



FALL 2024

Newsletter

DIRECTOR'S WELCOME

Celebrating 20 years of Global Computing Laboratory 2004-2024

Since 2004, the Global Computing Lab (GCLab) has been an integral part of my professional life. I started the GCLab at the University of Texas at El Paso with the aspiration that it be a place where motivation leads to innovation. I wanted the GCLab to have a transformative effect, where individuals develop their potential and envision an exciting future in computer science.



Taufer at ISC 2024 in Hamburg, Germany

Starting in 2018, GCLab has been situated at the University of Tennessee, Knoxville. Before that, GCLab spent nine years at the University of Delaware after relocating from the University of Texas at El Paso. At each of these institutions, the GCLab was able to thrive from a talented group of research associates, post-docs, graduate and undergraduate students. Many of them came from different parts of the globe, but all had the sole determination to advance their knowledge in the groundbreaking fields of computer science.

Even after 20 years, the work we do here at GCLab never ceases to be challenging. Many of the students and researchers who have been a part of it for the past two decades, have continued on with outstanding careers of their own. I wanted this newsletter to reflect on past alumni and celebrate their accolades.

Today, as the innovations in computer science continue to evolve, so does the GCLab. Our projects focus on high performance computing (HPC), and the design and testing of efficient computational algorithms and adaptive scheduling policies for scientific computing on GPUs, cloud computing, and volunteer computing. At the core of the GCLab, is a network of interdisciplinary research collaborations with the goal to produce trustworthy and influential outcomes.

Instilling the fundamental principles of engagement, perseverance, curiosity and adaptability, GCLab continues to strive for excellence from each of its members, and to prepare the next generation of researchers for success.

A handwritten signature in black ink that reads "Michela Taufer".

Michela Taufer, Ph.D.
Dongarra Professor in High Performance Computing
University of Tennessee, Knoxville, U.S.A.
Electrical Engineering and Computer Science



@TauferLab



<https://globalcomputing.group>

The evolution of the Global Computing Laboratory

Thank you for all those who have contributed to the GCLab throughout the years.

The University of Texas at El Paso 2004-2007



*Michela, Richard, Andre, Argo (back),
Daniel, Abel, David, Trilce, and Karina*

The University of Delaware Fall 2008



*Back: Dr. Taufer, Pat, Joe, Reed, and Abel
Front: Trilce, James, Kevin, and Adnan*

The University of Delaware Fall 2010



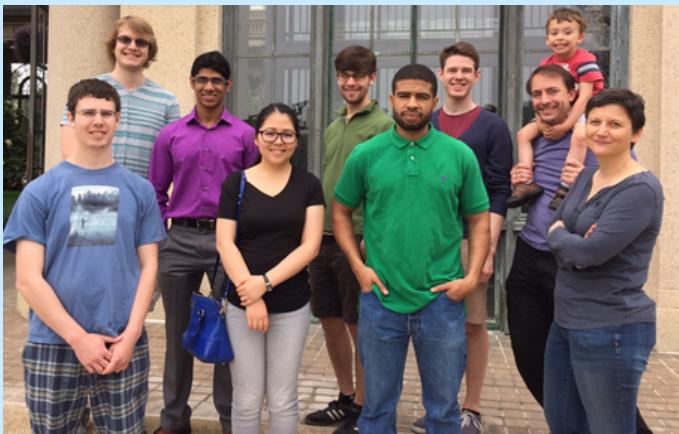
*Back: Dirk, Boyu, Dominik, Lifan, Trilce
Front: Reza, Kyle, Jeson, Narayan, and Dr. Taufer*

