Michela Taufer

ACM Distinguished Scientist
J.P. Morgan Chase Faculty Scholar
Associate Professor

University of Delaware
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Education:

Dec 2002   PhD in Computer Science, Swiss Federal Institute of Technology Zurich (ETH), Switzerland.

Thesis: *Inverting Middleware: Performance Analysis of Layered Application Codes in High Performance Distributed Computing.*

Thesis supervisors: Thomas M. Stricker (Chair), Daniel A. Reed

Dec 1996   MS (Laurea) in Computer Engineering, University of Padua, Italy.

Thesis: *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; scientific applications and their programmability on multi-core and many-core platforms; numerical reproducibility and stability of multithreaded applications; performance analysis, modeling, and optimization of multi-scale applications; cloud computing and volunteer computing; big data analytics and MapReduce.

Professional Experience:

Sep 2017 – present   Professor, University of Delaware, Newark, DE, USA.
- Department of Computer and Information Sciences
- Biomedical Engineering Program (Affiliated)
- Center for Bioinformatics & Computational Biology (Affiliated)

Sep 2012 – August 2017   Associate Professor, University of Delaware, Newark, DE, USA.
- Department of Computer and Information Sciences
- Biomedical Engineering Program (Affiliated)
- Center for Bioinformatics & Computational Biology (Affiliated)

Sep 2015 – Aug 2016   Acting Director at Center for Bioinformatics & Computational Biology (CBCB), Delaware Biotechnology Institute (DBI), Newark, DE, USA.

Jan 2013 – Aug 2016   David and Beverly J.C. Mills Career Development Chair, Depart. of Computer and Info. Sciences, University of Delaware, Newark, DE, USA.

Jun 2013 –   Visiting Faculty at the Oak Ridge National Laboratory, Computer Science and Mathematics

May 2014	Division. U.S. Department of Energy (DoE) Higher Education Research Experiences Faculty (HERE Faculty) Program, Oak Ridge, TN, USA.
Sep 2007 – *Aug 2012*	Assistant Professor, University of Delaware, Newark, DE, USA. Department of Computer and Information Sciences • Center for Bioinformatics & Computational Biology (Affiliated, Jun 2010- Aug 2012)
Jan 2005 – *Aug 2007*	Assistant Professor, Depart. of Computer Science, University of Texas, El Paso, TX, USA.
Jan 2003 – *Dec 2004*	Postdoctoral Researcher, Center for Theoretical Biological Physics (CTBP), University of California, San Diego. Affiliated to the Depart. of Molecular Biology at The Scripps Research Institute (TSRI), the San Diego Supercomputer Center (SDSC), and the Depart. of Computer Science and Engineering at the University of California at San Diego, San Diego, CA, USA.
Dec 1996 – *Dec 2002*	Research Student Assistant, Computer Systems Institute, Swiss Federal Institute of Technology Zurich (ETH), Switzerland.
Feb 1996 – *Dec 1996*	Visitor Scholar at the Swiss Center for Scientific Computing (SCSC/CSCS), Zurich, Switzerland.

Honors and Distinctions:

2017	UD Faculty Nomination for the Excellence in Undergraduate Academic Advising and Mentoring Award
Feb 2017 - present	J.P. Morgan Chase Faculty Scholar
Oct 2016	One of four Best Paper Finalists at the IEEE SBAC-PAD Conference, Los Angeles, CA
Sep 2016	Keynote at the IEEE Cluster Conference, Taipei, Taiwan
Jun 2016	Keynote at the 7th Workshop on Scientific Cloud Computing (ScienceCloud), Kyoto, Japan
2015	ACM (Association for Computing Machinery) Distinguished Scientist
May 2015	Keynote at the Fifth International Workshop on Accelerators and Hybrid Exascale Systems (AsHES), Hyderabad, India
2015	Winner of the 8th IEEE International Scalable Computing Challenge - Co-located with the IEEE/ACM CCGrid Conference
2014	ACM (Association for Computing Machinery) Senior Member
Sep 2014	One of six Best Paper Finalists at the IEEE Cluster Conference, Madrid, Spain
2014	UD Faculty Nomination for the Excellence in Undergraduate Academic Advising and Mentoring Award
2006	UTEP Young Investigator Award, Research and Sponsored Programs
2003 – 2004	La Jolla Interfaces in Science (LJIS) Interdisciplinary Fellowship - From January 1, 2003 to December 14, 2004 - Award: $50,000
1996	Erasmus Fellowship of the European Community (EU) for Graduate Students - From February 12, 1996 to December 12, 1996

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. Journal papers in which I am the senior author who provided the intellectual input and designed and approved the research in the study are marked with the tag *(Correspondent author)*.

Book Chapters:

1. P. Cicotti, S. Oral, G. Kestor, R. Gioiosa, S. Strande, **M. Taufer**, 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.* ISBN 9783319337401. 2016.
2. T. Estrada(*) and **M. Taufer**. Scheduling on Large Scale Volatile Desktop Grids, from Greedy and Naive to Intelligent and Adaptive Policies. Chapter in "Desktop Grid Computing", Christophe Cerin and Gilles Fedak (Eds.), Chapman and Hall/CRC, 2012.
3. R.S. Armen, E.R. May, and **M. Taufer**. Protein Docking. Chapter in "Encyclopedia of Parallel Computing", Padua, David (Ed.), Springer, 2011, ISBN 978-0-387-09765-7.
4. **M. Taufer** 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.

Journal Articles:

2017:

1. T. Johnston(#), B. Zhang(*), A. Liwo, S. Crivelli, and **M. Taufer**. In-Situ Data Analytics and Indexing of Protein Trajectories. *Journal of Computational Chemistry (JCC),* 38(16):1419-1430, *2017. (Correspondent author)*
2. B. Zhang(*), T. Estrada, P. Cicotti, P. Balaji, and **M. Taufer**. Enabling Scalable and Accurate Clustering of Distributed Ligand Geometries on Supercomputers. *Journal of Parallel Computing (ParCo),* 63: 38 – 60, 2017. *(Correspondent author)*
3. E. Deelman, T. Peterka, I. Altintas, C. Carothers, K. Kleese van Dam, K. Moreland, M. Parashar, L. Ramakrishnan, **M. Taufer**, and J. Vetter. The Future of Scientific Workflows. *International Journal of High Performance Computing Applications (IJHPCA), 2017. (*First Published April 26, 2017).
4. R. Searles, S. Herbein, T. Johnston, **M. Taufer**, 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), 2017. (Accepted)*

2016:

5. V. Stodden, M. McNutt, D. H. Bailey, E. Deelman, Y. Gil, B. Hanson, M. A. Heroux, J. P.A. Ioannidis, and **M. Taufer**. Enhancing Reproducibility for Computational Methods - Data, code and workflows should be available and cited. *Science,* 354(6317), December 9, 2016.
6. S. Herbein(+), S. McDaniel(+), N. Podhorszki, S. Klasky, and **M. Taufer**. Performance Characterization of Irregular I/O at the Extreme Scale. *Journal of Parallel Computing,* 51: 17 – 36, 2016. *(Correspondent author)*

2015:

7. T. Johnston(#), B. Zhang(*), A. Liwo, S. Crivelli, and **M. Taufer**. It-Situ Data Analysis of Protein Folding Trajectories. *CoRR abs/1510.08789*, pp. 1 – 40, October 30, 2015. *(Correspondent author)*
8. **M. Taufer** 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,* pp. 1 – 10, doi: 10.1177/1094342015594518, July 22, 2015. *(Correspondent author)*

9. S. Ou, D. Cui, M. Wezowicz(+), **M. Taufer**, 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.

2014:

10. S. Schlachter(+), S. Herbein(+), S. Ou, J.S. Logan, S. Patel, and **M. Taufer**. Pursuing Resource Utilization and Coordinated Progression in GPU-enabled Molecular Simulations. *IEEE Design&Test of Computers*, 31(1): 40 – 50, February 2014. *(Correspondent author)*

11. 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. Taufer**. 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.

