

The image shows a scenic landscape with a blue lake, mountains, and a town. Overlaid on the left is a dark blue vertical banner with the text 'iCAS 2024' in large white letters, and 'International Computing in the Atmospheric Sciences Symposium' in smaller white letters below it.

iCAS 2024

International Computing
in the Atmospheric
Sciences Symposium

iCAS 2024 Presentations

Schedule of presentations still to be determined.

Climate-resilient snowpack estimation with machine learning

Marianne Cowherd, University of California, Berkeley

As we progress into the 21st Century, warmer temperatures and shifting atmospheric circulation patterns are expected to lead to notable alterations in the timing, quantity, and spatial distribution of hydrological processes. This change affects water security and infrastructure and is also expected to negatively impact our ability to measure these same effects. In other words, climate change is detrimental to our ability to observe climate change. In this project, we use snowpack measurement networks in the United States as a case for exploring a) how network-based in situ measurements will change in representativity in the future and b) how we can use machine learning and gridded meteorological products to remedy the decline in sensor network usefulness. To do this, we investigate the performance of the Snow Telemetry network under a suite of dynamically downscaled CMIP6 models. We then use the WRF data to develop artificial intelligence-based models of snow distribution under future climates. Our primary focus is to discern the relative significance of model complexity and observational data in constraining snowpack estimates, especially when applied to downscaled climate models over the WUS. Our findings indicate that sufficiently intricate data-driven models are likely to sustain the accuracy of snowfall and snowpack estimates even under no-analog future climate scenarios. Additionally, these models can handle novel spatial and temporal correlations between predictors of snowfall and end-of-winter snowpack, allowing for reliable estimation in the face of unprecedented atmospheric conditions. By employing nimble artificial intelligence-based models, adept at incorporating partial and multi-modal snowpack information, we can effectively tackle these challenges. This approach ensures the resilience of end-of-winter snowpack estimation in the WUS, even as the climate evolves into uncharted territory. Lastly, we discuss strategies for similar implementations in other networks of environmental sensors; sensor networks and field measurements tend to follow political boundaries due to funding structures but hydrology does not recognize the same borders.

Towards accelerated computing in a Python framework

Anurag Dipankar, ETH Zürich

The modern exascale computing systems have given the climate and weather modeling community an opportunity for a step change in the simulation capabilities. One expects a resolution high enough to resolve the key atmospheric processes provided the machine is properly utilized. However, this is a non-trivial task. Given the complexities at various levels from the hardware to the software (model), a close collaboration between the computer scientists, software engineers, and domain experts is required to redesign the conventional model in a way that it fully utilizes the exascale capabilities while keeping the model easy to use. In EXCLAIM, we are developing a python-based framework that allows users to write code, debug, run the model, and visualize from within the framework. Computations are largely handled by the embedded DSL, GT4Py, whereas the driver code is envisioned to be in python. This approach decouples the hardware specific implementation choices made for efficiency, from the functional choices by the domain experts. The framework is expected to allow for interoperability with software components developed in other programming languages or other frameworks. The talk will give an overview of the progress we have made in the last years and challenges we have encountered.

Efficient resource usage for large-scale earth system model simulations on heterogeneous hardware

Jan Frederik Engels and Claudia Frauen, German Climate Computing Center (DKRZ)

On current exascale HPC systems most people only focus on GPUs, but all GPU nodes also contain CPUs, which are rarely utilized. Given this and the fact that not all codes are equally suited for running on GPUs we want to discuss approaches that go beyond the strategy of just porting everything to GPUs. Modern earth system models (ESMs) are becoming more complex by integrating more components. The different components of an ESM also have different computational characteristics, with some making good use of throughput devices like GPUs, while others, for example, only solve 2D problems, which have very low computational intensity. An example of such an ESM is the ICON model, which is used for km-scale simulations on various different hardware architectures. The atmospheric component of ICON is successfully running on GPUs but other components like the ocean model have not or only partially been ported to GPUs and might also not benefit to the same degree from running on GPUs. Thus, in this proposed talk we will discuss approaches to efficiently perform km-scale earth system simulations by optimally utilizing the available hardware resources. As a computing center, we are also interested in reducing energy consumption of simulations. Beyond savings by reducing run time as described above, we will also discuss strategies to optimise energy consumption for the full machine given our standard workload. As an outlook we also briefly touch on the idea of running every ESM component on the architecture suited best to its computational profile."