The University of Delaware Spring 2012



*Back: Boyu, Dr. Taufer, Trilce
Front: Sam, Jeff, Stephen, and Matt*

The University of Delaware Spring 2015

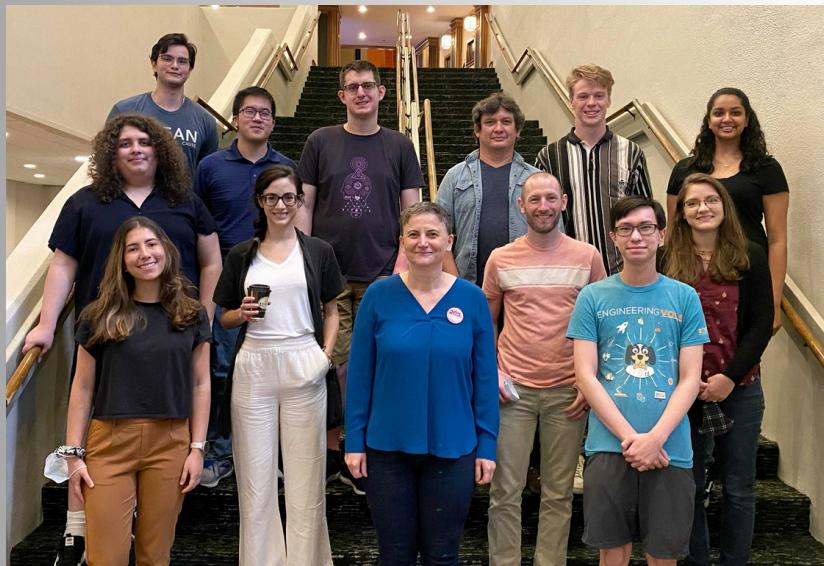
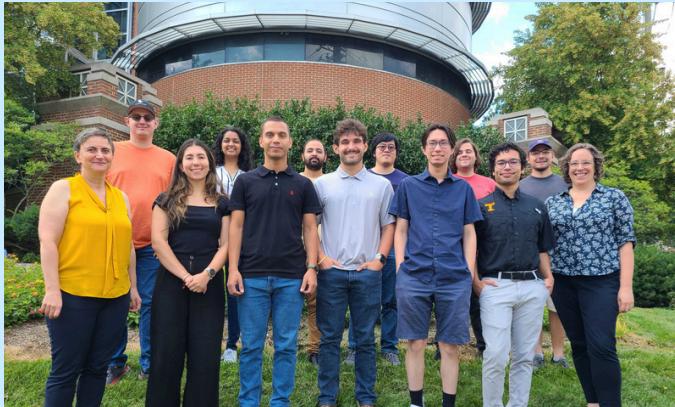


*Back: Stephen, Vivek, Dylan, Connor, Travis and David
Front: Ryan, Boyu, Sean, and Dr. Taufer*

The University of Delaware 2017



Josh, John, Sean, Tao, Dr. Taufer, Rachel, Dylan, Stephen

The evolution of the Global Computing Laboratory**University of Tennessee, Knoxville 2018****Joe, Mike, Dylan, Dr. Taufer, Stephen, Danny, Paula****University of Tennessee, Knoxville 2019****Paula, Danny, Dr. Taufer, Nigel, Neil, Kae, Dylan, Mike, Joe, Ian****University of Tennessee, Knoxville 2021****Kae, Paula, Silvina, Dr. Taufer, Ross, Brandan, Ariel, Jacob, Nigel, Ian, Leobardo, Dominic, Ria****University of Tennessee, Knoxville 2022****Jakob, Dr. Taufer, Silvina, Camila, Naweiluo, Georgia, Jack, Ria, Nigel, Dominic, Vanessa, Ian****University of Tennessee, Knoxville 2023****Dr. Taufer, Paula, Jack, Blake, Brandan, Gabriel, Lauren, Ian, Ria, Heberth, Nigel, Jay, Andrew****University of Tennessee, Knoxville 2024****Back: Nigel, Jay, Ian, Andrew, Kin and Lauren
Front: Dr. Taufer, Paula, Jack, Befikir, Amy and Gabriel**

The evolution of the Global Computing Laboratory



2008 MASPLAS
Princeton, New Jersey, U.S.A.



Tenure Celebration - Flight with Piper Cherokee Six (Fall 2012)
Greg (the pilot), Stephen, Sam, Michael, Michela, Boyu, and Trilce



Supercomputing 2014, New Orleans, Louisiana, U.S.A.



**Stephen Herbein at the 2016
Lawrence Livermore National Lab
Summer Poster Symposium**



Paula Olaya
at Supercomputing 2023

Supercomputing 2023, Denver, Colorado, U.S.A.