2013:

12. K. Benson(+), S. Schlachter(+), T. Estrada(*), **M. Taufer**, 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)*

13. B. Zhang(*), D. T. Yehdego(*), K. L. Johnson, M.-Y. Leung, and **M. Taufer**. 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)*

14. **M. Taufer**, 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)*

2012:

15. G. Arampatzis, M.A. Katsoulakis, P. Plechac, **M. Taufer**, and L. Xu(*). Hierarchical Fractional-step Approximations and Parallel Kinetic Monte Carlo Algorithms. *J. Computational Physics,* 231(23): 7795 – 7814, October 2012.

16. T. Estrada(*), B. Zhang(*), P. Cicotti, R. Armen, and **M. Taufer**. 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)*

2011:

17. N. Ganesan(#), B.A. Bauer, T. Lucas, S. Patel, and **M. Taufer**. 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)*

18. O. Rahaman(*), T. Estrada(*), D. Doren, **M. Taufer**, 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.

19. B.A. Bauer, J.E. Davis(*), **M. Taufer**, 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)*

2010:

20. J.J. Rosskopf, J.H. Upton, III, M.-Y. Leung, **M. Taufer**, 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.

2009:

21. T. Estrada(*), **M. Taufer**, and D. Anderson. Performance Prediction and Analysis of BOINC Projects: An Empirical Study with EmBOINC. *J. Grid Computing*, 7: 537 – 554, 2009. *(Leading author)*
22. **M. Taufer**, 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)*
23. **M. Taufer**, A. Licon(+), R. Araiza(*), D. Mireles, A. Gultyaev, 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)*

2008:

24. **M. Taufer**, 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)*
25. T. Estrada(*), O. Fuentes, and **M. Taufer**. A Distributed Evolutionary Method to Design Scheduling Policies for Volunteer Computing. *ACM SIGMETRICS Performance Evaluation Review Journal*, 36(3): 40 – 49, 2008. *(Correspondent author)*

2006:

26. K. Bhatia, **M. Taufer**, B. Stearn, R. Zamudio(*), and D. Catarino(+). Integrate GridFTP into Firefox - Build Grid Protocols into Mozilla-based Tools. *IBM developerWorks*, 10 October 2006.
27. **M. Taufer**, 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.

2005:

28. **M. Taufer**, 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.
29. P. Cicotti, **M. Taufer**, and A.A. Chien. DGMonitor: a Performance Monitoring Tool for Sandbox-based Desktop Grid Platforms. *J. Supercomputing,* 34(2): 113 – 133, 2005. *(Correspondent author)*
30. K. Baldridge, J.P. Greenberg, W. Sudholt, K. Bhatia, S. Mock, C. Amoreira, Y. Potier, and **M. Taufer**. 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):

2017:

1. 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. (*Rate:* 116/616, 18.8%)

2016:

2. 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. (*Rate:* 82/230, 35.6%)
3. T. Johnston(#), C. Zannin(+), and **M. Taufer**. HYPPO: A Hybrid, Piecewise Polynomial Modeling

Technique for Non-Smooth Surfaces. In *Proceedings of the 28th IEEEE 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%* – One of four Best Paper Candidates)

4. J. Benson, T. Estrada, A. Rosenberg, and **M. Taufer**. Scheduling Matters: Area-oriented Heuristics for Resource Management. . In *Proceedings of the 28th IEEEE 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%*)

5. 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%)

6. 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. (*Rate: 35% for full and short papers*)

7. 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%*)

8. S. Herbein(*), A. Dusia(*), A. Landwehr(*), S. McDaniel(*), J. Monsalve(*), Y. Yang(*), S. R. Seelam, and **M. Taufer**. 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. (*Rate: 25/60, 40%*)

2015:

9. T. Estrada, M. R. Wyatt, and **M. Taufer**. 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. (*Rate:* 82/230, 35.6%)

10. D. Chapp(*), T. Johnston, and **M. Taufer.** 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%)

11. V. Pallipuram(#), T. Estrada, and **M. Taufer**. 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%)

12. R. McKenna(+), V. Pallipuram(#), R. Vargas, and **M. Taufer**. 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.

13. T. Johnston(#), M. Alsulmi(*), P. Cicotti and **M. Taufer**. 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%)

14. B. Zhang(*), T. Estrada, P. Cicotti, P. Balaji, and **M. Taufer**. 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%)

2014:

15. M. Matheny(+), S. Herbein(+), N. Podhorszki, S. Klasky, and **M. Taufer**. 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%)

16. B. Javadi, B. Zhang(*), and **M. Taufer**. 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.

17. F. Raoking, J. Cohoon, K. Cooke, **M. Taufer**, 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.

18. V. K. Pallipuram(#), J. DiMarco(*), and M. **Taufer**. 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)

19. M. Portnoi(*), S. Schlachter(*), and **M. Taufer**. 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%)

20. B. Zhang(*), T. Estrada(#), P. Cicotti, and **M. Taufer**. 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%)

2013:

21. S. Herbein(+), M. Matheny(+), M. Wezowicz(+), J. Kroger, J.S. Logan, J. Kim, S. Klasky, **M. Taufer**. Performance Impact of I/O on QMCPack Simulations at the Petascale and Beyond. In *Proceedings of the 16th IEEE International Conferences on Computational Science and Engineering (CSE)*, pp. 92 – 99. Sydney, Australia. December 2013.

22. B. Zhang(*), T. Estrada(#), P. Cicotti, and **M. Taufer**. 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 16th IEEE International Conferences on Computational Science and Engineering (CSE)*, pp. 117 – 124. Sydney, Australia. December 2013.

23. S. Schlachter(*), S. Herbein(+), S. Ou, J. S. Logan, S. Patel, and **M. Taufer**. 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.