Rapid emergence and applications of AI/ML at NCI in the Earth System Sciences

Ben Evans, NCI Australia

Artificial Intelligence and Machine Learning (AI/ML) has been rapidly showing its potential as a new computation approach that either replaces or augments traditional modelling and data analysis. However, despite its power, these areas are not yet fully adopted and pervasive within the earth system

sciences research community or in production services. In this talk, I will describe our focus and progress in applying AI/ML, and new emerging areas that we are exploring.

Weather Prediction with ICON on GPUs

Marek Jacob, German Weather Service (DWD)

Graphics Processing Units (GPUs) have become integral components in the architecture of numerous world-leading supercomputers, offering energy efficient and powerful computational capabilities. The incorporation of GPUs, however, necessitates the adaptation of existing codes. In a collaborative international effort, the open-source weather prediction model ICON has been successfully ported to GPUs. MeteoSwiss scheduled the deployment of the ICON-GPU as its primary numerical weather prediction (NWP) system in mid-2024. Similarly, the German Weather Service (DWD) is gearing up for potential future GPU-based systems. Our presentation delves into the porting strategy of ICON using OpenACC compiler directives, highlighting recent successful ports essential for operational production. We also share insights into performance and experiences gained from deploying ICON on GPUs, as well as on recent NEC SX-Aurora Tsubasa Vector Engines installed as part of DWD's latest expansion stage in fall 2023. In addition to the porting of the classical ICON, the DWD applies GPU technology in artificial intelligence applications. Among various specialized applications, the DWD is actively involved in enhancing its NWP capabilities through the development of the "AICON" system. AICON utilizes machine learning and AI technologies to fully emulate the ICON-NWP model. This presentation introduces AICON-Graph, a graph neural network implementation within the AICON framework. AICON-Graph is a collaborative effort driven forward by the DWD and its partners.

From Super-Resolution to Downscaling - An Efficient Image-Inpainting Deep Neural Network for High Resolution Climate Models

Christopher Kadow, German Climate Computing Center (DKRZ)

Artificial Intelligence (AI) and Machine Learning (ML) are increasingly becoming integral components in the advancement of Earth System Models (ESMs), offering novel methodologies to address complex challenges in climate science. The integration of these technologies in and around climate modeling processes, particularly at the German Climate Computing Center (DKRZ), demonstrates their potential to enhance, complement, and in some cases revolutionize traditional modeling approaches. AI's role in improving the resolution of climate models through advanced downscaling techniques demonstrates its ability to refine model simulations. Using large datasets from initiatives such as CMIP6, AI techniques such as transfer learning and image inpainting are used not only to downscale model outputs, but also to reconstruct and enhance observational datasets, improving the quality and utility of climate data for research. We further investigate the application of our method to downscale quantities predicted by a numerical ocean model (ICON-O) to improve computational times. We focus on the ability of the model to predict eddies from low resolution data. Coupling ML models with ESMs such as ICON illustrates the ability of ML algorithms to emulate complex subgrid-scale processes such as the high-resolution ocean processes. By training on detailed simulations, these ML models can serve as cost-effective proxies, ensuring simulation stability and result plausibility through rigorous validation and benchmarking. The technical challenges of integrating ML models developed in high-level programming languages with ESMs written primarily in Fortran will be addressed through innovative coupling strategies, underscoring the technical feasibility and physical consistency of such hybrid approaches. The concept of Neural

Earth System Modeling further illustrates the transformative potential of AI/ML in climate science. By reimagining the integration of deep neural networks with ESMS, this approach aims to create self-validating, interpretable hybrid models that could significantly advance our understanding of Earth systems and potentially redefine the future of climate modeling.