The evolution of the Global Computing Laboratory



December 2004
GCLab begins at UTEP



Summer 2004
GCLab name was established in San Diego, California

September 2007
GCLab moves to



M.S. Graduate Students

- Prayook Tungjatoororrusame (co-advised, Dec 2006)
- David Flores (co-advised, May 2007)
- Richard Zamudio (May 2007)

M.S. Graduate Students

- Joseph Davis (co-advised, May 2009)
- Abel Licon (May 2010)
- Jeffrey DiMarco (May 2017)
- Dylan Chapp (May 2017)
- Rachel Kraft (Dec 2018)

September 2018
GCLab relocates to



M.S. Graduate Students

- Treece Burgess (July 2023)
- Vanessa Lama (May 2023)
- Kae Suarez (May 2022)
- Paula Olaya (May 2020)

Current M.S. Students

- Jay Ashworth (Aug 2023 - present)
- Gabriel Laboy (Aug 2023 - present)
- Zack Malkmus (Aug 2024 - present)

Ph.D. Graduate Students

- Trilce Estrada (May 2012)
- Boyu Zhang (May 2015)
- Sean McDaniel (August 2018)
- Stephen Herbein (August 2018)
- Dylan Chapp (June 2020)
- Michael Wyatt (June 2020)

Ph.D. Graduate Students

- Paula Olaya (July 2024)
- Nigel Tan (July 2024)

Current Ph.D. Students

- Ian Lumsden (Aug 2020 - present)
- Befikir Bogale (Aug 2024 - present)

Other Highlighted Alumni & Projects

Narayan Ganesan, Post-doctoral researcher 2010-2011,
Full MD simulations on GPU (Peptide penetration into cell membrane)

Michael Matheny, B.S. 2014, QMCPack performance modeling

Travis Johnston, Post-doctoral researcher 2014-2016, MD and in situ analysis

Ariel Rorabaugh, Post-doctoral researcher 2019-2022, Analytics for Neural Networks (A4NN)

Georgia Channing, B.S. 2023, A4NN applied to protein defraction

Silvina Caino, Post-doctoral researcher 2020-2023, Reproducibility of LIGO, ETH, and NICER findings

Jakob Luegau, Post-doctoral researcher 2021-2024, National Science Data Fabric

Awards & Recognition

Michela Taufer named American Association for the Advancement of Science (AAAS) Fellow in 2024

AAAS is one of the world's largest scientific societies and each year, there is a highly selective process to recognize those individuals who have made extraordinary achievements in their disciplines. Michela Taufer was honored for distinguished contributions to high-performance computing, particularly enabling trustworthiness to bridge computational and experimental research across scientific domains. [Read more about AAAS and Michela's recognition.](#)

Taufer invited to be member of Computing Community Consortium (CCC)

The CCC mission is "*to enable the pursuit of innovative, high-impact computing research that aligns with pressing national and global challenges*", and the organization recently selected Taufer to be one its newest members. [Learn more about the Computing Community Consortium.](#)

Michela Taufer served as the 2024 program chair for the International Supercomputing Conference (ISC) HPC conference held in Hamburg, Germany, May 12-16.



Over the course of four days, the ISC event which includes both a conference program and an exhibition, welcomed thousands of participants to Germany with a theme of **Reinventing HPC into ISC 2024**, with Taufer as program chair. [Find out more about the conference program here.](#)

[Read about Michela Taufer's vision for the ISC '24 in this HPC Wire article.](#)

Paula Olaya & Nigel Tan

Researchers' Corner

What is your PhD work about?

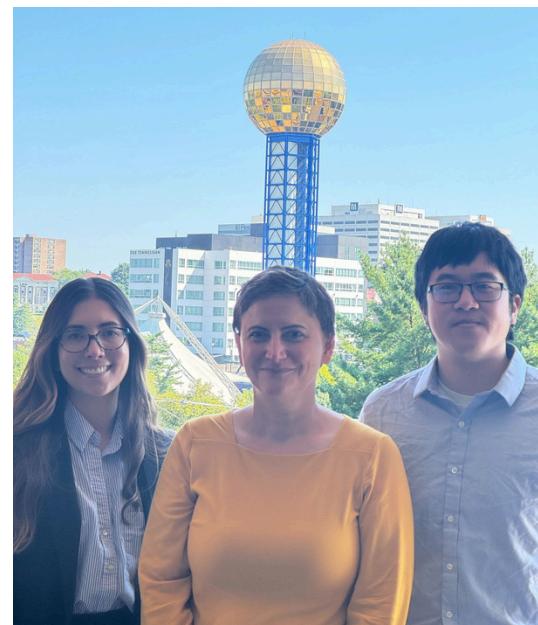
PAULA: My Ph.D. work is about codesigning scientific workflows and converged infrastructure to ensure robust science. This means that we develop software and computational environments that leverage HPC and cloud-converged infrastructure to accelerate scientific discovery while ensuring trustworthiness, reproducibility, and performance scalability.

