

## MICHELA TAUFER

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*Jack Dongarra Professor in High Performance Computing*  
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Research Group: Global Computing Laboratory <http://globalcomputing.group>

### 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* – Jack Dongarra Professor in High Performance Computing, Department of Electrical Engineering and Computer and Science, University of Tennessee Knoxville  
*present*
- Sep 2017* – Professor, Department of Computer and Information Sciences, University of Delaware (Affiliated with Biomedical Engineering and Center for Bioinformatics & Computational Biology)  
*May 2018*
- Sep 2012* – Associate Professor, Department of Computer and Information Sciences, University of Delaware, (Affiliated with Biomedical Engineering and Center for Bioinformatics & Computational Biology)  
*Aug 2017*
- Sep 2015* – Acting Director, Center for Bioinformatics & Computational Biology, Delaware Biotechnology Institute  
*Aug 2016*
- Jan 2013* – David and Beverly J.C. Mills Career Development Chair, Department of Computer and Information Sciences, University of Delaware  
*Aug 2016*
- Jun 2013* – Visiting Faculty, Computer Science and Mathematics Division, Oak Ridge National Laboratory.  
*May 2014*     U.S. Department of Energy Higher Education Research Experiences Faculty Program
- Sep 2007* – Assistant Professor, Department of Computer and Information Sciences, University of Delaware  
*Aug 2012*     (Affiliated with Center for Bioinformatics & Computational Biology Jun 2010 – 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 2020* Keynote at the EuroGraphics Symposium on Parallel Graphics and Visualization (EGPGV)
- Apr 2020* IEEE Senior Member
- Mar 2020* 2020 Tickle College of Engineering Faculty & Staff Award for Outstanding Service to the Discipline Category
- Dec 2019* Keynote at the 13<sup>th</sup> CHPC National Conference, Johannesburg, South Africa
- Nov 2019* General Chair of the ACM/IEEE International Conference for High Performance Computing, Networking, Storage, and Analysis (SC)
- Aug 2019* Keynote at the Euro-Par conference, Göttingen, Germany
- Feb 2019* IBM Faculty Award
- Feb 2019* HPCwire's 2019 Person to Watch
- Jun 2018* Jack Dongarra Professor in High Performance Computing
- May 2018* Keynote at the ACM SIGSIM Keynote at the Conference on Principles of Advanced Discrete Simulation (PADS), Rome, Italy
- Feb 2018* Keynote at the 9<sup>th</sup> IEEE International Workshop on Programming Models and Applications for Multicores and Many-cores (PMAM), Vosendorf, Austria
- Sep 2017* Keynote at the EuroMPI/USA 2017 Conference, Chicago, IL, USA
- Sep 2017* Keynote at the 12<sup>th</sup> International Conference on Parallel Processing and Applied Mathematics, Lublin, Poland
- 2017* Faculty Nomination for the Excellence in Undergraduate Academic Advising and Mentoring Award, University of Delaware
- May 2017* General Chair of the IEEE International Parallel and Distributed Processing Symposium (IPDPS)
- Feb 2017* – J.P. Morgan Chase Faculty Scholar, University of Delaware
- May 2018*
- Oct 2016* Best Paper Finalists at the IEEE International Symposium on Computer Architecture and High Performance Computing Conference (SBAC-PAD), Los Angeles, CA, USA
- Sep 2016* Keynote at the IEEE Cluster Conference, Taipei, Taiwan
- Jun 2016* Keynote at the 7<sup>th</sup> ACM Workshop on Scientific Cloud Computing (ScienceCloud), Kyoto, Japan
- 2015* ACM (Association for Computing Machinery) Distinguished Scientist
- Sep 2015* General co-Chair of the IEEE International Conference on Cluster Computing
- May 2015* Keynote at the 5<sup>th</sup> IEEE International Workshop on Accelerators and Hybrid Exascale Systems (ASHES), Hyderabad, India
- 2015* Winner of the 8<sup>th</sup> IEEE International Scalable Computing Challenge, Co-located with the IEEE/ACM CCGrid Conference

- 2014 ACM (Association for Computing Machinery) Senior Member
- Sep 2014 Best Paper Finalists at the IEEE Cluster Conference, Madrid, Spain
- 2014 Faculty Nomination for the Excellence in Undergraduate Academic Advising and Mentoring Award, University of Delaware
- 2012 – 2016 David and Beverly J.C. Mills Career Development Chair
- 2006 UTEP Young Investigator Award, Research and Sponsored Programs
- 2003 – 2004 La Jolla Interfaces in Science (LJIS) Interdisciplinary Fellowship.
- 1996 Erasmus Fellowship of the European Community (EU) for Graduate Students

## RESEARCH FUNDING

- 2020 *Study Performance Portability of the Vector Particle-In-Cell Project (VPIC) across architectures*  
**Source of Support:** Los Alamos National Laboratory  
**Total Amount:** \$92,373, Single PI  
**Project Period:** 05/01/2020 – 04/30/2021  
**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?”
- 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 – 03/31/2022  
**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.
- 2019 *JDRD: Empowering Training and Validation Stages in AI-Orchestrated Workflows*  
**Source of Support:** Science Alliance, University of Tennessee Knoxville  
**Total Amount:** \$108,750, Single PI  
**Project Period:** 10/01/2019 – 09/30/2020  
**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.
- 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 – 08/15/2021

**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 *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 – 05/31/2022

**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

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.

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.

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 – 09/30/2021

**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.

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.

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.

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 institutions: 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

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.
- 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.

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 201; 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.

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

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.

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.

## STUDENTS/PERSONNEL/JOB PLACEMENT

- Postdoctoral Associates* **Silvina Caíno-Lores** (Feb 2020 – present)  
**Leobardo Valera** (Jan 2020 – present)  
**Ariel Rorabaugh** (Oct 2019 – present)  
**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 National Laboratory  
**Vivek Pallipuram** (Jan 2014 – Jul 2015) First placement: Assistant Professor at the University of the Pacific  
**Trilce Estrada** (Jul 2012 – Jul 2013) First placement: Assistant Professor at University of New Mexico  
**Narayna Ganesan** (Jan 2010 – Jul 2011) First placement: Assistant Professor at Stevens Institute of Technology  
**Arun Rajendran** (Apr 2008 – Jul 2008)
- Postmaster Associate* **Samuel Schlachter** (Jun13 – Jul14) First placement: CTO at SNAPCARD, Inc
- PhD Students* **Ian Lumsden** (Aug 20 – present) Expected Preliminary Research Requirement on May 2023  
**Devon (Kae) Suarez** (Aug 20 – present) Expected Preliminary Research Requirement on May 2023

**Paula Olaya** (Fa20 – present) Expected Preliminary Research Requirement on May 2022

**Nigel Tan** (Fa19 – present) Expected Preliminary Research Requirement on May 2021

**Dylan Chapp** (graduated, June 2020) Thesis Title: *Modeling Non-Determinism of Scientific Applications*. First placement: Software Engineering at Glodon, USA.

**Michael Wyatt** (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** (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** (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

**Boyu Zhang** (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** (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 University of 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*

**Paula Olaya** (graduated, May 2020) Thesis Title: *Building containerized environments for reproducibility and traceability of scientific workflows*.

**Rachel Kraft** (graduated, Dec 2018)

**Dylan Chapp** (graduated, May 2017) Thesis Title: *Study of the Impact of Non-determinism on Numerical Reproducibility and Debugging at the Exascale*. First placement: PhD Student, University of Delaware

**Jeffrey DiMarco** (graduated, May 2017) First placement: Software developer at Fidessa

**Abel Licon** (graduated, May 2010) Thesis Title: *RNA/Lab 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** (graduated, May 2009) Co-advised with Sandeep Patel. First placement: Scientist Siemens Healthcare

**Prayook Tungjatooronrusame** (graduated, Dec 2006), Co-advised with Ming-Ying Leung

**David Flores** (graduated, May 2007) Co-advised with Patricia Teller. Thesis Title: *SimBA: A Discrete-event Simulator for Performance Prediction of Volunteer Computing Projects*. First placement: Software developer at Ximis

**Richard Zamudio** (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)

*Visiting  
Scholars*

**Ahmed Bin Zaman** (May 2019 – Jul 2019)

**Tao Gao** (Jan 2016 – Dec 2018)

**Julian A. Uran** (Jun 2014 – Nov 2014)

**Cindy Solano** (Jun 2013 – Aug 2013)

**Daniel T. Yehdego** (Jun 2013 – Aug 2013)

*Undergraduate  
Research  
Assistants*

**Clark Hathaway** (June 2020 – present)

**Sebastian Mobo** (June 2020 – present)

**Ria Patel** (Feb 2020 – present)

**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, University of Tennessee Knoxville

**Liz Racca** (Jun 2017 – Aug 2017)

**Rachel Kraft** (Jun 2017 – Aug 2017) First placement: Master's student, University of Delaware in CS at UD

**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, University of Massachusetts Amherst

**Sean McDaniel** (Jan 2014 – Dec 2014) First placement: PhD Student, University of 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, University of Delaware

**Michael Matheny** (Jan 2012-Aug 2014) First placement: PhD Student at University of Utah

**Samuel Schlachter** (Jun 2011 – May 2013) First placement: Researcher at University of Delaware

**Matthew Wezowicz** (Aug 2011-Aug 2013)

**Casey Casalnuovo** (Aug 2013 – Dec 2013)

**Haley Northrup** (Aug 2013 – Dec 2013)

**Ryan Huttman** (Aug 2011 – May 2013)

**Reza Hammond** (Aug 2010 – May 2011) First placement: PhD Student at University of Delaware

**Jason Park** (Jun 2010 – May 2011)

**Kyle Benson** (Jun 2010 – Aug 2011) First placement: PhD Student, University of California Irvine

**Dirk Mezger** (Aug 2010 – Dec 2010)

**Dominik Kimmel** (Aug 2010 – Dec 2010)

**Omar Padron** (Jun 2009- Aug 2009) First placement: PhD Student, University of 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, University of Delaware  
**Patrick McClory** (Jan 2008 – May 2009) First placement: PhD Student, University of 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, University of 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

*PhD / MS  
Committee  
Member  
external*

**Tu Mai Anh Do** (PhD Thesis supervisor: Ewa Deelman), PhD in Computer Science at USC Information Sciences Institute, 2022 (expected)  
**Craig Willis** (PhD Thesis supervisor: Victoria Stodden), PhD in Information Sciences at University of Illinois Urbana-Champaign, 2020 (expected)  
**Xi Luo** (PhD Thesis supervisor: Jack Dongarra and George Bosilca), PhD in Computer Science at University of Tennessee Knoxville, 2020  
**Mario Antonio Guevara Santamaria** (PhD Thesis supervisor: Rodrigo Vargas), PhD in Plant & Soil Sciences at University of Delaware, 2020  
**Thananon (Arm) Patinyasakdikul** (PhD Thesis supervisor: Jack Dongarra and George Bosilca), PhD in Computer Science at University of Tennessee Knoxville, 2019  
**Reazul Hoque** (PhD Thesis supervisor: Jack Dongarra and George Bosilca), PhD in Computer Science at University of Tennessee Knoxville, 2019  
**Robert Searles** (PhD Thesis supervisor: Sunita Chandrasekaran), PhD in Computer Science at University of 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 University of Delaware, 2017  
**Wei-Fan Chiang** (PhD Thesis supervisor: Ganesh Gopalakrishnan), PhD in Computer Science at University of Utah, 2016  
**Fan Yang** (PhD Thesis supervisor: Paul Amer), PhD in Computer Science at University of Delaware, 2015  
**Bryan Youse** (PhD Thesis supervisor: B. David Saunders), PhD in Computer Science at University of Delaware, 2015  
**Kevin McCormick** (PhD Thesis supervisor: Li Liao), PhD in Computer Science at University of Delaware, 2013  
**Daniel Orozco** (PhD Thesis supervisor: Guang R. Gao), PhD in Computer Engineering at University of Delaware, 2012

**Liang Gu** (PhD Thesis supervisor: Xiaoming Li), PhD in Computer Engineering at University of Delaware, 2011

**Kurt Ferreira** (PhD Thesis supervisor: Patrick Bridges), PhD in Computer Science at University of New Mexico, 2011

**Jayaraman Suresh Babu** (MS Thesis supervisor: Patricia J. Teller), MS in Computer Science at University of Texas El Paso, 2006

**Maria Gabriela Aguilera** (MS Thesis supervisor: Patricia J. Teller), MS in Computer Science at University of Texas El Paso, 2005

**Yash Dayal** (MS Thesis supervisor: Gregory Lush), MS in Electrical and Computer Engineering at University of Texas El Paso, 2005

**Javed Bilal Khan** (MS Thesis supervisor: John Chessa), MS in Mechanical Engineering at University of Texas El Paso, 2005

## STUDENT AWARDS AND RECOGNITIONS

### *National and International Level*

**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:** University of Tennessee Knoxville Graduate Student Fellowships, 2020 – present

**Devon (Kae) Suarez:** University of Tennessee Knoxville Graduate Student Fellowships, 2020 – present

**Nigel Tan:** University of Tennessee Knoxville Graduate Student Fellowships, 2019 – present

**Neil Lindquist:** University of Tennessee Knoxville Graduate Student Fellowships, 2019

**Paula Olaya:** University of Tennessee Knoxville Access and Diversity Fellowship, 2019

**Joe Teague:** University of Tennessee Knoxville Graduate student fellowships, 2018 – 2019

**Rachel Kraft:** University of Delaware University Graduate Scholar Award, 2017 – 2018

**Sean McDaniel:** University of Delaware University Graduate Scholar Award, 2015 – 2017

**Taylor Baldwin:** University of Delaware University Graduate Scholar Award, 2014 – 2015

**Omar Padron:** University of Delaware University Graduate Scholar Award, 2011 – 2012

**Trilce Estrada:** University of Delaware Graduate Fellow Award, 2010-2011

**Philip Saponaro:** University of Delaware University Graduate Scholar Award, 2010 – 2011

**Able Licon:** University of Delaware University Graduate Scholar Award, 2009 – 2011

**Trilce Estrada:** University of Delaware Alumni Enrichment Award, 2008

## PUBLICATIONS AND PRESENTATIONS

Mentored undergraduate co-authors are indicated with (+) in the author list; mentored graduate co-authors are indicated with (\*) in the author list; mentored post-doctoral researchers are indicated with (#) in the author list. It is my policy that my students' or postdoctoral researchers' name appear first on publications. I use the same author order as in computational chemistry and put the leading author at the end of the authorship list.

