on tasks.

NSCC Singapore regularly holds training and engagement workshops for users and the HPC community in Singapore. Keep an eye on our events page to stay updated on upcoming user workshops.

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Leveraging Supercomputing Resources for Net-Zero Research & Development

Researchers at the National University of Singapore (NUS) are exploring a high-fidelity numerical simulation of ammonia combustion to investigate the use of ammonia as a direct combustion fuel.
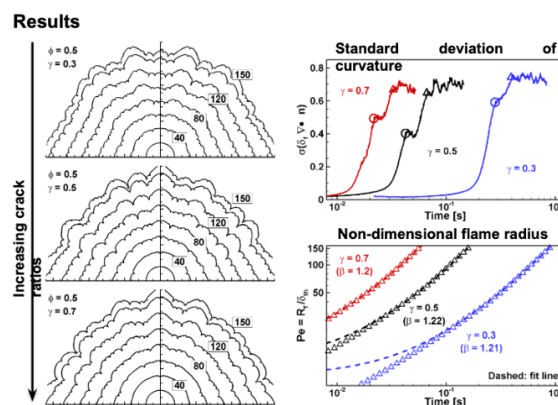
On 25 October 2022, Singapore announced its commitment to raise its national climate target, aiming for net-zero emissions by 2050 as part of its Long-Term Low-Emissions Development Strategy. Given the limited resources in Singapore, research into decarbonisation is essential to identify long-term solutions for achieving this goal.

A group of researchers from NUS is exploring the use of ammonia as an alternate energy source. This research is supported by Singapore's National Research Foundation (NRF), and A*STAR under the Directed Hydrogen Programme (DHP) in Low-Carbon Energy Research (LCER) Programme Phase 2.

The Research

Ammonia is an attractive alternative to fuel as it is carbon-free and has superior energy density. However, despite its significant decarbonization potential, its low reactivity impedes its widespread use as a direct

combustion fuel. Hence, the researchers from NUS are conducting high-fidelity numerical simulations to model the behaviour of ammonia flame under various conditions. These simulations will provide crucial insights to accelerate Singapore's transition to a low-carbon energy future.

The Technology

Flame modeling using OpenFOAM: Large-scale reactive flow simulations were conducted with OpenFOAM based solvers. This allows a detailed quantification of the combustion process including the formation of intermediate species and the interactions between fluid dynamics and chemical reactions across various time and length scales.

Understanding ammonia flame chemistry using AI techniques: The chemical kinetic mechanism for oxidation of ammonia was optimized with a deep reinforcement learning-based approach. The global deterministic search of reaction parameters was decomposed as a sequential local probabilistic optimization problem to speed up convergence and avoid the local optima. The optimized mechanism has demonstrated excellent agreements with experimental data.

GPU-Accelerated simulations for large scale ammonia gas turbine combustion: The adoption of CPU-GPU heterogeneous computing methods significantly accelerated the numerical solutions of ammonia combustion processes within gas turbines featuring billion-level grids. This high-efficiency computational approach enables rapid iteration in the design and optimization of ammonia gas turbines.

Benefits of HPC

- Exceptional scalability enables a wide range of computations from small-scale kinetic studies to large-scale direct numerical simulations.
- Powerful and massive computational nodes facilitating direct numerical simulation with over 1 million grids and a resolution of several micrometres.
- Accommodate large-scale simulations leveraging hybrid CPU-GPU platforms.
- Conduct direct numerical simulations with over 20 million grid cells and a grid resolution of several micrometres.

The Impact

By providing deeper insights into the combustion process, this research can facilitate the development of more efficient and cleaner ammonia-based power generation technologies in Singapore.

"Using HPC, we are able to capture intricate details of the combustion process, including the formation of intermediate species and the complex interplay between fluid dynamics and chemical reactions across multiple scales"

Zhang Huang Wei
Assistant Professor, Thermal Systems
NUS

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Digital Twin Consortium incorporates digital engineering methodologies

The Digital Twin Consortium (DTC) has announced a significant expansion of its scope to include the development and execution of advanced digital engineering methodologies throughout the digital twin lifecycle.

This progression builds upon the consortium's expertise in digital twin methodology and enabling technology. It expands the DTC's focus to cover the key domains and disciplines throughout the digital engineering ecosystem, including Model-Based System Engineering (MBSE), digital thread, and related strategies.

Credit: IOT Insider

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San Diego Supercomputer Centre Partners with CENIC to Boost AI Education Across Public Schools in California

The initiative reflects a deep-seated commitment to fostering the next generation of academics and thought leaders in the burgeoning field of AI.

In a significant move to bolster AI education across California, the San Diego Supercomputer Center (SDSC) at UC San Diego and the Corporation for Education Network Initiatives in California (CENIC) have joined forces to launch the CENIC AI Resource (CENIC AIR), a pivotal program aimed at weaving artificial intelligence and machine learning into the fabric of public education, encompassing K-12, community colleges, and university campuses.

Credits: Hoodline

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Switzerland unveils new supercomputer 'Alps,' already ranked sixth in the world

Switzerland has unveiled its new supercomputer "Alps," one of the most powerful machines of its kind in the world.

In the global supercomputer rankings published by Top 500 in June, Alps came in at number six behind electronic brains from the United States and Japan. The focus of "Alps" will be on scientific research, solving complex calculations in the fields of medicine, space research, and climatology.

Credit: Euro News

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