
MICHELA TAUFER

ACM Distinguished Scientist and IEEE Senior Member
Jack Dongarra Professor in High Performance Computing

Department of Electrical Engineering and Computer and Science
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EDUCATION

- Dec 2002** PhD in Computer Science, Swiss Federal Institute of Technology Zurich (ETH), Switzerland
Dissertation title: Inverting Middleware: Performance Analysis of Layered Application Codes in High Performance Distributed Computing.
Thesis supervisors: Thomas M. Stricker (Chair) and Daniel A. Reed
- Dec 1996** MS (Laurea) in Computer Engineering, University of Padua, Italy
Dissertation title: Development of the Parallelization of the Software Package OPAL for the Simulation of Dynamic Molecules on Supercomputers.
Thesis supervisors: Gianfranco Bilardi (Chair), Walter Gander, and Geppino Pucci

RESEARCH INTERESTS

High performance computing, cloud computing, and volunteer computing; algorithms and workflows for scientific applications; reproducibility, replicability, and transparency of scientific applications; performance analysis, modeling, and optimization of multi-scale applications; in situ and in transit data analytics.

ACADEMIC POSITIONS

- Jun 2018 – present* – Jack Dongarra Professor in High Performance Computing, Department of Electrical Engineering and Computer and Science, University of Tennessee Knoxville
- Sep 2017 – May 2018* – Professor, Department of Computer and Information Sciences, University of Delaware (Affiliated with Biomedical Engineering and Center for Bioinformatics & Computational Biology)
- Sep 2012 – Aug 2017* – Associate Professor, Department of Computer and Information Sciences, University of Delaware, (Affiliated with Biomedical Engineering and Center for Bioinformatics & Computational Biology)
- Sep 2015 – Aug 2016* – Acting Director, Center for Bioinformatics & Computational Biology, Delaware Biotechnology Institute
- Jan 2013 – Aug 2016* – David and Beverly J.C. Mills Career Development Chair, Department of Computer and Information Sciences, University of Delaware

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- Jun 2013* – Visiting Faculty, Computer Science and Mathematics Division, Oak Ridge National Laboratory. U.S. Department of Energy Higher Education Research Experiences Faculty Program
- May 2014*
- Sep 2007* – Assistant Professor, Department of Computer and Information Sciences, University of Delaware (Affiliated with Center for Bioinformatics & Computational Biology Jun 2010 – Aug 2012)
- Aug 2012*
- Jan 2005* – Assistant Professor, Department of Computer Science, University of Texas, El Paso
- Aug 2007*
- Jan 2003* – Postdoctoral Researcher, Center for Theoretical Biological Physics, University of California, San Diego (Affiliated with the Department of Molecular Biology, The Scripps Research Institute; San Diego Supercomputer Center; Department of Computer Science and Engineering, University of California San Diego)
- Dec 2004*
- Dec 1996* – Research Student Assistant, Computer Systems Institute, Swiss Federal Institute of Technology Zurich (ETH)
- Dec 2002*
- Feb 1996* – Visiting Scholar at the Swiss Center for Scientific Computing (SCSC/CSCS), Zurich
- Dec 1996*

HONORS AND DISTINCTIONS

- May 2022* 2022 IEEE Technical Community on Parallel Processing (TCPP) Outstanding Service and Contributions Award
- April 2022* Tickle College of Engineering Research Achievement Award, University of Tennessee Knoxville
- Dec 2021* IBM Faculty Award
- Aug 2021* R&D 100 Award Winner in Software/Services categories with the project "Flux : Next-Generation Workload Management Software Framework." Collaboration with Lawrence Livermore National Laboratory
- Jun 2021* Best Track Paper Award, International Conference on Computational Science (ICCS)
- Apr 2020* IEEE Senior Member
- Mar 2020* Tickle College of Engineering Faculty & Staff Award for Outstanding Service to the Discipline Category, University of Tennessee Knoxville
- Feb 2019* IBM Faculty Award
- Feb 2019* HPCwire's 2019 Person to Watch
- Jun 2018* Jack Dongarra Professor in High Performance Computing
- May 2017* Faculty Nomination for the Excellence in Undergraduate Academic Advising and Mentoring Award, University of Delaware
- Feb 2017* – J.P. Morgan Chase Faculty Scholar, University of Delaware
- May 2018*

<i>Oct 2016</i>	Best Paper Finalists at the IEEE International Symposium on Computer Architecture and High Performance Computing Conference (SBAC-PAD), Los Angeles, CA,USA
<i>2015</i>	ACM (Association for Computing Machinery) Distinguished Scientist
<i>2015</i>	Winner of the 8th IEEE International Scalable Computing Challenge, Co-located with the IEEE/ACM CCGrid Conference
<i>2014</i>	ACM (Association for Computing Machinery) Senior Member
<i>Sep 2014</i>	Best Paper Finalists at the IEEE Cluster Conference, Madrid, Spain
<i>May 2014</i>	Faculty Nomination for the Excellence in Undergraduate Academic Advising and Mentoring Award, University of Delaware
<i>2012 – 2016</i>	David and Beverly J.C. Mills Career Development Chair, University of Delaware
<i>May 2006</i>	UTEP Young Investigator Award, Research and Sponsored Programs, University of Texas El Paso
<i>Jan 2003 – Dec 2004</i>	La Jolla Interfaces in Science (LJIS) Interdisciplinary Fellows, University of California San Diego
<i>Feb 1996 – Dec 1996</i>	Erasmus Fellow, European Community (EU)

RESEARCH FUNDING

In progress:

- 2022 *SHF: Small: Methods, Workflows, and Data Commons for Reducing Training Costs in Neural Architecture Search on High-Performance Computing Platforms*
Source of Support: NSF #2223704
Total Amount: \$623,999, PI, with Silvina Caino-Lores (UTK) and Catherine Schuman (UTK).
Project Period: 10/01/2022 - 09/30/2025
Location of Project: University of Tennessee Knoxville
Description: This project addresses the urgent need to reduce the use of high-performance-computing resources for the training of neural networks, while assuring explainable, reproducible and nearly-optimal neural networks. To this end, the team of researchers proposes a flexible fitness-prediction method that uses parametric modeling to predict future fitness of neural networks and allow for early termination of the training process.
- 2021 *OAC: Piloting the National Science Data Fabric: A Platform Agnostic Testbed for Democratizing Data Delivery*
Source of Support: NSF #2138811
Total Amount: \$5,609,259 (\$750,000 at University of Tennessee Knoxville), co-PI.
Project Period: 10/01/2021 - 09/30/2024
Location of Project: University of Tennessee Knoxville
Description: This project aims to build a National Science Data Fabric (NSDF), a testbed experimenting with critical technology needed to democratize data-driven sciences by constructing a CI platform designed for equitable access. NSDF connects storage, compute, and networking components with a software stack that empowers end-users with scalable tools that are easy to use, integrate and scale. Community-driven education and outreach will guarantee equitable access to all resources and engage an open network of universities, including minority-serving institutions in a federated data fabric configurable for individual and shared scientific use.
- 2021 *Collaborative Research: Elements: SENSORY: Software Ecosystem for kNowledge diScOveRY - a data-driven framework for soil moisture applications*
Source of Support: National Science Foundation #2028923
Total Amount: \$600,000 (\$349,998 at University of Tennessee Knoxville), Lead PI. Collaborative research with Rodrigo Vargas, University of Delaware
Project Period: 06/01/2021 - 05/30/2024
Location of Project: University of Tennessee Knoxville
Description: This project connects multi-disciplinary advances across the scientific community (such as generating datasets at scale and supporting cloud-based cyber-infrastructure) to develop a data-driven software ecosystem for analyzing, visualizing, and extracting knowledge from the growing data collections (from fine-grained, in situ soil sensor information to coarse-grained, global satellite measurements) and releasing this knowledge to applications in environmental sciences.

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- 2021 *Leveraging Kokkos Abstractions to Automate Checkpointing*
Source of Support: Argonne National Laboratory
Total Amount: \$82,563, Single PI
Project Period: 05/01/2021 – 04/30/2023
Location of Project: University of Tennessee Knoxville
Description: This project focuses on what patterns the memory abstractions used by Kokkos form and how they can be efficiently captured and persistent with VELOC.
- 2020 *Leverage Containerized Environments for Reproducibility and Traceability of Scientific Workflows - the case study of Analytics for Neural Network Workflows*
Source of Support: Sandia National Laboratories
Total Amount: \$200,00, Single PI
Project Period: 07/15/2020 – 07/14/2023
Location of Project: University of Tennessee Knoxville
Description: This project builds a prototype of a containerized environment which encapsulates each component of a scientific workflow (i.e., data and applications) in individual container environment for transparent and automatic metadata collection and access, easy-to-read record trail, and tight connections between data and metadata.
- 2020 *Augmenting Hatchet to support scalability and replicability solutions for HPC applications*
Source of Support: Lawrence Livermore National Laboratory
Total Amount: \$200,000, Single PI
Project Period: 08/01/2020- 07/31/2023
Location of Project: University of Tennessee Knoxville
Description: This project uses Hatchet and its features (e.g., query language) to study scalability and replicability problems in applications of interest to LLNL at a large scale; and develops tooling to support the analysis and study of such problems to identify the source of the scalability and replicability problems.
- 2020 *Study Performance Portability of the Vector Particle-In-Cell Project (VPIC) across architectures*
Source of Support: Los Alamos National Laboratory
Total Amount: \$314,081, Single PI
Project Period: 05/01/2020 – 04/30/2023
Location of Project: University of Tennessee Knoxville
Description: This project studies aspect of performance portability associate to the Vector Particle-In-Cell Project or VPIC code across platforms by addressing questions such as “Is the execution of VPIC sensitive to new architectures on which it runs? How do we continue to extract as much performance as possible despite differences in hardware? What performance is lost when using a performance portability framework?”

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- 2020 *Flux Scheduler Specializations: Improving Workflow Performance with Scheduler Structure and Policy Tuning*
Source of Support: Lawrence Livermore National Laboratory
Total Amount: \$200,089, Single PI
Project Period: 04/01/2020 – 03/31/2023
Location of Project: University of Tennessee Knoxville
Description: This project studies how features of a user-level, highly-configurable scheduler like Flux can best be leveraged to maximize workflow performance. The project aims to answer this question through the development of a model that tunes scheduler settings to maximize workflow performance even under conditions of system stress such as scheduler fragmentation and resource drains.
- 2020 *Collaborative Research: PPOSS: Planning: Performance Scalability, Trust, and Reproducibility: A Community Roadmap to Robust Science in High-throughput Applications*
Source of Support: National Science Foundation #2028923
Total Amount: \$250,000 (\$90,000 at University of Tennessee Knoxville), Lead PI. Collaborative research with Ewa Deelman, University of South California; Trilce Estrada University of New Mexico; Mary Hall, University of Utah; and Victoria Stodden, University of Illinois at Urbana-Champaign
Project Period: 10/01/2020 - 09/30/2022
Location of Project: University of Tennessee Knoxville
Description: The project recruits a cross-disciplinary community working together in three virtual mini-workshops called virtual world cafes to define, design, implement, and use a set of solutions for robust science.
- 2020 *Collaborative Research: EAGER: Advancing Reproducibility in Multi-Messenger Astrophysics*
Source of Support: National Science Foundation #2041977
Total Amount: \$300,000 (\$100,000 at University of Tennessee Knoxville), Lead PI. Collaborative research with Ewa Deelman, University of South California, and Duncan Brown, Syracuse University
Project Period: 08/01/2020-07/31/2022
Location of Project: University of Tennessee Knoxville
Description: The project provides the astrophysics community with a transformative building block to a roadmap for reproducible open science. Findings about the reproducibility process of the EHT and NICER results are captured and disseminated through documentation, data products, and methods used.

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- 2019 *SHF: Medium: Collaborative Research: ANACIN-X: Analysis and Modeling of Non-determinism and Associated Costs in eXtreme Scale Applications*
Source of Support: National Science Foundation #1900888
Total Amount: \$1,199,940 (\$899,739 at University of Tennessee Knoxville), Leading PI. Collaborative research with Heike Jagode, University of Tennessee Knoxville and Sanjukta Bhowmick, University of North Texas
Total Project Period: 06/01/2019 – 05/31/2023
Location of Project: University of Tennessee Knoxville
Description: This project advances the study of nondeterministic HPC applications by studying the recording costs of Record-and-replay (R&R) tools and by defining strategy so that these tools can scale to the exascale domain.
Supplement: NSF Research Experiences for Undergraduates (REU), \$16,000, Summer 2019 and Summer 2020
- 2018 *BIGDATA: IA: Collaborative Research: In Situ Data Analytics for Next Generation Molecular Dynamics Workflows*
Source of Support: National Science Foundation #1741057/#1841758
Total Amount: \$1,993,043, (\$979,987 at University of Tennessee Knoxville), Leading PI.
Collaborative research with Trilce Estrada, University of New Mexico; Ewa Deelman and Rafael Ferreira da Silva, University of Southern California; Michel Cuendet and Harel Weinstein, Weill Medical College of Cornell University
Project Period: 10/01/2017 – 09/30/2023
Location of Project: University of Tennessee Knoxville
Description: This interdisciplinary project tackles the data challenge of data analysis of molecular dynamics simulations on the next-generation supercomputers. Specifically, this effort combines machine learning and data analytics approaches, workflow management methods, and high-performance computing techniques to analyze molecular dynamics data as it is generated.
- Completed:*
- 2019 *JDRD: Empowering Training and Validation Stages in AI-Orchestrated Workflows*
Source of Support: Science Alliance, University of Tennessee Knoxville
Total Amount: \$216,900, Single PI
Project Period: 10/01/2019 – 09/30/2021
Location of Project: University of Tennessee Knoxville
Description: This project studies AI-orchestrated workflows, including experimental, computational, and data manipulation steps in one or multiple domains, where an important component is one or more neural networks (NN) used for searching or decision making. The project's aim is to transform the process of training the NN in AI-orchestrated workflows from simulated data (clean, non-adversarial data) to deploying on real data (noisy, adversarial data) with the integration of mitigating methods.

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- 2019 *EAGER: Reproducibility in Computational and Data-Enabled Science - Paradigms, Practices, and Infrastructure*
Source of Support: National Science Foundation #1941443
Total Amount: \$300,000 (\$149,997 at University of Tennessee Knoxville), PI. Collaborative research with Victoria Stodden, University of Illinois at Urbana-Champaign
Total Project Period: 08/16/2019 – 08/15/2022
Location of Project: University of Tennessee Knoxville
Description: This project seeks to improve understanding of how the scientific community can adapt to the increasing use of computing and large-scale data resources. One challenge is ensuring that computational results, such as those from simulations, are "reproducible," that is, the same results are obtained when one re-uses the same input data, methods, software and analysis conditions. In 2019, the National Academies of Science, Engineering, and Medicine (NASEM) issued a report on "Reproducibility and Replication in Science" with a series of recommendations. The project assesses the implications of these recommendations on the scientific discovery process for computationally- and data-enabled research.
- 2019 *Study of Data-intensive Workflows on Next-generation Systems with Emphasis on Memory Access*
Source of Support: Sandia National Laboratories
Total Amount: \$99,999, Single PI
Project Period: 08/01/2019 – 07/31/2020
Location of Project: University of Tennessee Knoxville
Description: The project designs and implements a C++ suite of data-intensive mini- applications to study data management costs with emphasis on memory access times and use, power consumption, and replicability.
- 2019 *Building a "Miniature" Version of the ORNL's Summit supercomputer for Computational Science Research at UTK*
Source of Support: 2019 IBM Global University Program Shared University Research Award
Total Amount: \$472,536, Leading PI. Collaborative research with Jack Dongarra, Mark Dean, and Greg Peterson at University of Tennessee Knoxville
Total Project Period: 06/21/2019 - 06/20/2024
Location of Project: University of Tennessee Knoxville
Description: The award enabled the purchase of a supercomputer for computational science applications at University of Tennessee Knoxville.
- 2019 *Moving Towards Self-Adjusting Scheduling Policies for High Performance Workflows with Flux's Fully Hierarchical Scheduling*
Source of Support: Lawrence Livermore National Laboratory
Total Amount: \$63,107, Single PI
Project Period: 01/08/2019 – 03/31/2020
Location of Project: University of Tennessee Knoxville
Description: The project tackles scheduler specializations by systematically studying fully hierarchical scheduling models with Flux and defining models supporting a given workflow to employ the best scheduler specialization strategy at runtime.