NIGEL: My research revolves around "Enhancing Code Portability, Problem Scale, and Storage Efficiency in Exascale Applications". We explore a chain of development challenges that arise from large scale heterogeneous HPC platforms. We claim that developing HPC software on exascale supercomputers requires a cohesive approach to provide performance portability, increase problem size while preserving accuracy, and enhance storage efficiency by pruning redundancy.

What did you learn as a PhD student in the GCLab that you want to share with your peers?

PAULA: Resilience, perseverance, and teamwork will always be your allies when tackling challenges.

NIGEL: Time management and scheduling tools are vital. Prior to starting my PhD I could easily keep track of my courses, assignments, and events in my head because they were very regular. Research is much more dynamic, calendars and task lists are usually necessary. It is also important to isolate research from personal time. Not having a clear defined boundary is just asking for burnout.



Olaya, Taufer and Tan in 2024

What are your next professional steps?

PAULA: I will be joining IBM Research in New York as a research scientist in the hybrid cloud infrastructure team. This job would have not been possible without Dr. Taufer's connections in the industry and National Laboratories.

NIGEL: I will be staying at GCL for five months to help pass along research projects, organize my research data, and mentor other students. Starting in January I will take up a postdoctoral position at Los Alamos National Laboratory.

Would you like to share something about yourself outside work?

PAULA: I am an outdoors enthusiast. I love running, climbing, hiking, gardening, and everything that connects me to nature.

NIGEL: I'm a fan of Star Wars (Legends continuity only). The Darth Bane trilogy is one of my favorite book series.



GCLab members summer 2024

Meet our TEAM



Michela Taufer, Ph.D., Director

Jack Marquez, Ph.D., Research Assistant Professor

Kin Ng, Ph.D., Postdoctoral Researcher

**Michael Sutherlin, Ph.D.
Associate Director and Research Manager**

Dalal Sukkari, Ph.D., Senior Research Scientist

Befikir Bogale, Doctoral Student

Ian Lumsden, Doctoral Student

Paula Olaya, Doctoral Student

Nigel Tan, Doctoral Student

Jay Ashworth, Master's Student

Gabriel Laboy, Master's Student

Zackary Malkmus, Master's Student

**Ty Anderson, Undergraduate Student
Blake Milstead, Undergraduate Student**

**Barbara Fossum, Outreach Coordinator
Grace Wisser, Assistant Director**



GCLab members at SC '23 in Denver, Colorado

GCLab 2024 Summer Internships

Befikir Bogale and Ian Lumsden



Blake Milstead



Jay Ashworth



Pittsburgh Supercomputing Center

Gabriel Laboy



FRACTALE

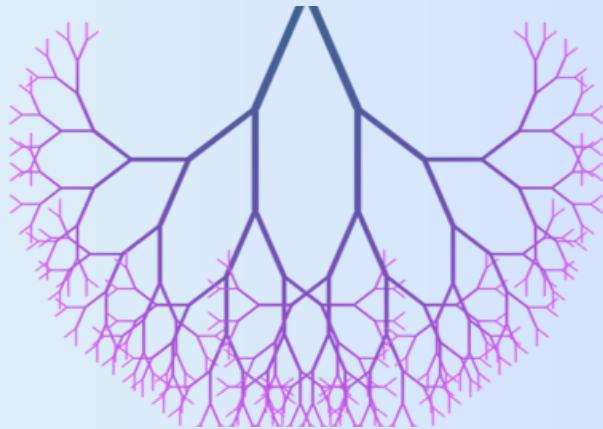
Reimagining HPC Efficiency

Project Spotlight



The Global Computing Lab has been fortunate to work with the Lawrence Livermore National Laboratory (LLNL) on multiple cutting-edge projects over the past ten years.

More recently, the group has joined efforts with collaborators at LLNL to reimagine a future where scientific breakthroughs happen twice as fast and where the complexity of managing HPC resources is a thing of the past through the **FRACTALE project — Fractal Resource Allocation for Center-wide Throughput Acceleration Leveraging Elasticity**.



FRACTALE transforms how scientific workflows are programmed and executed on HPC and Cloud platforms, unleashing unprecedented efficiency and productivity.