## BOOKS EDITED:



- E1. Future Trends of HPC in a Disruptive Scenario. Editors: L. Grandinetti, G.R. Joubert, K. Michielsen, S.L. Mirtaheri, **M. Tauffer**, and R. Yokota. Book Series: Volume 34 of Advances in Parallel Computing, ISBN: 978-1-61499-999-7. 2019.

#### BOOK CHAPTERS:

- B1. P. Cicotti, S. Oral, G. Kestor, R. Gioiosa, S. Strande, **M. Tauffer**, J. H. Rogers, H. Abbasi, J. Hill, and L. Carrington. Data Movement in Data-Intensive High Performance Computing. *Conquering Big Data with High Performance Computing*. Springer International Publishing AG. 2016. ISBN 9783319337401.
- B2. T. Estrada(\*) and **M. Tauffer**. Challenges in Designing Scheduling Policies in Volunteer Computing. Chapter in "Desktop Grid Computing", Christophe Cerin and Gilles Fedak (Eds.), Chapman and Hall/CRC, 2012.
- B3. R.S. Armen, E.R. May, and **M. Tauffer**. Protein Docking. Chapter in "Encyclopedia of Parallel Computing", Padua, David (Ed.), Springer, 2011, ISBN 978-0-387-09765-7.
- B4. **M. Tauffer** and C.L. Brooks III. Predictor@Home: A Protein Structure Prediction Supercomputer Based on Volunteer Computing. Distributed & Grid Computing – Science Made Transparent for Everyone. Principles, Applications and Supporting Communities (Weber, M.H.W., ed.). Rechenkraft.net, Marburg, 2008. (*On line book*)

#### JOURNAL ARTICLES:

- J1. M. Guevara, **M. Tauffer**, and R. Vargas. Gap-Free Annual Soil Moisture Global across 15km Grids: 1991-2016. *Earth System Science Data*, 2020. (*In Review*)
- J2. D. H. Ahn, N. Bass, A. Chu, J. Garlick, M. Grondona, S. Herbein, H. I. Ingolfsson, J. Koning, T. Patki, T. R. W. Scogland, B. Springmeyer, and **Michela Tauffer**. Flux: Overcoming Scheduling Challenges for Exascale Workflows. *Future Generation Computer Systems Journal*, 2020. (*Accepted*)
- J3. R. Llamas, M. Guevara, D. Rorabaugh (#), **M. Tauffer**, and R. Vargas. Spatial Gap-Filling of ESA CCI Satellite-Derived Soil Moisture based on Linear Geostatistics. *Remote Sensing*, 2020. (*Preprint*) (*Accepted*)
- J4. T. Gao(\*), Y. Guo, B. Zhang, P. Cicotti, Y. Lu, P. Balaji, and **M. Tauffer**. Memory-Efficient and Skew-Tolerant MapReduce over MPI for Supercomputing Systems. *Journal of IEEE Transactions on Parallel and Distributed Systems (IEEE TPDS)*, 2020. (*Correspondent author*) (*Accepted*)
- J5. H. Carrillo-Cabada, J. Benson, A. Razavi, B. Mulligan, M.A. Cuendet, H. Weinstein, **M. Tauffer**, and T. Estrada. A Graphic Encoding Method for Quantitative Classification of Protein Structure and Representation of Conformational Changes. *IEEE/ACM Transactions on Computational Biology and Bioinformatics (IEEE/ACM TCBC)*, 2020. (*Accepted*)
- J6. D. Chapp(\*), V. Stodden, and **M. Tauffer**. Building a Vision for Reproducibility in the Cyberinfrastructure Ecosystem: Leveraging Community Efforts. *Journal of Supercomputing Frontiers and Innovations*. 7(1): 112-129, 2020. (*Correspondent author*)
- J7. **M. Tauffer**, T. Estrada, and T. Johnston. A Survey of Algorithms for Transforming Molecular Dynamics Data into Metadata for *In Situ* Analytics based on Machine Learning Methods. *Issue of Philosophical Transactions A.*, 378(2166):1-11, 2020. (*Correspondent author*)
- J8. D. Chapp(\*), D. Rorabaugh(#), K. Sato, D. Ahn, and **M. Tauffer**. A Three-phase Workflow for General and Expressive Representations of Nondeterminism in HPC Applications. *International Journal of High Performance Computing Applications (IJHPCA)*, 33(6): 1175-1184. 2019. (*Correspondent author*)
- J9. R. Searles, S. Herbein(\*), T. Johnston(#), **M. Tauffer**, and S. Chandrasekaran. Creating a Portable, High-Level Graph Analytics Framework for Compute and Data-Intensive Applications. *International Journal of High Performance Computing and Networking (IJHPCN)*, 13(1): 105-118, 2019.
- J10. E. Deelman, T. Peterka, I. Altintas, C. Carothers, K. Kleese van Dam, K. Moreland, M. Parashar, L. Ramakrishnan, **M. Tauffer**, and J. Vetter. The Future of Scientific Workflows. *International Journal of High Performance Computing Applications (IJHPCA)*, 32(1): 159-175, 2018
- J11. D. Chapp(\*), K. Sato, D. Ahn, and **M. Tauffer**. Record-and-Replay Techniques for HPC Systems: A survey. *Journal of Supercomputing Frontiers and Innovations*, 5(1):11-30, 2018. (*Correspondent author*)
- J12. T. Johnston(#), B. Zhang(\*), A. Liwo, S. Crivelli, and **M. Tauffer**. In-Situ Data Analytics and Indexing of

- Protein Trajectories. *Journal of Computational Chemistry (JCC)*, 38(16):1419-1430, 2017. (Correspondent author)
- J13. B. Zhang(\*), T. Estrada, P. Cicotti, P. Balaji, and **M. Tauffer**. Enabling Scalable and Accurate Clustering of Distributed Ligand Geometries on Supercomputers. *Journal of Parallel Computing (ParCo)*, 63: 38 – 60, 2017. (Correspondent author)
- J14. **M. Tauffer** and A. L. Rosenberg. Scheduling DAG-based Workflows on Single Cloud Instances: High-performance and Cost Effectiveness with a Static Scheduler. *International Journal of High Performance Computing Applications (IJHPCA)*, 31(1): 19 – 31, 2017. (Correspondent author)
- J15. V. Stodden, M. McNutt, D. H. Bailey, E. Deelman, Y. Gil, B. Hanson, M. A. Heroux, J. P.A. Ioannidis, and **M. Tauffer**. Enhancing Reproducibility for Computational Methods - Data, code and workflows should be available and cited. *Science*, 354(6317), December 9, 2016.
- J16. S. Herbein(+), S. McDaniel(+), N. Podhorszki, S. Klasky, and **M. Tauffer**. Performance Characterization of Irregular I/O at the Extreme Scale. *Journal of Parallel Computing*, 51: 17 – 36, 2016. (Correspondent author)
- J17. T. Johnston(#), B. Zhang(\*), A. Liwo, S. Crivelli, and **M. Tauffer**. It-Situ Data Analysis of Protein Folding Trajectories. *CoRR abs/1510.08789*, pp. 1 – 40, October 30, 2015. (Correspondent author)
- J18. S. Ou, D. Cui, M. Wezowicz(+), **M. Tauffer**, and S. Patel. Free Energetics of Carbon Nanotube Association in Aqueous Inorganic NaI Salt Solutions: Temperature Effects using All-Atom Molecular Dynamics Simulations and High-Performance Graphical Processing Unit Based Resources. *Journal of Computational Chemistry*, 36(16): 1196 – 1212, 2015.
- J19. S. Schlachter(+), S. Herbein(+), S. Ou, J.S. Logan, S. Patel, and **M. Tauffer**. Pursuing Resource Utilization and Coordinated Progression in GPU-enabled Molecular Simulations. *IEEE Design&Test of Computers*, 31(1): 40 – 50, February 2014. (Correspondent author)
- J20. J. F. Lawrence, E.S. Cochran, A. Chung, A. Kaiser, C.M. Christensen, R. Allen, D. Anderson, J.W. Baker, B. Fry, T. Heaton, D. Kilb, M.D. Kohler, and **M. Tauffer**. Rapid Earthquake Characterization Using MEMS Accelerometers and Volunteer Hosts Following the *M*7.2 Darfield, New Zealand, Earthquake. *Bulletin of the Seismological Society of America*, 104(1): 184 – 192, doi: 10.1785/0120120196. February 2014.
- J21. K. Benson(+), S. Schlachter(+), T. Estrada(\*), **M. Tauffer**, E. Cochran, and J. Lawrence. On the Powerful Use of Simulations in the Quake-Catcher Network to Efficiently Position Low-cost Earthquake Sensors. *Future Generation Computer Systems*, 29(8): 2128–2142, October 2013. (Correspondent author)
- J22. B. Zhang(\*), D. T. Yehdego(\*), K. L. Johnson, M.-Y. Leung, and **M. Tauffer**. Enhancement of Accuracy and Efficiency for RNA Secondary Structure Prediction by Sequence Segmentation and MapReduce. *BMC Structural Biology*, 13(Suppl 1): S3, pp. 1 – 24, November 8, 2013. (Correspondent author with Leung)
- J23. **M. Tauffer**, N. Ganesan(#), and S. Patel. GPU-enabled Macromolecular Simulation: Challenges and Opportunities. *IEEE Computing in Science and Engineering (CiSE)*, 15(1): 64 – 64, 2013. (Correspondent author)
- J24. G. Arampatzis, M.A. Katsoulakis, P. Plechac, **M. Tauffer**, and L. Xu(\*). Hierarchical Fractional-step Approximations and Parallel Kinetic Monte Carlo Algorithms. *J. Computational Physics*, 231(23): 7795 – 7814, October 2012.
- J25. T. Estrada(\*), B. Zhang(\*), P. Cicotti, R. Armen, and **M. Tauffer**. A Scalable and Accurate Method for Classifying Protein-Ligand Binding Geometries Using a MapReduce Approach. *Comp. in Bio. and Med.*, 42(7): 758 – 771, July 2012. (Correspondent author)
- J26. N. Ganesan(#), B.A. Bauer, T. Lucas, S. Patel, and **M. Tauffer**. Structural, Dynamic, and Electrostatic Properties of Fully Hydrated DMPC Bilayers from Molecular Dynamics Simulations Accelerated with Graphical Processing Units (GPUs). *J. Computational Chemistry*, 32(14): 2958 – 2973, 2011. (Correspondent author with Patel)
- J27. O. Rahaman(\*), T. Estrada(\*), D. Doren, **M. Tauffer**, C. L. Brooks III, and R.S. Armen. Evaluation of Several Two-Step Scoring Functions Based on Linear Interaction Energy, Effective Ligand Size, and Empirical Pair Potentials for Prediction of Protein-Ligand Binding Geometry and Free Energy. *J. Chemical Information and Modeling*, 51(9): 2047 – 65, 2011.
- J28. B.A. Bauer, J.E. Davis(\*), **M. Tauffer**, and S. Patel. Molecular Dynamics Simulations of Aqueous Ions at