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- 2018 *Driving Next-Generation Schedulers with Machine Learning-Based Application Patterns*
Source of Support: Lawrence Livermore National Laboratory
Total Amount: \$199,570, Single PI
Project Period: 08/01/2018 – 07/31/2020
Location of Project: University of Tennessee Knoxville
Description: This project develops methods to identify and understand irregular HPC job patterns and integrates knowledge of these irregular HPC patterns into multi-objective schedulers. The work leverages results of a previous award from Lawrence Livermore National Laboratory.
- 2018 *Collaborative: EAGER: Exploring and Advancing the State of the Art in Robust Science in Gravitational Wave Physics*
Source of Support: National Science Foundation #1823372
Total Amount: \$299,410 (\$75,000 at University of Tennessee Knoxville), PI. Collaborative research with Ewa Deelman, University of Southern California; Duncan Brown, Syracuse University; and Von Welch, Indiana University
Project Period: 05/31/2018 – 04/30/2020
Location of Project: University of Tennessee Knoxville
Description: The project develops and uses a survey to collect information about LIGO workflows that are composed of a series of experimental, computational, and data manipulation steps.
- 2017 *CIF21 DIBBs: PD: Cyberinfrastructure Tools for Precision Agriculture in the 21st Century*
Source of Support: National Science Foundation #1724843/#1854312
Total Amount: \$574,999 (\$339,497 at University of Tennessee Knoxville), Leading PI. Collaborative research with Rodrigo Vargas, University of Delaware
Project Period: 07/01/2017 – 06/30/2021
Location of Project: University of Tennessee Knoxville
Description: This interdisciplinary project applies computer science approaches and computational resources to large multidimensional environmental datasets and synthesizes this information into ecoinformatics, a branch of informatics that analyzes ecological and environmental science variables such as information on landscapes, soils, climate, organisms, and ecosystems.
- 2017 *Investigating Massively Scalable I/O-Aware Job Scheduling in Support of Flux (III)*
Source of Support: Lawrence Livermore National Laboratory
Total Amount: \$112,014, Single PI
Project Period: 06/01/2017 – 05/31/2018
Location of Project: University of Delaware
Description: This project investigates distinct—yet complementary—techniques to overcome challenges that can preclude I/O-aware schemes from effectively scheduling massively large- scale systems. The work leverages results of a previous award from Lawrence Livermore National Laboratory.

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- 2016 *HAKEr-HPC: HArnessing Knowledge for Environmental Research using High Performance Computing (HPC) Solutions*
Source of Support: University of Delaware Research Foundation
Total Amount: \$45,000, Senior Personnel Project Period: 12/01/2016 – 05/31/2018
Location of Project: University of Delaware
Description: This award aims to build preliminary results on the development of HPC-based tools for the analysis of moisture in soil data at the large scale.
- 2016 *Student Support: IEEE Cluster 2017 Conference*
Source of Support: National Science Foundation #1648617
Total Amount: \$20,000, Single PI
Project Period: 08/01/2016 – 07/31/2018
Location of Project: University of Delaware
Description: This award supports 20 students from American institutions to attend the IEEE Cluster 2017 conference.
- 2016 *Performance Characterization and Optimization of the MapReduce-MPI Framework*
Source of Support: Argonne National Laboratory
Total Amount: \$14,760, Single PI
Project Period 09/01/2016 – 09/30/2016
Location of Project: University of Delaware
Description: This project studies the performance of MapReduce-MPI on high-end clusters and identifies the performance bottlenecks for a selected number of popular benchmarks.
- 2016 *Development of a Scalable Method for Identifying Dietary Clusters in the National Health and Nutrition Examination Survey using MapReduce*
Source of Support: University of Delaware - UDRF
Total Amount: \$38,500, PI (previous PI Mia Papas)
Project Period: 06/01/2016 – 05/31/2018
Location of Project: University of Delaware
Description: This award aims to build preliminary results on the development of MapReduce- based tools for the analysis of dietary data at the large scale.
Supplement: NSF REU \$3,500, Summer 2017
- 2016 *Investigating Massively Scalable I/O-Aware Job Scheduling in Support of Flux (Part II)*
Source of Support: Lawrence Livermore National Laboratory
Total Amount: \$103,626, single PI
Project Period: 03/31/2016 – 05/31/2017
Location of Project: University of Delaware
Description: This project investigates distinct—yet complementary—techniques to overcome challenges that can preclude I/O-aware schemes from effectively scheduling massively large- scale systems. The work leverages results of a previous award from Lawrence Livermore National Laboratory.

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- 2015 *BD Hubs: Collaborative Proposal: SOUTH: A Big Data Innovation Hub for the South Region*
Source of Support: National Science Foundation #1550305
Total Amount: \$750,712 (Funds only to leading hub instructions: Georgia Tech and University of North Carolina, Chapel Hill), Senior Personnel
Project Period: 09/15/15 – 09/30/18
Location of Project: University of Delaware
Description: This award establishes the South Big Data Regional Innovation Hub (South BD Hub) with lead institutions, Georgia Institute of Technology (GT) and the University of North Carolina at Chapel Hill (UNC-CH). The South BD Hub serves as the primary vehicle for interdisciplinary, multi-stakeholder partnerships designed to pursue BD projects of interest to the South region by engaging academic institutions from 16 states in the South, including the University of Delaware
- 2015 *Student Support: IEEE Cluster 2015-2016 Conference*
Source of Support: National Science Foundation #1550348 Total Amount: \$20,000, Single PI
Project Period: 08/01/2015 – 07/31/2018
Location of Project: University of Delaware
Description: This award supports 20 students from American institutions to attend the IEEE Cluster 2015 and Cluster 2016 conferences.
- 2015 *Comprehensive Study of I/O Performance at the Extreme Scale*
Source of Support: Army Research Office #W911NF-15-2-0033 Total Amount: \$297,015, Single PI
Project Period: 06/01/2015 – 05/31/2018
Location of Project: University of Delaware
Description: This award involves studying aspects of I/O performance and in situ analysis for applications relevant to the Army.
- 2015 *SHF: Medium: Collaborative Research: A Comprehensive Methodology to Pursue Reproducible Accuracy in Ensemble Scientific Simulations on Multi- and Many-core Platforms*
Source of Support: National Science Foundation #1513025/#1841552
Total Amount: \$814,733 (\$443,878 at University of Delaware and University of Tennessee Knoxville), Leading PI. Collaborative research with Michela Becchi, North Carolina State University
Total Project Period: 06/15/2015 – 05/31/2019
Location of Project: University of Delaware and University of Tennessee Knoxville
Description: This project tackles numerical errors due to limited arithmetic precision and non-determinism associated with multithreading; the goal is defining methodologies to enable reproducible accuracy of large ensemble simulations on exascale platforms.
Supplement: NSF REU, \$16,000, Summer 2016

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- 2014 *Becoming the Online Resource Center for Ethics Education in Engineering and Science*
Source of Support: National Science Foundation #1355547
Total Amount: \$1,199,918 (\$209,239 at University of Delaware), Co-PI. Collaborative research with Thomas Powers, University of Delaware
Project Period: 02/01/2014 – 05/31/2018
Location of Project: University of Delaware
Description: This University of Delaware award subcontract supports the Online Ethics Center for Engineering and Science (OEC), which is an expansion of the existing National Academy of Engineering's (NAE) Online Ethics Center for Engineering and Research (OEC) to include international best practices in ethics for engineers and scientists at the global level.
- 2014 *Investigating Massively Scalable I/O-Aware Job Scheduling in Support of Flux*
Source of Support: Lawrence Livermore National Laboratory
Total Amount: \$64,118, Single PI
Project Period: 11/05/2014 – 03/31/2016
Location of Project: University of Delaware
Description: This project investigates distinct—yet complementary—techniques to overcome challenges that can preclude I/O-aware schemes from effectively scheduling massively large- scale systems.
- 2014 *Student Support: IEEE Cluster 2014 Conference*
Source of Support: National Science Foundation #1441397
Total Amount: \$20,000, Single PI
Project Period: 07/01/2014 – 06/01/2016
Location of Project: University of Delaware
Description: This award supports 20 students from American institutions to attend the IEEE Cluster 2014 and Cluster 2015 Conferences.
- 2014 *EAGER: Assessment of the Numerical Reproducibility in Large-Scale Scientific Simulations on Multicore Architectures*
Source of Support: National Science Foundation #1446794
Total Amount: \$89,999, Single PI
Project Period: 06/15/2014 – 06/01/2016
Location of Project: University of Delaware
Description: This project studies the impact of rounding errors on result reproducibility when concurrent executions burst and workflow determinism vanishes in cutting-edge multicore architectures.
- 2014 *Evaluating, Analyzing, and Improving the Performance of Data-intensive Applications*
Source of Support: Argonne National Laboratory
Total Amount: \$28,657, Single PI
Project Period: 06/09/2014 – 01/15/2015
Location of Project: University of Delaware
Description: This project studies various data-intensive computing frameworks, including MR- MPI and DataMPI, and investigates their performance characteristics, particularly in the context of processing very large data.

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- 2013 *SHF: Small: Collaborative Research: Modeling and Analyzing Big Data on Peta- and Exascale Distributed Systems supported by MapReduce Methodologies*
Source of Support: National Science Foundation #1318417
Total Amount: \$512,038.00 (\$459,000 at UD, PI, with Pietro Cicotti co-PI, SDSC)
Project Period: 09/01/2013 – 08/31/2017
Location of Project: University of Delaware
Description: This project develops transformative analysis methodology to model the properties of large scientific datasets in a distributed manner on petascale and exascale systems.
Supplements: NSF REU, \$16,000, Summer 2014; NSF REU, \$16,000, Summer 2015
- 2012 *CSR: Small: Collaborative: Pursuing High Performance on Clouds and Other Dynamically Heterogeneous Computing Platforms*
Source of Support: National Science Foundation #1217812
Total Amount: \$500,000 (\$192,487 at University of Delaware). Co-PI: Arnold L. Rosenberg, Northeastern University
Project Period: 10/01/2012 – 09/30/2015
Location of Project: University of Delaware
Description: This project develops a transformative computing paradigm that enables high- performance computing on computing clouds and many genres of computing grids.
Supplement: NSF REU, \$8,000, Fall 2013
- 2012 *Scalable Aero-Load and Aero-Elasticity Solvers for Massively Parallel Heterogeneous Computing Architectures (Phase II)*
Source of Support: Air Force Office of Scientific Research Small Business Technology Transfer Program (AFOSR SBTT): Highly Scalable Computational-Based Engineering Algorithms for Emerging Parallel Machine Architectures (Topic BT13)
Total Amount: \$700,000 (\$162,000 at University of Delaware), PI. Collaborative research with Eric Kelmelis, EM Photonics
Project Period: 09/01/2012 – 08/31/2014
Location of Project: University of Delaware
Description: This project supports development of innovative algorithms for scientific computing, modeling, and simulation in a multi-GPU environment with an emphasis on parallelization of scientific applications across multiple GPUs.
- 2012 *Scalable Aero-Load and Aero-Elasticity Solvers for Massively Parallel Heterogeneous Computing Architectures (Phase I)*
Source of Support: Air Force Office of Scientific Research Small Business Technology Transfer Program (AFOSR SBTT) Program: Highly Scalable Computational-Based Engineering Algorithms for Emerging Parallel Machine Architectures (Topic BT13)
Total Amount: \$200,000 (\$59,997 at University of Delaware), PI. Collaborative research with Eric Kelmelis, EM Photonics
Project Period: 03/01/2012 – 03/01/2013
Location of Project: University of Delaware
Description: This award supports the development of innovative algorithms for scientific computing, modeling, and simulation in a multi-GPU environment with an emphasis on parallelization of scientific applications across multiple GPUs.

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- 2010 *Collaborative Research: CDI-Type II: From Data to Knowledge: The Quake-Catcher Network*
Source of Support: National Science Foundation #1027807
Total Amount: \$1,841,104 (\$101,513 at University of Delaware), PI. Collaborative research with Jesse F. Lawrence, Stanford University; Elizabeth S. Cochran, University of California, Riverside; Richard Allen, University of California, Berkeley; Jack Baker, Stanford University; Tomas Heaton, California Institute of Technology; Deborah Kilb, Scripps Institution of Oceanography
Project Period: 10/01/2010 – 09/30/2014
Location of Project: University of Delaware
Description: This award develops Volunteer Computing cyber-infrastructures to process and analyze large new seismic data sets in near-real time and to foster collaboration between thousands of researchers and interested participants around the world.
Supplement: NSF REU, \$7,500, Fall 2011; NSF REU, \$6,000, Fall 2013
- 2010 *Collaborative Research: SoCS - ExSciTecH: An Interactive, Easy-to-Use Volunteer Computing System to Explore Science, Technology, and Health*
Source of Support: National Science Foundation #0968350
Total Amount: \$683,199 (\$308,719 at University of Delaware), Leading PI. Collaborative research with Garry M. Zoppetti, Millersville University and Johan Cohoon, University of Virginia
Project Period: 09/01/2010 – 08/31/2014
Location of Project: University of Delaware
Description: This award supported the development of interactive methods for engaging new communities as volunteer citizen-scientists and building a mutually beneficial infrastructure for their interaction with professional scientists working on volunteer computing projects in biology and medicine.
Supplement: NSF REU, \$7,500, Summer 2012; NSF REU, \$7,500, Summer 2011
- 2010 *Collaborative Research: Accelerated Linear Algebra Solvers for Multi-Core GPU-Based Computing Architecture*
Source of Support: Air Force Office of Scientific Research Small Business Technology Transfer Program (AFOSR SBTT) program - Highly-Scalable Computational-Based Engineering Algorithms for Emerging Parallel Machine Architectures (Topic BT13)
Total Amount: \$99,000 (\$34,125 at University of Delaware), PI. Collaborative research with Eric Kelmelis, EM Photonics
Project Period: 06/08/2010 – 06/07.2011
Location of Project: University of Delaware
Description: This award supports the development of innovative algorithms for scientific computing, modeling, and simulation on a multi-GPU environment with an emphasis on algorithms related to sparse and dense linear algebra problems.

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- 2010 *ExSciTech: An Interactive, Easy-to-Use Volunteer Computing System to Explore Science, Technology, and Health*
Source of Support: University of Delaware Research Foundation
Total Amount: \$35,000, Single PI
Project Period: 06/01/2010 – 05/31/2012
Location of Project: University of Delaware
Description: This seed award aims to build an interactive, easy-to-use VC system to explore science, technology, and health that motivates and facilitates diverse volunteers to donate their resources to VC projects, thereby aiding scientific discovery.
Supplement: University of Delaware Research Foundation REU, \$3,500, single PI, Summer 2011
- 2009 *CDI-Type I: Bridging the Gap Between Next-Generation Hybrid High Performance Computers and Physics Based Computational Models for Quantitative Description of Molecular Recognition*
Source of Support: National Science Foundation #0941318
Total Amount: \$538,740, co-PI. Collaborative research with Sandeep Patel, University of Delaware
Project Period: 10/01/2009 – 09/30/2013
Location of Project: University of Delaware
Description: This project designs and implements advanced algorithms and middleware packages for polarizable force fields on multicore and GPU systems supported by the MapReduce paradigm.
- 2009 *Acquisition of a Facility for Computational Approaches to Molecular-Scale Problems*
Source of Support: National Science Foundation #0922657
Total Amount: \$451,051, Co-PIs: Douglas Doren, University of Delaware; Sandeep Patel, University of Delaware; and Dionisios Vlachos, University of Delaware
Project Period: 09/15/2009 – 09/14/2012
Location of Project: University of Delaware
Description: This award supports the acquisition of a hybrid-computing cluster, with GPU- accelerated computing nodes, for theoretical and experimental researchers at the University of Delaware to study a number of problems in chemical sciences.
- 2009 *Computer-Aided Design for Drugs on Emerging Hybrid High Performance Computers*
Source of Support: Army Research Office #54723-CS
Total Amount: \$306,750, single PI
Project Period: 06/01/2009 – 05/31/2013
Location of Project: University of Delaware
Description: This project developed accurate and efficient protein-ligand docking applications for hybrid computer systems in HPC, including multicore architectures and GPGPUs.
Supplements: ARO Undergraduate Research Program, \$3,750, single PI, Summer 2012; ARO High School Apprenticeship Program, \$3,000, single PI, Summer 2010

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- 2009 *CRA Mentor, Distributed Mentor Project for Undergraduate Summer Research*
Source of Support: Computing Research Association (CRA)
Total Amount: \$6,000, single PI
Total Project Period: 06/01/2009 – 08/31/2000
Location of Project: University of Texas El Paso
Description: This project supports 2 undergraduate students for 10 weeks of research under my supervision. The research targets biological applications and their efficient migration to distributed systems.
- 2008 *Collaborative Research: Mathematical Models for RNA*
Source of Support: National Science Foundation #0800266
Total Amount: \$621,193 (\$205,561 at University of Delaware). Co-PIs: Ming-Ying Leung, University of Texas El Paso and Kyle L. Johnson, University of Texas El Paso
Project Period: 06/01/2008 – 05/31/2012
Location of Project: University of Delaware
Description: This project develops probabilistic models to study the inversion distribution in RNA sequences and to combine the results with the general theory of excursions in order to maximize the prediction accuracy using an optimal RNA segment length. My group addresses the computational component with grid computing systems.
- 2008 *CRA Mentor, Distributed Mentor Project for Undergraduate Summer Research*
Source of Support: Computing Research Association (CRA)
Total Amount: \$6,000, single PI
Total Project Period: 06/01/2008 – 08/31/2008
Location of Project: University of Texas El Paso
Description: This project supports 2 undergraduate students for 10 weeks of research under my supervision. The research targets biological applications and their efficient migration to distributed systems.
- 2007 *Computational Prediction of RNA Viral Genome Structures*
Source of Support: National Institute of Health (NIH)
Total Amount: \$581,329, co-PI. Collaborative research with Ming-Ying Leung, University of Texas El Paso
Project Period: 09/01/2007 – 08/31/2011
Location of Project: University of Texas El Paso
Description: This project designed and implemented mathematical methods and computation tools for RNA secondary structure prediction in viral genomics.