24. J. DiMarco (*) and M. **Taufer**. 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.

2012:

25. T. Estrada(*) and **M. Taufer**. 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%)

26. T. Estrada(*), B. Zhang(*), P. Cicotti, R. Armen, and **M. Taufer**. 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%)

27. M. Wezowicz(+), B. D. Saunders, and **M. Taufer**. 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.

2011:

28. K. Benson(+), T. Estrada(*), **M. Taufer**, 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%)

29. T. Estrada(*) and **M. Taufer**. Providing Application-Level Quality of Science in Volunteer Computing. In *Proceedings of the 13th IEEE High Performance Computing and Communications (HPCC) Conference*, pp. 68 – 77. Banff, Canada. September 2011. (*Acceptance Rate:* 59/271, 21.7%)

30. N. Ganesan(#), R.D. Chamberlain, J. Buhler, and **M. Taufer**. 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.

2010:

31. T. Estrada(*), R. Armen, and **M. Taufer**. 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%)

32. N. Ganesan(#), R.D. Chamberlain, J. Buhler, and **M. Taufer**. Breaking the Sequential Dependency Bottleneck: Extracting Data Parallelism in the Presence of Serializing Data Dependencies. 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%)

33. **M. Taufer**, 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%)

34. L. Xu(*), **M. Taufer**, 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%)

35. Licon(*), **M. Taufer**, 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%)

2009:

36. J. Atlas(*), T. Estrada(*), K. Decker, and **M. Taufer**. 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%)

37. T. Estrada(*), **M. Taufer**, and K. Reed. Modeling Job Lifespan Delays in Volunteer Computing Projects. In *Proceedings of the 9th IEEE International Symposium on Cluster Computing and Grid (CCGrid),* pp. 331 – 338. Shanghai, China. May 2009. (*Acceptance Rate*: 57/271, 21%)

38. J.E. Davis(*), A. Ozsoy(*), S. Patel, and **M. Taufer**. 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%)

2008:

39. T. Estrada(*), O. Fuentes, and **M. Taufer**. 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%)

2007:

40. G. Lopez(+), **M. Taufer**, 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.
41. R. Araiza(*), **M. Taufer**, 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 26th International Conference of the North American Fuzzy Information Processing Society (NAFIPS),* pp. 520 − 525. San Diego, California, USA. June 2007.

2006:

42. T. Estrada(*), D.A. Flores(*), **M. Taufer**, 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%)

2005:

43. **M. Taufer**, 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%)

2004:

44. D. Kondo, **M. Taufer**, 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%).

2003:

45. **M. Taufer**, 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%)
46. B. Uk, **M. Taufer**, 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%).
47. B. Uk, **M. Taufer**, 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%)

2002:

48. **M. Taufer**, T. Stricker, and R. Weber. Scalability and Resource Usage of an OLAP Benchmark on Clusters of PCs. In *Proceedings of the 14th ACM Symposium on Parallel Algorithms and Architectures (SPAA),* pp. 83 − 94. Winnipeg, Manitoba, Canada. August 2002.

49. **M. Taufer**, 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%)

50. **M. Taufer**, 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%)

1998:

51. **M. Taufer**, 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.

1996:

52. P. Arbenz, M. Billeter, P. Guentert, P. Luginbuehl, **M. Taufer**, and U. von Matt. Molecular Dynamics Simulations on Cray Clusters using the Sciddle-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):

2014:

1. S. Herbein(+), S. Klasky, and **M. Taufer**. 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%)

2013:

2. T. Estrada(#), K. Pusecker, M. Torres, J. Cohoon, and **M. Taufer**. Benchmarking Gender Differences in Volunteer Computing Projects. In the *Proceedings of the 3ʳᵈ Workshop on Analyzing and Improving Collaborative eScience with Social Networks (eSoN)*, pp. 342 – 349. Beijing, China. October 2013.

3. M. Wezowicz(+), T. Estrada(#), S. Patel, and **M. Taufer**. Performance Dissection of a MD Code across CUDA and GPU Generations. In *Proceedings of the 14ᵗʰ 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%)

4. D. Yehdego(*), B. Zhang(*), V. K. R. Kodimala, K. Johnson, **M. Taufer**, and M.-Y. Leung. Secondary Structure Predictions for Long RNA Sequences based on Inversion Excursions and MapReduce. In *Proceedings of 12ᵗʰ IEEE International Workshop on High Performance Computational Biology (HiCOMB),* pp. 545 – 547. Boston, Massachusetts, USA. April 2013. (*Acceptance Rate*: 9/17, 52%)

2012:

5. M. Matheny(+), S. Schlachter(+/*), L. Crouse, E. Kimmel, T. Estrada(*), M. Schumann, R. Armen, G. Zoppetti, and **M. Taufer**. ExSciTecH: Expanding Volunteer Computing to Explore Science, Technology, and Health. In *Proceedings of the 2ⁿᵈ Workshop on Analyzing and Improving Collaborative eScience with Social Networks (eSoN),* pp. 1 – 8. Chicago, Illinois, USA. October 2012.

6. B. Zhang(*), D. Yehdego(*), K. Johnson, M.-Y. Leung, and **M. Taufer**. 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%)

2011:

7. R. Riesen, K. Ferreira, M. Ruiz Varela(*), **M. Taufer**, and A. Rodrigues. Simulating Application Resilience at Exascale. In the *Proceedings of the 4ᵗʰ 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.

8. N. Ganesan(#), B.A. Bauer(*), S. Patel, and **M. Taufer**. FEN ZI: GPU-enabled Molecular Dynamics Simulations of Large Membrane Regions based on the CHARMM Force Field and PME. In *Proceedings of the 10ᵗʰ IEEE International Workshop on High Performance Computational Biology (HiCOMB),* pp. 472 – 480. Anchorage, Alaska, USA. May 2011. (*Acceptance Rate:* 11/21, 52.3%)

2009:

9. P. McClory(+), E. Kissel, D.M. Swany, and **M. Taufer**. MNEOMIC: Network Environment for Measurement and Observation for Network Interaction and Control. In *Proceedings of the 1ˢᵗ Workshop on Grid and P2P Systems and Applications (GridPeer),* held together with the *18ᵗʰ IEEE International Conference on Computer Communications and Networks* (ICCCN), pp. 1 – 7. August 2009.

10. S. Kamboj(*), T. Estrada(*), **M. Taufer**, 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.

11. T. Estrada(*), **M. Taufer**, 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.

2008:

12. **M. Taufer**, 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 7ᵗʰ 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%)

2007:

13. **M. Taufer**, 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%)

14. M. Taufer, 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 6ᵗʰ 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%)

15. **M. Taufer**, 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.

16. R. Zamudio(*), D. Catarino, **M. Taufer**, K. Bhatia, and B. Stearn. Topaz: Extending Firefox to Accommodate the GridFTP Protocol. In *Proceedings of the 4ᵗʰ High-Performance Grid Computing Workshop (HPGC),* in conjunction with IPDPS, pp. 1 – 8. Long Beach, California, USA. March 2007.