- the Liquid-Vapor Interface Accelerated Using Graphics Processors. *J. Computational Chemistry*, 32(3): 375 – 385, 2011. (Correspondent author with Patel)
- J29. J.J. Rosskopf, J.H. Upton, III, M.-Y. Leung, **M. Tauffer**, and K.L. Johnson. 3' Terminal Stem-loop Structure in Nodamura Virus RNA2 Forms an Essential Cis-acting Signal for RNA Replication. *Virus Research*, 150: 12 – 21, 2010.
- J30. T. Estrada(\*), **M. Tauffer**, and D. Anderson. Performance Prediction and Analysis of BOINC Projects: An Empirical Study with EmBOINC. *J. Grid Computing*, 7: 537 – 554, 2009. (Leading author)
- J31. **M. Tauffer**, R.S. Armen, J. Chen, P.J. Teller, and C.L. Brooks III. Computational Multi-Scale Modeling in Protein-Ligand Docking. *IEEE Engineering in Medicine and Biology Magazine*, 28(2): 58 – 69, 2009. (Correspondent author)
- J32. **M. Tauffer**, A. Licon(+), R. Araiza(\*), D. Mireles, A. Gulyaev, F.H.D. Van Batenburg, and M-Y Leung. PseudoBase++: An Extension of PseudoBase for Easy Searching, Formatting, and Visualization of Pseudoknots. *Nucleic Acids Research*, Database Issue, 37, pp. 1 – 9, 2009. (Correspondent author)
- J33. **M. Tauffer**, M-Y. Leung, T. Solorio, A. Licon(+), D. Mireles(+), R. Araiza(\*), and K.J. Johnson. RNAVLab: A Virtual Laboratory for Studying RNA Secondary Structures based on Grid Computing Technology. *J. Parallel Computing*, 34: 661 – 680, 2008. (Leading author)
- J34. T. Estrada(\*), O. Fuentes, and **M. Tauffer**. A Distributed Evolutionary Method to Design Scheduling Policies for Volunteer Computing. *ACM SIGMETRICS Performance Evaluation Review Journal*, 36(3): 40 – 49, 2008. (Correspondent author)
- J35. K. Bhatia, **M. Tauffer**, B. Stearn, R. Zamudio(\*), and D. Catarino(+). Integrate GridFTP into Firefox - Build Grid Protocols into Mozilla-based Tools. *IBM developerWorks*, 10 October 2006.
- J36. **M. Tauffer**, C. An, A. Kerstens, and C.L. Brooks III: Predictor@Home. A Protein Structure Prediction Supercomputer Based on Global Computing. *IEEE Transactions on Parallel and Distributed Systems*, 17(8): 786 – 796, 2006.
- J37. **M. Tauffer**, M. Crowley, D. Price, A.A. Chien, and C.L. Brooks III. Study of an Accurate and Fast Protein-Ligand Docking Algorithm based on Molecular Dynamics. *Concurrency and Computation: Practice and Experience*, 17(14): 1627 – 1641, 2005.
- J38. P. Cicotti, **M. Tauffer**, and A.A. Chien. DGMonitor: a Performance Monitoring Tool for Sandbox-based Desktop Grid Platforms. *J. Supercomputing*, 34(2): 113 – 133, 2005. (Correspondent author)
- J39. K. Baldridge, J.P. Greenberg, W. Sudholt, K. Bhatia, S. Mock, C. Amoreira, Y. Potier, and **M. Tauffer**. The Computational Chemistry Prototyping Environment. *Proceedings of the IEEE - Special Issue on Grid Computing*, 93(3): 510 – 521, 2005.

## RESEARCH PAPERS IN REFEREED CONFERENCES AND SYMPOSIUMS (PEER-REVIEWED):

(Acceptance rates are provided when known.)

- C1. T. Mai Anh Do, L. Pottier, S. Thomas (#), R. Ferreira da Silva, M. A. Cuendet, H. Weinstein, T. Estrada, **M. Tauffer**, and E. Deelman. A Novel Metric to Evaluate In Situ Workflows. In *Proceedings of the International Conference on Computational Science (ICCS)*, pp. 1 – 14. Amsterdam, The Netherlands. 2020.
- C2. M.R. Wyatt II (\*), S. Herbein, K. Shoga, T. Gamblin, and **M. Tauffer**. CanarIO: Sounding the Alarm on IO-Related Performance Degradation. In *Proceedings of the 34<sup>th</sup> IEEE International Parallel and Distributed Processing Symposium (IPDPS)*, pp. 1-12. New Orleans, LA, USA. May 18-22, 2020. (Acceptance Rate: 45/110, 24.7%)
- C3. S. Thomas (#), M. Wyatt, T. M. Anh Do, L. Pottier, R. Ferreira da Silva, H. Weinstein, M. A. Cuendet, T. Estrada, E. Deelman, and **M. Tauffer**. Characterization of In Situ and In Transit Analytics of Molecular Dynamics Simulations for Next-generation Supercomputers. In *Proceedings of the IEEE eScience Conference*, pp.1-12. San Diego, CA, USA. September 24-27, 2019.
- C4. D. Rorabaugh (#), M. Guevara, R. Llamas, J. Kitson, R. Vargas, and **M. Tauffer**. SOMOSPIE: A Modular SOil MOisture SPatial Inference Engine based on Data Driven Decisions. In *Proceedings of the IEEE eScience Conference*, pp. 1-10. San Diego, CA, USA. September 24-27, 2019.
- C5. J. Davis (+), T. Gao (\*), S. Chandrasekaran, J. Heike, D. Anthony, B. Pavan, J. Dongarra, and **M. Tauffer**. Characterization of Power Usage and Performance in Data-Intensive Applications using MapReduce over

- MPI. In *Proceedings of the International Conference on Parallel Computing (ParCo)*, pp. 1-16. Prague, Check Republic. September 10-13, 2019.
- C6. T. Gao (\*), Y. Guo, B. Zhang, P. Cicotti, Y. Lu, P. Balaji, and **M. Taufer**. On the Power of Combiner Optimizations in MapReduce over MPI Workflows. In *Proceedings of the IEEE 24th International Conference on Parallel and Distributed Systems (ICPADS)*, pp. 441-448. Singapore. December 11-13, 2018. (Acceptance Rate: 257/97, 37.7%)
- C7. T. Estrada, J. Benson, H. Carrillo-Cabada, A. Razavi, M. Cuendet, H. Weinstein, E. Deelman, and **M. Taufer**. Graphic Encoding of Proteins for Efficient High-Throughput Analysis. In *Proceedings of the 9th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (BCB)*, pp. 315 – 324. Washington, DC, USA. August 29 - September 1, 2018. (Acceptance Rate: 27%)
- C8. M.R. Wyatt II (\*), S. Herbein (\*), T. Gamblin, A. Moody, D. Ahn, and **M. Taufer**. PRIONN: Predicting Runtime and IO using Neural Networks. In *Proceedings of the International Conference on Parallel Processing (ICPP)*, pp. 1 – 12. Eugene, OR, USA. August 13-16, 2018. (Acceptance Rate: 305/99, 32.5%)
- C9. X. Chen, M. Peterson, J. Benson, **M. Taufer**, and T. Estrada. KeyBin2: Distributed Clustering for Scalable and In-Situ Analysis. In *Proceedings of the International Conference on Parallel Processing (ICPP)*, pp. 1 – 10. Eugene, OR, USA. August 13-16, 2018. (Acceptance Rate: 305/99, 32.5%)
- C10. S. McDaniel (\*), D. L. Boothe, D. R. Shires, A. B. Yu, and **M. Taufer**. Leveraging In Situ Analysis to Enable Computational Steering of Brain's Neocortex Simulations with GENESIS. In *Proceedings of the International Symposium on Advances in High Performance Computing and Networking (AHPCN)*, pp. 873-880. Exeter, England, UK. June 28-30, 2018.
- C11. T. Gao (\*), Y. Guo, Y. Wei, B. Wang, Y. Lu, P. Cicotti, P. Balaji, and **M. Taufer**. Bloomfish: A Highly Scalable Distributed K-mer Counting Framework. In *Proceedings of the IEEE 23rd International Conference on Parallel and Distributed Systems (ICPADS)*. Shenzhen, China. December 15-17, 2017. (Acceptance Rate: 271/89, 32.8%)
- C12. T. Gao(\*), Y. Guo, B. Zhang, P. Cicotti, Y. Lu, P. Balaji, and **M. Taufer**. Mimir: Memory-Efficient and Scalable MapReduce for Large Supercomputing Systems. In *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS)*. Orlando, Florida, USA. May 29 – Jun 2, 2017. (Acceptance Rate: 116/616, 18.8%)
- C13. S. McDaniel(\*), D. L. Boothe, J. C. Crone, S. Jun Park, D. R. Shires, A. B. Yu, and **M. Taufer**. Study of Neocortex Simulations with GENESIS on High Performance Computing Resources. In *Proceedings of the 22th IEEE International Conference on Parallel and Distributed Systems (ICPADS)*, pp. 924-931. Wuhan, China. December 14 – 16, 2015. (Acceptance Rate: 82/230, 35.6%)
- C14. T. Johnston(#), C. Zannin(+), and **M. Taufer**. HYPPO: A Hybrid, Piecewise Polynomial Modeling Technique for Non-Smooth Surfaces. In *Proceedings of the 28th IEEE International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD)*, pp. 1 – 8. Los Angeles, CA, USA. October 26 – 28, 2016. (Acceptance Rate: 27/77, ~35% – One of four Best Paper Candidates)
- C15. J. Benson, T. Estrada, A. Rosenberg, and **M. Taufer**. Scheduling Matters: Area-oriented Heuristics for Resource Management. . In *Proceedings of the 28th IEEE International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD)*, pp. 1 – 8. Los Angeles, CA, USA. October 26 – 28, 2016. (Rate: 27/77, ~35%)
- C16. M. Wyatt (\*), T. Johnston(#), M. Papas, and **M. Taufer**. Development of a Scalable Method for Creating Food Groups Using the NHANES Dataset and MapReduce. In *Proceedings of the ACM Bioinformatics and Computational Biology Conference (BCB)*, pp. 1 – 10. Seattle, WA, USA. October 2 – 4, 2016. (Acceptance Rate: 47/112, 42%)
- C17. R. McKenna (+), S. Herbein (\*), A. Moody, T. Gamblin, and **M. Taufer**. Machine Learning Predictions of Runtime and IO Traffic on High-end Clusters. *IEEE Cluster Conference*, pp. 1 – 4. Taipei, Taiwan. September 12 – 16, 2016. (Acceptance Rate: 35% for full and short papers)
- C18. S. Herbein (\*), D. H. Ahn, D. Lipari, T. R.W. Scogland, M. Stearman, M. Grondona, J. Garlick, B. Springmeyer, and **M. Taufer**. Scalable I/O-Aware Job Scheduling for Burst Buffer Enabled HPC Clusters. In *Proceedings of the ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC)*, pp. 1 – 10. Kyoto, Japan. May 30 – Jun 4, 2016. (Rate: 20/129, 15.5%)

- C19. S. Herbein (\*), A. Dusia (\*), A. Landwehr (\*), S. McDaniel (\*), J. Monsalve (\*), Y. Yang (\*), S. R. Seelam, and **M. Tauffer**. Resource Management for Running HPC Applications in Container Clouds In *Proceedings of the International Supercomputing Conference (ISC)*, pp. 1 – 19. Frankfurt, Germany. June 19 – 23, 2016. (Acceptance Rate: 25/60, 40%)
- C20. T. Estrada, M. R. Wyatt, and **M. Tauffer**. A Genetic Programming Approach to Design Resource Allocation Policies for Heterogeneous Workflows in the Cloud. In *Proceedings of the 21th IEEE International Conference on Parallel and Distributed Systems (ICPADS)*, pp. 372 – 379. Melbourne, Australia. December 14 – 16, 2015. (Acceptance Rate: 82/230, 35.6%)
- C21. D. Chapp (\*), T. Johnston, and **M. Tauffer**. The Strong Case for Pursuing Numerical Reproducibility through Intelligent Runtime Selection of Reduction Algorithms at the Extreme Scale. In *Proceedings of IEEE Cluster Conference*, pp. 166 – 175. Chicago, Illinois, USA. September 8 – 11, 2015. (Acceptance Rate: 38/157, 24%)
- C22. V. Pallipuram (#), T. Estrada, and **M. Tauffer**. A Testing Engine for High-Performance and Cost-Effective Workflow Execution in the Cloud. In *Proceedings of the International Conference on Parallel Processing (ICPP)*, pp. 849 – 858. Beijing, China. September 1 – 4, 2015. (Acceptance Rate: 99/305, 32.5%)
- C23. R. McKenna (+), V. Pallipuram (#), R. Vargas, and **M. Tauffer**. From HPC Performance to Weather Modeling: Transforming Methods for HPC Predictions Into Models of Extreme Climate Conditions. In *Proceedings of the Tenth IEEE International Conference on e-Science and Grid Technologies (eScience)*, pp. 108 – 117. Munich, Germany. August 31 – September 4, 2015.
- C24. T. Johnston (#), M. Alsulmi (\*), P. Cicotti and **M. Tauffer**. Performance Tuning of MapReduce Jobs Using Surrogate-Based Modeling. In *Proceedings of the International Conference on Computational Science (ICCS)*, pp. 49 – 59. Reykjavik, Iceland. June 1 – 3, 2015. (Acceptance Rate: 26%)
- C25. B. Zhang (\*), T. Estrada, P. Cicotti, P. Balaji, and **M. Tauffer**. Accurate Scoring of Drug Conformations at the Extreme Scale. In *Proceedings of 8th IEEE International Scalable Computing Challenge - Co-located with IEEE/ACM CCGrid*, pp. 817 – 822. Shenzhen, China. 4 – 7 May 2015. (Award Winners. Acceptance Rate: 5/15, 33%)
- C26. M. Matheny (+), S. Herbein (+), N. Podhorszki, S. Klasky, and **M. Tauffer**. Using Surrogate-based Modeling to Predict Optimal I/O Parameters of Applications at the Extreme Scale. In *Proceedings of the 20th IEEE International Conference on Parallel and Distributed Systems (ICPADS)*, pp. 568 – 575. Hsinchu, Taiwan. December 16 – 19, 2014. (Acceptance Rate: 96/322, 29.8%)
- C27. B. Javadi, B. Zhang (\*), and **M. Tauffer**. Bandwidth Modeling in Large Distributed Systems for Big Data Applications. In *Proceedings of the 15th International Conference on Parallel and Distributed Computing, Applications and Technologies (PDCAT)*, pp. 21 – 27. Hong Kong, China. December 9 – 11, 2014.
- C28. F. Raoking, J. Cohoon, K. Cooke, **M. Tauffer**, and T. Estrada(#). Gender and Volunteer Computing. In *Proceedings of the 44th Annual Frontiers in Education (FIE) Conference*, pp. 1 – 5. Madrid, Spain. October 22 – 25, 2014.
- C29. V. K. Pallipuram (#), J. DiMarco (\*), and **M. Tauffer**. Applying Frequency Analysis Techniques to DAG-based Workflows to Benchmark and Predict Resource Behavior on Non-Dedicated Clusters. In *Proceedings of the IEEE Cluster 2014 Conference*, pp. 29 – 37. Madrid, Spain, September 22 – 26, 2014. (Acceptance Rate: 29/122, 23.8% - One of four Best Paper Candidates)
- C30. M. Portnoi (\*), S. Schlachter (\*), and **M. Tauffer**. Study the Network Impact on Earthquake Early Warning in the Quake-Catcher Network Project. In *Proceedings of the International Conference on Computational Science (ICCS)*, pp. 453 – 464. Cairns, Queensland, Australia. June 10 – 12, 2014. (Acceptance Rate: 197/65, 33%)
- C31. B. Zhang (\*), T. Estrada (#), P. Cicotti, and **M. Tauffer**. Enabling In-situ Data Analysis for Large Protein Folding Trajectory Datasets. In *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS)*, pp. 221 – 230. Phoenix, Arizona, USA. May 19 – 23, 2014. (Acceptance Rate: 114/541, 21%)
- C32. S. Herbein (+), M. Matheny (+), M. Wezowicz (+), J. Kroger, J.S. Logan, J. Kim, S. Klasky, **M. Tauffer**. Performance Impact of I/O on QMCPack Simulations at the Petascale and Beyond. In *Proceedings of the 16<sup>th</sup> IEEE International Conferences on Computational Science and Engineering (CSE)*, pp. 92 – 99.