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- 2006 *S-STEM - SHiPPER: Spreading High Performance Computing Participation in Undergraduate Education and Research*
Source of Support: National Science Foundation #0631168
Total Amount: \$275,856, Leading PI. Collaborative research with Patricia Teller, University of Texas El Paso
Project Period: 10/01/2006 – 01/31/2011
Location of Project: University of Texas El Paso
Description: The award creates and consolidates a community of undergraduate and graduate students pursuing advanced degrees in fields that combine expertise in high-performance computing and other scientific and engineering disciplines.
- 2006 *RNA Secondary Structure Prediction Using a Grid of Heterogeneous Computers*
Source of Support: Texas Higher Education Coordinating Board, Advanced Research Program #003661-0008-2006
Total Amount: \$99,982. Co-PI: Min-Ying Leung, University of Texas El Paso
Total Project Period: 05/15/2006 – 05/14/2008
Location of Project: University of Texas El Paso
Description: This project builds an adaptive grid computing system that, at runtime, identifies and exploits computer resources across the University of Texas at El Paso campus to predict secondary structures of large numbers of RNA segments using a variety of prediction programs.
- 2006 *Collaborative Research: DAPLDS: a Dynamically Adaptive Protein-Ligand Docking System based on Multi-Scale Modeling*
Source of Support: National Science Foundation #0506429/#0802650
Total Amount: \$1,220,036 (\$382,558 at University of Delaware and \$273,068 at University of Texas El Paso). Co-PIs: Charles L. Brooks III, The Scripps Research Institute (TSRI) and D.P. Anderson, University of California Berkeley
Project Period: 09/01/2005 – 08/31/2009
Location of Project: University of Delaware and University of Texas El Paso
Description: This project explores the multiscale nature of algorithmic adaptations in protein- ligand docking and development of cyber-infrastructures based on computational methods and models that efficiently accommodate these adaptations.
Supplement: NSF REU, \$6,250, Summer 2009
- 2005 *High Performance Modular FEM/hp-FEM System (HERMES)*
Source of Support: University of Texas El Paso Seed Funds
Total Amount: \$23,400, Co-PI. Collaborative research with Pavel Solin
Total Project Period: 06/01/2005 – 08/31/2005
Location of Project: University of Texas El Paso
Description: This project studies feasibility of parallelization of FEM algorithms.

2005

Performance via Autonomicity, Analysis, Virtualization, and Micro-partitioning, and Research in Life Sciences and Bioinformatics

Source of Support: 2005 IBM Global University Program Shared University Research Award

Total Amount: \$600,000, co-PI. Collaborative research with Patricia Teller

Total Project Period: 05/2005

Location of Project: University of Texas El Paso

Description: The award enables the purchase of a supercomputer for biology and bioinformatics applications at University of Texas El Paso.

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BOOK CHAPTERS

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- [1] Ricardo M Llamas, Leobardo Valera*, Paula Olaya+, **Michela Taufer**, and Rodrigo Vargas. Downscaling Satellite Soil Moisture using a Modular Spatial Inference Framework. *Remote Sensing in Geology, Geomorphology and Hydrology*, 2022. (Accepted).
- [2] Tu Mai Anh Do, Loïc Pottier, Rafael Ferreira da Silva, Silvina Caíno-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)*, 2022. (Accepted).
- [3] Ariel Keller Rorabaugh*, Silvina Cano-Lores*, Travis Johnston, and **Michela Taufer**. Building High-throughput Neural Architecture Search Workflows via a Decoupled Fitness Prediction Engine. *IEEE Trans. Parallel Distributed Syst. (TPDS)*, 33(11):2913–2926, 2022.
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- [6] Nigel Tan+, Robert Bird, Guangye Chen, Scott V. Luedtke, Brian Albright, and **Michela Taufer**. Analysis of Vector Particle-In-Cell (VPIC) Memory Usage Optimizations on Cutting-Edge Computer Architectures. *Journal of Computational Science*, 60:101566, 2022.
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- [98] Bennet Uk, **Michela Taufer**, Thomas Stricker, Giovanni Settanni, Andrea Cavalli, and Amedeo Caflisch. Combining Task- and Data Parallelism to Speed up Protein Folding on a Desktop Grid Platform. In *Proceedings of the 3rd IEEE International Symposium on Cluster Computing and the Grid (CCGrid)*, pages 240–247, Tokyo, Japan, May 2003. IEEE Computer Society. (*Acceptance Rate: 39/114, 34.2%*).
- [99] **Michela Taufer** and Thomas Stricker. A Performance Monitor Based on Virtual Global Time for Clusters of PCs. In *Proceedings of the 2003 IEEE International Conference on Cluster Computing (CLUSTER)*, pages 64–72, Kowloon, Hong Kong, China, December 2003. IEEE Computer Society. (*Acceptance Rate: 48/164, 29.3%*).

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- [100] Bennet Uk, **Michela Taufer**, Thomas Stricker, Giovanni Settanni, and Andrea Cavalli. Implementation and Characterization of Protein Folding on a Desktop Computational Grid - Is CHARMM a Suitable Candidate for the United Devices MetaProcessor? In *Proceedings of the 17th International Parallel and Distributed Processing Symposium (IPDPS)*, pages 50–, April, Nice, France 2003. IEEE Computer Society. (*Acceptance Rate: 119/407, 29.2%*).
- [101] **Michela Taufer**, Thomas Stricker, Gerard Roos, and Peter Güntert. On the Migration of the Scientific Code Dyana from SMPs to Clusters of PCs and on to the Grid. In *Proceedings of the 2nd IEEE International Symposium on Cluster Computing and the Grid (CCGrid)*, pages 93–101, Berlin, Germany, May 2002. IEEE Computer Society. (*Acceptance Rate: 25.0%*).
- [102] **Michela Taufer**, Egon Perathoner, Andrea Cavalli, Amedeo Caflisch, and Thomas Stricker. Performance Characterization of a Molecular Dynamics Code on PC Clusters: Is There Any Easy Parallelism in CHARMM? In *Proceedings of the 16th International Parallel and Distributed Processing Symposium (IPDPS)*, Fort Lauderdale, FL, USA, April 2002. IEEE Computer Society. (*Acceptance Rate: 98/258, 38%*).
- [103] **Michela Taufer**, Thomas Stricker, and Roger Weber. Scalability and Resource Usage of an OLAP Benchmark on Clusters of PCs. In *Proceedings of the Fourteenth Annual ACM Symposium on Parallel Algorithms and Architectures (SPAA)*, pages 83–94, Winnipeg, Manitoba, Canada, August 2002. ACM.
- [104] **Michela Taufer** and Thomas Stricker. Accurate Performance Evaluation, Modelling and Prediction of a Message Passing Simulation Code based on Middleware. In *Proceedings of the ACM/IEEE Conference on Supercomputing (SC)*, pages 52–, Orlando, FL, USA, November 1998. IEEE Computer Society.
- [105] Peter Arbenz, Martin Billeter, Peter Güntert, Peter Luginbühl, **Michela Taufer**, and Urs von Matt. Molecular Dynamics Simulations on Cray Clusters using the SCIDDLE-PVM Environment. In *Proceedings of the Parallel Virtual Machine - EuroPVM'96, Third European PVM Conference*, volume 1156 of *Lecture Notes in Computer Science*, pages 142–149, München, Germany, October 1996. Springer.

REPORTS

- [1] Connor Scully-Allison, Ian Lumsden, Katy Williams, Jesse Bartels, **Michela Taufer**, Stephanie Brink, Abhinav Bhatele, Olga Pearce, and Katherine E. Isaacs. Designing an Interactive, Notebook-Embedded, Tree Visualization to Support Exploratory Performance Analysis. *CoRR*, abs/2205.04557, 2022.
- [2] Ria Patel, Brandan Roachell, Silvina Caíno-Lores, Ross Ketron, Jacob Leonard, Nigel Tan, Duncan A. Brown, Ewa Deelman, and **Michela Taufer**. Reproducibility of the First Image of a Black Hole in the Galaxy M87 from the Event Horizon Telescope (EHT) Collaboration. *CoRR*, abs/2205.10267, 2022.
- [3] Ariel Keller Rorabaugh, Silvina Caíno-Lores, Michael R. Wyatt II, Travis Johnston, and **Michela Taufer**. Peng4nn: An accurate performance estimation engine for efficient automated neural network architecture search. *CoRR*, abs/2101.04185, 2021.
- [4] Robert F. Bird, Nigel Tan, Scott V. Luedtke, Stephen Lien Harrell, **Michela Taufer**, and Brian J. Albright. VPIC 2.0: Next generation particle-in-cell simulations. *CoRR*, abs/2102.13133, 2021.

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- [5] Mark Asch, François Bodin, Micah Beck, Terry Moore, **Michela Taufer**, and Jean-Pierre Vilotte. Cybercosm: New foundations for a converged science data ecosystem. *CoRR*, abs/2105.10680, 2021.
 - [6] Paula Olaya, Jay F. Lofstead, and **Michela Taufer**. Building containerized environments for reproducibility and traceability of scientific workflows. *CoRR*, abs/2009.08495, 2020.
 - [7] Duncan A. Brown, Karan Vahi, **Michela Taufer**, Von Welch, and Ewa Deelman. Reproducing GW150914: the first observation of gravitational waves from a binary black hole merger. *CoRR*, abs/2010.07244, 2020.
 - [8] Joshua Hoke Davis, Tao Gao, Sunita Chandrasekaran, and **Michela Taufer**. Studying the impact of power capping on mapreduce-based, data-intensive mini-applications on intel KNL and KNM architectures. *CoRR*, abs/1903.11694, 2019.
 - [9] Dylan Chapp, Danny Rorabaugh, Duncan A. Brown, Ewa Deelman, Karan Vahi, Von Welch, and **Michela Taufer**. Applicability study of the PRIMAD model to LIGO gravitational wave search workflows. *CoRR*, abs/1904.05211, 2019.
 - [10] Danny Rorabaugh, Mario Guevara, Ricardo M. Llamas, Joy Kitson, Rodrigo Vargas, and **Michela Taufer**. SOMOSPIE: A modular soil moisture spatial inference engine based on data driven decision. *CoRR*, abs/1904.07754, 2019.
 - [11] Travis Johnston, Boyu Zhang, Adam Liwo, Silvia Crivelli, and **Michela Taufer**. It-situ data analysis of protein folding trajectories. *CoRR*, abs/1510.08789, 2015.

POSTERS AND ABSTRACTS

- [1] Silvina Caino-Lores, Michel Cuendet, Trilce Estrada, Ewa Deelman, Harel Weinstein, and **Taufer, Michela**. High-Throughput In-Situ Workflows for Ensemble Molecular Dynamics. In *Proceedings of the 18th IEEE International Conference on e-Science (eScience)*, pages 1–1, Salt Lake City, Utah, USA, October 2022. IEEE Computer Society.
- [2] Nauweiluo Zhou, Jakob Luettgau, Rahul Reddy Kancharla, Joshua Kane, Brendan Croom, Robert Wheeler, Pania Newell, Giorgio Scorzelli, Valerio Pascucci, and **Taufer, Michela**. A Software Framework for Scientific Workflow Orchestration at Large Scale. In *Proceedings of the 18th IEEE International Conference on e-Science (eScience)*, pages 1–1, Salt Lake City, Utah, USA, October 2022. IEEE Computer Society.
- [3] Jakob Luettgau, Giorgio Scorzelli, Nauweiluo Zhou, Glenn Tarcea, Jay Lofstead, Valerio Pascucci, and **Taufer, Michela**. Toward a Lightweight Indexing Service for the National Science Data Fabric. In *Proceedings of the 18th IEEE International Conference on e-Science (eScience)*, pages 1–1, Salt Lake City, Utah, USA, October 2022. IEEE Computer Society.
- [4] Clark Hathaway, Sebastian Mobo, Silvina Caíno-Lores, Travis Johnston, and **Michela Taufer**. A Framework for Linking Urban Traffic and Vehicle Emissions in Smart Cities. In *Poster at the 33rd ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. IEEE Computer Society, November 2020. (*Best UG Poster Candidate*).
- [5] Ian Lumsden, Stephanie Brink, Michael R. Wyatt II, Todd Gamblin, and **Michela Taufer**. Enabling Graph-Based Profiling Analysis using Hatchet. In *Poster at the 33rd ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. IEEE Computer Society, November 2020. (*Best UG Poster*).

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- [6] Nigel Tan, Robert F. Bird, and **Michela Taufer**. Optimizing Vector Particle-In-Cell (VPIC) for Memory Constrained Systems Using Half-Precision. In *Poster at the 33rd ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. IEEE Computer Society, November 2020. (*Best Graduate Poster Candidate*).
 - [7] Paula Olaya, Jay Lofstead, and **Michela Taufer**. Containerized Environment for Reproducibility and Traceability of Scientific Workflows. In *Poster at the 33rd ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. IEEE Computer Society, November 2020.
 - [8] Paula Olaya, Michael Wyatt, Silvina Caino-Lores, Piotr Luszczek, Osamu Miyashita, Florence Tama, and **Michela Taufer**. XPSI: XFEL-based Protein Structure Identifier. In *Poster at the 33rd ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. IEEE Computer Society, November 2020.
 - [9] Nigel Tan, **Michela Taufer**, Scott Luedtke, Robert Bird, and Brian Albright. Expanding VPIC Portability to Large Scale GPU Systems. In *Abstract in Proceedings of the 62nd Annual Meeting of the APS Division of Plasma Physics*. IEEE Computer Society, November 2020.
 - [10] Rodrigo M Llamas, Mario Guevara, Danny Rorabaugh, **Michela Taufer**, and Rodrigo Vargas. Large-Scale Soil Moisture Modeling Based on Linear Geostatistics and Remotely Sensed Data. In *Abstract in AGU 100 – Advanced Earth and Space Science – Fall Meeting*, Washington DC, USA, December 2018. IEEE Computer Society.
 - [11] Dylan Chapp, Danny Rorabaugh, and **Michela Taufer**. Modeling Record-and-Replay for Non-deterministic Applications on Exascale Systems. In *Poster at ModSim 2018: Workshop on Modeling simulation of Systems and Applications*, Seattle, WA, USA, August 2018.
 - [12] Robert Searles, Stephen Herbein, Travis Johnston, **Michela Taufer**, and Sunita Chandrasekaran. Creating a Portable, High- Level Graph Analytics Paradigm For Compute and Data-Intensive Applications. In *Poster in 2018 GPU Technology Conference (GTC)*, San Jose, CA, USA, March 2018.
 - [13] S. Herbein, T. Patki, D. H. Ahn, D. Lipari, T. Dahlgren, D. Domyancic, and **Michela Taufer**. Fully Hierarchical Scheduling: Paving the Way to Exascale Workloads. In *Poster at the 29th ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*, Denver, CO, USA, November 2017. IEEE Computer Society. (*Best Poster Candidate*).
 - [14] S. Herbein, M. Matheny, M. Wezowicz, J. Kroger, J.S. Logan, J. Kim, S. Klasky, and **Michela Taufer**. Predictions of Large-scale QMCPack I/Os on Titan using Skel. In *Poster at the 24th ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*, Denver, CO, USA, November 2013. IEEE Computer Society. (*Acceptance Rate: 40%*).
 - [15] M. Wezowicz and **Michela Taufer**. On the Cost of a General GPU Framework - The Strange Case of CUDA 4.0 vs. CUDA 5.0. In *Poster at the 23th ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. IEEE Computer Society, November 2012. (*Acceptance Rate: 47%*).
 - [16] T. Estrada, K. Pusecker, M. Torres, J. Cohoon, and **Michela Taufer**. Benchmarking Gender Differences in Voluntary Computer Projects. In *Poster at 2012 Grace Hopper Celebration of Women in Computing (GHC12)*, Baltimore, Maryland, USA, October 2012.

