

ART@SC24 Agenda Nov. 15-16

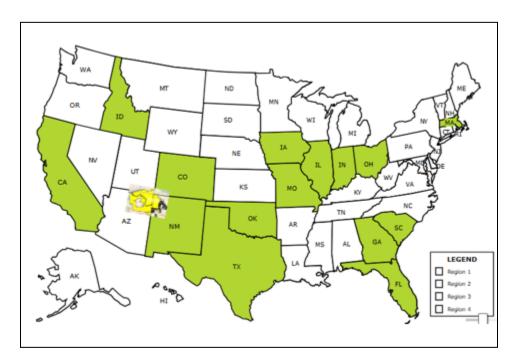
Friday, Nov. 15: Jet Lag Day: International delegates will visit Georgia Tech. Details shared separately with invited attendees.

Saturday, Nov. 16, 2024 9:00 a.m. to 3:45 p.m. Workshop at World Congress Convention Center, Room B206.

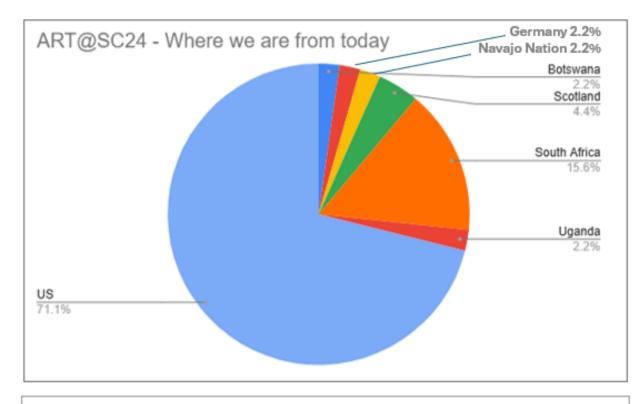
9:00 a.m. Check-in, welcome and orientation. Elizabeth Leake, Texas A&M University and STEM-Trek Nonprofit. Our sixth SC co-workshop, ART@SC24, will explore a variety of topics related to high-performance computing (HPC) and artificial intelligence (AI).

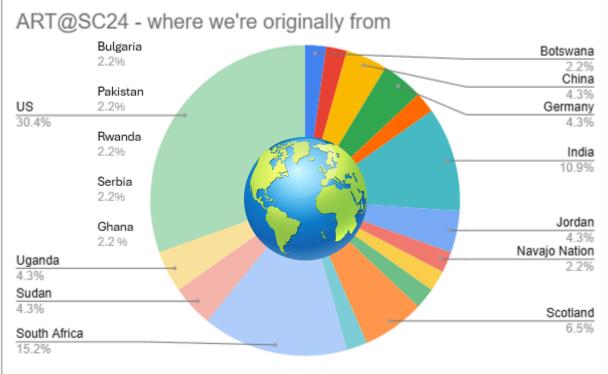


9:15-10:00: Introductions. This is our biggest cohort ever! This year, we're expanding the global footprint of innovation and discovery with 41 attendees representing 16 nations and 13 US states. Political geography aside, we're all from the same tribe - the one with a passion for solving global grand challenges with science, technology, education and collaborations!



Where is everyone from?





10-10:45 a.m. Training Panel. Facilitated by Elizabeth Leake, Texas A&M/STEM-Trek Nonprofit



From left: <u>Mary Thomas</u> (San Diego Supercomputing Center, SDSC), <u>Bryan Johnston</u> (Centre for High-Performance Computing, CHPC), <u>Linda Akli</u> and <u>Lena Duplechin-Seymour</u> (Texas Advanced Computing Center, TACC). Each center will present a 10-minute flash talk about their training programs, followed by a 15-minute Q&A session. Seed questions: How is your center preparing the workforce for Al? Do you conduct K-12 outreach; how do you explain complex concepts to children? Do you share your training materials; where? What is your biggest hurdle when it comes to provisioning Tribal Colleges and Universities, and other Minority-Serving Institutions in remote regions? What are you doing to prepare teachers?

10:45-11:00 a.m. - Break

11:00-11:30 a.m. - Hakizumwami Birali Runesha (UChicago Global).