Sydney, Australia. December 2013.

- C33. B. Zhang (\*), T. Estrada (#), P. Cicotti, and **M. Tauffer**. On Efficiently Capturing Scientific Properties in Distributed Big Data without Moving the Data - A Case Study in Distributed Structural Biology using MapReduce. In *Proceedings of the 16<sup>th</sup> IEEE International Conferences on Computational Science and Engineering (CSE)*, pp. 117 – 124. Sydney, Australia. December 2013.
- C34. S. Schlachter (\*), S. Herbein (+), S. Ou, J. S. Logan, S. Patel, and **M. Tauffer**. Efficient Sodium dodecyl sulfate (SDS) Simulations on Multi-GPU Nodes of XSEDE High-end Clusters. In *Proceedings of the Eighth IEEE International Conference on e-Science and Grid Technologies (eScience)*, pp. 116 – 123. Beijing, China. October 2013.
- C35. J. DiMarco (\*) and **M. Tauffer**. Performance Impact of Dynamic Parallelism on Clustering Algorithms on GPUs. In *Proceedings of the DSS11 SPIE Defense, Security, and Sensing Symposium - Modeling and Simulation for Defense Systems and Applications VI*, pp. 1 – 8. Baltimore, Maryland, USA. May 2013.
- C36. T. Estrada (\*) and **M. Tauffer**. On the Effectiveness of Application-aware Self-management for Scientific Discovery in Volunteer Computing Systems. In *Proceedings of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC)*, pp. 1 – 11. Salt Lake City, Utah, USA. November 2012. (Acceptance Rate: 100/472, 21%)
- C37. T. Estrada (\*), B. Zhang (\*), P. Cicotti, R. Armen, and **M. Tauffer**. Reengineering High-throughput Molecular Datasets for Scalable Clustering using MapReduce. In *Proceedings of the 14th IEEE International Conference on High Performance Computing and Communications (HPCC-2012)*, pp. 351 – 359. Liverpool, England, UK. June 2012. (Acceptance Rate: 104/395, ~26.2%)
- C38. M. Wezowicz (+), B. D. Saunders, and **M. Tauffer**. Dealing with Performance/Portability and Performance/Accuracy Trade-offs in Heterogeneous Computing Systems: A Case study with Matrix Multiplication Modulo Primes. In *Proceedings of the DSS11 SPIE Defense, Security, and Sensing Symposium - Modeling and Simulation for Defense Systems and Applications VI*, pp. 1 – 10. Baltimore, Maryland, USA. April 2012.
- C39. K. Benson (+), T. Estrada(\*), **M. Tauffer**, E. Cochran, and J. Lawrence. On the Powerful Use of Simulations in the Quake-Catcher Network to Efficiently Position Low-cost Earthquake Sensors. In *Proceedings of the Seventh IEEE International Conference on e-Science and Grid Technologies (eScience)*, pp. 77 – 84. Stockholm, Sweden. December 2011. (Acceptance Rate: 54/110, 50%)
- C40. T. Estrada (\*) and **M. Tauffer**. Providing quality of science in volunteer computing. In *Proceedings of the 13<sup>th</sup> IEEE High Performance Computing and Communications (HPCC) Conference*, pp. 68 – 77. Banff, Canada. September 2011. (Acceptance Rate: 59/271, 21.7%)
- C41. N. Ganesan (#), R.D. Chamberlain, J. Buhler, and **M. Tauffer**. Rolling Partial Prefix-Sums To Speedup Evaluation of Uniform and Affine Recurrence Equations. In *Proceedings of the DSS11 SPIE Defense, Security, and Sensing Symposium - Modeling and Simulation for Defense Systems and Applications VI*, pp. 1 – 8. Orlando, Florida, USA. April 2011.
- C42. T. Estrada (\*), R. Armen, and **M. Tauffer**. Automatic Selection of Near-Native Protein-Ligand Conformations using a Hierarchical Clustering and Volunteer Computing. In *Proceedings of the ACM International Conference on Bioinformatics and Computational Biology (BCB)*, pp. 204 – 213. New York, USA. August 2010. (Acceptance Rate: 37/136, 28%)
- C43. N. Ganesan (#), R.D. Chamberlain, J. Buhler, and **M. Tauffer**. Accelerating HMMER on GPUs by implementing hybrid data and task parallelism. In *Proceedings of the ACM International Conference on Bioinformatics and Computational Biology (BCB)*, pp. 418-421. New York, USA. August 2010. (Short Paper – Acceptance Rate: 30/99, 33%)
- C44. **M. Tauffer**, O. Padron (+), P. Saponaro (+), and S. Patel. Improving Numerical Reproducibility and Stability in Large-Scale Numerical Simulations on GPUs. In *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS)*, pp. 1 – 9. Atlanta, Georgia, USA. April 2010. (Acceptance Rate: 127/527, 24%)
- C45. L. Xu (\*), **M. Tauffer**, S. Collins, and D. G. Vlachos. Parallelization of Tau-Leap Coarse-Grained Monte Carlo Simulations on GPUs. In *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS)*, pp. 1 – 9. Atlanta, Georgia, USA. April 2010. (Acceptance Rate: 127/528,

24%)

- C46. A. Licon (\*), **M. Tauffer**, M.-Y. Leung, and K.L. Johnson. A Dynamic Programming Algorithm for Finding the Optimal Segmentation of an RNA Secondary Structure Prediction. In *Proceedings of the International Conference on Bioinformatics and Computational Biology (BICoB)*, pp. 165-170. Honolulu, Hawaii, USA. March 2010. (Acceptance Rate: 45%)
- C47. J. Atlas (\*), T. Estrada (\*), K. Decker, and **M. Tauffer**. Balancing Scientist Needs and Volunteer Preferences in Volunteer Computing using Constraint Optimization. In *Proceedings of the International Conference on Computational Science (ICCS)*, pp. 143 – 152. Baton Rouge, Louisiana, USA. May 2009. (Acceptance Rate: ~30%)
- C48. T. Estrada (\*), **M. Tauffer**, and K. Reed. Modeling Job Lifespan Delays in Volunteer Computing Projects. In *Proceedings of the 9<sup>th</sup> IEEE International Symposium on Cluster Computing and Grid (CCGrid)*, pp. 331 – 338. Shanghai, China. May 2009. (Acceptance Rate: 57/271, 21%)
- C49. J.E. Davis (\*), A. Ozsoy (\*), S. Patel, and **M. Tauffer**. Towards Large-Scale Molecular Dynamics Simulations on Graphics Processors. In *Proceedings of the International Conference on Bioinformatics and Computational Biology (BICoB)*, pp. 176 – 186. New Orleans, Louisiana, USA. April 2009. (Acceptance Rate: 30/72, 41.6%)
- C50. T. Estrada (\*), O. Fuentes, and **M. Tauffer**. A Distributed Evolutionary Method to Design Scheduling Policies for Volunteer Computing. In *Proceedings of ACM Computing Frontiers (CF)*, pp. – . Ischia, Italy. May 2008. (Acceptance Rate: 30/110, 27%)
- C51. G. Lopez (+), **M. Tauffer**, and P.J. Teller. Evaluation of IEEE 754 Floating-Point Arithmetic Compliance Across a Wide Range of Heterogeneous Computers. In *Proceedings of the 2007 Richard Tapia Celebration of Diversity in Computing Conference*, pp. 313 – 322. Orlando, Florida, USA. October 2007.
- C52. R. Araiza (\*), **M. Tauffer**, and M.-Y. Leung. Towards Optimal Scheduling for Global Computing Under Probabilistic, Interval, and Fuzzy Uncertainty, with Potential Applications to Bioinformatics. In *Proceedings of the 26<sup>th</sup> International Conference of the North American Fuzzy Information Processing Society (NAFIPS)*, pp. 520 – 525. San Diego, California, USA. June 2007.
- C53. T. Estrada (\*), D.A. Flores (\*), **M. Tauffer**, P.J. Teller, A. Kerstens, and D. Anderson. The Effectiveness of Threshold-based Scheduling Policies in BOINC Projects. In *Proceedings of the Second IEEE International Conference on e-Science and Grid Technologies (eScience)*, pp. 1 – 12. Amsterdam, The Netherlands. December 2006. (Acceptance Rate: 60/160, 37.5%)
- C54. **M. Tauffer**, P.J. Teller, D.P. Anderson, and C.L. Brooks III. Metrics for Effective Resource Management in Global Computing Environments. In *Proceedings of the First IEEE International Conference on e-Science and Grid Technologies (eScience)*, pp. 1 – 8. Melbourne, Australia. December 2005. (Acceptance Rate: 54/171, 31.6%)
- C55. D. Kondo, **M. Tauffer**, C.L. Brooks III, H. Casanova, and A.A. Chien. Characterizing and Evaluating Desktop Grids: An Empirical Study. In *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS)*, pp. 1 – 10. Santa Fe, New Mexico, USA. April 2004. (Acceptance Rate: 31.7%)
- C56. **M. Tauffer**, and T. Stricker. A Performance Monitor based on Virtual Global Time for Clusters of PCs. In *Proceedings of the IEEE International Conference on Cluster Computing 2003 (Cluster)*, pp. 64 – 72. Hong Kong, China. December 2003. (Acceptance Rate: 48/164, 29.3%)
- C57. B. Uk, **M. Tauffer**, T. Stricker, G. Settanni, A. Cavalli, and A. Caflisch. Combining Task- and Data Parallelism to Speed up Protein Folding on a Desktop Grid Platform - Is efficient protein folding possible with CHARMM on the United Devices MetaProcessor? In *Proceedings the IEEE International Symposium on Cluster Computing and the Grid (CCGRID)*, pp. 240 – 247. Tokyo, Japan. May 2003. (Acceptance Rate: 39/114, 34.2%)
- C58. B. Uk, **M. Tauffer**, T. Stricker, G. Settanni, and A. 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 IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS)*, pp. 1 – 10. Nice, France. April 2003. (Acceptance Rate: 119/407, 29.2%)
- C59. **M. Tauffer**, T. Stricker, and R. Weber. Scalability and Resource Usage of an OLAP Benchmark on Clusters



- of PCs. In *Proceedings of the 14<sup>th</sup> ACM Symposium on Parallel Algorithms and Architectures (SPAA)*, pp. 83 – 94. Winnipeg, Manitoba, Canada. August 2002.
- C60. **M. Tauber**, T. Stricker, G. Roos, P. Guentert. On the Migration of the Scientific Code DYANA from SMPs to Clusters of PCs and on to the Grid. In *Proceedings of the IEEE International Symposium on Cluster Computing and the Grid (CCGRID)*, pp. 93 – 101. Berlin, Germany. May 2002. (Acceptance Rate: 25.0%)
- C61. **M. Tauber**, E. Perathoner, A. Cavalli, A. Caflisch, and T. Stricker. Performance Characterization of a Molecular Dynamics Code on PC Clusters - Is there any easy parallelism in CHARMM? In *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS)*, pp. 1 – 10. Fort Lauderdale, Florida, USA. April 2002. (Acceptance Rate: 98/258, 38%)
- C62. **M. Tauber**, and T. Stricker. Accurate Performance Evaluation, Modeling and Prediction of a Message Passing Simulation Code based on Middleware. In *Proceedings of the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. Orlando, Florida, USA. November 1998.
- C63. P. Arbenz, M. Billeter, P. Guentert, P. Luginbuehl, **M. Tauber**, and U. von Matt. Molecular Dynamics Simulations on Cray Clusters using the Scidde-PVM Environment. *Lecture Notes in Computer Science, Parallel Virtual Machine — EuroPVM '96*. Lecture Notes in Computer Science 1156 A. Bode, J. Dongarra, T. Ludwig, V. Sunderam (Eds.) *Presented at the Parallel Virtual Machine – EuroPVM'96, Third European PVM Conference*, Munich, Germany. October 1996.