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- [18] T. Estrada, B. Zhang, R.S. Armen, and **Michela Taufer**. Study of Protein-ligand Binding Geometries using a Scalable and Accurate Octree-based Algorithm in MapReduce. In *Poster at the 21th ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*, Seattle, Washington, USA, November 2011. IEEE Computer Society. (Acceptance Rate: 40%).
- [19] O. Rahaman, R. Armen, T. Estrada, D. Doren, **Michela Taufer**, and C. L. Brooks III. Binding Free Energy Prediction by Molecular Dynamics Based Docking and Volunteer Computing. In *Poster at Division of Computers in Chemistry for the 238th ACS National Meeting*, Washington, DC, USA, August 2009. IEEE Computer Society.
- [20] N. Ganesan, S. Patel, and **Michela Taufer**. Simulations of Large Membrane Regions using GPU-enabled Computations - Preliminary Results. In *Poster at the 2010 Symposium on Application Accelerators in High Performance Computing (SAAHPC)*, Knoxville, Tennessee, USA, July 2010.
- [21] L. Xu, S. Collin, **Michela Taufer**, and D.G. Vlachos. Parallelization of Tau-Leaping Coarse-Grained Monte Carlo Method for Efficient and Accurate Simulations on GPUs. In *Poster at the 19th ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*, Portland, Washington, USA, November 2009. IEEE Computer Society.
- [22] K.S. Hogle, J.H. Upton, A. Licon, M.-Y. Leung, **Michela Taufer**, and K.L. Johnson. Role of RNA secondary structure in replication of Nodamura virus RNA2. In *Poster at the 27th Annual Meeting of American Society for Virology*, Cornell University, Ithaca, NY, USA, July 2008. IEEE Computer Society.
- [23] T. Estrada, **Michela Taufer**, and K. Reed. Performance analysis of Volunteer Computing Trace. In *Poster at the ACM/IEEE International Conference for High Performance Computing, Network, Storage, and Analysis conference (SC)*, Reno, Nevada, USA, November 2007. IEEE Computer Society. (Acceptance Rate: 24.5%).
- [24] David A. Flores, Trilce Estrada, **Michela Taufer**, Patricia J. Teller, and Andre Kerstens. SimBA: a discrete event simulator for performance prediction of volunteer computing projects. In *Poster at the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*, Tampa, FL, USA, November 2006. IEEE Computer Society.
- [25] C. An, **Michela Taufer**, and C.L. Brooks III. Predictorhome: A Multiscale, Distributed Approach for Protein Structure Prediction. In *Poster at 229th ACM National Meeting*, San Diego, California, USA, March 2005. IEEE Computer Society.
- [26] C. An, **Michela Taufer**, and C.L. Brooks III. Predictorhome: A Multiscale, Distributed Approach for Protein Structure Prediction. In *Poster at 6th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP6)*, Gaeta, Italy, December 2004.
- [27] Matthew Wezowicz and **Michela Taufer**. On the Cost of a General GPU Framework: The Strange Case of CUDA 4.0 vs. CUDA 5.0. In *Poster at the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*, pages 1535–1536, Salt Lake City, UT, USA, November 10-16 2012. IEEE Computer Society. (Best UG Poster Candidate).

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- [28] Trilce Estrada, Boyu Zhang, Pietro Cicotti, Roger S. Armen, and **Michela Taufer**. Study of Protein-ligand Binding Geometries using a Scalable and Accurate Octree-based Algorithm in MapReduce. In *Poster at the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*, pages 39–40, Seattle, WA, USA, November 12-18 2011. ACM.

THESIS

- [1] **Michela Taufer**. *Inverting Middleware: Performance Analysis of Layered Application Codes in High Performance Distributed Computing*. PhD thesis, ETH Zurich, 2002.
- [2] **Michela Taufer**. *Development of the Parallelization of the Software Package OPAL for the Simulation of Dynamic Molecules on Supercomputers*. Master’s thesis, University of Padova, 1996.

PATENTS

System and Methods for Graphic Encoding of Macromolecules for Efficient High-Throughput Analysis
UNMRI Ref. No. 2018-036-03.

TALKS

KEYNOTES

- Dec 2022* In Situ Data Analytics For Next Generation Molecular Dynamics Workflows. 15 IEEE/ACM International Conference on Utility and Cloud Computing (UCC2022), Portland, OR, USA.
- Sep 2022* Studying Degree And Sources Of Non-Determinism In MPI Applications Via Graph Kernels. Latin America High Performance Computing Conference (CARLA), Porto Alegre, RS, Brazil.
- Sep 2022* In Situ Data Analytics For Next Generation Molecular Dynamics Workflows. Parallel Processing and Applied Mathematics (PPAM), Gdańsk, Poland.
- Dec 2021* AI4IO: A Suite of AI-based Tools For IO-aware HPC Resource Management. International Conference on High Performance Computing, Data and Analytics (HiPC) – Virtual conference.
- Oct 2021* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. Seventh International Conference on Big Data and Information Analytics (BigDIA 2021). October 29-31, 2021. Chongqing, China – Virtual conference.
- Oct 2021* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD). Oct 26-29, 2021 – Virtual conference.
- Feb 2021* AI4IO: A Suite of AI-based Tools For IO-aware HPC Resource Management. First International Symposium on Checkpointing for Supercomputing (SuperCheck) – Virtual conference.
- Nov 2020* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. Fifteen Workshop on Workflows in Support of Large-Scale Science (WORKS) – Virtual conference.
- May 2020* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. EuroGraphics Symposium on Parallel Graphics and Visualization – Virtual conference.
- Dec 2019* Scientific Applications and Heterogeneous Architectures – Data Analytics and the Intersection of HPC and Edge Computing. Thirteenth CHPC National Conference, Johannesburg, South Africa.
- Aug 2019* Scientific Applications and Heterogeneous Architectures – Data Analytics and the Intersection of HPC and Edge Computing. EuroPar Conference, Göttingen, Germany.
- May 2018* Modeling the Next-Generation High Performance Schedulers. ACM Conference on Principles of Advanced Discrete Simulation (PADS), Rome, Italy.
- Feb 2018* Building the next Generation of MapReduce Programming Models over MPI to Fill the Gaps between Data Analytics and Supercomputers. Ninth International Workshop on Programming Models and Applications for Multicores and Many-cores (PMAM), Vosendorf, Austria.

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- Sep 2017* Building the next Generation of MapReduce Programming Models over MPI to Fill the Gaps between Data Analytics and Supercomputers. Keynote at the EuroMPI/USA 2017 Conference, Chicago, IL, USA.
- Sep 2017* Challenges in Big Data Computing on HPC Platforms. Parallel Processing and Applied Mathematics (PPAM), Lublin, Poland.
- Sep 2016* Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. IEEE Cluster Conference, Taipei, Taiwan.
- Jun 2016* Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. Keynote at the 7th Workshop on Scientific Cloud Computing (ScienceCloud), Kyoto, Japan.
- May 2015* The Numerical Reproducibility Fair Trade: Facing the Concurrency Challenges at the Extreme Scale. Fifth International Workshop on Accelerators and Hybrid Exascale Systems (AsHES), Hyderabad, India.

INVITED TALKS

- Sep 2022* The Curious Case of Reproducing Scientific Results about Black Holes. Workshop on Clusters, Clouds, and Data for Scientific Computing (CCDSC). Chemin de Chanzé, France.
- Jul 2022* The Curious Case of Reproducing Scientific Results about Black Holes. High Performance Computing Conference 2022, Cetraro, Italy.
- Jul 2022* A Containerized Environment for Reproducibility and Traceability of Scientific Workflows. 2022 IEEE World Congress on SERVICES - Hybrid conference.
- Jun 2022* AI4IO: A Suite of AI-Based Tools for IO-Aware HPC Resource Management. Sparse Days 2022, Saint-Girons, Ariège, France.
- Oct 2021* AI4IO: A Suite of AI-Based Tools for IO-Aware HPC Resource Management. Seminar at the Università della Svizzera Italiana – Virtual seminar.
- Sep 2020* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. SIGHPC ASCAN Chapter Seminar – Virtual seminar.
- Sep 2020* AI4IO: A Suite of AI-Based Tools for IO-Aware HPC Resource Management. Joint Laboratory for Extreme Scale Computing (JLESC) Workshop – Virtual workshop.
- Jul 2020* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. IBM TJ Watson – Virtual seminar.
- Feb 2020* Cyberinfrastructure Tools for Precision Agriculture in the 21st Century. NSF CSSI PI Meeting. Seattle, WA, USA.
- Feb 2020* Transparency and Reproducibility: Case Studies, Formalisms, and Structured Guidance in Scientific Applications at Scale. SIAM Conference on Parallel Processing for Scientific Computing (PP20), February 12-15, 2020, Seattle, Washington. USA.
- Nov 2019* Algorithms for In Situ Data Analytics of Next Generation Molecular Dynamics Workflows. 5th International Workshop on Data Analysis and Reduction for Big Scientific Data (DRBSD-5), Denver, CO, USA.

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- Oct 2019* PRIONN: Predicting Runtime and I/O using Neural Networks. Big Data and Extreme-scale Computing Workshop, San Diego, CA, USA.
- Sep 2019* Scientific Applications and Heterogeneous Architectures – Data Analytics and the Intersection of HPC and Edge Computing. IEEE eScience Conference, San Diego, CA, USA.
- Jul 2019* Scientific Applications and Heterogeneous Architectures – Data Analytics and the Intersection of HPC and Edge Computing. Argonne Training Program on Extreme-Scale Computing, Chicago, IL. USA.
- Jul 2019* Convergence of Data Generation and Analytics in the Era of Heterogeneous Applications and Edge Computing. Sandia National Laboratories, Albuquerque, NM, USA.
- Jun 2019* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. HPC ISC Conference, Frankfurt, Germany.
- Apr 2019* Convergence of Data Generation and Analytics in the Era of Heterogeneous Applications and Edge Computing. DoE Salishan Conference on High Speed Computing, Salishan, Oregon.
- Apr 2019* Characterization of Power and Performance in Data-Intensive Applications using MapReduce over MPI. Joint Laboratory for Extreme Scale Computing (JLESC) Workshop, Knoxville, USA.
- Apr 2019* Algorithms for In Situ Data Analytics of Next Generation Molecular Dynamics Workflows. Numerical Algorithms for High-Performance Computational Science Workshop, The Royal Society, London, UK.
- Mar 2019* Filling the Gaps between Data Analytics and High Performance Computing with (some help from) MPI. Inaugural MPI-Beyond Workshop, University of Tennessee Chattanooga, Chattanooga, Tennessee, USA.
- Feb 2019* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. Minisymposium on "Computational Tools and Precision Medicine," SIAM CSE, Spokane, Oregon, USA.
- Feb 2019* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. Big Data and Extreme-scale Computing Workshop, Kobe, Japan.
- Nov 2018* PRIONN: Predicting Runtime and IO using Neural Networks and GPUs. NVIDIA booth at SC18. Dallas, Texas, USA.
- Oct 2018* Cyberinfrastructure Tools for Precision Agriculture in the 21st Century. Big Data and Extreme-scale Computing Workshop, Indiana University, Bloomington, Indiana, USA.
- Sep 2018* Modeling Record-and-Replay Costs for Nondeterministic Applications on Exascale Systems. Clusters and Computational Data for Scientific Computing Workshop, Lyon, France.
- Aug 2018* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. Los Alamos National Laboratory, USA.

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- Jul 2018* Challenges in Big Data Analytics on High Performance Computing Systems. 13th Scheduling for Large Scale Systems Workshop, Cetraro, Italy.
- Jul 2018* Building the Next-Generation HPC Schedulers. 13th Scheduling for Large Scale Systems Workshop, Cetraro, Italy.
- Jun 2018* Building the Next-Generation HPC Schedulers. HPC ISC Conference, Frankfurt, Germany.
- Jun 2018* Modeling the Next-Generation HPC Batch-Job Schedulers. 13th Scheduling for Large Scale Systems Workshop. Lawrence Berkeley National Laboratory, Berkeley, CA, USA.
- May 2018* Convergence Opportunities and Limits in Big Data and Simulations. Workshop on Converging Simulation and Data-Driven Science. National Academy of Sciences, Engineering, and Medicine. Washington, D.C., USA.
- Mar 2018* Transitioning Data Analytics of MD Simulations Toward the Exascale Era. Session on Data Analytics in HPC: An Applications' Perspective. SIAM Conference on Parallel Processing (SIAM PP), Tokyo, Japan.
- Dec 2017* Challenges in Big Data Analytics on High Performance Computing Systems. Workshop on Data Intensive Computing. Shenzhen Institutes of Advanced Technology. Shenzhen, China.
- Oct 2017* Challenges in Big Data Computing on HPC Platforms. Department of Electrical Engineering and Computer Science, The University of Tennessee at Knoxville, Knoxville, TN, USA.
- Aug 2017* Impacts of Non-determinism on Numerical Reproducibility and Debugging at the Exascale. Analysis and Synthesis of Floating-point Programs Seminar, Dagstuhl, Germany.
- Aug 2017* Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. Information Sciences Institute, Marina del Rey, CA, USA.
- Apr 2017* Leveraging MapReduce and Machine Learning Technologies in Support of Big Data Analytics to Examine Food Nutrient Content. Value Institute, Christina Care Health System. Wilmington, DE, USA.
- Apr 2017* Cyberinfrastructures for Big Data Analytics: Trends and Opportunities. University of Alabama, Birmingham. Birmingham, AL, USA.
- Mar 2017* The Three Rs of Work in Scientific Papers: Repeatability, Replicability, and Reproducibility. High Performance Distributed Computing Technical Program Committee Workshop, Tampa, FL, USA.
- Feb 2017* The Numerical Reproducibility Fair Trade: Facing the Concurrency Challenges at the Extreme Scale. SIAM Conference on Computational Science and Engineering (CSE17), Atlanta, GA, USA.
- Feb 2017* Cyberinfrastructures for Big Data Analytics: Trends and Opportunities. Institute for Financial Services Analytics, University of Delaware, Newark, DE, USA.

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- Nov 2016* The Three Rs of Work in Scientific Papers: Repeatability, Replicability, and Reproducibility. Numerical Reproducibility at Exascale Workshop (NRE2016). In cooperation with SC16, Salt Lake City, UT, USA.
- Nov 2016* Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. ExaIO Workshop. In cooperation with SC16, Salt Lake City, UT, USA.
- Oct 2016* The Numerical Reproducibility Fair Trade: Facing the Concurrency Challenges at the Extreme Scale. 2016 CCL Workshop on Scalable Computing, University of Notre Dame, IN, USA.
- Oct 2016* In-Situ Data Analytics and Indexing of Protein Trajectories. National Supercomputing Center - Guangzhou, Guangzhou, China.
- Oct 2016* In-Situ Data Analytics and Indexing of Protein Trajectories. International Workshop on HPC Architecture, Software, and Application at an Extreme Scale. National Supercomputing Center - Wuxi, Wuxi, China.
- Oct 2016* In Situ Data Analysis of Protein Trajectories. Clusters, Clouds, and Data for Scientific Computing (CCDSC). Chemin de Chanzé, France.
- Aug 2016* In-Situ Data Analytics and Indexing of Protein Trajectories. Lawrence Livermore National Laboratory, Livermore, CA, USA.
- Aug 2016* Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. Research Computing Center Seminar, University of Queensland, Brisbane, Australia.
- Mar 2016* In-Situ Data Analysis of Protein-folding Trajectories. 251st ACS National Meeting & Exposition - Division of Computers in Chemistry: From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules, San Diego, CA, USA.
- Mar 2016* Resource Management for Running HPC Applications in Container Clouds. Recent Advances in HPDC Research Workshop, Pittsburg, PA, USA.
- Mar 2016* Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. Rensselaer Polytechnic Institute, Troy, NJ, USA.
- Dec 2015* In-Situ Data Analysis of Protein-folding Trajectories. University of Queensland, Brisbane, Australia.
- May 2015* Enabling In-situ Analysis of Ligand Geometries in Drug Design Simulations on Supercomputers. 14th Workshop on High Performance Computational Biology, Hyderabad, India.
- Apr 2015* Enabling In-Situ and Scalable Data Analysis of Folding Trajectories on Distributed Memory Systems. Novel Tools in Computational Chemistry Coding (NTC3) Meeting, Rutgers University, Piscataway, NJ, USA.
- Mar 2015* Numerical Reproducibility Challenges on Extreme Scale Multi-threading GPUs. NVIDIA GPU Technology Conference, San Jose, CA, USA.