At its core, FRACTALE shifts the burden of resource management from users to intelligent software. Instead of manually configuring every detail, scientists specify their expected outcomes, such as completing a complex simulation in a set amount of time. FRACTALE optimizes resource allocation across the HPC center, ensuring seamless and efficient execution.

Building on the success of the R&D 100 award-winning Flux resource manager with Dr. Taufer, one of the Flux Team winning the award in 2021, FRACTALE integrates this new paradigm into existing HPC environments and at the HPC cloud convergence. The project significantly improves turnaround time and user productivity by allowing workflows to span multiple systems. Imagine running mission-critical simulations in half the time across various hardware types, with minimal manual intervention.

The Global Computing Laboratory has been fortunate to work with several colleagues at LLNL, including Tom Scogland, Olga Pierce, Dan Milroy, Jae Seung Yeon, and Tapasya Patki.

Research supported by: Under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

2023-2024 Journal Articles

Click the title to link to the article

Michela Taufer, Daniel Milroy, Todd Gamblin, Andrew Jones, Bill Magro, Heidi Poxon, and Seetharami Seelam.

HPC and Cloud Convergence Beyond Technical Boundaries: Strategies for Economic Sustainability, Standardization, and Data Accessibility.

IEEE Computer, 2024.

10.1109/MC.2024.3387013. (open access)

Connor Scully-Allison, Ian Lumsden, Katy Williams, Jesse Bartels, Michela Taufer, Stephanie Brink, Abhinav Bhatele, Olga Pearce, and Katherine E. Isaacs.

Design Concerns for Integrated Scripting and Interactive Visualization in Notebook Environments.

IEEE Transactions on Visualization and Computer Graphics, pages 1-13, 2024.

10.1109/TVCG.2024.3354561.

Chaitanya Afle, Patrick Miles, Silvina Caino-Lores, Collin Capano, Ingo Tews, Karan Vahi, Ewa Deelman, Michela Taufer, and Duncan Brown.

Reproducing the Results for NICER Observation of PSR J0030+0451.

IEEE Computing in Science and Engineering (CiSE), pages 1-13, 2024.

10.1109/MCSE.2024.3381080. (open access)

Michela Taufer, Heberth Martinez, Jakob Luettgau, Lauren Whitnah, Giorgio Scorzelli, Pania Newell, Aashish Panta, Timo Bremer, Doug Fils, Christine R. Kirkpatrick, and Valerio Pascucci.

Integrating FAIR Digital Objects into the National Science Data Fabric to Scientific Discovery.

IEEE Computing in Science and Engineering (CiSE), 25:39-47, 2023.

10.1109/MCSE.2024.3363828. (open access)

Tu Mai Anh Do, L  c Pottier, Rafael Ferreira da Silva, Silvina C  no-Lores, Michela Taufer, and Ewa Deelman.

Performance Assessment of Ensembles of In Situ Workflows under Resource Constraints.

Journal of Concurrency and Computation: Practice and Experience (CCPE), 35(40):e7111, 2023.

10.1002/cpe.7111.

Naweiluo Zhou, Giorgio Scorzelli, Jakob Luettgau, Rahul Reddy Kancharla, Joshua Kane, Robert Wheeler, Brendan Croom, Pania Newell, Valerio Pascucci, and Michela Taufer.

Orchestration of Materials Science Workflows for Heterogeneous Resources at Large Scale.

International Journal of High-Performance Computing Applications (IJHPCA), 3-4(37):260-271, 2023.

10.1177/10943420231167800.

2023-2024 Journal Articles

Sanjukta Bhowmick, Patrick Bell, and Michela Taufer.

A Survey of Graph Comparison Methods with Applications to Nondeterminism in High-Performance Computing

International Journal of High-Performance Computing Applications (IJHPCA), 3-4(37):306-327, 2023.
10.1177/10943420231166610

Paula Olaya, Dominic Kennedy, Ricardo Llamas, Leobardo Valera, Rodrigo Vargas, Jay Lofstead, and Michela Taufer.

Building Trust in Earth Science Findings through Data Traceability and Results Explainability.

IEEE Trans. Parallel Distributed Syst. (TPDS), 34(2):704-717, 2023.
10.1109/TPDS.2022.3220539. (open access)

Stephen Herbein, Tapasya Patki, Dong H. Ahn, Sebastian Mobo, Clark Hathaway, Silvina Caino-Lores, James Corbett, David Domyancic, Thomas R. W. Scogland, Bronis R. de Supinski, and Michela Taufer.