## RESEARCH PAPERS IN REFEREED WORKSHOP (PEER-REVIEWED):

(Acceptance rates are provided when known.)

- W1. V. Welch, V. Stodden, E. Deelman, and **M. Tauber**. Initial Thoughts on Cybersecurity And Reproducibility. In *Proceedings of the 2<sup>nd</sup> International Workshop on Practical Reproducible Evaluation of Computer Systems (P-REC)*, co-located with the ACM HPDC Conference, 1-6. Phoenix, AZ, June 2019.
- W2. D. Chapp (+), D. Rorabaugh (#), D. Brown, E. Deelman, K. Vahi, V. Welch, and **M. Tauber**. Applicability study of the PRIMAD model to LIGO gravitational wave search workflows. In *Proceedings of the 2<sup>nd</sup> International Workshop on Practical Reproducible Evaluation of Computer Systems (P-REC)*, co-located with the ACM HPDC Conference, 1-6. Phoenix, AZ, June 2019.
- W3. D. H. Ahn, N. Bass, A. Chu, J. Garlick, M. Grondona, S. Herbein, J. Koning, T. Patki, T. R. W. Scogland, B. Springmeyer, and **M. Tauber**. Flux: Overcoming Scheduling Challenges for Exascale Workflows. In *Proceedings of the 13th Workshop on Workflows in Support of Large-Scale Science (WORKS)*, Dallas, TX, November 2018, (Acceptance Rate: 8/19, 42%).
- W4. S. Herbein (+), S. Klasky, and **M. Tauber**. Benchmarking the Performance of Scientific Applications with Irregular I/O at the Extreme Scale. In *Proceedings of the Seventh International Workshop on Parallel Programming Models and Systems Software for High-End Computing (P2S2)*, pp. 291 – 301. Minneapolis, MN, USA. September 2014. (Acceptance Rate: 25/13, 52%)
- W5. T. Estrada (#), K. Pusecker, M. Torres, J. Cohoon, and **M. Tauber**. Benchmarking Gender Differences in Volunteer Computing Projects. In the *Proceedings of the 3<sup>rd</sup> Workshop on Analyzing and Improving Collaborative eScience with Social Networks (eSoN)*, pp. 342 – 349. Beijing, China. October 2013.
- W6. M. Wezowicz(+), T. Estrada(#), S. Patel, and **M. Tauber**. Performance Dissection of a MD Code across CUDA and GPU Generations. In *Proceedings of the 14<sup>th</sup> IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC)*, pp. 1355 – 1364. Boston, Massachusetts, USA. April 2013. (Acceptance Rate: 16/42, 38%)
- W7. D. Yehdego (\*), B. Zhang (\*), V. K. R. Kodimala, K. Johnson, **M. Tauber**, and M.-Y. Leung. Secondary Structure Predictions for Long RNA Sequences based on Inversion Excursions and MapReduce. In *Proceedings of 12<sup>th</sup> IEEE International Workshop on High Performance Computational Biology (HiCOMB)*, pp. 545 – 547. Boston, Massachusetts, USA. April 2013. (Acceptance Rate: 9/17, 52%)
- W8. M. Matheny (+), S. Schlachter (+), L. Crouse, E. Kimmel, T. Estrada(\*), M. Schumann, R. Armen, G. Zoppetti, and **M. Tauber**. ExSciTech: Expanding Volunteer Computing to Explore Science, Technology, and Health. In *Proceedings of the 2<sup>nd</sup> Workshop on Analyzing and Improving Collaborative eScience with Social Networks (eSoN)*, pp. 1 – 8. Chicago, Illinois, USA. October 2012.



- W9. B. Zhang (\*), D. Yehdego (\*), K. Johnson, M.-Y. Leung, and **M. Tauffer**. A Modularized MapReduce Framework to Support RNA Secondary Structure Prediction and Analysis Workflows. In *Proceedings of the 2012 Computational Structural Bioinformatics Workshop (CSBW)*, pp. 86 – 93. Philadelphia, Pennsylvanian, USA. October 2012. (Acceptance Rate: 11/33, 33%)
- W10. R. Riesen, K. Ferreira, M. Ruiz Varela(\*), **M. Tauffer**, and A. Rodrigues. Simulating Application Resilience at Exascale. In the *Proceedings of the 4<sup>th</sup> Workshop on Resiliency in High Performance Computing (Resilience) in Clusters, Clouds, and Grids*, in conjunction with the 17th International European Conference on Parallel and Distributed Computing (Euro-Par), pp. 221 – 230. Bordeaux France. August 2011.
- W11. N. Ganesan (#), B.A. Bauer (\*), S. Patel, and **M. Tauffer**. FEN ZI: GPU-enabled Molecular Dynamics Simulations of Large Membrane Regions based on the CHARMM Force Field and PME. In *Proceedings of the 10<sup>th</sup> IEEE International Workshop on High Performance Computational Biology (HiCOMB)*, pp. 472 – 480. Anchorage, Alaska, USA. May 2011. (Acceptance Rate: 11/21, 52.3%)
- W12. P. McClory (+), E. Kissel, D.M. Swany, and **M. Tauffer**. MNEOMIC: Network Environment for Measurement and Observation for Network Interaction and Control. In *Proceedings of the 1<sup>st</sup> Workshop on Grid and P2P Systems and Applications (GridPeer)*, held together with the 18<sup>th</sup> IEEE International Conference on Computer Communications and Networks (ICCCN), pp. 1 – 7. August 2009.
- W13. S. Kamboj (\*), T. Estrada(\*), **M. Tauffer**, and K. Decker. Applying Organizational Self-Design to a Real-world Volunteer Computing System. In *Proceedings of the Agent Design: Advancing from Practice to Theory Workshop (ADAPT)*, held together with AAMAS'09, pp. 1 – 10. Budapest, Hungary. May 2009.
- W14. T. Estrada (\*), **M. Tauffer**, K. Reed, and D. Anderson. EmBOINC: An Emulator for Performance Analysis of BOINC Projects. In *Proceedings of the Third Workshop on Large-Scale, Volatile Desktop Grids (PCGrid)*, in conjunction with IPDPS 2009, pp. 1 – 8. Rome, Italy. May 2009.
- W15. **M. Tauffer**, T. Solorio, A. Licon (+), D. Mireles (+), and M.-Y. Leung. On the Effectiveness of Rebuilding RNA Secondary Structures from Sequence Chunks. In *Proceedings of the 7<sup>th</sup> IEEE International Workshop on High Performance Computational Biology (HiCOMB)*, in conjunction with IPDPS 2008, pp. 1 – 8. Miami, Florida, USA. April 2008. (Acceptance Rate: 10/25, 40%)
- W16. **M. Tauffer**, A. Kerstens, T. Estrada (\*), D.A. Flores(\*), and P.J. Teller. SimBA: a Discrete Event Simulator for Performance Prediction of Volunteer Computing Projects. In *Proceedings of the International Workshop on Principles of Advanced and Distributed Simulation 2007 (PADS)*, pp. 1 – 9. San Diego, California, USA. June 2007. (Acceptance Rate: 37/24, 65%)
- W17. M. Tauffer, M.-Y. Leung, K. L. Johnson, A. Licon(+). RNAVLab: A Unified Environment for Computational RNA Structure Analysis based on Grid Computing Technology. In *Proceedings of the 6<sup>th</sup> IEEE International Workshop on High Performance Computational Biology (HiCOMB)*, in conjunction with IPDPS, pp. 1 – 8. Long Beach, California, USA. March 2007. (Acceptance Rate: 43%)
- W18. **M. Tauffer**, A. Kerstens, T. Estrada (\*), D.A. Flores (\*), R. Zamudio (\*), P.J. Teller, R. Armen, and C.L. Brooks III. Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling. In *Proceedings of the First Workshop on Large-Scale, Volatile Desktop Grids (PCGrid)*, in conjunction with IPDPS, pp. 1 – 8. Long Beach, California, USA. March 2007.
- W19. R. Zamudio (\*), D. Catarino, **M. Tauffer**, K. Bhatia, and B. Stearn. Topaz: Extending Firefox to Accommodate the GridFTP Protocol. In *Proceedings of the 4<sup>th</sup> High-Performance Grid Computing Workshop (HPGC)*, in conjunction with IPDPS, pp. 1 – 8. Long Beach, California, USA. March 2007.
- W20. T. Estrada (\*), A. Licon(+), and **M. Tauffer**. CompPknets: a Framework for Parallel Prediction and Comparison of RNA Secondary Structures with Pseudoknots. In *Proceedings of First Frontier on High Performance Computing and Networking Workshop (FHPCN)*, in conjunction with ISPA, pp. 1 – 8. Sorrento, Italy. December 2006.
- W21. K. Bhatia, B. Stearn, **M. Tauffer**, R. Zamudio(\*), and D. Catarino. Extending Grid Protocols onto the Desktop using the Mozilla Framework. In *Proceedings of the Second International Workshop on Grid Computing Environments (GCE)*, in conjunction with SC 2006, pp. 1 – 8. Tampa, Florida, USA. November 2006.
- W22. G. Aguilera (\*), P.J. Teller, **M. Tauffer**, and F. Wolf. A Systematic Multi-step Methodology for Performance Analysis of Communication Traces of Distributed Applications based on Hierarchical Clustering. In

*Proceedings of 5<sup>th</sup> International Workshop on Performance Modeling, Evaluation, and Optimization of Parallel and Distributed Systems (PMEO-PDS)*, in conjunction with IPDPS, pp. 1 – 8. Rhodes Island, Greece. April 2006.

- W23. **M. Tauffer**, C. An A. Kerstens, and C.L. Brooks III. Predictor@Home: A "Protein Prediction Supercomputer" Based on Public-Resource Computing. In *Proceedings 4<sup>th</sup> IEEE International Workshop on High Performance Computational Biology (HiCOMB)*, in conjunction with IPDPS 2005, pp. 1 – 8. Denver, Colorado, USA. April 2005. (Acceptance Rate: 10/32, 31.5%)
- W24. **M. Tauffer**, D.P. Anderson, P. Cicotti, and C.L. Brooks III. Homogeneous redundancy: a technique to ensure integrity of molecular simulation results using public computing. In *Proceedings of the 14<sup>th</sup> Heterogeneous Computing Workshop (HCW)*, in conjunction with IPDPS 2005, pp. 1 – 8. Denver, Colorado, USA. April 2005. (Acceptance Rate: 14/29, 47%)
- W25. **M. Tauffer**, M. Crowley, D. Price, A.A. Chien, and C.L. Brooks III. Study of an Accurate and Fast Protein-Ligand Docking Algorithm based on Molecular Dynamics. In *Proceedings of the Third IEEE International Workshop on High Performance Computational Biology (HiCOMB)*, in conjunction with IPDPS 2004, pp. 1 – 8. Santa Fe, New Mexico, USA. April 2004.
- W26. P. Cicotti, **M. Tauffer**, and A.A. Chien. DGMonitor: a Performance Monitoring Tool for Sandbox-based Desktop Grid Platforms. In *Proceedings of the Third International Workshop on Performance Modeling, Evaluation, and Optimization of Parallel and Distributed Systems (PMEO-PDS)*, in conjunction with IPDPS, pp. 1 – 8. Santa Fe, New Mexico, USA. April 2004.

#### DOE REPORTS:

- R1. M.A. Heroux, L.A. Barba, M. Parashar, V. Stodden, and **M. Tauffer**. Toward a Compatible Reproducibility Taxonomy for Computational and Computing Sciences. *Sandia Report SAND2018-11186*. Sandia National Laboratories. Albuquerque, New Mexico, USA. October 2018.
- R2. E. Deelman, T. Peterka, I. Altintas, C. Carothers, K.K. van Dam, K. Moreland, M. Parashar, L. Ramakrishnan, **M. Tauffer**, and J. Vetter. The Future of Scientific Workflows. *Report of the DOE NGNS/CS Scientific Workflows Workshop*. Rockville, Maryland, USA. April 20-21, 2015.

#### EDUCATIONAL PAPERS (SELECTED):

- E1. **M. Tauffer**, P.J. Teller, A. Kerstens, and R. Romero. Collaborative Research Tools for Students, Staff, and Faculty. In *Proceedings of the International SUN Conference on Teaching and Learning*, El Paso, Texas. March 2006.

#### ABSTRACTS, EXTENDED ABSTRACTS, AND POSTERS IN PEER-REVIEWED CONFERENCES, SYMPOSIUMS, AND WORKSHOPS:

(Acceptance rates are provided when known.)