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- Mar 2015* Enabling Scalable Data Analysis of Large Computational Structural Biology Datasets on Distributed Memory Systems. 2015 Hot Topics in High-Performance Distributed Computing Workshop, IBM Almadena, California, USA.
- Feb 2015* Enabling Scalable Data Analysis of Large Computational Structural Biology Datasets on Distributed Memory Systems. Delaware Bioinformatics Institute, Newark, DE, USA.
- Jan 2015* Enabling Scalable Data Analysis of Large Computational Structural Biology Datasets on Distributed Memory Systems. National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA.
- Oct 2014* Enabling Scalable Data Analysis of Large Computational Structural Biology Datasets on Distributed Memory Systems. Virginia Tech, Blacksburg, VA, USA.
- Oct 2014* Enabling Scalable Data Analysis of Large Computational Structural Biology Datasets on Distributed Memory Systems. Rensselaer Polytechnic Institute (RPI), Troy, NY, USA.
- Sep 2014* Performance and Cost Effectiveness of DAG-based Workflow Executions on the Cloud. Clusters, Clouds, and Data for Scientific Computing (CCDSC). Chemin de Chanzé, France.
- Jul 2014* The Numerical Reproducibility Fair Trade: Facing the Concurrency Challenges at the Extreme Scale. Challenges in 21st Century Experimental Mathematical Computation. Institute for Computational and Experimental Research in Mathematics (ICERM). Providence, RI, USA.
- May 2014* Enabling Scalable Data Analysis of Large Computational Structural Biology Datasets on Distributed Memory Systems. Stony Brook University, Stony Brook, NY, USA.
- Apr 2014* Enabling Scalable Data Analysis of Large Computational Structural Biology Datasets on Distributed Memory Systems. Rutgers University, Piscataway, NJ, USA.
- Mar 2014* Performance Impact of Dynamic Parallelism on Clustering Algorithms on GPUs. NVIDIA GPU Technology Conference, San Jose, CA, USA.
- Mar 2014* Enabling Scalable Data Analysis of Large Computational Structural Biology Datasets on Distributed Memory Systems. University of Chicago, IL, USA.
- Oct 2013* Enabling Scalable I/O and In-situ Analysis in Scientific Simulations at the Petascale. U.S. Army Research Laboratory at the Aberdeen Proving Ground, Aberdeen, MD, USA.
- Sep 2013* On the Effectiveness of Application-aware Self-management for Scientific Discovery in Distributed Systems. ScalPerf '13 - Scalable Approaches to High Performance and High Productivity, Bertinoro, Italy.
- Aug 2013* On the Effectiveness of Application-aware Self-management for Scientific Discovery in Volunteer Computing Systems. The University of Tennessee at Knoxville, Knoxville, TN, USA.

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- Aug 2013* On the Effectiveness of Application-aware Self-management for Scientific Discovery in Volunteer Computing Systems. Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, USA.
- May 2013* A Scalable and Accurate Method for Classifying Protein–ligand Binding Geometries using a MapReduce Approach. Novartis, Boston, MA, USA.
- Mar 2013* Transforming Computing Algorithms and Paradigms in HPC to Enable more Science out of our Day-to-day Simulations, Florida State University, Tallahassee, FL, USA.
- Mar 2013* Application-aware Resource Management in Volunteer Computing. Workshop on Trends in High-Performance Distributed Computing, Rutgers University, Piscataway, NJ, USA.
- Mar 2013* GPU-enabled Studies of Molecular Systems on Keeneland at ORNL - On pursuing high resource utilization and coordinated simulations' progression. NVIDIA GPU Technology Conference, San Jose, CA, USA. (With Sandeep Patel)
- Oct 2012* Transforming Computing Algorithms and Paradigms in HPC to Enable more Science out of our Day-to-day Simulations, Oak Ridge national Laboratory, Oak Ridge, TN, USA.
- Oct 2012* Transforming Computing Algorithms and Paradigms in HPC to Enable more Science out of our Day-to-day Simulations, Argonne National Laboratory, Chicago, IL, USA.
- Jul 2012* Volunteer Computing for Drug Design, UD K-12 Engineering, University of Delaware, Newark, DE, USA.
- May 2012* GPU-enabled Macromolecular Simulation: Challenges and Opportunities. NVIDIA GPU Technology Conference, San Jose, CA, USA. (With Sandeep Patel)
- Mar 2012* GPU-enabled Macromolecular Simulation: Challenges and Opportunities, 2012 HPC Symposium at Lehigh University, Bethlehem, PA, USA.
- Mar 2012* Reengineering High-throughput Molecular Datasets for Scalable Clustering using MapReduce, Workshop on Trends in High-Performance Distributed Computing, Vrije Universiteit, Amsterdam, Netherlands.
- Feb 2012* GPU-enabled Macromolecular Simulation: Challenges and Opportunities, NVIDIA Headquarter, San Jose, CA, USA.
- Dec 2011* GPU-enabled Macromolecular Simulation: Challenges and Opportunities, NVIDIA webinar, San Jose, CA, USA.
- Mar 2011* Enabling Faster Large-Scale Simulations with GPU Programming, Aberdeen Army Research Laboratory, Aberdeen, MD, USA.
- Oct 2010* Enabling Faster Molecular Dynamics Simulations and Protein Motif-Finding with GPU Programming. Enabling Discovery with Dell HPC GPU Solutions, Harvard Medical School, MA, USA.
- Sep 2010* MD Simulations of Large Membranes. NVIDIA GPU Technology Conference, San Jose, CA, USA. (With Sandeep Patel and Narayan Ganesan)

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- Jun 2009* Computational Multi-Scale Modeling in Protein-Ligand Docking. Colloquium at IBM T.J. Watson, York Town, NY, USA.
- Jan 2008* Computational Multi-Scale Modeling in Protein-Ligand Docking. Invited speaker at the 20th Annual CSU Biotechnology Symposium Information, Special Session on Interface between Computer Science and Biotechnology, Oakland CA, USA.
- Apr 2007* DAPLDS: a Dynamically Adaptive Protein-Ligand Docking System based on Multi-Scale Modeling. Invited speaker at the Multiscale Modeling (MSM) PI Consortium Meeting, NIH, Bethesda, MD, USA.
- Mar 2007* Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling. Department Colloquium - Department of Computer Science, Mississippi State University, Starkville, MS, USA.
- Mar 2007* Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling. Department Colloquium - Department of Computer and Information Sciences, University of Delaware, Newark, DE, USA.
- Mar 2007* Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling. Department Colloquium – Department of Computer Science, University of Pittsburgh, Pittsburgh, PA, USA.
- Mar 2007* Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling. Department Colloquium - Department of Computer Science, University of New Mexico, Albuquerque, NM, USA.
- Feb 2007* Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling. Department Colloquium – Department of Computer Science and Engineering, University of South Florida, Tampa, FL, USA.
- Dec 2006* High-Performance Computing: An Increasingly Powerful Tool for Biomedical Science - what can HPC do for Cancer Research? Colloquium - San Antonio Cancer Institute Seminar Series - via AccessGrid.
- Oct 2006* Predictor@Home: A “Protein Structure Prediction Supercomputer Based on Volunteer Computing.” Invited speaker at the 19th Rocky Mountain Regional Meeting of The American Chemical Society, Tucson, AZ, USA.
- Sep 2006* Moving Volunteer Computing Towards Data-Driven, Knowledge-Constructed Capabilities. Department Colloquium – Department of Computer Science at the University of Houston, Houston, TX, USA.
- Apr 2006* Predictor@Home: A “Protein Structure Prediction Supercomputer” Based on Global Computing. Bioinformatics Colloquium – Universality of Texas at El Paso, El Paso, TX, USA.
- Feb 2006* Predictor@Home: A “Protein Structure Prediction Supercomputer” Based on Global Computing. Colloquium – High Performance Computing Center, Texas Tech University, Lubbock, TX, USA.
- Dec 2005* Metrics for Effective Resource Management in Global Computing Environments. Colloquium at National ICT, Australia, Sydney, Australia.

CONFERENCE/WORKSHOPS TALKS

- Sep 2019* Characterization of Power Usage and Performance in Data-Intensive Applications using MapReduce over MPI. International Conference on Parallel Computing (ParCo) 2019 Conference. Prague, Czech Republic.
- Dec 2018* On the Power of Combiner Optimizations in MapReduce over MPI Workflows. In IEEE 24th International Conference on Parallel and Distributed Systems (ICPADS), Singapore.
- Oct 2016* HYPPO: A Hybrid, Piecewise Polynomial Modeling Technique for Non-Smooth Surfaces. 28th IEEE International Symposium on Computer Architecture and High-Performance Computing (SBAC-PAD), Los Angeles, CA, USA.
- Jun 2016* Resource Management for Running HPC Applications in Container Clouds. International Supercomputing Conference (ISC), Frankfurt, Germany.
- Apr 2016* In-Situ Data Analysis of Protein-folding Trajectories. Short talk at the Salishan Conference on High Speed Computing, Gleneden Beach, OR, USA.
- Dec 2015* A Genetic Programming Approach to Design Resource Allocation Policies for Heterogeneous Workflows in the Cloud. 21th IEEE International Conference on Parallel and Distributed Systems (ICPADS), Melbourne, Australia.
- Sep 2015* A Resource-selection Heuristic for High-performance and Cost-effective Workflow Execution on the Cloud. International Conference on Parallel Processing (ICPP), Beijing, China.
- Aug 2015* From HPC Performance to Weather Modeling: Transforming Methods for HPC Predictions Into Models of Extreme Climate Conditions. Tenth IEEE International Conference on e-Science and Grid Technologies (eScience), Munich, Germany.
- May 2015* Accurate Scoring of Drug Conformations at the Extreme Scale. Eight IEEE International Scalable Computing Challenge - Co-located with IEEE/ACM CCGrid, Shenzhen, China.
- Sep 2014* Applying Frequency Analysis Techniques to DAG-based Workflows to Benchmark and Predict Resource Behavior on Non-Dedicated Clusters. IEEE Cluster Conference. Madrid, Spain.
- Jun 2014* Study the Network Impact on Earthquake Early Warning in the Quake-Catcher Network Project. International Conference on Computational Science (ICCS), Cairns, Australia.
- Dec 2013* Performance Impact of I/O on QMCPack Simulations at the Petascale and Beyond. 16th IEEE International Conferences on Computational Science and Engineering (CSE), Sydney, Australia.
- Dec 2013* On Efficiently Capturing Scientific Properties in Distributed Big Data without Moving the Data - A Case Study in Distributed Structural Biology using MapReduce. 16th IEEE International Conferences on Computational Science and Engineering (CSE), Sydney, Australia.

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- Oct 2013* Efficient Sodium dodecyl sulfate (SDS) Simulations on Multi-GPU Nodes of XSEDE High-end Clusters. Eighth IEEE International Conference on e-Science and Grid Technologies (eScience), Beijing, China.
- Oct 2013* Benchmarking Gender Differences in Volunteer Computing Projects. Third Workshop on Analyzing and Improving Collaborative eScience with Social Networks (eSoN). Beijing, China.
- Oct 2012* ExSciTech: Expanding Volunteer Computing to Explore Science, Technology, and Health. Second workshop on Analyzing and Improving Collaborative eScience with Social Networks (eSoN), Chicago, IL, USA.
- Oct 2012* A Modularized MapReduce Framework to Support RNA Secondary Structure Prediction and Analysis Workflows. 2012 Computational Structural Bioinformatics Workshop (CSBW), Philadelphia, PA, USA.
- Sep 2011* Providing Application-Level Quality of Science in Volunteer Computing. 13th IEEE High Performance Computing and Communications (HPCC) Conference, Banff, Canada.
- May 2011* FEN ZI: GPU Enabled Molecular Dynamics Simulation of Large Membrane Regions Based on CHARMM Force Field and PME. Tenth IEEE Workshop on Hi-Performance Computational Biology (HiCOMB), Anchorage, AK, USA.
- May 2011* FEN ZI: GPU Enabled Molecular Dynamics Simulation of Large Membrane Regions Based on CHARMM Force Field and PME. Tenth IEEE Workshop on Hi-Performance Computational Biology (HiCOMB), Anchorage, AK, USA.
- Apr 2010* Improving Numerical Reproducibility and Stability in Large-Scale Numerical Simulations on GPUs. IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS), Atlanta, GA, USA.
- Mar 2007* Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling. First Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), Long Beach, CA, USA.
- Dec 2006* The Effectiveness of Threshold-based Scheduling Policies in BOINC Projects. Second IEEE International Conference on e-Science and Grid Technologies (eScience), Amsterdam, The Netherlands.
- Mar 2006* Web-based Tools to Facilitate Collaboration. International SUN Conference on Teaching and Learning, El Paso, Texas, USA.
- Dec 2005* Metrics for Effective Resource Management in Global Computing Environments. First IEEE International Conference on e-Science and Grid Technologies (e-Science). Melbourne, Australia.
- Apr 2005* Homogeneous Redundancy: a Technique to Ensure Integrity of Molecular Simulation Results Using Public Computing. 14th Heterogeneous Computing Workshop (HCW), Denver, CO, USA.

Apr 2005 Predictor@Home: A "Protein Structure Prediction Supercomputer" Based on Public- Resource Computing. Fourth IEEE International Workshop on High Performance Computational Biology (HiCOMB), Denver, CO, USA.

EXPERT PANELS

Nov 2021 Hierarchical Parallelism for Exascale Computing. Second Workshop on Hierarchical Parallelism for Exascale Computing, hosted the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC21), St. Louis, MO, USA.

Aug 2020 The Future of HPC Systems in the Presence of AI. (Keynote Panel) Smoky Mountains Computational Science and Engineering Conference, Virtual Conference.

Nov 2019 The National Academies' report on Reproducibility and Replicability in Science: Inspirations for the SC Reproducibility Initiative. The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC19), Denver, CO, USA.

Jun 2019 Exascale and Beyond: Challenges in Productive and Sustainable Software. SIGHPC Platform for Advanced Scientific Computing (PASC) Conference. Zurich, Switzerland.

Aug 2018 Skills and Competencies for Modeling and Simulations. ModSim 2018: Workshop on Modeling & simulation of Systems and Applications. Seattle, WA, USA.

Nov 2017 Reproducibility and Uncertainty in High Performance Computing? The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC17), Denver, CO, USA.

Nov 2017 Blurring the Lines: High-End Computing and Data Science. The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC17), Denver, CO, USA.

Sep 2017 MPI on Post-Exascale Systems. EuroMPI/USA 2017 Conference, Chicago, IL, USA. Sep 2016 HPC vs. Big Data: Different Worlds or Common Ground? IEEE Cluster Conference 2016, Taipei, Taiwan.

Feb 2016 Integration with the Scholarly Record: Case Studies and Lessons Learned. Panel moderator in AAAS workshop on Software Reproducibility, Washington DC, USA.

Jun 2008 A Day in the life of a researcher in Graduate School, Academia, and Industry. Panelist at CRA-W/CDC Systems Research Mentoring Workshop, University of Delaware, Newark, Delaware, USA.

Nov 2003 What we DO need to make Desktop Grids a Success in Practice. Panelist in panel discussion: "The Great Academia/Industry Grid Debate", 4th International Workshop on Grid Computing (Grid 2003), Phoenix, Arizona.

MINISYMPOSIUM SPEAKER

Feb 2022 Managing High-Throughput Application Workloads: Findings and Recommendations. Mini-symposium on "A Roadmap to Robust Science for High-throughput Applications: The Developers' Perspective." SIAM Conference on Parallel Processing for Scientific Computing (PP22), February 23-26, 2022, Seattle, WA, USA.

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- Jul 2021* A4MD: In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. Mini-symposium on “Building a Community Roadmap to Robust Science based on Performance Scalability, Trust, and Reproducibility in High-throughput Applications.” Platform for Advanced Scientific Computing (PASC) Conference, July 5-9, 2021. Virtual Event.
- Mar 2021* Reproducibility vs. Scalability in Containerized Workflows – The SOMPOSPIE Use Case. Mini-symposium on “Building a Community Roadmap to Robust Science in High-Throughput Applications.” SIAM Conference on Computational Science and Engineering (CSE21), March 1-5, 2021. Virtual Event.
- Feb 2020* Transparency and Reproducibility: Case Studies, Formalisms, and Structured Guidance in Scientific Applications at Scale. Mini-symposium on “Transparency, Reproducibility, Sustainability, and Security: The Four Pillars of the Next Generation Scientific Software Stack.” SIAM Conference on Parallel Processing for Scientific Computing (PP20), February 12-15, 2020, Seattle, Washington. USA.
- Mar 2019* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. Mini-symposium on “Computational Tools and Precision Medicine.” SIAM Conference on Computational Science and Engineering (CSE18), February 25 – March 1, 2019. Spokane, Oregon, USA

MINISYMPOSIUM ORGANIZER

- Feb 2022* A Roadmap to Robust Science for High-throughput Applications: The Developers’ Perspective. SIAM Conference on Parallel Processing for Scientific Computing (PP22), February 23-26, 2022, Seattle, WA, USA.
- Jul 2021* Building a Community Roadmap to Robust Science based on Performance Scalability, Trust, and Reproducibility in High-throughput Applications. Platform for Advanced Scientific Computing (PASC) Conference, July 5-9, 2021. Virtual Event.
- Mar 2021* Building a Community Roadmap to Robust Science in High-Throughput Applications. SIAM Conference on Computational Science and Engineering (CSE21), March 1-5, 2021. Virtual Event.
- Feb 2020* Transparency, Reproducibility, Sustainability, and Security: The Four Pillars of the Next Generation Scientific Software Stack. SIAM Conference on Parallel Processing for Scientific Computing (PP20), February 12-15, 2020, Seattle, Washington. USA.
- Mar 2018* Data Analytics in HPC: An Applications’ Perspective. SIAM Conference on Parallel Processing for Scientific Computing (PP18), March 7-10, 2018, Waseda University in Tokyo, Japan.