2006:

17. T. Estrada(*), A. Licon(+), and **M. Taufer**. CompPknots: 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.

18. K. Bhatia, B. Stearn, **M. Taufer**, 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.

19. G. Aguilera(*), P.J. Teller, **M. Taufer**, and F. Wolf. A Systematic Multi-step Methodology for Performance Analysis of Communication Traces of Distributed Applications based on Hierarchical Clustering. In *Proceedings of 5th 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.

2005:

20. **M. Taufer**, C. An A. Kerstens, and C.L. Brooks III. Predictor@Home: A "Protein Prediction Supercomputer" Based on Public-Resource Computing. In *Proceedings 4th 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%)

21. **M. Taufer**, D.P. Anderson, P. Cicotti, and C.L. Brooks III. Homogeneous Technique to Ensure Integrity of Molecular Simulation Results Using Public Resources. In *Proceedings of the 14th Heterogeneous Computing Workshop (HCW),* in conjunction with IPDPS 2005, pp. 1 – 8. Denver, Colorado, USA. April 2005. (*Acceptance Rate:* 14/29, 47%)

2004:

22. **M. Taufer**, 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.

23. P. Cicotti, **M. Taufer**, 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.

Birds of a Feathers (BoFs) (peer-review):

1. 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.

DOE Reports:

1. Ewa Deelman (co-organizer), Tom Peterka (co-organizer), Ilkay Altintas, Christopher Carothers, Kerstin Kleese van Dam, Kenneth Moreland, Manish Parashar, Lavanya Ramakrishnan, **Michela Taufer**, and Jeffrey 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):

1. **M. Taufer**, 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 and Posters in Peer-Reviewed Conferences, Symposiums, and Workshops:

1. Ayush Dusia(*), Yang Yang(*), and **Michela Taufer**. Network Quality of Service in Docker Containers. In *Proceedings of the IEEE Cluster 2015 Conference.* Chicago, Illinois, USA. September 2015.

2. Jose Manuel Monsalve Diaz(*), Aaron Landwehr(*), and **Michela Taufer**. 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.

3. Sean McDaniel(*), Stephen Herbein(*), and **Michela Taufer**. 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.

4. S. Herbein(+), M. Matheny(+), M. Wezowicz(+), J. Kroger, J.S. Logan, J. Kim, S. Klasky, and **M. Taufer.** 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%)

5. M. Wezowicz(+) and **M. Taufer**. 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%)

6. D.T. Yehdego(*), V. K. R. Kodimala, S. Viswakula, B. Zhang(*), R. Vegesna, K. L. Johnson, **M. Taufer** 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.

7. T. Estrada(*), K. Pusecker, M. Torres, J. Cohoon, and **M. Taufer**. 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.

8. B. Zhang(*), P. Cicotti, and **M. Taufer**. 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.

9. T. Estrada(*), B. Zhang(*), R.S. Armen, and **M. Taufer**. 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%)

10. O. Rahaman(*), R. Armen, T. Estrada(*), D. Doren, **M. Taufer**, 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 238th ACS National Meeting*. Washington, DC, USA. August 16-20, 2009.

11. N. Ganesan(#), S. Patel, and **M. Taufer**. 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.

12. L. Xu(*), S. Collin, **M. Taufer**, 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.

13. K.S. Hogle, J.H. Upton, A. Licon(+/*), M.-Y. Leung, **M. Taufer**, and K.L. Johnson. Role of RNA secondary structure in replication of Nodamura virus RNA2. *American Society for Virology, 27th Annual Meeting*, Cornell University, Ithaca, NY, USA. July 12-16, 2008.

14. T. Estrada(*), **M. Taufer**, 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%)

15. D. Flores(*), T. Estrada(*), **M. Taufer**, 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%)

16. C. An, **M. Taufer**, and C.L. Brooks III. Predictor@home: A Multiscale, Distributed Approach for Protein Structure Prediction. *229ᵗʰ ACM National Meeting,* San Diego, California, USA. March 2005.

17. C. An, **M. Taufer**, and C.L. Brooks III. Predictor@home: A Multiscale, Distributed Approach for Protein Structure Prediction. *6ᵗʰ Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP6)*, Gaeta, Italy. December 2004.

Theses:

1. **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.

2. **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 were advertised at the hosting instruction level; conference talks were listed in the event program and open to all event attendees.

Keynotes:

Sep 2016	Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. Keynote at the IEEE Cluster Conference, Taipei, Taiwan.
Jun 2016	Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. Keynote at the 7th Workshop on Scientific Cloud Computing (ScienceCloud), Kyoto, Japan.
May 2015	The Numerical Reproducibility Fair Trade: Facing the Concurrency Challenges at the Extreme Scale. Keynote at the Fifth International Workshop on Accelerators and Hybrid Exascale Systems (AsHES), Hyderabad, India.

Invited Talks:

April 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.
April 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*, the 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. *Laurence Livermore National Laboratory*, Livermore, CA, USA.
Aug 2016	Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. *Research Computing Center Seminar, University of Queensland*, Brisbane, Australia.
Mar 2016	*In-Situ* Data Analysis of Protein-folding Trajectories. *251st ACS National Meeting & Exposition - Division of Computers in Chemistry: From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules*, San Diego, CA, USA.
Mar 2016	Resource Management for Running HPC Applications in Container Clouds. *Recent Advances in HPDC Research Workshop*, Pittsburg, PA, USA.
Mar 2016	Who is Afraid of I/O? - Exploring I/O Challenges and Opportunities at the Exascale. *Rensselaer Polytechnic Institute*, Troy, NJ, USA.
Dec 2015	*In-Situ* Data Analysis of Protein-folding Trajectories. *University of Queensland, Brisbane*, Australia.
May 2015	Enabling *In-situ* Analysis of Ligand Geometries in Drug Design Simulations on Supercomputers. *14th Workshop on High Performance Computational Biology*, Hyderabad, India.
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:

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

Beijing, China.

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

Peer-reviewed Panel:

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.

Invited Panel:

Sep 2016   *HPC vs. Big Data: Different Worlds or Common Ground?* IEEE Cluster Conference 2016, Taipei, Taiwan.

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

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

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

Funding and Awards

Awards Summary:

SOURCE	GRANT ID	TOTAL	INSTITUTION	GROUP	REU	START	END	TYPE	ROLE
UD (2012 - present)									
NSF	OAC#1724843	$499,999	$499,999	$250,000		7/1/17	6/31/2019	Research	PI
DoE	LLNL Sub-Contract	$301,490	$301,490	$301,490		6/1/17	5/30/19	Research	PI
UD	UDRF	$38,500	$38,500			12/1/16	11/30/18	Research	co-PI
UD	UDRF	$38,500	$38,500	$38,500	$3,500	6/1/16	5/30/18	Research	PI
NSF	CCF#1648617	$20,000	$20,000	$20,000		9/1/16	8/31/18	Training	PI
DoE	ANL Sub-Contract	$14,760	$14,760	$14,760		9/1/16	9/30/16	Research	PI
DoE	LLNL Sub-Contract	$164,271	$164,271	$164,271		3/31/16	3/30/18	Research	PI
NSF	IIS#1550305	$750,712				9/15/15	9/30/18	Research	Senior Per.
NSF	CNS#1318417	$814,733	$443,878	$443,878	$23,800	6/15/15	5/31/18	Research	PI
ARO	W911NF-15-2-0033	$297,015	$297,015	$297,015		6/1/15	5/31/18	Research	PI
NSF	CCF#1550348	$20,000	$20,000	$20,000		7/7/15	6/13/16	Training	PI
DoE	LLNL Sub-Contract	$64,118	$64,118	$64,118		11/5/14	3/31/16	Research	PI
NSF	CCF#1446794	$89,999	$89,999	$89,999		6/15/14	6/1/16	Research	PI
DoE	ANL Sub-Contract	$28,657	$28,657	$28,657		6/9/14	1/15/15	Research	PI
NSF	CCF#1441397	$20,000	$20,000	$20,000		6/1/14	6/1/16	Training	PI
NSF	SES#1355547 Sub-Contract	$1,199,918	$209,239			2/1/14	1/31/19	Training	co-PI at UD
NSF	CNS#1318417	$512,038	$459,000	$459,000	$32,000	9/1/13	8/31/16	Research	PI
NSF	CNS#1217812	$500,000	$192,487	$192,487	$8,000	11/1/12	9/30/15	Research	co-PI
UD (2007 - 2012)									
AFOSR	EM Photinica Sub-Contract	$700,000	$16,200	$16,200		8/1/12	7/31/14	Research	co-PI
NSF	EAR#1027807	$1,841,104	$100,961	$100,961	$13,500	10/1/10	9/30/14	Research	co-PI
NSF	IIS#0968350	$683,199	$308,719	$308,719	$15,000	9/1/10	8/31/14	Research	PI
NSF	DMS#0800266	$621,193	$205,561	$205,561		6/1/08	5/31/12	Research	co-PI
NSF	CDI#0941318	$538,740	$538,740	$269,370		10/1/09	9/31/13	Research	co-PI
ARO	#54723-CS	$306,750	$306,750	$306,750	$6,750	6/1/09	5/31/13	Research	PI
AFOSR	EM Photinica Sub-Contract	$200,000	$59,997	$59,997		3/1/12	3/1/13	Research	co-PI
NSF	MRI#0922657	$451,051	$451,051			9/15/09	9/14/12	Infrastrcutres	co-PI
UDRF		$35,000	$35,000	$306,750	$3,500	6/1/10	5/31/12	Research	PI
AFOSR	EM Photinica Sub-Contract	$99,000	$34,125	$306,750		6/8/10	6/7/11	Research	co-PI
CRA/NSF		$6,000	$6,000	$306,750		6/1/09	8/31/09	Training	PI
CRA/NSF		$6,000	$6,000	$306,750		6/1/08	8/31/08	Training	PI
NSF	SCI#0802650 (SCI#0506429)		$388,808	$388,808		9/1/07	8/31/09	Research	PI
UTEP (2005 - 2007)									
NSF	SCI#0506429	$1,220,036	$273,068	$273,068		9/1/05	8/31/07	Research	PI
ARP	Texas High Education Grant	$99,982	$99,982	$49,991	$6,250	5/15/06	5/14/08	Research	PI
IBM		$600,000	$600,000			5/1/05		Infrastrcutres	co-PI
UTEP	Seed Money	$23,400	$23,400	$11,700		6/1/05		Research	co-PI
NSF	DUE#0631168	$275,856	$275,856	$137,928		10/1/06	1/31/11	Training	PI
NIH	SCORE	$581,329	$581,329	$290,665		9/1/07	8/31/11	Research	co-PI
		TOTAL ($)	**TO UD ($)**	**TO MY GROUP ($)**	**REU ($)**				
Total Awards		$13,663,350	$7,213,460	$6,050,892	$112,300				
Awards after tenure at UD		$5,374,710	$2,901,913	$2,404,175	$67,300				
Awards before tenure at UD		$5,488,037	$2,457,912	$2,883,366	$38,750				
Awards before tenure at UTEP		$2,800,603	$1,853,635	$763,352	$6,250				

Awards in Progress (12):

NSF OAC#1724843, $4999,999, PI (with Rodrigo Vargas co-PI, D)
Title: *CIF21 DIBBs: PD: Cyberinfrastructure Tools for Precision Agriculture in the 21st Century*
Duration: July 1, 2017 – May 30, 2020
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.

Lawrence Livermore National Laboratory Subcontract, $301,490, single PI
Title: *Investigating Massively Scalable I/O-Aware Job Scheduling in Support of Flux (Part III)*

Duration: June 1, 2017 – May 31, 2019
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.

UDRF-SI, $45,000, Senior Faculty
HAKER-HPC: HArnessing Knowledge for Environmental Research using High Performance Computing (HPC) Solutions
Duration: December 1, 2016 – November 30, 2018
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.

UDRF, $38,500, PI (previous PI was Mia Papas now at Christina Care Health System)
Title: Development of a Scalable Method for Identifying Dietary Clusters in the National Health and Nutrition Examination Survey using MapReduce
Duration: June 1, 2016 – May 30, 2018
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.
• NSF REU Supplement, $3,500, single PI, Summer 2017

NSF CCF#1648617, $20,000, single PI
Title: *Student Support: IEEE Cluster 2017 Conference*
Duration: August 1, 2016 – July 31, 2018
Description: This award supports 20 students from American institutions to attend the IEEE Cluster 2017 conference.

NSF CCF#1550348, $20,000, single PI
Title: *Student Support: IEEE Cluster 2015-2016 Conferences*
Duration: August 1, 2015 – July 31, 2018
Description: This award supports 20 students from American institutions to attend the IEEE Cluster 2015 and Cluster 2016 conferences.

NSF IIS #1550305, $750,712 (Funds to leading hub instructions GeorgiaTech and UNC-CH), Senior personnel.
Title: *BD Hubs: Collaborative Proposal: SOUTH: A Big Data Innovation Hub for the South Region*
Duration: 9/15/15 – 9/30/18
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, multistakeholder partnerships designed to pursue BD projects of interest to the South region by engaging academic institutions from 16 states in the South region and the District of Columbia including the University of Delaware.

NSF CNS#1513025, $814,733 ($443,878 at UD), PI (with Michela Becchi co-PI, University of Missouri-Columbia)
Title: *SHF:Medium:Collaborative Research: A Comprehensive Methodology to Pursue Reproducible Accuracy in Ensemble Scientific Simulations on Multi- and Many-core Platforms*
Duration: June 15, 2015 – May 31, 2018
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 Supplement, $16,000, single PI, Summer 2016

ARO # W911NF-15-2-0033, $297,015, single PI
Title: *Comprehensive Study of I/O Performance at the Extreme Scale*
Duration: June 1, 2015 – May 31, 2018
Description: This award involves studying aspects of I/O performance and *in situ* analysis for applications relevant to the Army.