Supporting an Evolving HPC Community at NCAR

Rory Kelly, NSF NCAR

"The National Center for Atmospheric Research (NCAR) has a long and rich history with high-performance computing (HPC), having been a pivotal early adopter and having procured over 40 HPC machines since the early 1960s. Owing to this extensive history, the majority of modeling codes at NCAR have been developed for CPU architectures, although our CPU modeling community has navigated substantial technological transitions through scalar, SIMD, wide-vector, shared-memory, and distributed-memory cluster architectures. The industry's increasing adoption of GPU computing, further propelled by advancements in artificial intelligence and machine learning, is leading to another technological shift for our user community. Our latest HPC procurement, NWSC-3, was the first to mandate inclusion of a GPU-capable compute partition, accounting for a significant fraction of the machine's overall computational capacity. This presentation will cover the development of the NWSC-3 benchmark suite, aimed at procuring a machine meeting several key objectives: supporting existing CPU-based modeling workflows, encouraging our developer community to embrace code modernization for GPU architectures, and providing a substantial compute resource for our emerging GPU computing community, capable of supporting production science on the GPU partition. We will discuss the benchmarks and metrics, including the creation of the Cheyenne Sustained Equivalent Performance (CSEP) metric, used to compare the aggregate performance of a machine with both CPU and GPU-based nodes to Cheyenne, our previous CPU-based HPC cluster. We will review the procurement outcomes and look at the resultant machine, Derecho, to evaluate how well the benchmark suite achieved its goals. Additionally, we'll examine usage patterns on Derecho's CPU and GPU partitions during the first year of production, highlighting community adoption patterns, efforts to support code modernization and GPU readiness, and potential implications for a Derecho follow-on machine.

All data everywhere all at once

Richard Lawrence, The Met Office

The Met Office plans a fundamental shift in how it will curate and share data. This presentation will outline how the Met Office will change its focus to making data available followed by ensuring it is as accurate, consistent and useful as possible. Utilising the partnerships we have with the cloud hyperscalers and UK and international weather and climate agencies we look to define and share plans for increasing the reach of our weather and climate data. The presentation will close with how we see data architecture evolving in the coming years and how it will adapt to ML data driven models upending the traditional paradigms of data transfer and data proximate computation.

Challenges and Opportunities Represented by Computational Modeling and AI/ML Workloads

Tsengdar Lee, Laura Carriere, Dan Duffy, NASA

We have seen unprecedented changes in computing architecture and resources in recent years. First, managers at high-end computing centers are facing significant challenges but these also present new opportunities for scientific research. We need to support the traditional CPU based workloads, provide the resources and manpower for transitioning the legacy model codes to CPU-GPU based heterogeneous architectures, while at the same time there are more and more users demanding GPU-based systems for AI/ML workloads. These are just the technological challenges and opportunities. Programmatically, NASA Earth science has launched an Earth Science to Action (ES2A) initiative that would dramatically change the focus of our modeling program and the use of analytical tools. In this talk, we will go over the recent activities at NASA with the emphasis on the integration of modeling, on-prem computing, cloud computing, and the software stack. Join us as we present our vision toward an integrated ES2A environment.

Pivoting to NSF NCAR's Next Generation Geoscience Data Exchange, Integrated Research Data Commons

Doug Schuster, NSF NCAR

This presentation will highlight NSF NCAR's plans to develop and deploy the Next Generation Geoscience Data Exchange, Integrated Research Data Commons (NG-GDEX). NG-GEX will provide data science infrastructure that can overcome the research challenges described above and position NSF NCAR to bolster its integration with NSF's National Discovery Cloud for Climate and be well positioned to support the National Artificial Intelligence Research Pilot Program, by connecting community model generated products with datasets produced through NSF's Facilities for Atmospheric Research and Education program. It is envisioned that NG-GDEX will democratize computational and data-driven research approaches, promote open science and broaden participation—from experienced scientists to early career researchers—through community-driven data sharing, with a focus on promoting best practices for curation of digital assets (FAIR and CARE principles, Analysis Ready (AR) and Artificial Intelligence (AI) ready data structures), and by providing simplified access to analysis-oriented resources and services through web based applications, including computational notebooks.