TUTORIALS

- Jul 2019* Introduction of Practical Approaches to Data Analytics for HPC with Spark. ACM Europe Summer School, Barcelona Supercomputer Center – HPC Architectures for AI and Dedicated Applications, Barcelona, Spain. (Half day tutorial)
- Nov 2018* Introduction of Practical Approaches to Data Analytics for HPC with Spark. International Conference for High Performance Computing, Networking, Storage, and Analysis (SC18). (Half day tutorial)

BIRDS OF A FEATHERS (BOFS)

Nov 2015 M. Leaser, D. Ahn, and M. Taufer. Reproducibility of High Performance Codes and Simulations – Tools, Techniques, Debugging. BoF Session at the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2015. Austin, TX, USA.

GROUP MEMBERS

Research Associates

- *Naweiluo Zhou* (Dec 2021 – present)
- *Jakob Luettgau* (Oct 2021 – present)
- *Nick Bell* (Sep 2020 – present)
- *Silvina Caíno-Lores* (Feb 2020 – present)
- *Ariel Rorabaugh* (Oct 2019 – present)

- *Leobardo Valera* (Jan 2020 – Dec 2021)
- *Danny Rorabaugh* (Jan 2018 – Feb 2020)
- *Stephen Thomas* (Aug 2018 – May 2019)
First placement: Engineer at Celgene
- *Wei-Fan Chien* (Sep 2016 – Mar 2017)
- *Travis Johnston* (Sep 2014 – Jul 2016)
First placement: Researcher at Oak Ridge Nat. Lab.
- *Vivek Pallipuram* (Jan 2014 – Jul 2015)
First placement: Assistant Professor at the U. Pacific
- *Samuel Schlachter* (Jun 13 – Jul 14)
First placement: CTO at SNAPCARD, Inc
- *Trilce Estrada* (Jul 2012 – Jul 2013)
First placement: Assistant Professor at U. New Mexico
- *Narayna Ganesan* (Jan 2010 – Jul 2011)
First placement: Assistant Prof. at Stevens I. of Tech.
- *Arun Rajendran* (Apr 2008 – Jul 2008)

Consultants & Associates

- *Grace Wisser* (Sep 2020 – present) Event Coordinator and Journal Manager
- *Barbara Fossum* (Sep 2019 – present) Outreach Coordinator
- *Lauren Whitnah* (Jun 2019 – present) Technical Writer

PhD Students

- *Ian Lumsden* (Aug 2020 – present) Preliminary Research Exam on May 2023
- *Paula Olaya* (Aug 2020 – present) Preliminary Research Exam on May 2022
- *Nigel Tan* (Aug 2019 – present) Preliminary Research Exam on May 2022

- *Dylan Chapp* (UDel graduated, June 2020)
Thesis Title: Modeling Non-Determinism of Scientific Applications. First placement: Software Engineering at Glodon, USA
- *Michael Wyatt* (UDel graduated, June 2020)
Thesis Title: AI4IO: A Suite of AI-Based Tools for IO-Aware HPC Resource Management. First placement: Scientist at LLNL
- *Stephen Herbein* (UDel graduated, August 2018)
Thesis Title: Scalable I/O-Aware Job Scheduling for Burst Buffer Enabled HPC Clusters. First placement: Scientist at LLNL. Award: IEEE TCSC Outstanding PhD Dissertation Award, 2019
- *Sean McDaniel* (UDel graduated, August 2018)
Thesis Title: Computational Steering for Spike-coupled Neuronal Network Simulations on High-performance Computing Resources. First placement: Post-doctoral researcher at John Hopkins

University

- *Boyue Zhang* (UDel graduated, May 2015)
Thesis Title: Enabling Scalable Data Analysis for Large Computational Structural Biology Datasets on Large Distributed Memory Systems supported by the MapReduce Paradigm. First placement: Data analyst at Purdue University
- *Trilce Estrada* (UDel graduated, May 2012)
Thesis Title: On the Effectiveness of Application-aware Self-management for Scientific Discovery on Volunteer Computing System. First placement: Post-doctoral associate at U. Delaware

Research Graduate Students

- *Neil Lindquist* (Aug 2019 – Feb 2020)
- *Joseph Teague* (Aug 2018 – Dec 2019)
- *Mohammad Alsulmi* (Jan 2014 – Dec 2014)
- *Taylor Baldwin* (Jan 2014 – Aug 2014)
- *Marcos Portnoi* (Jan 2013 – Dec 2013)
- *William Killian* (Jun 2011 – May 2012)
- *Omar Padron* (Jun 2011 – May 2012)
- *Maria Ruiz* (Jan 2010 – Dec 2011)
- *Lifan Xu* (Jan 2019 – Dec 2010)
- *Kevin Kreiser* (Jun 2008 – Aug 2009)
- *Obaidur Rahaman* (Jun 2008 – May 2010)
- *James Atlas* (Jun 2008 – Aug 2009)
- *Adnan Ozsoy* (Aug 2008 – Dec 2008)
- *Roberto Araiza* (Jan 2007 – Dec 2007)

MS Students

- *Treece Burgess* (Aug 2021 – present)
- *Vanessa Lama* (May 2021 – present)
- *Kae Suarez* (UTK graduated, May 2022)
- *Paula Olaya* (UTK graduated, May 2020)
Thesis Title: Building containerized environments for reproducibility and traceability of scientific workflows.
- *Rachel Kraft* (UDel graduated, Dec 2018)
- *Dylan Chapp* (UDel graduated, May 2017)
Thesis Title: Study of the Impact of Non-determinism on Numerical Reproducibility and Debugging at the Exascale. First placement: PhD Student, U. Delaware
- *Jeffrey DiMarco* (UDel graduated, May 2017)
First placement: Software developer at Fidessa
- *Abel Licon* (UDel graduated, May 2010)
Thesis Title: RNAVLab 2.0: Combining Web Applications, Grid Computing, and Dynamic Programming to Overcome Resource Limitations in RNA Secondary Structure Analysis. First placement: Researcher at Thermo Fisher Scientific
- *Joseph Davis* (UDel graduated, May 2009)
Co-advised with Sandeep Patel. First placement: Scientist Siemens Healthcare
- *Prayook Tungjatoornrusame* (UTEP graduated, Dec 2006)
Co-advised with Ming-Ying Leung
- *David Flores* (UTEP graduated, May 2007)

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- Thesis Title: SimBA: A Discrete-event Simulator for Performance Prediction of Volunteer Computing Projects. Co-advised with Patricia Teller. First placement: Software developer at Ximis
- *Richard Zamudio* (UTEP graduated, May 2007)
- Thesis Title: TOPAZ: A Firefox Protocol Extension for GridFTP. First placement: Software developer at Rockwell Collins. Outstanding Thesis in Computer Science 2006-2007 (UTEP)

Undergraduate Research Assistants

- *Lauren Proctor* (Jan 2022 – present)
 - *Cole Johnston* (Jan 2022 – present)
 - *Juliet Bradford* (Jan 2022 – present)
 - *Georgia Channing* (Jan 2022 – present)
 - *Dominic Kennedy* (Aug 2021 – present)
 - *Brandon Roachell* (Jan 2021 – present)
 - *Ria Patel* (Feb 2020 – present)
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- *Jacob Leonard* (Jan 2021 – present)
 - *Ross Ketron* (Jan 2021 – present)
 - *Clark Hathaway* (June 2020 – August 2021)
 - *Sebastian Mobo* (Jun 2020 – May 2021)
 - *Ian Lumsden* (Jun 2019 – Jul 2020)
 - *Devon (Kae) Suarez* (Jan 2019 – May 2020)
 - *Antonio Vega* (Aug 2019 – Dec 2019)
 - *Matthew Dixon* (Jan 2019 – Aug 2019)
 - *Josh Davis* (Aug 2017 – May 2019)
 - *Joy Kitson* (Jun 2017 – May 2018)
 - *John Bounds* (Jun 2016 – May 2018)
 - *Paula Olaya* (Jun 2017 – Aug 2017)
First placement: PhD Student, U.Tennessee Knoxville
 - *Liz Racca* (Jun 2017 – Aug 2017)
 - *Rachel Kraft* (Jun 2017 – Aug 2017)
First placement: MS student, U. Delaware in CS at UDel
 - *Connor Zanin* (Jan 2015 – May 2016)
Senior Thesis: Tuning MapReduce with Surrogate- Based Modeling. First placement: PhD Student, Northeastern University
 - *Ryan McKenna* (Aug 2014 – May 2016)
Senior Thesis: Predicting Performance Variability in Parallel File Systems. First placement: PhD Student, U. Massachusetts Amherst
 - *Sean McDaniel* (Jan 2014 – Dec 2014) First placement: PhD Student, U. Delaware
 - *Stephen Herbein* (Aug 2014 – Aug 2014)
Senior Thesis: Benchmarking and Auto-tuning I/O Intensive Applications at the Extreme Scale. First placement: PhD Student, U. Delaware
 - *Michael Matheny* (Jan 2012-Aug 2014)
First placement: PhD Student at U. Utah
 - *Samuel Schlachter* (Jun 2011 – May 2013)
First placement: Researcher at U. Delaware
 - *Matthew Wezowicz* (Aug 2011-Aug 2013)
 - *Casey Casalnuovo* (Aug 2013 – Dec 2013)
 - *Haley Northrup* (Aug 2013 – Dec 2013)

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- *Ryan Huttman* (Aug 2011 – May 2013)
 - *Reza Hammond* (Aug 2010 – May 2011) First placement: PhD Student at U. Delaware
 - *Jason Park* (Jun 2010 – May 2011)
 - *Kyle Benson* (Jun 2010 – Aug 2011)
First placement: PhD Student, U. California Irvine
 - *Dirk Mezger* (Aug 2010 – Dec 2010)
 - *Dominik Kimmel* (Aug 2010 – Dec 2010)
 - *Omar Padron* (Jun 2009- Aug 2009)
First placement: PhD Student, U. Delaware
 - *Philip Saponaro* (Jan 2009 – May 2010)
Senior Thesis: An Efficient Arbitrary Precision Mathematical Library for Accurate and Fast MD Simulations in Single Precision GPUs. First placement: PhD Student, U. Delaware
 - *Patrick McClory* (Jan 2008 – May 2009)
First placement: PhD Student, U. Pittsburgh
 - *Reed Matz* (Jun 2008 – Dec 2008)
 - *Jason Parrott* (Aug 2007 – May 2008)
First placement: Factset Research Systems
 - *Robert Keller* (Aug 2007 – May 2008)
First placement: Vanguard
 - *Brenda Medina* (Jun 2008 – Aug 2008)
 - *David Mireles* (Aug 2006 – Aug 2007, Jun 2008-Aug 2008)
 - *Vladimir Soto* (Jan 2007 – Aug 2007)
 - *Princess Trillo* (Jan 2007 – Aug 2007)
 - *David Gomez-Leon* (Aug 2006 – May 2007)
 - *Karina Escapita* (Jan 2006 – Aug 2007)
 - *Guillermo Lopez* (Aug 2006 – Aug 2007)
 - *Abel Licon* (Aug 2006 – Aug 2007)
First placement: MS Student, U. Delaware
 - *Daniel Catarino* (Jan 2006 – Dec 2006)
First placement: Exxon Mobil

High School Student

- *Lou Fogel* (Jun 2010 – Aug 2010)
First placement: BS, Worcester Polytechnic Institute

Visiting Scholars

- *Ahmed Bin Zaman* (May 2019 – Jul 2019)
- *Tao Gao* (Jan 2016 – Dec 2017)
- *Julian A. Uran* (Jun 2014 – Nov 2014)
- *Cindy Solano* (Jun 2013 – Aug 2013)
- *Daniel T. Yehdego* (Jun 2013 – Aug 2013)

PhD / MS Committee Member

- *Zhixiu Lu* (PhD Thesis supervisor: (Scott Emrich)
PhD in Computer Science at U. Tennessee Knoxville, 2023 (Expected)
- *Tanner Hobson* (PhD Thesis supervisor: Jian Huang)
PhD in Computer Science at U. Tennessee Knoxville, 2023 (Expected)

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- *Ricardo llamas* (PhD Thesis supervisor: Rodrigo Vargas)
PhD in Plant Soil Sciences at U. Delaware, 2022 (Expected)
 - *Tu Mai Anh Do* (PhD Thesis supervisor: Ewa Deelman)
PhD in Computer Science at USC Information Sciences Institute, 2022 (Expected)
 - *Angelica Walker* (PhD Thesis supervisor: Daniel Jacobson)
PhD in Data Sciences at U. Tennessee Knoxville, 2022
 - *Craig Willis* (PhD Thesis supervisor: Victoria Stodden)
PhD in Information Sciences at U. Illinois Urbana-Champaign, 2020
 - *Xi Luo* (PhD Thesis supervisor: Jack Dongarra and George Bosilca)
PhD in Computer Science at U. Tennessee Knoxville, 2020
 - *Mario Antonio Guevara Santamaria* (PhD Thesis supervisor: Rodrigo Vargas)
PhD in Plant Soil Sciences at U. Delaware, 2020
 - *Thananon (Arm) Patinyasakdikul* (PhD Thesis supervisor: Jack Dongarra and George Bosilca)
PhD in Computer Science at U. Tennessee Knoxville, 2019
 - *Reazul Hoque* (PhD Thesis supervisor: Jack Dongarra and George Bosilca)
PhD in Computer Science at U. Tennessee Knoxville, 2019
 - *Robert Searles* (PhD Thesis supervisor: Sunita Chandrasekaran)
PhD in Computer Science at U. Delaware, 2019
 - *Valentin Reis* (PhD Thesis supervisor: Denis Trystram)
PhD in Computer Science at Institute for Research in Computer Science and Automation (INRIA)
2018
 - *Arnov Sinha* (MS Thesis supervisor: Sunita Chandrasekaran)
MS in Computer Science at U. Delaware, 2017
 - *Wei-Fan Chiang* (PhD Thesis supervisor: Ganesh Gopalakrishnan)
PhD in Computer Science at U. Utah, 2016
 - *Fan Yang* (PhD Thesis supervisor: Paul Amer)
PhD in Computer Science at U. Delaware, 2015
 - *Bryan Youse* (PhD Thesis supervisor: B. David Saunders)
PhD in Computer Science at U. Delaware, 2015
 - *Kevin McCormick* (PhD Thesis supervisor: Li Liao)
PhD in Computer Science at U. Delaware, 2013
 - *Daniel Orozco* (PhD Thesis supervisor: Guang R. Gao)
PhD in Computer Engineering at U. Delaware, 2012
 - *Liang Gu* (PhD Thesis supervisor: Xiaoming Li)
PhD in Computer Engineering at U. Delaware, 2011
 - *Kurt Ferreira* (PhD Thesis supervisor: Patrick Bridges)
PhD in Computer Science at U. New Mexico, 2011
 - *Jayaraman Suresh Babu* (MS Thesis supervisor: Patricia J. Teller)
MS in Computer Science at U. Texas El Paso, 2006
 - *Maria Gabriela Aguilera* (MS Thesis supervisor: Patricia J. Teller)
MS in Computer Science at U. Texas El Paso, 2005
 - *Yash Dayal* (MS Thesis supervisor: Gregory Lush)
MS in Electrical and Computer Engineering at U. Texas El Paso, 2005
 - *Javed Bilal Khan* (MS Thesis supervisor: John Chessa)
MS in Mechanical Engineering at U. Texas El Paso, 2005