- A1. D. Chapp (\*), D. Rorabaugh (#), and **M. Tauffer**. Modeling Record-and-Replay for Nondeterministic Applications on Exascale Systems. In *ModSim 2018: Workshop on Modeling & simulation of Systems and Applications*. Seattle, WA, USA. August 15-17, 2018.
- A2. R. M Llamas, M. Guevara, D. Rorabaugh(#), **M. Tauffer**, and Rodrigo Vargas. Large-Scale Soil Moisture Modeling Based on Linear Geostatistics and Remotely Sensed Data. In *AGU 100 – Advanced Earth and Space Science – Fall Meeting*. Washington DC. December 10-14, 2018.
- A3. R. Searles, S. Herbein (\*), T. Johnston, **M. Tauffer**, and S. Chandrasekaran. Creating a Portable, High-Level Graph Analytics Paradigm For Compute and Data-Intensive Applications. In *2018 GPU Technology Conference (GTC)*. San Jose, CA, USA. March 26-28, 2018.
- A4. Thomas Kitson(+), Paula Olaya(+), Elizabeth Racca(+), Michael R. Wyatt II(\*), Mario Guevara, Rodrigo Vargas, and **Michela Tauffer**. Data Analytics for Modeling Soil Moisture Patterns across United States Ecoclimatic Domains. In *Proceedings of the 2017 IEEE International Conference on Big Data*. pp 1-3. Boston, MA, USA. December 2017.
- A5. S. Herbein (\*), T. Patki, D. H. Ahn, D. Lipari, T. Dahlgren, D. Domyancic, and **M. Tauffer**. Fully Hierarchical Scheduling: Paving the Way to Exascale Workloads. In *29th ACM/IEEE International*

- Conference for High Performance Computing and Communications conference (SC)*, Denver, CO, USA. November 2017. (*Best Poster Candidate*)
- A6. Ayush Dusia (\*), Yang Yang(\*), and **M. Tauffer**. Network Quality of Service in Docker Containers. In *Proceedings of the IEEE Cluster 2015 Conference*. Chicago, Illinois, USA. September 2015.
- A7. Jose Manuel Monsalve Diaz (\*), Aaron Landwehr (\*), and **M. Tauffer**. Resource Management Layers for Dynamic CPU Resource Allocation in Containerized Cloud Environments. In *Proceedings of the IEEE Cluster 2015 Conference*. Chicago, Illinois, USA. September 2015.
- A8. Sean McDaniel (\*), Stephen Herbein (\*), and **M. Tauffer**. A Two-Tiered Approach to I/O Quality of Service in Linux. In *Proceedings of the IEEE Cluster 2015 Conference*. Chicago, Illinois, USA. September 2015.
- A9. S. Herbein(+), M. Matheny(+), M. Wezowicz(+), J. Kroger, J.S. Logan, J. Kim, S. Klasky, and **M. Tauffer**. Predictions of Large-scale QMCPack I/Os on Titan using Skel. In *Proceedings of the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. Denver, Colorado, USA. November 2013. (*Acceptance Rate: 40%*)
- A10. M. Wezowicz(+) and **M. Tauffer**. On the Cost of a General GPU Framework - The Strange Case of CUDA 4.0 vs. CUDA 5.0. In *Proceedings of the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. Salt Lake City, Utah, USA. November 2012. (*Acceptance Rate: 47%*)
- A11. D.T. Yehdego(\*), V. K. R. Kodimala, S. Viswakula, B. Zhang(\*), R. Vegesna, K. L. Johnson, **M. Tauffer** and M.-Y. Leung. Secondary Structure Predictions for Long RNA Sequences Based on Inversion Excursions – Preliminary Results. In *Proceedings of the ACM Conference on Bioinformatics, Computational Biology and Biomedicine (ACM-BCB)*. Orlando, FL, October 7-10, 2012.
- A12. T. Estrada (\*), K. Pusecker, M. Torres, J. Cohoon, and **M. Tauffer**. Benchmarking Gender Differences in Voluntary Computer Projects. In *Proceedings of the 2012 Grace Hopper Celebration of Women in Computing (GHC12)*. Baltimore, Maryland, USA. October 2012.
- A13. B. Zhang (\*), P. Cicotti, and **M. Tauffer**. MapReduce clustering on large datasets using SSDs and virtual shared memory. In *Proceeding of the Extreme Science and Engineering Discovery Environment (XSEDE)*. Chicago, Illinois, USA. July 2012.
- A14. T. Estrada (\*), B. Zhang (\*), R.S. Armen, and **M. Tauffer**. Study of Protein-ligand Binding Geometries using a Scalable and Accurate Octree-based Algorithm in MapReduce. In *Proceedings of the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*. Seattle, Washington, USA. November 2011. (*Acceptance Rate: 40%*)
- A15. O. Rahaman (\*), R. Armen, T. Estrada(\*), D. Doren, **M. Tauffer**, C. L. Brooks III. Binding Free Energy Prediction by Molecular Dynamics Based Docking and Volunteer Computing. Presented at the *Division of Computers in Chemistry for the 238<sup>th</sup> ACS National Meeting*. Washington, DC, USA. August 16-20, 2009.
- A16. N. Ganesan (#), S. Patel, and **M. Tauffer**. Simulations of Large Membrane Regions using GPU-enabled Computations - Preliminary Results. In *Proceedings of the 2010 Symposium on Application Accelerators in High Performance Computing (SAAHPC)*, University of Tennessee Conference Center, Knoxville, Tennessee, USA. July 13-15, 2010.
- A17. L. Xu (\*), S. Collin, **M. Tauffer**, and D.G. Vlachos. Parallelization of Tau-Leaping Coarse-Grained Monte Carlo Method for Efficient and Accurate Simulations on GPUs. Poster in *Proceedings of the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*, Portland, Washington, USA. November 2009.
- A18. K.S. Hogle, J.H. Upton, A. Licon(+/\*), M.-Y. Leung, **M. Tauffer**, and K.L. Johnson. Role of RNA secondary structure in replication of Nodamura virus RNA2. *American Society for Virology, 27<sup>th</sup> Annual Meeting*, Cornell University, Ithaca, NY, USA. July 12-16, 2008.
- A19. T. Estrada (\*), **M. Tauffer**, and K. Reed, Performance Analysis of Volunteer Computing Traces. In *Proceedings of the ACM/IEEE International Conference for High Performance Computing, Network, Storage, and Analysis conference (SC)*, Reno, Nevada, USA. November 2007. (*Acceptance Rate: 24.5%*)
- A20. D. Flores (\*), T. Estrada(\*), **M. Tauffer**, P. Teller, and A. Kerstens. SimBA: a Discrete Event Simulator for Performance Prediction of Volunteer Computing Projects. In *Proceedings of the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC)*, Tampa, Florida, USA.

November 2006. (*Acceptance Rate: 25%*)

- A21. C. An, **M. Taufer**, and C.L. Brooks III. Predictor@home: A Multiscale, Distributed Approach for Protein Structure Prediction. *229<sup>th</sup> ACM National Meeting*, San Diego, California, USA. March 2005.
- A22. C. An, **M. Taufer**, and C.L. Brooks III. Predictor@home: A Multiscale, Distributed Approach for Protein Structure Prediction. *6<sup>th</sup> Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP6)*, Gaeta, Italy. December 2004.

## THESES:

- T1. **M. Taufer**. Inverting Middleware: Performance Analysis of Layered Application Codes in High Performance Distributed Computing. Dissertation ETH No. 14845, Institute for Computer Systems, Swiss Federal Institute of Technology Zurich (ETH), Zurich, Switzerland. Published by Hartung Gorre Verlag Konstanz, Germany, ISBN 3-89649-821-5 ISSN 1611-0943. December 2002.
- T2. **M. Taufer**. Development of the Parallelization of the Software Package OPAL for the Simulation of Dynamic Molecules on Supercomputers. Master Thesis, Department of Computer Science, University of Padova, Padova, Italy. December 1996.

## TECHNICAL TALKS AND INVITED SEMINARS

I have given a series of invited and conference presentations at national and international conferences, universities, and government laboratories since 2005, when appointed at the rank of assistant professor. Invited talks at universities were advertised at the hosting institution level; conference talks were listed in the event program and open to all event attendees.

## KEYNOTES:

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| <i>May 2020</i> | In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. <i>Keynote of the EuroGraphics Symposium on Parallel Graphics and Visualization</i> , Virtual conference.   |
| <i>Dec 2019</i> | Scientific Applications and Heterogeneous Architectures – Data Analytics and the Intersection of HPC and Edge Computing. <i>Keynote at the 13<sup>th</sup> CHPC National Conference</i> , Johannesburg, South Africa.  |
| <i>Aug 2019</i> | Scientific Applications and Heterogeneous Architectures – Data Analytics and the Intersection of HPC and Edge Computing. <i>Keynote at the EuroPar Conference</i> , Göttingen, Germany.  |
| <i>May 2018</i> | Modeling the Next-Generation High Performance Schedulers. <i>Keynote at the ACM Conference on Principles of Advanced Discrete Simulation (PADS)</i> , Rome, Italy.   |
| <i>Feb 2018</i> | Building the next Generation of MapReduce Programming Models over MPI to Fill the Gaps between Data Analytics and Supercomputers. <i>Keynote at the 9th International Workshop on Programming Models and Applications for Multicores and Many-cores (PMAM)</i> , Vösendorf, Austria. |
| <i>Sep 2017</i> | Building the next Generation of MapReduce Programming Models over MPI to Fill the Gaps between Data Analytics and Supercomputers. <i>Keynote at the EuroMPI/USA 2017 Conference</i> , Chicago, IL, USA.  |
| <i>Sep 2017</i> | Challenges in Big Data Computing on HPC Platforms. <i>Keynote at the Parallel Processing and Applied Mathematics (PPAM)</i> , Lublin, Poland.  |
| <i>Sep 2016</i> | Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. <i>Keynote at the IEEE Cluster Conference</i> , Taipei, Taiwan.  |

*Jun 2016* Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. *Keynote at the 7<sup>th</sup> Workshop on Scientific Cloud Computing (ScienceCloud)*, Kyoto, Japan.

*May 2015* The Numerical Reproducibility Fair Trade: Facing the Concurrency Challenges at the Extreme Scale. *Keynote at the Fifth International Workshop on Accelerators and Hybrid Exascale Systems (AsHES)*, Hyderabad, India.

#### INVITED TALKS:

*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. *5<sup>th</sup> International Workshop on Data Analysis and Reduction for Big Scientific Data (DRBSD-5)*, Denver, CO, USA.

*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.

*Feb 2019* In Situ Data Analytics for Next Generation Molecular Dynamics Workflows. *Mini-symposium 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.
- 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
- 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*, Pittsburgh, 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. *14<sup>th</sup> Workshop on High Performance Computational Biology*, Hyderabad, India.
- April 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.
- 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.
- 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)
- 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*, Glenden 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. *16<sup>th</sup> 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. *16<sup>th</sup> IEEE International Conferences on Computational Science and Engineering (CSE)*, Sydney, Australia.
- 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. *13<sup>th</sup> 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. *14<sup>th</sup> 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 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”, 4<sup>th</sup> International Workshop on Grid Computing (Grid 2003), Phoenix, Arizona.

## MINISYMPOSIUM ORGANIZER

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.

Nov 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 2019 *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. Leeser, 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.

## SOFTWARE PACKAGES:

Group GitHub Repository: <https://github.com/TauferLab>

Selected projects:

- 2020 - present **SOMOSPIE** – A modular SOil MOisture SPatial Inference Engine based on data driven decisions that leverages machine-learning techniques coupled with other sources of environmental information (e.g., topography) to generate gap-free information and at a finer spatial resolution (i.e., increased granularity).  
URL: <https://github.com/TauferLab/SOMOSPIE>
- 2016 - present **Mimir** – New implementation of MapReduce over MPI. Mimir inherits the core principles of existing MapReduce frameworks, such as MR-MPI, while redesigning the execution model to incorporate a number of sophisticated optimization techniques that achieve similar or better performance with significant reduction in the amount of memory used.  
URL: <https://github.com/TauferLab/Mimir>
- 2016- present **In-Situ-Protein-Analytics** – This software targets MD simulations at the exascale and proposes a novel technique for in situ data analysis and indexing of MD trajectories. Our technique maps individual trajectories' substructures (i.e., alpha-helices, beta-strands) to metadata frame by frame. The metadata captures the conformational properties of the substructures.  
URL: <https://github.com/TauferLab/In-Situ-Protein-Analytics>

- 2016 - 2018*      **NHANES-Analytics** – This repository contains code for analysis of the NHANES dataset. Specifically, it contains code that will examine the unique food items in the NHANES dietary data. The food items are clustered based on nutrient similarities into new food groups.  
URL: <https://github.com/TauferLab/NHANES-Analytics>
- 2010 - 2016*      **QCN Explorer** – Development of a simulator of the Quake Catcher Network, a volunteer computing project out of Stanford University. The goal of this project is to educate people about seismology and increase the awareness of QCN. QCN Explorer allows users to simulate how the QCN responds to an earthquake with a larger number of sensors than the network currently supports.  
Webpage: <http://qcnexplorer.org>  
Code: <https://github.com/TauferLab/QCN-Explorer>
- 2009 – 2016*      **ExSciTech** – 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.  
Webpage: <http://exscitech.org>  
Code: <https://github.com/TauferLab/ExSciTech>
- 2007 - 2016*      **FEN ZI (yun dong de FEN ZI or moving molecules)** – Parallelization paradigm shifting for large-scale Molecular Dynamics on emerging technologies i.e., GPUs and multi-core architectures.  
Webpage: <http://gcl.cis.udel.edu/projects/fenzi>  
Code: <https://github.com/TauferLab/fen-zi>
- 2005 – 2014*      **Docking@Home** – A world-community experiment and effort to use distributed world-wide-web volunteer resources to assemble a supercomputer able to study protein-ligand docking for drug discovery.  
Webpage: <http://docking.cis.udel.edu>  
Data download: <http://docking.gcl.cis.udel.edu/resultsDownload/>
- 2005 – 2014*      **RNAVLab** – A virtual environment based on mathematical models and grid technology for computational RNA structure analysis, i.e., prediction, alignment, comparison, and classification.  
Webpage: <http://rnavlab.utep.edu>
- 2005 – 2010*      **jTopaz** – An open-source extension to the Firefox browser that provides users with a familiar and user-friendly interface to access arbitrary GridFTP servers.  
Webpage: <http://gcl.cis.udel.edu/projects/topaz>
- 2006 – 2007*      **SHiPPER** – A community of undergraduate and graduate students who will pursue advanced degrees in fields that combine expertise in high-performance computing and other scientific and engineering disciplines.  
Webpage: <http://gcl.cis.udel.edu/projects/shipper>
- 2004 – 2005*      **Predictor@Home** – A world-community experiment and effort to use distributed world-wide-web volunteer resources to assemble a supercomputer able to predict protein structure from protein sequence.  
Webpage: <http://predictor.scripps.edu>