Future of Canada's Hydrometeorological Supercomputing Service

Charles Schwartz, Shared Services Canada

The trend in acquiring and operating larger and larger supercomputing infrastructure to support national hydrometeorological programs has been fairly consistent over the last several decades. This trend has reached its limit and is no longer sustainable given modern realities by power constraints, Moore's Law slowdown and financial considerations. Disruptive approaches have arrived that bring with them new opportunities – AI, machine learning, cloud – and new costs and considerations. We have a shared duty to help scientists model climate, while reducing the environmental impact it causes. One factor is the growing importance of data – its use in AI and machine learning is essential but storing data is costly. Migrating from one platform to another is also rapidly becoming unthinkable complex – Canada will have more than 1 Exabyte of meteorological data stored by 2025. Technologies to support

AI and machine learning workloads are expensive both financially and ecologically. What does this mean for the future of hydrometeorological supercomputing systems? Canada's current supercomputing infrastructure for hydrometeorological services is sunsetting soon and we are preparing for the future. What should the next generation systems look like? We will discuss alternative approaches that we deemed unthinkable only a few years ago: heterogeneity of computing platforms and on-premises and cloud systems; the divergence of a forward-looking R&D environment that is not aligned with the existing operational systems to fork development of new technologies and approaches; and re-thinking our data management practices.

DART: 20 Years of Collaboration for Advancing Earth System Science

Marlee Smith, NSF NCAR

The Data Assimilation Research Testbed (DART) is an open-source software facility for ensemble data assimilation that has been at the cutting edge for over 20 years, supporting a diverse community of Earth system scientists. DA combines information from numerical forecasts with measurements of the Earth system to enhance the value of both. Applications include generating initial conditions for forecasts and predictability studies, diagnosing model error and bias, and assessing the value of existing and planned observations. This presentation will detail several impactful collaborations and further explore the capabilities and innovations in the DART software that enable, support, and welcome collaborations in the context of ever-evolving technologies, software practices, and science. Concluding discussion will focus on the importance of providing student and early-career opportunities and mentoring in research software engineering, especially due to its interdisciplinary nature at the convergence of software and science. DART interfaces with many Earth system models and observations, as diverse as ocean biogeochemistry and space weather. The software implements uniquely powerful DA algorithms like novel methods for pollutants, sea ice concentration, and soil moisture. We deploy flexible, robust tools to handle ever higher-resolution models, increasingly large numbers of ensemble members, and soaring numbers of observations. DART is also crucial to the application of innovative artificial intelligence approaches to forecasting by generating reanalysis datasets. Focusing on accessibility to support a diverse user community, our software is carefully engineered to run efficiently on systems ranging from laptops to supercomputers and be compatible with most compilers. DART facilitates adding new models and observation types and deploying state-of-the-art DA systems. We strive for the democratization of Earth system science by working with contributors ranging from high school students to renowned researchers, with institutions including the Euro-Mediterranean Centre for Climate Change, KAUST, the University of Hamburg, and the University of Vienna.

GT4Py: A Python Framework for the Development of High-Performance Weather and Climate Applications

Hannes Vogt, CSCS (ETH Zurich)

GT4Py is a Python framework for weather and climate applications simplifying the development and maintenance of high-performance codes in prototyping and production environments. GT4Py separates model development from hardware architecture dependent optimizations, instead of intermixing both together in source code, as regularly done in lower-level languages like Fortran, C, or C+. Domain scientists focus solely on numerical modeling using a declarative embedded domain

specific language supporting common computational patterns of dynamical cores and physical parametrizations. An optimizing toolchain then transforms this high-level representation into a finely-tuned implementation for the target hardware architecture. This separation of concerns allows performance engineers to implement new optimizations or support new hardware architectures without requiring changes to the application, increasing productivity for domain scientists and performance engineers alike. We will present recent developments in the project: support for interactive debugging, new compiler passes that optimize data-movement, an improved frontend with support for high-level constructs and new backends connecting GT4Py with existing HPC frameworks (DaCe, Jax).

Asynchronous IO and optimized data compression workflow

Haiying Xu, NSF NCAR

Object storage technologies are emerging because such storage offers easier access and unlimited scaling, to petabytes and beyond. These features allow object storage can meet the necessities of the large volume data of scientific computing. However, if scientists want to incorporate object store data format in their simulations, they need to put a lot of effort into modifying their simulation software. Our workflow can let simulations generate object store data or traditional file system data without significant changes. Also, using this workflow, we introduce a compression workflow to compress petabyte-scale scientific data in the fastest way by various compressors with slow or fast compression speed. We tested this workflow on the MURaM simulation model and achieved very good performance results and scalability.