An Analytical Performance Model of Generalized Hierarchical Scheduling.

International Journal of High-Performance Computing Applications (IJHPCA), 36(3):289-306, 2022.
10.1177/10943420211051039.

2023 - 2024 Refereed Conferences, Symposiums and Workshops

Ian Lumsden, Hariharan Devarajan, Jack Marquez, Stephanie Brink, David Boehme, Olga Pearce, Jae-Seung Yeom, and Michela Taufer.

Empirical Study of Molecular Dynamics Workflow Data Movement: DYAD vs. Traditional I/O Systems.

In Proceedings of the 19th International Parallel and Distributed Processing Symposium (IPDPS) - Workshop Proceedings (HiCOMB),
San Francisco, CA, USA, May 2024. IEEE Computer Society.

Camila Roa, Mats Rynge, Paula Olaya, Karan Vahi, Todd Miller, John Goodhue, James Griffoen, David Hudak, Shelley Knuth, Ricardo Llamas, Rodrigo Vargas, Miron Livny, Ewa Deelman, and Michela Taufer.

End-to-end Integration of Scientific Workflows on Distributed Cyberinfrastructures: Challenges and Lessons Learned with an Earth Science Application.

In Proceedings of the 15th IEEE/ACM International Conference on Utility and Cloud Computing (UCC), pages 1-10, Taormina (Messina), Italy, December 2023.
IEEE Computer Society. (Acceptance Rate: 20/50, 40%).



Recent Publications

2023-2024 Refereed Conferences, Symposia and Workshops

Jakob Luetgau, Paula Olaya, Heberth Martinez, Giorgio Scorzelli, Glenn Tarcea, Jay Lofstead, Christine Kirkpatrick, Valerio Pascucci, and Michela Taufer.

NSDF-Services: Integrating Networking, Storage, and Computing Services into a Testbed for Democratization of Data Delivery.

In Proceedings of the 15th IEEE/ACM International Conference on Utility and Cloud Computing (UCC), pages 1-10, Taormina (Messina), Italy, December 2023.

IEEE Computer Society. (Acceptance Rate: 20/50, 40%).

Nigel Tan, Scott Luedtke, Michela Taufer, and Brian Albright. Efficient Particle Tracing for Scalable Kinetic Plasma Simulation Analysis.

In Proceedings of the IEEE Cluster Conference (CLUSTER), pages 1-2, Santa Fe, New Mexico, October 2023. IEEE Computer Society. (Short paper).

Seoyoung An, Georgia Channing, Catherine Schuman, and Michela Taufer. Visual Analytics Interactive Tool for Neural Network Archaeology.

In Proceedings of the IEEE Cluster Conference (CLUSTER), pages 1-2, Santa Fe, New Mexico, October 2023. IEEE Computer Society. (Short paper).

Harshita Sahni, Hector Carrillo-Cabada, Ekaterina Kots, Silvina Caino-Lores, Jack Marquez, Ewa Deelman, Michel Cuendet Harel Weinstein, Michela Taufer, and Trilce Estrada.

Online Boosted Gaussian Learners for in-situ Detection and Characterization of Protein Folding States in Molecular Dynamics Simulations.

In Proceedings of the 19th IEEE International Conference on e-Science (eScience), pages 1-10, Limassol, Cyprus, October 2023. IEEE Computer Society. (Acceptance Rate: 40/81, 50%).

Nigel Tan, Bogdan Nicolae, Jakob Luetgau, Jack Marquez, Keita Teranishi, Nicolas Morales, Sanjukta Bhowmick, Michela Taufer, and Franck Cappello.

Scalable Checkpointing of Applications with Sparsely Updated Data. In Proceedings of the 52nd International Conference Parallel Processing (ICPP), pages 1-10, Salt Lake City, UT, USA, August 2023. ACM. (Acceptance Rate: 29%).

Georgia Channing, Ria Patel, Paula Olaya, Ariel Rorabaugh, Osamu Miyashita, Silvina Caino-Lores, Catherine Schuman, Florence Tama, and Michela Taufer.

Composable Workflow for Accelerating Neural Architecture Search Using In Situ Analytics for Protein Characterization. In Proceedings of the 52nd International Conference on Parallel Processing (ICPP), pages 1-10, Salt Lake City, UT, USA, August 2023. ACM. (Acceptance Rate: 29%).