NSF SES #1355547, $1,199,918 ($209,239), co-PI of sub-contract at UD (with T. Powers as PI of sub-contract at UD)
Title: *Becoming the Online Resource Center for Ethics Education in Engineering and Science*
Duration: February 1, 2014 – January 31, 2019
Description: The UD 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.

NSF CNS#1318417, $512,038.00 ($459,000 at UD), PI, with Pietro Cicotti (co-PI, SDSC)
Title: *SHF: Small: Collaborative Research: Modeling and Analyzing Big Data on Peta- and Exascale Distributed Systems supported by MapReduce Methodologies*
Duration: September 1, 2013 – August 31, 2016
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 Supplement, $16,000, single PI, Summer 2014
- NSF REU Supplement, $16,000, single PI, Summer 2015

Awards Completed (22):

Lawrence Livermore National Laboratory Subcontract, $103,626, single PI
Title: *Investigating Massively Scalable I/O-Aware Job Scheduling in Support of Flux (Part II)*
Duration: March 31, 2016 – May 31, 2017
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.

Argonne National Laboratory Sub-contract, $14,760, single PI
Title: Performance Characterization and Optimization of the MapReduce-MPI Framework
Duration: September 1, 2016 – September 30, 2016
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.

NSF CCF# 1441397, $20,000, single PI
Title: *Student Support: IEEE Cluster 2014 Conference; Madrid Spain; September 22-26, 2014*
Duration: July 1, 2014 – June 1, 2016
Description: This award supported 20 students from American institutions to attend the IEEE Cluster 2014 and Cluster 2015 Conferences.

NSF CCF# 1446794, $89,999, single PI
Title: *EAGER: Assessment of the Numerical Reproducibility in Large-Scale Scientific Simulations on Multicore Architectures*
Duration: June 15, 2014 – July 1, 2016

Description: This project studied the impact of rounding errors on result reproducibility when concurrent executions burst and workflow determinism vanishes in cutting-edge multicore architectures.

Lawrence Livermore National Laboratory Sub-contract, $64,118, single PI
Title: *Investigating Massively Scalable I/O-Aware Job Scheduling in Support of Flux*
Duration: November 5, 2014 – March 31, 2016
Description: This project investigated distinct—yet complementary—techniques to overcome challenges that can preclude I/O-aware schemes from effectively scheduling massively large-scale systems.

NSF CNS#1217812, $500,000 ($192,487 at UD), co-PI, with Arnold L. Rosenberg (PI, Northeastern University) and Rajmohan Rajaraman (co-PI Northeastern University)
Title: *CSR: Small: Collaborative: Pursuing High Performance on Clouds and Other Dynamically Heterogeneous Computing Platforms*
Duration: October 1, 2012 – September 30, 2015
Description: This project developed a transformative computing paradigm that enables high-performance computing on computing clouds and many genres of computing grids.
Supplement:
  • NSF REU Supplement, $8,000, single PI, Fall 2013

Argonne National Laboratory Sub-contract, $28,657, single PI
Title: *Evaluating, Analyzing, and Improving the Performance of Data-intensive Applications*
Duration: June 9, 2014 – January 15, 2015
Description: This project studied various data-intensive computing frameworks, including MR-MPI and DataMPI, and investigated their performance characteristics, particularly in the context of processing very large data.

AFOSR STTR Program - Highly Scalable Computational-Based Engineering Algorithms for Emerging Parallel Machine Architectures (Topic BT13): $700,000 ($162,000 at UD), co-PI, with Eric Kelmelis (PI, EM Photonics).
Title: *Scalable Aero-Load and Aero-Elasticity Solvers for Massively Parallel Heterogeneous Computing Architectures (Phase II)*
Duration: September 1, 2012 – August 31, 2014
Description: This project supported development of innovative algorithms for scientific computing, modeling, and simulation in a multi-GPU environment. Emphasis was on parallelization of scientific applications across multiple GPUs.

NSF EAR#1027807, $1,841,104 ($101,513 at UD), co-PI, with Jesse F. Lawrence (PI, Stanford University), Elizabeth S. Cochran (co-PI, University of California, Riverside), Richard Allen (co-PI, University of California, Berkeley), Jack Baker (co-PI, Stanford University), Tomas Heaton (co-PI, California Institute of Technology), Deborah Kilb (co-PI, Scripps Institution of Oceanography)
Title: *Collaborative Research: CDI-Type II: From Data to Knowledge: The Quake-Catcher Network*
Duration: October 1, 2010 – September 30, 2014
Description: This award developed 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.
Supplements:
  • NSF REU Supplement, $7,500, single PI, Fall 2012
  • NSF REU Supplement, $6,000, single PI, Fall 2013

NSF IIS#0968350, $683,199 ($308,719 at UD), PI, with G.M. Zoppetti (co-PI, Millersville University) and J. Cohoon (co-PI, University of Virginia)

Title: *Collaborative Research: SoCS - ExSciTecH: An Interactive, Easy-to-Use Volunteer Computing System to Explore Science, Technology, and Health*
Duration: September 1, 2010 – August 31, 2014
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.
Supplements:
- NSF REU Supplement, $7,500, single PI, Summer 2012
- NSF REU Supplement, $7,500, single PI, Summer 2011

NSF CDI#0941318, $538,740, co-PI, with Sandeep Patel (PI, UD)
Title: *CDI-Type I: Bridging the Gap Between Next-Generation Hybrid High Performance Computers and Physics Based Computational Models for Quantitative Description of Molecular Recognition*
Duration: October 1, 2009 – September 30, 2013
Description: This project designed and implemented advanced algorithms and middleware packages for polarizable force fields on multicore and GPU systems, supported by the MapReduce paradigm.

NSF DMS#0800266, $621,193 ($205,561 at UD), co-PI, with Ming-Ying Leung (PI, UTEP) and Kyle L. Johnson (co-PI, UTEP).
Title: *Collaborative Research: Mathematical Models for RNA*
Duration: June 1, 2008 – May 31, 2012
Description: This project developed 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 addressed the computational component with grid computing systems.

ARO #54723-CS, $306,750, single PI
Title: *Computer-Aided Design for Drugs on Emerging Hybrid High Performance Computers*
Duration: June 1, 2009 – May 31, 2013
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 (URP), $3,750, single PI, Summer 2012
- ARO – High School Apprenticeship Program (HSAP), $3,000, single PI, Summer 2010

AFOSR STTR program – Highly Scalable Computational-Based Engineering Algorithms for Emerging Parallel Machine Architectures (Topic BT13), $200,000 ($59,997 at UD), co-PI, with J. Humphrey (PI, EM Photonics)
Title: *Scalable Aero-Load and Aero-Elasticity Solvers for Massively Parallel Heterogeneous Computing Architectures (Phase I)*
Duration: March 1, 2012 – March 1, 2013
Description: This award supported the development of innovative algorithms for scientific computing, modeling, and simulation in a multi-GPU environment. Emphasis was on parallelization of scientific applications across multiple GPUs.