**TEACHING ACTIVITIES**

Created and taught advanced graduate computer science course on Molecular Dynamics and HPC, 2007 – 2011

Created and taught advanced graduate computer science course on Big Data and HPC, 2014 – present

**COURSES TAUGHT AT UTK (2018 – ):****Graduate Courses Taught (Semester, Course Title, Enrolment, Credits):**

<i>Sp20</i>	<i>COSC526: Introduction to Data Mining</i>	<i>18</i>	<i>3</i>
<i>Fa18</i>	<i>COSC690 (001) / COSC 594 (007): Big Data Analytics</i>	<i>28</i>	<i>3</i>

**COURSES TAUGHT AT UD (2007 – 2018):****Graduate Courses Taught (Semester, Course Title, Enrolment, Credits):**

<i>Sp18</i>	<i>CISC 879: Advanced Topics in Arch. and Softw. Systems: Big Data Analytics</i>	<i>10</i>	<i>3</i>
<i>Fa17</i>	<i>CISC 879: Advanced Topics in Arch. and Softw. Systems: Big Data Analytics for Financial Systems</i>	<i>9</i>	<i>3</i>
<i>Fa16</i>	<i>CISC 879: Advanced Topics in Arch. and Softw. Systems: Big Data Analytics for Health and Nutritional Datasets</i>	<i>23</i>	<i>3</i>
<i>Fa15</i>	<i>CISC 879: Advanced Topics in Arch. and Softw. Systems: HPC and Data AnALyTICS</i>	<i>11</i>	<i>3</i>
<i>Sp15</i>	<i>CISC 663: OPERATING SYSTEMS</i>	<i>8</i>	<i>3</i>
<i>Fa14</i>	<i>CISC 879: Advanced Topics in Arch. and Softw. Systems: HPC and Data AnALyTICS</i>	<i>13</i>	<i>3</i>
<i>Sp13</i>	<i>CISC 663: OPERATING SYSTEMS</i>	<i>10</i>	<i>3</i>
<i>Fa12</i>	<i>CISC 662: ARCHITECTURE</i>	<i>19</i>	<i>3</i>
<i>Sp12</i>	<i>CISC 663: OPERATING SYSTEMS</i>	<i>7</i>	<i>3</i>
<i>Fa11</i>	<i>CISC 662: ARCHITECTURE</i>	<i>13</i>	<i>3</i>
<i>Sp11</i>	<i>CISC 879: High Performance Parallel Algorithms for Computational Science</i>	<i>9</i>	<i>3</i>
<i>Fa10</i>	<i>CISC 662: ARCHITECTURE</i>	<i>27</i>	<i>3</i>
<i>Fa09</i>	<i>CISC 662: ARCHITECTURE</i>	<i>27</i>	<i>3</i>
<i>Sp09</i>	<i>CISC 849: High Performance Parallel Algorithms for Computational Science</i>	<i>9</i>	<i>3</i>
<i>Fa08</i>	<i>CISC 662: ARCHITECTURE</i>	<i>25</i>	<i>3</i>
<i>Sp07</i>	<i>CISC 849: Analysis of Bio. Simulations</i>	<i>7</i>	<i>3</i>
<i>Fa07</i>	<i>CISC 662: ARCHITECTURE</i>	<i>19</i>	<i>3</i>

**Undergraduate Courses Taught (Semester, Course Title, Enrolment, Credits):**

<i>Sp17</i>	<i>CISC 361: OPERATING SYSTEMS</i>	<i>44</i>	<i>3</i>
<i>Fa15</i>	<i>CISC 361: OPERATING SYSTEMS</i>	<i>28</i>	<i>3</i>
<i>Sp15</i>	<i>CISC 361: OPERATING SYSTEMS</i>	<i>40</i>	<i>3</i>
<i>Sp10</i>	<i>CISC 361: OPERATING SYSTEMS</i>	<i>40</i>	<i>3</i>
<i>Fa09</i>	<i>CISC 360: ARCHITECTURE</i>	<i>39</i>	<i>3</i>
<i>Fa08</i>	<i>CISC 360: ARCHITECTURE</i>	<i>16</i>	<i>3</i>
<i>Fa07</i>	<i>CISC 360: ARCHITECTURE</i>	<i>19</i>	<i>3</i>

**COURSES TAUGHT AT UTEP (2005 – 2007):**

*CS 3320: Computer Architecture II: Advanced Computer Design and Implementation* (Undergraduate course):  
Sp07, Fa06, Sp06, Fa05

*CS 3335: Systems Programming* (Undergraduate course): Fa06

*CS 5334: Parallel and Concurrent Programming* (Graduate course): Sp05, Sp06,

*CS 5341: Analysis and Modeling of Biological Structures* (Graduate course – cross-listed with the Bioinformatics Program and the Chemistry Department): Sp07

## PROFESSIONAL SERVICES AND ACTIVITIES

### EDITORIAL AFFILIATIONS:

- 2015 – present* Editorial Board, International Journal of High Performance Computing Applications (IJHPCA)
- 2015 – present* Associate Editor, Journal of Parallel Computing (ParCo), Elsevier
- 2015 – present* Subject Area Editor, Supercomputing Frontiers and Innovations Journal
- 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 of the Special Issue of Parallel and Distributed Computing (ParCo) titled “Computing Frontiers 2014: Best Papers.”
- 2009* Guest Editor of the Special Issue of Computer Communications on Information and Future Communication Security, Elsevier.

### STEERING COMMITTEES AND ADVISORY COMMITTEES:

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

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

**2019:**



1. *General Chair* of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2019, Denver, CO, USA.

**2017:**

2. *Finance Chair* of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2017, Denver, CO, USA.
3. *Technical Paper Area Co-Chair for Applications and Algorithms* of the IEEE Cluster Conference, September 2017, Honolulu, Hawaii, USA.
4. *Workshop Chair* of the 32<sup>nd</sup> ISC High Performance Conference, June 2017, Frankfurt, Germany.
5. *General Chair* of the IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2017, Orlando, FL, USA.
6. *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:**

7. *Panel Chair* of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2016. Salt Lake City, UT, USA.
8. *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.
9. *Technical Paper Area Chair* of the "Multicore and Many-core Parallelism" Track – EuroPar, August 2016, Grenoble, France.
10. *Workshop co-Chair* of the 31<sup>st</sup> ISC High Performance Conference, June 19 – June 23, 2016, Frankfurt, Germany.
11. *Technical Paper Area Chair* of the "Performance" Track – International Conference on Parallel Processing (ICPP), August 2016, Philadelphia, PA, USA.

**2015:**

12. *Workshop Chair* of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2015. Austin, TX, USA.
13. *General co-Chair* of the IEEE International Conference on Cluster Computing 2015, September 2015, Chicago, IL, USA.
14. *Technical Program co-Chair* of the 24<sup>th</sup> ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 15-19, 2015, Portland, OR, USA.

**2014:**

15. *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.
16. *Technical Paper Area Chair* of the "Cluster Design, Configuration and Administration" Track - IEEE International Conference on Cluster Computing (Cluster), September 2014, Madrid, Spain.

**2013:**

17. *Technical Poster Chair* of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2013. Denver, CO, USA.

**2012:**

18. *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:**

19. *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:

20. *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.
21. *Technical Paper Area Chair* of "Distributed Systems and Applications" of the 12<sup>th</sup> IEEE International Conference on High Performance Computing and Communications (HPCC), September 2010, Melbourne, Australia.

#### 2009:

22. *Technical Program vice-Chair* of the topic "Distributed Systems and Applications" Track - 11<sup>th</sup> IEEE International Conference on High Performance Computing and Communications (HPCC), June 2009, Seoul, South Korea.
23. *Technical Program Chair* of the 8<sup>th</sup> IEEE International Workshop on High Performance Computational Biology (HiCOMB), May 2009, Rome, Italy.

#### 2003:

24. *Workshop co-Chair* of the First Advanced Topics Workshop on Desktop Grids: Critical Systems and Applications Research (DGRID). November 2003, Phoenix, Arizona, USA.

### COMMITTEE MEMBER - CONFERENCES / WORKSHOPS / SYMPOSIUMS / SCHOLARSHIPS:

#### 2020:

1. *Technical Program Committee Member* of the 3<sup>rd</sup> International Workshop on Reproducible Evaluation of Computer Systems (P-RECS), June 2020. Stockholm, Sweden.
2. *Technical Program Committee Member* of the 28<sup>th</sup> International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2020. Stockholm, Sweden.
3. *Tutorial Committee Member* of the 35<sup>th</sup> ISC High Performance Conference. June 21-25, 2020, Frankfurt, Germany.
4. *Technical Program Committee Member* of the 20<sup>th</sup> International Workshop on High Performance Computational Biology (HiCOMB), May 2020, New Orleans, LA, USA.
5. *Technical Program Committee Member* of the International SC Asia Conference, February 2020, Singapore.

#### 2019:

6. *Technical Program Committee Member* of the 5<sup>th</sup> International Workshop on Container Technologies & Container Clouds (WoC), December 2019. Davis, CA, USA.
7. *Technical Program Committee Member* of the 2<sup>nd</sup> International Workshop on Reproducible Evaluation of Computer Systems (P-RECS), June 2019. Phoenix Arizona, USA.
8. *Technical Program Committee Member* of the 27<sup>th</sup> International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2019. Phoenix, AZ, USA.
9. *Technical Program Committee Member* of the 32<sup>nd</sup> IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2019. Rio de Janeiro, Brazil.

#### 2018:

10. *Technical Program Committee Member* of the of the 2018 IEEE International Conference on Bioinformatics and Biomedicine (BIBM18), December 2018, Madrid, Spain.
11. *Technical Program Committee Member* of the of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2019, Dallas, TX, USA.
12. *Technical Program Committee Member* of the 1<sup>st</sup> International Workshop on Reproducible Evaluation of Computer Systems (RECS), June 2018. Washington DC, USA.

13. *Technical Program Committee Member* of the 27<sup>th</sup> International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2018. Phoenix, AZ, USA.
14. *Technical Program Committee Member* of the 33<sup>rd</sup> ISC High Performance Conference. June 18-22, 2017, Frankfurt, Germany.
15. *Technical Program Committee Member* of the 32<sup>nd</sup> IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2018. Vancouver, Canada.
16. *Workshop Committee Member* of the International Conference on Computational Science (ICCS). June 11-13, 2017, Wuxi, China.

**2017:**

17. *Panel Committee Member* of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2017. Denver, CO, USA.
18. *Technical Program Committee Member* of the 26<sup>th</sup> International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2017, Washington DC, USA.
19. *Technical Program Committee Member* of the 32<sup>nd</sup> ISC High Performance Conference. June 18-22, 2017, Frankfurt, Germany.
20. *Workshop Committee Member* of the International Conference on Computational Science (ICCS). June 12-14, 2017, Zurich, Switzerland.
21. *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.

**2016:**

22. *Technical Program Committee* of the 23<sup>rd</sup> IEEE International Conference on High Performance Computing, Data and Analytics (HiPC), December 19-22, 2016, Hyderabad, India.
23. *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.
24. *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.
25. *Technical Program Committee Member* of the System Track - IEEE International Conference on Cluster Computing, September 2016, Taipei, Taiwan.
26. *Technical Program Committee Member* ISC High Performance Conference. June 19-23, 2016, Frankfurt, Germany.
27. *Technical Program Committee Member* of the 25<sup>nd</sup> International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2016, Kyoto, Japan.
28. *Technical Program Committee Member* of the 16th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid), May 2016, Cartagena, Colombia.
29. *Technical Program Committee Member* of the ACM International Conference on Computing Frontiers (CF), May 2016, Como, Italy.
30. *Technical Program Committee Member* of the 6th International Workshop on Adaptive Self-tuning Computing Systems (ADAPT), January 2016, Prague, Czech Republic.

**2015:**

31. *Technical Program Committee Member* of the 21th IEEE International Conference on Parallel and Distributed Systems (ICPADS), December 2015, Melbourne, Australia.
32. *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.
33. *Technical Program Committee Member* of the IA<sup>3</sup> 2015: 5th Workshop on Irregular Applications: Architectures and Algorithms. November 2015. Austin, TX, USA.
34. *Technical Program Committee Member* of the EduHPC-15: Workshop on Education for High-

Performance Computing, November 2015, Austin, TX, USA.

35. *Technical Program Committee Member* of 11<sup>nd</sup> IEEE International Conference on e-Science and Grid Technologies (eScience), August 2015, Munich, Germany.
36. *Technical Program Committee Member* of the 2014 ACM International Conference on Supercomputing (ICS), June 2015, Long Beach, USA.
37. *Technical Program Committee Member* of the ACM Computing Frontiers (CF), May 2015, Ischia, Italy.
38. *Technical Program Committee Member* of 2015 ACM/IEEE CS George Michael HPC Fellowship.
39. *Technical Program Committee Member* of Workshop and Tutorials at the 2015 Richard Tapia Celebration of Diversity in Computing Conference, Boston, MA, USA.