STUDENT AWARDS

International Level

- *Ian Lumsden*: First Place at the ACM Student Poster Competition (UG) at SC20
- *Sebastian Mobo and Clark Hathaway*: Third Place at the ACM Student Poster Competition (UG) at SC20
- *Nigel Tan*: Third Place at the ACM Student Poster Competition (Graduate) at SC20
- *Stephen Herbein*: IEEE TCSC Outstanding PhD Dissertation Award, 2019
- *Dylan Chapp*: Best Student Poster at the ACM HPDC Conference, 2019
- *Josh Davis*: Second Place at the ACM Student Poster Competition (UG) at SC18
- *Sean McDaniel*: First Place at the ACM Student Poster Competition (UG) at SC14
- *Stephen Herbein*: Second Place at the ACM Student Poster Competition (UG) at SC13
- *Matthew Wezowicz*: Second Place at the ACM Student Poster Competition (UG) at SC12
- *Philip Saponaro and Omar Padron*: Dr. Robert M. Panoff Award (UG) at SC09
- *Abel Licon*: Google Hispanic Scholarship Fund Scholarship, 2008
- *David Mireles*: Google Hispanic Scholarship Fund Scholarship, 2007
- *Daniel Catarino*: Google Hispanic Scholarship Fund Scholarship, 2006

University Level

- *Ian Lumsden*: U. Tennessee Knoxville Graduate Student Fellowships, 2020 – present
- *Devon (Kae) Suarez*: U. Tennessee Knoxville Graduate Student Fellowships, 2020 – present
- *Nigel Tan*: U. Tennessee Knoxville Graduate Student Fellowships, 2019 – present
- *Neil Lindquist*: U. Tennessee Knoxville Graduate Student Fellowships, 2019 -2020
- *Paula Olaya*: U. Tennessee Knoxville Access and Diversity Fellowship, 2019
- *Joe Teague*: U. Tennessee Knoxville Graduate student fellowships, 2018 – 2019
- *Rachel Kraft*: U. Delaware University Graduate Scholar Award, 2017 – 2018
- *Sean McDaniel*: U. Delaware University Graduate Scholar Award, 2015 – 2017
- *Taylor Baldwin*: U. Delaware University Graduate Scholar Award, 2014 – 2015
- *Omar Padron*: U. Delaware University Graduate Scholar Award, 2011 – 2012
- *Trilce Estrada*: U. Delaware Graduate Fellow Award, 2010-2011
- *Philip Saponaro*: U. Delaware University Graduate Scholar Award, 2010 – 2011
- *Abel Licon*: U. Delaware University Graduate Scholar Award, 2009 – 2011
- *Trilce Estrada*: U. Delaware Alumni Enrichment Award, 2008

TEACHING

COURSES AT UTK (2018 –):

Graduate Courses – Semester, Course Title, Enrolment (Credits):

Sp22 COSC526: Introduction to Data Mining 32 (3)

Sp21 COSC526: Introduction to Data Mining 19 (3)

Sp20 COSC526: Introduction to Data Mining 18 (3)

Fa18 COSC690(001) / COSC594(007): Big Data Analytics 28 (3)

Undergraduate Courses – Semester, Course Title, Enrolment (Credits):

Sp22 COSC426: Introduction to Data Mining 24 (3)

COURSES AT UD (2007 – 2018):

Graduate Courses – Semester, Course Title, Enrolment (Credits):

Sp18 CISC879: Adv. Topics in Arch. and Softw. Systems: Big Data Analytics 10 (3)

Fa17 CISC879: Adv. Topics in Arch. and Softw. Systems: Big Data Analytics 9 (3)

Fa16 CISC879: Adv. Topics in Arch. and Softw. Systems: Big Data Analytics 23 (3)

Fa15 CISC879: Adv. Topics in Arch. and Softw. Systems: Big Data Analytics 11 (3)

Sp15 CISC663: Operating Systems 8 (3)

Fa14 CISC879: Adv. Topics in Arch. and Softw. Systems 13 (3)

Fa13 CISC663: Operating Systems 10 (3)

Fa12 CISC662: Computer Architecture 19 (3)

Sp12 CISC663: Operating Systems 7 (3)

Fa11 CISC662: Computer Architecture 13 (3)

Sp11 CISC879: High Performance Parallel Algorithms for Computational Science 9 (3)

Fa10 CISC662: Computer Architecture 27 (3)

Fa09 CISC662: Computer Architecture 27 (3)

Sp09 CISC849: High Performance Parallel Algorithms for Computational Science 9 (3)

Fa08 CISC662: Computer Architecture 25 (3)

Sp07 CISC849: Analysis of Bio. Simulations 7 (3)

Fa07 CISC 662: Computer Architecture 19 (3)

Undergraduate Courses – Semester, Course Title, Enrolment (Credits):

Sp17 CISC361: Operating Systems 44 (3)

Fa15 CISC361: Operating Systems	28 (3)
Sp15 CISC361: Operating Systems	40 (3)
Sp10 CISC361: Operating Systems	40 (3)
Fa09 CISC360: Computer Architecture	39 (3)
Fa08 CISC360: Computer Architecture	16 (3)
Fa07 CISC360: Computer Architecture	19 (3)

COURSES AT UTEP (2005 – 2007):

Graduate courses – Semester, Course Title:

Sp05, Sp06 CS5334: Parallel and Concurrent Programming

Sp07 CS5341: Analysis and Modeling of Biological Structures

Undergraduate courses – Semester, Course Title:

Sp07, Fa06, Sp06, Fa05 CS3320: Computer Architecture II

Fa06 CS3335: Systems Programming

SERVICES

EDITORIAL AFFILIATIONS

- 2021* – Editor in Chief, Future Generation Computer Systems (FGCS), Elsevier
present
- 2015* – Subject Area Editor, International Journal of High-Performance Computing Applications (IJHPCA), Sage
present
- 2015* – Associate Editor, Journal of Parallel Computing (ParCo), Elsevier
present
- 2015* – Subject Area Editor, Supercomputing Frontiers and Innovations Journal (SuperFI), Sage
present
- 2014 – 2017* Associate Editor, Journal of Parallel and Distributed Computing (JPDC), Elsevier
- 2014* Subject Area Editor, Journal of Parallel and Distributed Computing (ParCo), Elsevier
- 2014* Guest Editor, Special Issue of Parallel and Distributed Computing (ParCo) titled “Computing Frontiers 2014: Best Papers.”
- 2009* Guest Editor, Special Issue of Computer Communications on Information and Future Communication Security, Elsevier

STEERING AND ADVISORY COMMITTEES

- 2022* – Treasurer, IEEE Computer Society
present
- 2022* - Vice-Chair, ACM Special Interest Group on High Performance Computing (SIGHPC) – member elected 2 consecutive times
present
- 2021* – Steering Committee Member, South African CHPC National Conference
present
- 2021 - 2024* Advisory Board Member, EuroHPC project ADMIRE: Adaptive multi-tier intelligent data manager for Exascale
- 2021* - Scientific Advisory Committee Member of Helmholtz Imaging Platform and the Helmholtz Association (18 German research centers employing more than 40,000 staff)
present
- 2020* – Steering Committee Chair, IEEE International Conference on Cluster Computing (IEEE Cluster)
present
- 2020* – Advisory Board Member, Anvil Project, Purdue University
present
- 2020* Steering Committee Chair, IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC)
- 2019* – Steering Committee Chair, NSF-founded South Big Data Hub Coordination Council
present

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- 2019 – 2021* Chair, IEEE-CS Technical Meeting Request Committee (TMRC) for the Technical & Conference Activities Board
 - 2019* Chair, ACM Senior Member Committee
 - 2018* – Steering Committee Member, ACM PASC conference
 - present*
 - 2016* – Committee Member, Executive Committee of NSF-funded South Hub
 - present*
 - 2016 – 2022* Member-at-Large, ACM Special Interest Group on High Performance Computing (SIGHPC) – member elected 2 consecutive times
 - 2016 – 2021* Steering Committee Member, ISC High Performance Computing
 - 2016 – 2019* Member, NSF Advisory Committee for Cyberinfrastructure
 - 2016 – 2018* Member, ACM Senior Member Committee
 - 2016 - 2018* Steering Committee Member, IEEE International Parallel and Distributed Processing Symposium (IPDPS)
 - 2015 – 2021* Steering Committee Member, ACM International Symposium on High-Performance Parallel and Distributed Computing (ACM HPDC)
 - 2015 – 2018* Member, Advisory Group on Reproducibility - Advisory to the SC Conference, ACM, and IEEE
 - 2014* – Steering Committee Member, IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (IEEE/ACM SC)
 - present*
 - 2014 – 2020* Steering Committee Member, IEEE International Conference on Cluster Computing (IEEE Cluster)

CHAIR AND CO-CHAIR - CONFERENCES / WORKSHOPS / SYMPOSIUMS / SCHOLARSHIPS (SELECTED ACTIVITIES)

- 2022* Technical Program Co-Chair of the IEEE eScience Conference. October 2022, Salt Lake City, Utah, USA
- 2021* Workshop Chair of the IEEE eScience Conference. September 2021, Innsbruck, Austria
- Technical Program Track Chair of the IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2021, Portland, OR, USA
- 2019* General Chair of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2019, Denver, CO, USA
- 2017* Finance Chair of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2017, Denver, CO, USA

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- Technical Paper Area Co-Chair for Applications and Algorithms of the IEEE Cluster Conference, September 2017, Honolulu, Hawaii, USA
- Workshop Chair of the 32nd ISC High Performance Conference, June 2017, Frankfurt, Germany
- General Chair of the IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2017, Orlando, FL, USA
- SCALE Challenge Co-Chair of the 17th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing, to be held in May 2017, Madrid, Spain
- 2016* Panel Chair of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2016. Salt Lake City, UT, USA
- Technical Paper Area Chair of the "Applications" Track - 28th International Symposium on Computer Architecture and High-Performance Computing (SBAC-PAD)", October 26-28, 2016, Los Angeles, CA, USA
- Technical Paper Area Chair of the "Multicore and Many-core Parallelism" Track – EuroPar, August 2016, Grenoble, France
- Workshop co-Chair of the 31st ISC High Performance Conference, June 19 – June 23, 2016, Frankfurt, Germany
- Technical Paper Area Chair of the "Performance" Track – International Conference on Parallel Processing (ICPP), August 2016, Philadelphia, PA, USA
- 2015* Workshop Chair of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2015. Austin, TX, USA
- General co-Chair of the IEEE International Conference on Cluster Computing 2015, September 2015, Chicago, IL, USA
- Technical Program Co-Chair of the 24th ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 15-19, 2015, Portland, OR, USA
- 2014* Technical Program Co-Chair of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2014. New Orleans, LA, USA
- Technical Paper Area Chair of the "Cluster Design, Configuration and Administration" Track - IEEE International Conference on Cluster Computing (Cluster), September 2014, Madrid, Spain
- 2013* Technical Poster Chair of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2013. Denver, CO, USA

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- 2012* Birds of a Feather (BoF) Chair of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2012, Salt Lake City, UT, USA
- 2011* Deputy Birds of a Feather (BoF) Chair of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2011, Seattle, WA, USA
- 2010* Technical Paper Area Co-Chair of the System Software technical track at the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2010, New Orleans, LA, USA
- Technical Paper Area Chair of "Distributed Systems and Applications" of the 12th IEEE International Conference on High Performance Computing and Communications (HPCC), September 2010, Melbourne, Australia
- 2009* Technical Program vice-Chair of the topic "Distributed Systems and Applications" Track - 11th IEEE International Conference on High Performance Computing and Communications (HPCC), June 2009, Seoul, South Korea
- Technical Program Chair of the 8th IEEE International Workshop on High Performance Computational Biology (HiCOMB), May 2009, Rome, Italy
- 2003* Workshop co-Chair of the First Advanced Topics Workshop on Desktop Grids: Critical Systems and Applications Research (DGRID). November 2003, Phoenix, Arizona

COMMITTEE MEMBER - CONFERENCES / WORKSHOPS / SYMPOSIUMS / SCHOLARSHIPS

1. Technical Program Committee Member of the IEEE Cluster Conference (Cluster), September 2022, Heidelberg, Germany.
2. Technical Program Committee Member of the 51st IEEE International Conference on Parallel Processing (ICPP), August 2022, Bordeaux, France.
3. Technical Program Committee Member of the 34nd IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2022, Nice, France.
4. Technical Program Committee Member of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2021, St Louis, MO, USA.
5. Technical Program Committee Member of the IEEE International Conference on Cluster Computing (Cluster), September 2021, Portland, OR, USA.
6. Technical Program Committee Member of the IEEE International Conference on Parallel Processing (ICPP), August 2021, Argonne National Laboratory, IL, USA.
7. Technical Program Committee Member of the 41st IEEE International Conference on Distributed Computing Systems (ICDCS 2021), July 2021, Washington DC, USA.
8. Technical Program Committee Member of the 28th International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2021. Stockholm, Sweden.

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9. Technical Program Committee Member of the 21st IEEE/ACM International Symposium on Cluster, Cloud and Internet Computing (CCGrid), May 2021, Melbourne, Australia.
 10. Technical Program Committee Member of the 2020 IEEE International Symposium on Workload Characterization (IISWC), October 2020, Virtual Conference.
 11. Technical Program Committee Member of the 40th IEEE International Conference on Distributed Computing Systems (ICDCS), July 2020, Singapore.
 12. Technical Program Committee Member of the 3rd International Workshop on Reproducible Evaluation of Computer Systems (P-RECS), June 2020. Stockholm, Sweden.
 13. Technical Program Committee Member of the 28th International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2020. Stockholm, Sweden.
 14. Tutorial Committee Member of the 35rd ISC High Performance Conference. June 21-25, 2020, Frankfurt, Germany.
 15. Technical Program Committee Member of the 20th International Workshop on High Performance Computational Biology (HiCOMB), May 2020, New Orleans, LA, USA.
 16. Technical Program Committee Member of the International SC Asia Conference, February 2020, Singapore.
 17. Technical Program Committee Member of the 5th International Workshop on Container Technologies and Container Clouds (WoC), December 2019. Davis, CA, USA.
 18. Technical Program Committee Member of the 2st International Workshop on Reproducible Evaluation of Computer Systems (P-RECS), June 2019. Phoenix Arizona, USA.
 19. Technical Program Committee Member of the 27th International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2019. Phoenix, AZ, USA.
 20. Technical Program Committee Member of the 32nd IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2019. Rio de Janeiro, Brazil.
 21. Technical Program Committee Member of the of the 2018 IEEE International Conference on Bioinformatics and Biomedicine (BIBM), December 2018, Madrid, Spain.
 22. Technical Program Committee Member of the of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2018, Dallas, TX, USA.
 23. Technical Program Committee Member of the 1st International Workshop on Reproducible Evaluation of Computer Systems (RECS), June 2018. Washington DC, USA.
 24. Technical Program Committee Member of the 27th International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2018. Phoenix, AZ, USA.
 25. Technical Program Committee Member of the 33rd ISC High Performance Conference. June 18-22, 2017, Frankfurt, Germany.
 26. Technical Program Committee Member of the 32nd IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2018. Vancouver, Canada.
 27. Workshop Committee Member of the International Conference on Computational Science (ICCS). June 11-13, 2017, Wuxi, China.

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28. Panel Committee Member of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2017. Denver, CO, USA.
 29. Technical Program Committee Member of the 26th International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2017, Washington DC, USA.
 30. Technical Program Committee Member of the 32nd ISC High Performance Conference. June 18-22, 2017, Frankfurt, Germany.
 31. Workshop Committee Member of the International Conference on Computational Science (ICCS). June 12-14, 2017, Zurich, Switzerland.
 32. Technical Program Committee of the 2017 IEEE International Symposium on Performance Analysis of Systems and Software. April 23-25, 2017 San Francisco Bay Area, California, USA.
 33. Technical Program Committee of the 23rd IEEE International Conference on High Performance Computing, Data and Analytics (HiPC), December 19-22, 2016, Hyderabad, India.
 34. Workshop Committee Member of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2016. Salt Lake City, UT, USA.
 35. Student Cluster Competition Reproducibility Committee Member of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2016. Salt Lake City, UT, USA.
 36. Technical Program Committee Member of the System Track - IEEE International Conference on Cluster Computing, September 2016, Taipei, Taiwan.
 37. Technical Program Committee Member ISC High Performance Conference. June 19-23, 2016, Frankfurt, Germany.
 38. Technical Program Committee Member of the 25th International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2016, Kyoto, Japan.
 39. Technical Program Committee Member of the 16th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid), May 2016, Cartagena, Colombia.
 40. Technical Program Committee Member of the ACM International Conference on Computing Frontiers (CF), May 2016, Como, Italy.
 41. Technical Program Committee Member of the 6th International Workshop on Adaptive Self-tuning Computing Systems (ADAPT), January 2016, Prague, Czech Republic.
 42. Technical Program Committee Member of the 21th IEEE International Conference on Parallel and Distributed Systems (ICPADS), December 2015, Melbourne, Australia.
 43. Technical Program Committee Member (Data Analytics and Visualization Track) of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2015. Austin, TX, USA.
 44. Technical Program Committee Member of the IA³ 2015: 5th Workshop on Irregular Applications: Architectures and Algorithms. November 2015. Austin, TX, USA.
 45. Technical Program Committee Member of the EduHPC-15: Workshop on Education for High-Performance Computing. November 2015. Austin, TX, USA.