NSF MRI#0922657, $451,051, co-PI, with Douglas Doren (PI, UD), Sandeep Patel (co-PI, UD), Dionisios Vlachos (co-PI, UD).
Title: *Acquisition of a Facility for Computational Approaches to Molecular-Scale Problems*
Duration: September 15, 2009 - September 14, 2012
Description: This award supported the acquisition of a hybrid-computing cluster, with GPU-accelerated computing nodes, for theoretical and experimental researchers at UD to study a number of problems in chemical sciences.

University of Delaware Research Foundation (UDRF), $35,000, single PI
Title: *ExSciTecH: An Interactive, Easy-to-Use Volunteer Computing System to Explore Science, Technology, and Health*
Duration: June 1, 2010 – May 31, 2012
Description: This seed award aimed 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 (UDRF) REU, $3,500, single PI, Summer 2011

AFOSR STTR program - Highly-Scalable Computational-Based Engineering Algorithms for Emerging Parallel Machine Architectures (Topic BT13), $99,000 ($34,125 at UD), co-PI, with E. Kelmelis (PI, EM Photonics)
Title: *Collaborative Research: Accelerated Linear Algebra Solvers for Multi-Core GPU-Based Computing Architecture*
Duration: June 8, 2010 – June 7, 2011
Description: This award supported the development of innovative algorithms for scientific computing, modeling, and simulation on a multi-GPU environment. Emphasis was on algorithms related to sparse and dense linear algebra problems.

NSF SCI#0506429/#0802650, $1,220,036 ($382,558 at UD and $273,068 at UTEP), PI, with C.L. Brooks III (co-PI, TSRI(and D.P. Anderson (co-PI, UC Berkeley)
Title: *Collaborative Research: DAPLDS - a Dynamically Adaptive Protein-Ligand Docking System based on Multi-Scale Modeling*
Duration: September 1, 2005 – August 31, 2009
Description: This project explored 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 Supplement, $6,250, single PI, Summer 2009

CRA/NSF (sponsored by CRA, funded by NSF), $6,000, single PI
Title: *CRA Mentor, Distributed Mentor Project for undergraduate summer research*
Duration: Summer 2009, 10 weeks
Description: This project supported 1 undergraduate student for 10 weeks of research under my supervision. The research targeted arbitrary precision libraries for GPUs.

CRA/NSF (sponsored by CRA, funded by NSF), $6,000, single PI
Title: *CRA Mentor, Distributed Mentor Project for undergraduate summer research*
Duration: Summer 2008, 10 weeks
Description: This project supported 2 undergraduate students for 10 weeks of research under my supervision. The research targeted biological applications and their efficient migration to distributed systems.

ARP #003661-0008-2006, Advanced Research Program (ARP) - Texas Higher Education Coordinating Board, $99,982 (no-overhead), PI, with M.-Y. Leung (co-PI, UTEP)
Title: *RNA Secondary Structure Prediction Using a Grid of Heterogeneous Computers*
Duration: May 15, 2006 – May 14, 2008
Description: This project built an adaptive grid computing system that, at runtime, identified and exploited computer resources across the University of Texas at El Paso (UTEP) campus to predict secondary structures of large numbers of RNA segments using a variety of prediction programs.

IBM Shared University Research Award Program, over $600,000 retail value, co-PI, with P. Teller (PI, UTEP) and other UTEP faculty
Title: *Performance via Autonomicity, Analysis, Virtualization, and Micro-partitioning, and Research in Life Sciences and Bioinformatics*
Duration: May 2005
Description: The award enabled the purchase of a supercomputer for biology and bioinformatics applications at UTEP.

UTEP Seed Funds, $23,400, co-PI, with P. Solin (PI, UTEP)
Title: *High Performance Modular FEM/hp-FEM System (HERMES)*
Duration: Summer 2005
Description: This project was a feasibility study of parallelization of FEM algorithms.

Awards not transferred to UD from UTEP (2):

NSF DUE#0631168, $275,856, PI, with P. Teller (co-PI, UTEP)
Title: *S-STEM - SHiPPER: Spreading High Performance computing Participation in undergraduate Education and Research*
Duration: October 1, 2006 – January 31, 2011
Description: The award created and consolidated a community of UG and graduate students pursuing advanced degrees in fields that combine expertise in high-performance computing and other scientific and engineering disciplines.

SCORE-NIH, $581,329, co-PI, with M.-Y. Leung (PI, UTEP)
Title: *Computational Prediction of RNA Viral Genome Structures*
Duration: September 1, 2007 – August 31, 2011
Description: This project designed and implemented mathematical methods and computation tools for RNA secondary structure prediction in viral genomics.

Academic Gifts:

2012:

Hardware gift: 1 nVidia graphic cards Kepler K20, Professor Partnership Program. Award amount: approx. $3,199.

Hardware gift: 2 nVidia graphic cards Tesla M2090, Professor Partnership Program. Award amount: approx. $2,500 each.

2010:

Hardware gift: 4 nVidia graphic cards Tesla C2050, Professor Partnership Program. Award amount: approx. $2,500 each.

2009:

Hardware gift: 4 nVidia graphic cards Tesla C1060, Professor Partnership Program. Award amount: approx. $2,400 each.

Hardware gift: 1 Tesla S1070, Professor Partnership Program. Award amount: approx. $6,500.

2008:

Hardware gift: 2 nVidia graphic cards GeForce GTX280, Professor Partnership Program. Award amount: approx. $900 each.

Hardware gift: 2 nVidia graphic cards GeForce 9800 GX2, Professor Partnership Program. Award amount: approx. $1,200 each.

Hardware gift: 2 nVidia graphic cards FX5600, Professor Partnership Program. Award amount: approx. $6,000.

2006:

Software gift from Innobase Oy: perpetual InnoDB Hot Backup license for Linux. Award amount: $1,300.

2005:

Software gift from University of Harvard: CHARMM license for the DAPLDS project. Award amount: $600.

Travel Scholarship:

2012: NSF travel support to participate in the workshop: "Grid Computing - the Next Decade", Zakapane (Poland) – on invitation only

2006: NIH/PSC travel award to attend the workshop "MARC: Developing Bioinformatics Programs", Pittsburgh Supercomputing Center, July 17-28

2005: NSF travel award to attend the CRA Women Workshop for Women in Academic Career, Washington D.C., Virginia

2004: Travel award to attend the 6th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP6), Gaeta, Italy

Software Packages:

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

Selected projects:

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 - present	**NHANES-Analytics** – This repository contains cone 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 - present	**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 - present	**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 - present	**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

Students and Mentoring Activities:

Post-Doctoral Advisees:

Current: (Name, Period of support)
Open position

Former: (Name, Period of support, First position)
Wei-Fan Chien   Sep16 –Mar17
Travis Johnston   Sep14-Jul16   Researcher at Oak Ridge National Laboratory
Vivek Pallipuram   Jan14-Jul15   Assistant Professor at the University of the Pacific
Trilce Estrada   Jul12-Jul13   Assistant Professor at University of New Mexico
Narayna Ganesan   Jan10-Jul11   Assistant Professor at Stevens Institute of Technology
Arun Rajendran   Apr08-Jul08

Post-Master Advisees:

Former: (Name, Period of support, First position)
Samuel Schlachter   Jun13-Jul14   CTO at SNAPCARD, Inc.