#### 2014:

40. *Technical Program Committee Member* of the 13<sup>th</sup> IEEE International Conference on Ubiquitous Computing and Communications (IUCC) December 2014, Chengdu, China.
41. *Technical Program Committee Member* of 10<sup>nd</sup> IEEE International Conference on e-Science and Grid Technologies (eScience), October 2014, Guarujá, San Paulo, Brazil.
42. *Technical Program Committee Member* of the 2<sup>nd</sup> Workshop on Parallel and Distributed Agent-Based Simulations (PADABS), 25-29 August 2014, Porto, Portugal.
43. *Technical Program Committee Member* of the 2014 ACM International Conference on Supercomputing (ICS), June 2014, Munich, Germany.
44. *Technical Program Committee Member* of the 23<sup>rd</sup> International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2014, Vancouver, Canada.
45. *Technical Program Committee Member* of the ACM International Conference on Computing Frontiers 2014 (CF), May 2014, Cagliari, Italy.
46. *Technical Program Committee Member* of the 14<sup>th</sup> IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid), May 2014, Chicago, USA.

#### 2013:

47. *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.
48. *Technical Program Committee Member* of the 13<sup>th</sup> International Workshop on High Performance Computational Biology (HiCOMB), May 2013, Phoenix, Arizona, USA.
49. *Technical Program Committee Member* of the 6th IEEE/ACM International Conference on Utility and Cloud Computing (UCC), December 2013, Dresden, Germany.
50. *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.
51. *Technical Program Committee Member* of the Workshop on Parallel Computational Biology (PBC), held in conjunction with PPAM 2013, September 8-11, 2013, Warsaw, Poland.
52. *Technical Program Committee Member* of the 1<sup>st</sup> Workshop on Parallel and Distributed Agent-Based Simulations (PADABS), August 2013, Aachen, Germany.
53. *Technical Program Committee Member* of the 22<sup>nd</sup> International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2013, New York, NY, USA.
54. *Technical Program Committee Member* of the 12<sup>th</sup> International Workshop on High Performance Computational Biology (HiCOMB), May 2013, Boston, MA, USA.
55. *Technical Program Committee Member* of the 13<sup>th</sup> IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid), May 2013, Delft, The Netherlands.

#### 2012:

56. *Technical Program Committee Member* of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2012, Salt Lake City, UT, USA.
57. *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.

58. *Technical Program Committee Member* of the High Performance Computing Conference (HiPC), December 2012, Pune, India.
59. *Technical Program Committee Member* of the 5<sup>th</sup> IEEE/ACM International Conference on Utility and Cloud Computing (UCC), November 2012, Chicago, IL, USA.
60. *Technical Program Committee Member* of the Grace Hopper Conference (GHC) Panels, Workshops, and Presentations (PWP) Committee, October 2012, Baltimore, MD, USA.
61. *Technical Program Committee Member* of 8<sup>nd</sup> IEEE International Conference on e-Science and Grid Technologies (eScience), October 2012, Chicago, IL, USA.
62. *Technical Program Committee Member* of Symposium on Application Accelerators in High-Performance Computing (SAAHPC), July 2012, Argonne National Laboratory, IL, USA.
63. *Technical Program Committee Member* of the 21<sup>st</sup> ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2012, Delft, The Netherlands.
64. *Technical Program Committee Member* of the 12<sup>th</sup> IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid), May 2012, Ottawa, Canada.
65. *Technical Program Committee Member* of the 2012 ACM International Conference on Computing Frontiers (CF), May 15-17, 2012, Cagliari, Italy.
66. TCPP Travel Award Committee of the 26<sup>th</sup> IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 21 – 25, 2012, Shanghai, China.
67. *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.

## 2011:

68. *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.
69. *Technical Program Committee Member* of the 13<sup>th</sup> IEEE International Conference on High Performance Computing and Communications (HPCC) in Biological/Molecular Computing Track, September 2 – 4, 2011, Banff, Alberta, Canada.
70. *Technical Program Committee Member* of the IEEE Cluster 2011 Conference (Cluster), September 26 – 30, 2011, Austin, TX, USA.
71. *Technical Program Committee Member* of the Workshop on Parallel Computational Biology (PBC), held in conjunction with PPAM 2011, September 11-14, 2011, Torun, Poland.
72. *Technical Program Committee Member* of the 11<sup>th</sup> IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 23 – 26, 2011, Los Angeles, CA, USA.
73. *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.
74. *Technical Program Committee Member* of the 7<sup>th</sup> International Workshop on High Performance Computational Biology (HiCOMB), May 16, 2011, Anchorage, AK, USA.
75. *Technical Program Committee Member* of the 4<sup>th</sup> Annual Workshop for General-Purpose Computation on Graphics Processing Units (GPGPU), March 5, 2011, Newport Beach, California, USA.
76. *Technical Program Committee Member* of the 18<sup>th</sup> Euromicro Conference on Parallel, Distributed and Network-Based Processing (PDP), February 9-11, 2011, Ayia Napa, Cyprus.

## 2010:

77. *Technical Program Committee Member* of the 2010 IEEE 6<sup>th</sup> International Conference on e-Science (eScience), December 7 – 10, 2010, Brisbane, Australia.
78. *Technical Program Committee Member* of the International Conference of Computer Design (ICCD), October 3-6, 2010, Amsterdam, The Netherlands.

79. *Technical Program Committee Member* of the 22<sup>nd</sup> International Symposium on Computer Architecture and High-Performance Computing (SBAC-PAD), October 2010, Petropolis, Brazil.
80. *Technical Program Committee Member* of the Workshop on Parallel Programming and Applications on Accelerator Clusters (PPAAC), September 2010, Heraklion, Greece.
81. *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.
82. *Technical Program Committee Member* of the 2010 ACM International Symposium on High Performance Distributed Computing (HPDC), June 2010, Chicago, IL, USA.
83. *Technical Program Committee Member* of the ACM Computing Frontiers Conference (CF), May 2010, Bertinoro, Italy.
84. *Technical Program Committee Member* of the 10<sup>th</sup> IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 2010, Melbourne, Australia.
85. *Technical Program Committee Member* of the Second Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2010, Melbourne, Australia.
86. *Technical Program Committee Member* of the 18<sup>th</sup> Euromicro Conference on Parallel, Distributed and Network-Based Processing (PDP), February 2010, Pisa, Italy.

## 2009:

87. *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.
88. *Technical Program Committee Member* of the International Conference of Computer Design (ICCD), November 4 – 7, 2009, Lake Tahoe, CA, USA.
89. *Scholarship Committee Member* of the Grace Hopper Celebration of Women in Computing 2009, October 2009, Tucson, AZ, USA.
90. *Technical Program Committee Member* of the 2009 IEEE International Conference on Cluster Computing (Cluster), August 29 – September 4, 2009, New Orleans, LA, USA.
91. *Technical Program Committee Member* of the 12<sup>th</sup> IEEE International Conference on Computational Science and Engineering (CSE), August 29 – 31, 2009, Vancouver, Canada.
92. *Technical Program Committee Member* of 9<sup>th</sup> IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 2009, Shanghai, China.
93. *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.
94. *Technical Program Committee Member* of the Second Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2009, Rome, Italy.
95. *Technical Program Committee Member* of the 2009 Richard Tapia Celebration of Diversity in Computing Conference, April 2009, Portland, OR, USA.
96. *Technical Program Committee Member* of the 17<sup>th</sup> Euromicro Conference on Parallel, Distributed and Network-Based Processing (PDP), February 2009, Bauhaus-University Weimar in Thuringia, Germany.

## 2008:

97. *Technical Program Committee Member* of the Intl. Conference on Advanced Computing and Communications, December 2008, Chennai, India.
98. *Technical Program Committee Member* of the Computational Structural Bioinformatics Workshop 2008 November 2008, Philadelphia, PA, USA.
99. *Technical Program Committee Member* of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2008, Austin, TX, USA.
100. *Technical Program Committee Member* of the Grace Hopper Celebration of Women in Computing 2008, October 2008, Denver CO, USA.
101. *Technical Program Committee Member* of the IEEE Intl. Conference on Computer Design (ICCD),

October 2008, Lake Tahoe, CA, USA.

102. *Technical Program Committee Member* of the 10<sup>th</sup> IEEE International Conference on High Performance Computing and Communications (HPCC), September 2008, DaLian, China.
103. *Technical Program Committee Member* of the International Conference on Computational Science (ICCS), June 2008, Krakow, Poland.
104. *Technical Program Committee Member* of the ACM Computing Frontiers (CF), May 2008, Ischia, Italy.
105. *Technical Program Committee Member* of the Global and Peer-to-Peer Computing (GP2PC), May 2008, Lyon, France.
106. *Technical Program Committee Member* of the 7<sup>th</sup> International Workshop on High Performance Computational Biology (HiCOMB), May 2008, Miami, FL, USA.
107. *Technical Program Committee Member* of the 9<sup>th</sup> IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC), May 2008, Miami, FL, USA.
108. *Technical Program Committee Member* of the 2<sup>nd</sup> Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2008, Miami, Florida, USA.
109. *Technical Program Committee Member* of the 22<sup>nd</sup> IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2008, Miami, FL, USA.
110. *Technical Program Committee Member* of the Euromicro Conference on Parallel, Distributed and Network based Processing (PDP) February 2008, Toulouse, France.

## 2007:

111. *Technical Poster Committee Member* of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2007, Reno, NV, USA.
112. *Technical Program Committee Member* of the First Computational Structural Bioinformatics Workshop, November 2007, San Jose, CA, USA.
113. *Technical Poster Committee Member* of the 2007 Richard Tapia Celebration of Diversity in Computing Conference, October 2007, Orlando, FL, USA.
114. *Scholarship Committee Member* of the Grace Hopper Celebration of Women in Computing 2007, October 2007, Orlando, FL, USA.
115. *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.
116. *Technical Program Committee Member* of the International Conference on Computational Science 2007 (ICCS), May 2007, Beijing, China.
117. *Technical Program Committee Member* of the 6<sup>th</sup> International Workshop on Global and Peer-to-Peer Computing (GP2P), May 2007, Rio de Janeiro, Brazil.
118. *Technical Program Committee Member* of 26<sup>th</sup> IEEE International Performance Computing and Communications Conference (IPCCC), April 2007 - New Orleans, LA, USA.
119. *Technical Program Committee Member* of the First Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), March 2007, Long Beach, CA, USA.

## 2006:

120. *Technical Program Committee Member* of the 4<sup>th</sup> IEEE International Symposium on Parallel and Distributed Processing and Applications (ISPA), December 2006, Sorrento, Italy.
121. *Technical Program Committee Member* of the 2<sup>nd</sup> IEEE International Conference on e-Science and Grid Technologies (eScience), December 2006, Amsterdam, The Netherlands.
122. *Technical Program Committee Member* of the 5<sup>th</sup> International Workshop on Global and Peer-to-Peer Computing (GP2P), May 2006, Singapore.
123. *Technical Program Committee Member* of the 20<sup>th</sup> IEEE International Parallel and Distributed Processing Symposium (IPDPS), April 2006, Rhodes, Greece.
124. *Technical Program Committee Member* of the 5<sup>th</sup> IEEE International Workshop on High Performance Computational Biology (HiCOMB), April 2006, Rhodes, Greece.

**2005:**

125. *Technical Program Committee Member* of the 1<sup>st</sup> IEEE International Conference on e-Science and Grid Technologies (eScience), December 2005, Melbourne, Australia.
126. *Technical Program Committee Member* of the 2005 IEEE International Conference on Cluster Computing (Cluster), September 2005, Boston, MA, USA.
127. *Technical Program Committee Member* of the 2005 International Conference on High Performance Computing and Communications (HPCC), September 2005, Sorrento, Italy.
128. *Technical Program Committee Member* of the 5<sup>th</sup> 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.

**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.

**SERVICES TO THE UNIVERSITY, COLLEGE, AND DEPARTMENT (SELECTED)*****At UTK:***

- |                       |  |
|-----------------------|--|
| <i>2019 – present</i> | Member, Committees to review faculty for their post-tenure performance (College Committee)   |
| <i>2018 – 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)
<i>2012 – 2013</i>	Member, Biomedical Engineering Graduate Committee (BME Program)
<i>2012 – 2013</i>	Chair, Distinguished Speaker Series Committee (CIS Department)
<i>2010</i>	Organizer, CIS Research Day (CIS Department)
<i>2009 – 2013</i>	Member, Bioinformatics Program Committee (University Committee)
<i>2009 – 2011</i>	Member, Research Computing Task Force (University Committee)
<i>2009 – 2010</i>	Member, Graduate Recruiting Committee (CIS Department)
<i>2008 – 2009</i>	Member, Graduate Committee (CIS Department)
<i>2007 – 2009</i>	Advisor, Student ACM Chapter (CIS Department)
<i>2007 – 2008</i>	Member, Graduate Recruiting Committee (CIS Department)
<b><i>At UTEP:</i></b>	
<i>2006 – 2007</i>	Member, Bioinformatics Research Committee and Bioinformatics Colloquium Committee (University Committee)
<i>2005 – 2007</i>	Member, High-End Computing Along the Rio Grande Consortium
<i>2005 – 2007</i>	Member, Computer System Curriculum Committee and the Facilities Committee
<i>2006</i>	Member, NSF-CSEMS Scholarship Committee at the University of Texas at El Paso, 2006

**PROFESSIONAL AFFILIATIONS**

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