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46. Technical Program Committee Member of 11nd IEEE International Conference on e-Science and Grid Technologies (eScience), August 2015, Munich, Germany.
 47. Technical Program Committee Member of the 2014 ACM International Conference on Supercomputing (ICS), June 2015, Long Beach, USA.
 48. Technical Program Committee Member of the ACM Computing Frontiers (CF), May 2015, Ischia, Italy.
 49. Technical Program Committee Member of 2015 ACM/IEEE CS George Michael HPC Fellowship.
 50. Technical Program Committee Member of Workshop and Tutorials at the 2015 Richard Tapia Celebration of Diversity in Computing Conference, Boston, MA, USA.
 51. Technical Program Committee Member of the 13th IEEE International Conference on Ubiquitous Computing and Communications (IUCC) December 2014, Chengdu, China.
 52. Technical Program Committee Member of 10nd IEEE International Conference on e-Science and Grid Technologies (eScience), October 2014, Guarujá, San Paulo, Brazil.
 53. Technical Program Committee Member of the 2nd Workshop on Parallel and Distributed Agent-Based Simulations (PADABS), 25-29 August 2014, Porto, Portugal.
 54. Technical Program Committee Member of the 2014 ACM International Conference on Supercomputing (ICS), June 2014, Munich, Germany.
 55. Technical Program Committee Member of the 23rd International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2014, Vancouver, Canada.
 56. Technical Program Committee Member of the ACM International Conference on Computing Frontiers 2014 (CF), May 2014, Cagliari, Italy.
 57. Technical Program Committee Member of the 14th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid), May 2014, Chicago, USA.
 58. Technical Program Committee Member (System Software Track) of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2013, Denver, Colorado, USA.
 59. Technical Program Committee Member of the 13th International Workshop on High Performance Computational Biology (HiCOMB), May 2013, Phoenix, Arizona, USA.
 60. Technical Program Committee Member of the 6th IEEE/ACM International Conference on Utility and Cloud Computing (UCC), December 2013, Dresden, Germany.
 61. Technical Program Committee Member of the 2013 IEEE International Conference on Big Data (IEEE Big Data 2013), October 6-9, 2013, Silicon Valley, CA, USA.
 62. Technical Program Committee Member of the Workshop on Parallel Computational Biology (PBC), held in conjunction with PPAM 2013, September 8-11, 2013, Warsaw, Poland.
 63. Technical Program Committee Member of the 1st Workshop on Parallel and Distributed Agent-Based Simulations (PADABS), August 2013, Aachen, Germany.
 64. Technical Program Committee Member of the 22nd International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2013, New York, NY, USA.

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65. Technical Program Committee Member of the 12th International Workshop on High Performance Computational Biology (HiCOMB), May 2013, Boston, MA, USA.
 66. Technical Program Committee Member of the 13th IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid), May 2013, Delft, The Netherlands.
 67. Technical Program Committee Member of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2012, Salt Lake City, UT, USA.
 68. Technical Program Committee Member (Programming Systems Track) of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2012, Salt Lake City, UT, USA.
 69. Technical Program Committee Member of the High Performance Computing Conference (HiPC), December 2012, Pune, India.
 70. Technical Program Committee Member of the 5th IEEE/ACM International Conference on Utility and Cloud Computing (UCC), November 2012, Chicago, IL, USA.
 71. Technical Program Committee Member of the Grace Hopper Conference (GHC) Panels, Workshops, and Presentations (PWP) Committee, October 2012, Baltimore, MD, USA.
 72. Technical Program Committee Member of 8nd IEEE International Conference on e-Science and Grid Technologies (eScience), October 2012, Chicago, IL, USA.
 73. Technical Program Committee Member of Symposium on Application Accelerators in High- Performance Computing (SAAHPC), July 2012, Argonne National Laboratory, IL, USA.
 74. Technical Program Committee Member of the 21st ACM International Symposium on High- Performance Parallel and Distributed Computing (HPDC), June 2012, Delft, The Netherlands.
 75. Technical Program Committee Member of the 12th IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid), May 2012, Ottawa, Canada.
 76. Technical Program Committee Member of the 2012 ACM International Conference on Computing Frontiers (CF), May 15-17, 2012, Cagliari, Italy.
 77. TCPP Travel Award Committee of the 26th IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 21 – 25, 2012, Shanghai, China.
 78. Technical Program Committee Member of the Workshop Innovative Parallel Computing: Foundations and Applications of GPU, Many-core, and Heterogeneous Systems (InPar), May 2012, San Jose, CA, USA.
 79. Technical Program Committee Member (System Software Track) of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2011, Seattle, WA, USA.
 80. Technical Program Committee Member of the 13th IEEE International Conference on High Performance Computing and Communications (HPCC) in Biological/Molecular Computing Track, September 2 – 4, 2011, Banff, Alberta, Canada.
 81. Technical Program Committee Member of the IEEE Cluster 2011 Conference (Cluster), September 26 – 30, 2011, Austin, TX, USA.

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82. Technical Program Committee Member of the Workshop on Parallel Computational Biology (PBC), held in conjunction with PPAM 2011, September 11-14, 2011, Torun, Poland.
 83. Technical Program Committee Member of the 11th IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 23 – 26, 2011, Los Angeles, CA, USA.
 84. Technical Program Committee Member of the 2011 Symposium on Application Accelerators in High Performance Computing (SAAHPC), July 19 – 20, 2011, University of Tennessee Conference Center, TN, USA.
 85. Technical Program Committee Member of the 7th International Workshop on High Performance Computational Biology (HiCOMB), May 16, 2011, Anchorage, AK, USA.
 86. Technical Program Committee Member of the 4th Annual Workshop for General-Purpose Computation on Graphics Processing Units (GPGPU), March 5, 2011, Newport Beach, California, USA.
 87. Technical Program Committee Member of the 18th Euromicro Conference on Parallel, Distributed and Network- Based Processing (PDP), February 9-11, 2011, Ayia Napa, Cyprus.
 88. Technical Program Committee Member of the 2010 IEEE 6th International Conference on e-Science (eScience), December 7 – 10, 2010, Brisbane, Australia.
 89. Technical Program Committee Member of the International Conference of Computer Design (ICCD), October 3-6, 2010, Amsterdam, The Netherlands.
 90. Technical Program Committee Member of the 22nd International Symposium on Computer Architecture and High-Performance Computing (SBAC-PAD), October 2010, Petropolis, Brazil.
 91. Technical Program Committee Member of the Workshop on Parallel Programming and Applications on Accelerator Clusters (PPAAC), September 2010, Heraklion, Greece.
 92. Technical Program Committee Member of the 2010 Symposium on Application Accelerators in High Performance Computing (SAAHPC), July 13 – 15, 2010, University of Tennessee Conference Center, TN, USA.
 93. Technical Program Committee Member of the 2010 ACM International Symposium on High Performance Distributed Computing (HPDC), June 2010, Chicago, IL, USA.
 94. Technical Program Committee Member of the ACM Computing Frontiers Conference (CF), May 2010, Bertinoro, Italy.
 95. Technical Program Committee Member of the 10th IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 2010, Melbourne, Australia.
 96. Technical Program Committee Member of the Second Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2010, Melbourne, Australia.
 97. Technical Program Committee Member of the 18th Euromicro Conference on Parallel, Distributed and Network- Based Processing (PDP), February 2010, Pisa, Italy.
 98. Technical Program Committee Member (System Software Track) of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2009, Portland, OR, USA.

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99. Technical Program Committee Member of the International Conference of Computer Design (ICCD), November 4 – 7, 2009, Lake Tahoe, CA, USA.
 100. Scholarship Committee Member of the Grace Hopper Celebration of Women in Computing 2009, October 2009, Tucson, AZ, USA.
 101. Technical Program Committee Member of the 2009 IEEE International Conference on Cluster Computing (Cluster), August 29 – September 4, 2009, New Orleans, LA, USA.
 102. Technical Program Committee Member of the 12th IEEE International Conference on Computational Science and Engineering (CSE), August 29 – 31, 2009, Vancouver, Canada.
 103. Technical Program Committee Member of 9th IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 2009, Shanghai, China.
 104. Technical Program Committee Member of the Workshop on Using Emerging Parallel Architectures for Computational Science, held in conjunction with the ICCS 2009, May 2009, Baton Rouge, LA, USA.
 105. Technical Program Committee Member of the Second Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2009, Rome, Italy.
 106. Technical Program Committee Member of the 2009 Richard Tapia Celebration of Diversity in Computing Conference, April 2009, Portland, OR, USA.
 107. Technical Program Committee Member of the 17th Euromicro Conference on Parallel, Distributed and Network- Based Processing (PDP), February 2009, Bauhaus-University Weimar in Thuringia, Germany.
 108. Technical Program Committee Member of the Intl. Conference on Advanced Computing and Communications, December 2008, Chennai, India.
 109. Technical Program Committee Member of the Computational Structural Bioinformatics Workshop 2008 November 2008, Philadelphia, PA, USA.
 110. Technical Program Committee Member of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2008, Austin, TX, USA.
 111. Technical Program Committee Member of the Grace Hopper Celebration of Women in Computing 2008, October 2008, Denver CO, USA.
 112. Technical Program Committee Member of the IEEE Intl. Conference on Computer Design (ICCD), October 2008, Lake Tahoe, CA, USA.
 113. Technical Program Committee Member of the 10th IEEE International Conference on High Performance Computing and Communications (HPCC), September 2008, DaLian, China.
 114. Technical Program Committee Member of the International Conference on Computational Science (ICCS), June 2008, Krakow, Poland.
 115. Technical Program Committee Member of the ACM Computing Frontiers (CF), May 2008, Ischia, Italy.
 116. Technical Program Committee Member of the Global and Peer-to-Peer Computing (GP2PC), May 2008, Lyon, France.

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117. Technical Program Committee Member of the 7th International Workshop on High Performance Computational Biology (HiCOMB), May 2008, Miami, FL, USA.
 118. Technical Program Committee Member of the 9th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC), May 2008, Miami, FL, USA.
 119. Technical Program Committee Member of the 2nd Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2008, Miami, Florida, USA.
 120. Technical Program Committee Member of the 22nd IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2008, Miami, FL, USA.
 121. Technical Program Committee Member of the Euromicro Conference on Parallel, Distributed and Network based Processing (PDP) February 2008, Toulouse, France.
 122. Technical Poster Committee Member of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2007, Reno, NV, USA.
 123. Technical Program Committee Member of the First Computational Structural Bioinformatics Workshop, November 2007, San Jose, CA, USA.
 124. Technical Poster Committee Member of the 2007 Richard Tapia Celebration of Diversity in Computing Conference, October 2007, Orlando, FL, USA.
 125. Scholarship Committee Member of the Grace Hopper Celebration of Women in Computing 2007, October 2007, Orlando, FL, USA.
 126. Technical Program Committee Member of the 5th IEEE International Symposium on Parallel and Distributed Processing and Applications (ISPA), August-September, 2007, Niagara Falls, Ontario, Canada.
 127. Technical Program Committee Member of the International Conference on Computational Science 2007 (ICCS), May 2007, Beijing, China.
 128. Technical Program Committee Member of the 6th International Workshop on Global and Peer-to-Peer Computing (GP2P), May 2007, Rio de Janeiro, Brazil.
 129. Technical Program Committee Member of 26th IEEE International Performance Computing and Communications Conference (IPCCC), April 2007 - New Orleans, LA, USA.
 130. Technical Program Committee Member of the First Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), March 2007, Long Beach, CA, USA.
 131. Technical Program Committee Member of the 4th IEEE International Symposium on Parallel and Distributed Processing and Applications (ISPA), December 2006, Sorrento, Italy.
 132. Technical Program Committee Member of the 2nd IEEE International Conference on e-Science and Grid Technologies (eScience), December 2006, Amsterdam, The Netherlands.
 133. Technical Program Committee Member of the 5th International Workshop on Global and Peer-to-Peer Computing (GP2P), May 2006, Singapore.
 134. Technical Program Committee Member of the 20th IEEE International Parallel and Distributed Processing Symposium (IPDPS), April 2006, Rhodes, Greece.
 135. Technical Program Committee Member of the 5th IEEE International Workshop on High Performance Computational Biology (HiCOMB), April 2006, Rhodes, Greece.

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136. Technical Program Committee Member of the 1st IEEE International Conference on e-Science and Grid Technologies (eScience), December 2005, Melbourne, Australia.
 137. Technical Program Committee Member of the 2005 IEEE International Conference on Cluster Computing (Cluster), September 2005, Boston, MA, USA.
 138. Technical Program Committee Member of the 2005 International Conference on High Performance Computing and Communications (HPCC), September 2005, Sorrento, Italy.
 139. Technical Program Committee Member of the 5th International Workshop on Global and Peer-to-Peer Computing (GP2P), May 2005, Cardiff, UK.

JOURNAL AND BOOK REFEREE

Since 2005, I have reviewed several articles for journal and book editors, including IEEE Transactions on Parallel and Distributed Systems, Journal of Computational Chemistry, Parallel and Distributed Computing, and Journal of Bioinformatics.

SERVICES TO THE UNIVERSITY, COLLEGE, AND DEPARTMENT (SELECTED)

At UTK:

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|-------------------------------|--|
| <i>2020</i> | Member, Committee to review StAR proposals. (University Committee) |
| <i>2019</i>
<i>present</i> | – Member, Committee to review faculty for their post-tenure performance (College Committee) |
| <i>2018</i>
<i>present</i> | – Member, Faculty Search (Department) Committee |
| <i>2018</i> | Member, Organization Committee of the NIMBioS Investigative Workshop Scientific Collaboration Enabled by High Performance Computing (University Committee) |

At UD:

- | | |
|--------------------|---|
| <i>2016 – 2018</i> | Chair, Publicity/Awards/Development Activity Committee (CIS Department) |
| <i>2016 – 2018</i> | Faculty Secretary, College of Engineering (CoE) |
| <i>2007 – 2018</i> | Coordinator, CIS/ECE booth at the Supercomputing Conference (CIS Department) |
| <i>2017 – 2018</i> | Member, Faculty Recruitment Committee (CIS Department) |
| <i>2016 – 2017</i> | Member, Ad-hoc College of Engineering Committee on Server Room Relocation (CoE) |
| <i>2015 – 2016</i> | Acting Director, Center for Bioinformatics & Computational Biology (CBCB), Delaware Biotechnology Institute (DBI) |
| <i>2015 – 2016</i> | Member, Faculty Recruitment Committee (ECE Department) |
| <i>2014 – 2016</i> | Member, Bioinformatics Steering Committee (Bioinformatics Program) |
| <i>2014 – 2016</i> | Advisor, Bioinformatics Student Association (Bioinformatics Program) |
| <i>2015</i> | Member, Undergraduate Committee (CIS Department) |
| <i>2014 – 2015</i> | Chair, Distinguished Speaker Series Committee (CIS Department) |
| <i>2014</i> | Chair, Faculty Recruitment Committee (CIS Department) |

2012 – 2013 Member, Biomedical Engineering Graduate Committee (BME Program)
2012 – 2013 Chair, Distinguished Speaker Series Committee (CIS Department)
2010 Organizer, CIS Research Day (CIS Department)
2009 – 2013 Member, Bioinformatics Program Committee (University Committee)
2009 – 2011 Member, Research Computing Task Force (University Committee)
2009 – 2010 Member, Graduate Recruiting Committee (CIS Department)
2008 – 2009 Member, Graduate Committee (CIS Department)
2007 – 2009 Advisor, Student ACM Chapter (CIS Department)
2007 – 2008 Member, Graduate Recruiting Committee (CIS Department)

At UTEP:

2006 – 2007 Member, Bioinformatics Research Committee and Bioinformatics Colloquium Committee (University Committee)
2005 – 2007 Member, High-End Computing Along the Rio Grande Consortium
2005 – 2007 Member, Computer System Curriculum Committee and the Facilities Committee
2006 Member, NSF-CSEMS Scholarship Committee at the University of Texas at El Paso, 2006

SERVICE TO FEDERAL AGENCIES

Panelist for National Science Foundation (NSF), National Institutes of Health (NIH), Department of Energy (DoE), Army Research Office (ARO)

Note: The single panels are not provided to assure the confidentiality of the review process

PROFESSIONAL AFFILIATIONS

- ACM, ACM SIGHPC
- IEEE, IEEE-CS
- SIAM, SIAM-SC
- AAAS