2023-2024 Refereed Conferences, Symposia and Workshops

Paula Olaya, Jakob Luettgau, Camila Roa, Ricardo Llamas, Rodrigo Vargas, Sophia Wen, I-Hsin Chung, Seetharami Seelam, Yoonho Park, Jay Lofstead, and Michela Taufer.

Enabling Scalability in the Cloud for Scientific Workflows: An Earth Science Use Case.

In Proceedings of IEEE CLOUD, pages 1-10, Chicago, IL, USA, June 2023. IEEE Computer Society.
(Acceptance Rate: 21.6%).

Silvina Caino-Lores, Michel A. Cuendet, Jack Marquez, Trilce Estrada, Ewa Deelman, Harel Weinstein, and Michela Taufer.

Runtime Steering of Molecular Dynamics Simulations Through In Situ Analysis and Annotation of Collective Variables. In Proceedings of Platform for Advanced Scientific Computing (PASC) Conference, pages 1-10, Davos, Switzerland, June 2023. ACM.

Camila Roa, Paula Olaya, Ricardo Llamas, Rodrigo Vargas, and Michela Taufer.

GEOtiled: A Scalable Workflow for Generating Large Datasets of High-Resolution Terrain Parameters. In Proceedings of the 32nd International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC), pages 1-2, Orlando, Florida, USA, June 2023. ACM.
(Short paper).

Jakob Luettgau, Heberth Martinez, Glenn Tarcea, Giorgio Scorzelli, Valerio Pascucci, and Michela Taufer.

Studying Latency and Throughput Constraints for Geo-Distributed Data in the National Science Data Fabric. In Proceedings of the 32nd International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC), pages 1-2, Orlando, Florida, USA, June 2023. ACM.
(Short paper).

Stephanie Brink, Michael McKinsey, David Boehme, W. Daryl Hawkins, Connor Scully-Allison, Ian Lumsden, Treece Burgess, Vanessa Lama, Katherine E. Isaacs, Jakob Luettgau, Michela Taufer, and Olga Pearce.

Thicket: Seeing the Performance Experiment Forest for the Individual Run Trees.

In Proceedings of the 32nd International ACM Symposium on High-Performance Parallel and Distributed Computing (HPDC), pages 1-10, Orlando, Florida, USA, June 2023. ACM. (Acceptance Rate: 21/101, 20.7%).

Jakob Luettgau, Giorgio Scorzelli, Valerio Pascucci, and Michela Taufer.

Development of Large-Scale Scientific Cyberinfrastructure and the Growing Opportunity to Democratize Access to Platforms and Data. In Proceedings of the 25TH International Conference On Human-Computer Interaction (HCII), Copenhagen, Denmark, July 2023. Springer.

2023 - 2024 Keynote & Invited Talks

Advancing Scientific Discovery with the National Scientific Data Fabric: Democratizing Data Access and Use through Reproducibility, Analytical Tools, and User-Focused Services.

Keynote speaker. 53nd International Conference on Parallel Processing (ICPP), Gotland, Sweden. August 2024

The National Science Data Fabric: Democratizing Data Access for Science and Society.

High Performance Computing Conference 2023, Cetraro, Italy. June 2024

National Science Data Fabric: A Platform Agnostic Testbed for Democratizing Data Delivery.

HPC ISC Conference, Hamburg, Germany. May 2024

Composable Workflow for Accelerating Neural Architecture Search Using In Situ Analytics - A Use Case for 2D Protein Diffraction (PD) Patterns.

Joint Laboratory for Extreme Scale Computing (JLESC), Osaka, Japan. April 2024

Advancing Science with the National Scientific Data Fabric: Democratizing Data Access and Use through Reproducibility, Analytical Tools, and User-Focused Services.

SOS'26, Cocoa Beach, FL, USA. March 2024

An Introduction to the National Science Data Fabric.

The Fourth National Science Data Fabric (NSDF) in-person meeting, San Diego, CA. February 2024

Analytics4NN: Accelerating Neural Architecture Search through Modeling and High-Performance Computing Techniques.

The 6th R-CCS International Symposium, Kobe, Japan. January 2024

Building Trust in Scientific Applications through Data Traceability and Results Explainability.

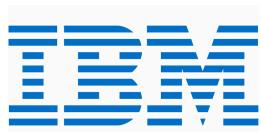
High Performance Computing Conference 2023, Cetraro, Italy. June 2023



Sponsors



National
Science
Foundation



@TauferLab



<https://globalcomputing.group>