As associate vice president for research computing and director of the Research Computing Center, Dr. Hakizumwami Birali Runesha provides leadership and vision for advancing all aspects of research computing strategies at the University. He is responsible for the design, configuration, and administration of the centrally managed high-performance computing (HPC) systems and related services across the University of Chicago. In addition, he provides access to advanced technical expertise, user support, advice, and training to the research community.

11:30 a.m. -12:00 noon - Spencer Bryngelson (Georgia Tech).



Spencer Bryngelson is an assistant professor in the School of Computational Science and Engineering at Georgia Tech. Prior to GT, he worked at California Institute of Technology, MIT, and the Center for Exascale Simulation of Plasma Coupled Combustion. Bryngelson received his Ph.D. in Theoretical and Applied Mechanics from University of Illinois at Urbana-Champaign and B.S. degrees in Mechanical Engineering and Mathematics from the University of Michigan. His research group, Computational Physics @ Georgia Tech (https://comp-physics.group),

develops models, fast numerics, and scalable algorithms for solving problems in health, defense, and energy.

Dr. Bryngelson's presentation title/abstract: Competitive neural networks enable learning accurate PDE surrogates.

Neural networks can be trained to solve partial differential equations (PDEs) by using the PDE residual as the loss function. This strategy is called "physics-informed neural networks" (PINNs), but it currently cannot produce high-accuracy solutions, typically attaining about 0.1% relative error. We present an adversarial approach that overcomes this limitation, which we call competitive PINNs (CPINNs). CPINNs train a discriminator that is rewarded for predicting mistakes the PINN makes. The discriminator and PINN participate in a zero-sum game with the exact PDE solution as an optimal strategy. This approach avoids squaring the large condition numbers of PDE discretizations, which is the likely reason for failures of previous attempts to decrease PINN errors even on benign differential equations. Numerical experiments on a Poisson problem show that CPINNs achieve errors four orders of magnitude smaller than the best-performing PINN. We observe relative errors on the order of single-precision accuracy, consistently decreasing with each epoch. To our knowledge, this is the first time this level of accuracy and convergence behavior has been achieved.

Lunch 12:00-12:45 p.m. In the room, or somewhere in the center, TBD.

12:45-1:15 p.m. - Report from Jetlag day @Ga Tech: Bryan Johnston (CHPC South Africa), John Poole (Clemson U), Brian Kyanjo (Georgia Tech postdoctoral scholar; PhD Boise State University).



1:15-1:45 p.m - Marumo "Happy" Sithole, CSIR (NICIS/CHPC, South Africa). Dr. Sithole is the director of the Centre for High Performance Computing at the CSIR. He completed his PhD in materials science, focusing on electronic and atomistic simulation of iron sulfides, at the University of Limpopo. He has applied high-performance computing to solve problems in mining industries and nuclear power plant designs. Sithole also sits on several international steering committees of high-performance computing meetings. He is the Chairperson of the ICT Committee of the National Library Board.Dr. Sithole will tell us about

CHPC's new system (how it will excel with AI workflows in mining, climate, and other domains that South Africa dominates, etc.).



1:45-2:15 p.m. Vasilka Chergarova is an IT Assistant Director at the Center for Internet Augmented Research and Assessment (CIARA) at Florida International University (FIU). She holds a Ph.D. in Information Systems with a focus on security from Nova Southeastern University, where she researched the factors influencing Software Defined Networking (SDN) adoption by research and educational networks. Her career at FIU includes roles as Research Coordinator II and System Administrator at CIARA, where she contributed to NSF grant projects, outreach programs, and academic research in cyberinfrastructure and

SDN. She has international research experience from her collaboration with the UNESP Center for Scientific Computing in Brazil. Chergarova is also involved in mentoring and is an active member of professional societies such as the Golden Key International Honour Society and the Society for Women in Engineering.

Dr. Chergarova's presentation abstract:

The rapid evolution of artificial intelligence (AI) and machine learning (ML) research demands extensive and versatile computing resources. The AMPATH-supported National Research Platform (NRP), Open Science Grid (OSG), ACCESS, and FABRIC collectively provide robust cyberinfrastructure that accelerates AI research across diverse domains. The NRP, led by the University of California San Diego, offers the Nautilus cluster—a distributed computing environment with CPU, GPU, and FPGA resources designed to meet the demands of AI, ML, and data science applications. The OSG provides high-throughput computing services through the Open Science Pool (OSPool) and storage access via the Open Science Data Federation (OSDF), enabling scalable compute and data-sharing capabilities for U.S.-affiliated researchers.

ACCESS, supported by the National Science Foundation, grants academic researchers streamlined access to high-performance computing systems and large-scale storage, facilitating resource allocation tailored to computational requirements. FABRIC, an international testbed infrastructure, further expands experimental opportunities by connecting 29 high-performance sites with specialized networks in areas like 5G, IoT, and cloud computing. These shared resources collectively underpin a transformative environment for AI research, offering accessible, high-performance computing, data-sharing, and experimentation capacities essential for advancing AI methodologies and applications at scale.

2:15-2:30 p.m. Break



2:30-3:15 p.m. - Collaborations and programs that support Al. Honggao Liu (Texas A&M/ACES), Suresh Marru (ARTISAN/Ga Tech), DK Panda (The Ohio State U/ICICLE). Each will present a 10-minute overview of their project and resources, with 15 minutes of Q&A. Moderator: Bryan Johnston (CHPC).

Dr. Liu will talk about **ACES** (Accelerating Computing for Emerging Sciences), an innovative advanced computational prototype developed by Texas A&M University, and supported by the U.S. National Science Foundation. ACES features a menu of accelerators, agile memory and a composable fabric that allows users to select the best possible combination for their Al/ML workflow.

Dr. Marru is the Director of Georgia Tech's **ARTISAN** Center. His team is at the forefront of pioneering efforts to integrate AI into diverse scientific domains; they're dedicated to bridging the gap between theory, experimentation, and computation by fostering open-source integration frameworks. These frameworks automate research processes, optimize complex models, and integrate disparate scientific data with simulation engines.

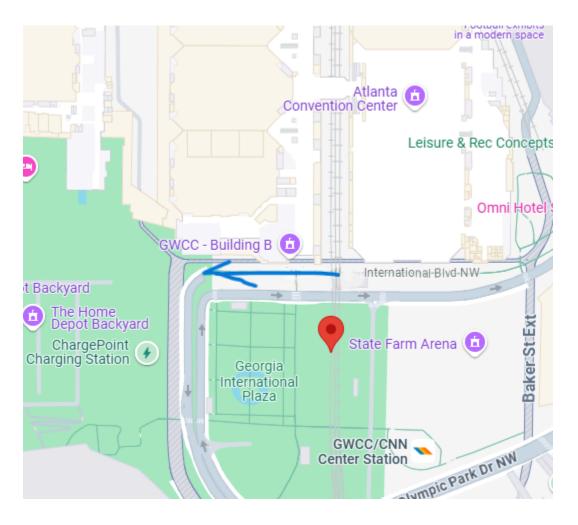
Dr. Panda directs the National Science Foundation-funded AI institute for Intelligent CI with Computational Learning in the Environment (ICICLE). **ICICLE** will build the next generation of Cyberinfrastructure to render AI more accessible to everyone and drive its further democratization in the larger society. The widespread adoption of AI fueling advances in science, education, and commerce has been driven not only by the ability to aggregate data from a wide range of sources, but also by the availability of increasingly powerful DI supporting AI advances.

3:15 p.m. Closing Remarks and group photo. Elizabeth Leake

3:30 board the bus bound for Medieval Times - parked outside of doors "B" across from the State Farm Arena.

Medieval Times Dinner & Tournament Dinner & Tournament

Our group visited Medieval Times in Dallas before SC22, and everyone loved it so much we decided to return! One in our group even received a proposal of marriage from a mounted Knight who spotted her in the front row. We will have VIP seating in the "Queens Box" so there's a chance your Knight in Shining Armor will find you there! If you love horses, a good meal and history, you'll enjoy Medieval Times.



5:00 p.m. to 7 p.m. Dinner and entertainment at Medieval Times - sponsored by Dell and Intel. Meet outside the convention center promptly at 3:30 p.m. Fun evening out; a good meal and more! The bus should return to the WCC by 8:30 p.m.



Thank you, ART@SC24 Sponsors and friends!