PhD Advisees (2 PhD Theses completed, 3 PhD Theses in progress):

Current: (Name, Period of support, PhD status)
Stephen Herbein   Fa14 – present   Research Proposal on May 2017 (passed)
Sean McDaniel   Sp15 – present   Preliminary Research Requirement on May 2016 (passed)
Michael Wyatt   Sp16 – present   Preliminary Research Requirement on December 2016 (passed)
Dylan Chapp   Su17 – present   Preliminary Research Requirement on May 2017 (passed)

Former: (Name, Period of support, First position, Thesis title)
Boyu Zhang   Fa09-Su15   Big Data Analyst at Purdue U.
                     Thesis Title: *Enabling Scalable Data Analysis for Large Computational Structural Biology Datasets on Large Distributed Memory Systems supported by the MapReduce Paradigm*
Trilce Estrada   Sp06-Su12   Assistant Professor at University of New Mexico
                     Thesis Title: *On the Effectiveness of Application-aware Self-management for Scientific Discovery on Volunteer Computing System*

Other PhD Students mentored: (Name, Period of support)
Mohammad Alsulmi   Sp14-Fa14
Taylor Baldwin   Sp14-Su14
Marcos Portnoi   Sp13-Fa13
William Killian   Su11-Sp12
Omar Padron   Su11-Sp12
Maria Ruiz   Sp10-Fa11
Lifan Xu   Sp09-Fa10
Obaidur Rahaman   Su08-Sp10
James Atlas   Su08-Su09
Adnan Ozsoy   Fa08
Roberto Araiza   Sp07-Fa07

Number of preliminary research requirement exams supervised: 5 (Baldwin, Alsulmi, Herbein, McDaniel, Wyatt, and Chapp)

MS Advisees (7 students, 4 MS Theses):

Current: (Name, Period of support)
Rachel Kraft   Su17 – present

Former: (Name, Period of support, First position, Thesis title when applicable)
Dylan Chapp   Fa14 – Sp17
         Thesis Title: *Study of the Impact of Non-determinism on Numerical Reproducibility and Debugging at the Exascale*
Jeffrey DiMarco   Fa12-Fa14   Fidessa
Abel Licon   Sp08-Sp10   Thermo Fisher Scientific
         Thesis Title: *RNAVLab 2.0: Combining Web Applications, Grid Computing, and Dynamic Programming to Overcome Resource Limitations in RNA Secondary Structure Analysis*
Kevin Kreiser   Su08-Su09   MapQuest
Joseph Davis   Sp08-Su09   Siemens Healthcare
         Co-advised with Sandeep Patel (Dept. of Chemistry and Biochemistry, UD)
Prayook   Sp06-Fa06
Tungjatooronrusame   Co-advised with Ming-Ying Leung (Bioinformatics Program, UTEP)
David Flores   Sp06-Sp07   Ximis, El Paso, Texas.
         Thesis Title: *SimBA: A Discrete-event Simulator for Performance Prediction of Volunteer Computing Projects*
         Co-advised with Patricia Teller (Dept. of Computer Science, UD)
Richard Zamudio   Fa05-Sp07   Rockwell Collins, Iowa
         Thesis Title: *TOPAZ: A Firefox Protocol Extension for GridFTP - Outstanding Thesis in Computer Science 2006-2007 (UTEP)*

Graduate Visitor Scholars (4 students):

Current: (Name, Period of support, Affiliation)
Tao Gao   Jan16 – present   NUDT, China

Former: (Name, Period of support, Affiliation)
Julian A. Uran   Jun14-Nov14   University of Los Andes, Colombia
Cindy Solano   Su13   Universidad Industrial de Santander, Colombia
Daniel T. Yehdego   Su11   University of Texas at El Paso

UG Advisees (31 students, 4 Senior Theses):

Current (Name, Period of support, Funding, Thesis title when applicable)
John Bounds   Su16 – present   NSF REU
Liz Racca   Su17 – present   NSF REU
Thomas Kitson   Su17 – present   NSF REU
Paula Olaya   Su17   NSF REU

Former: (Name, Period of support, First position, Funding, Thesis title when applicable)
Rachel Kraft   Su17-present   NSF REU
Connor Zanin   Sp15-Sp16   PhD Student at Northeastern U.   NSF REU

	Senior Thesis: *Tuning MapReduce with Surrogate-Based Modeling*		
Ryan McKenna	Fa14-Sp16	PhD Student at UMass Amherst	NSF REU
	Senior Thesis: *Predicting Performance Variability in Parallel File Systems*		
Sean McDaniel	Sp14-Fa14	PhD Student at UD	NSF REU
Stephen Herbein	Fa12-Su14	PhD Student at UD	NSF REU
	Senior Thesis: *Benchmarking and Auto-tuning I/O Intensive Applications at the Extreme Scale*		
Michael Matheny	Sp12-Su14	PhD Student at U. Utah	NSF REU
Samuel Schlachter	Su11-Sp13	Post-Master at UD	NSF REU
Matthew Wezowicz	Fa11-Su13		NSF REU
Casey Casalnuovo	Fa13		NSF REU
Haley Northrup	Fa13		NSF REU
Ryan Huttman	Fa11-Sp13		NSF REU
Reza Hammond	Fa10-Sp11	PhD Student at UD	NSF REU
Jason Park	Su10-Sp11		NSF REU
Kyle Benson	Su10-Su11	PhD Student at UCI	NSF REU
Dirk Mezger	Fa10		
Dominik Kimmel	Fa10		
Omar Padron	Su09	PhD Student at UD	CRA-DMP
Philip Saponaro	Sp09-Sp10	PhD Student at UD	NSF REU
	Senior Thesis: *An Efficient Arbitrary Precision Mathematical Library for Accurate and Fast MD Simulations in Single Precision GPUs*		
Patrick McClory	Sp08-Sp09	PhD Student a UPitt	NSF REU
Reed Matz	Su08-Fa08		NSF REU
Jason Parrott	Fa07-Sp08	Factset Resarch Systems	NSF REU
Robert Keller	Fa07-Sp08	Vanguard	NSF REU
Brenda Medina	Su08		CRA-DMP
David Mireles	Fa06-Su07, Su08		NSF REU, CRA-DMP
Vladimir Soto	Sp07-Su07		NSF REU
Princess Trillo	Sp07-Su07		NSF REU
David Gomez-Leon	Fa06-Sp07		NSF REU
Karina Escapita	Sp06-Su07		NSF REU
Guillermo Lopez	Fa06-Su07		NSF REU
Abel Licon	Fa06-Su07	MS at UD	NSF REU
Daniel Catarino	Sp06-Fa06	Exxon Mobil	NSF REU

High School Advisees:

Former: (Name, Period of support, First position, Funding)

Lou Fogel	Su10	B.S. CS at Worcester Polytechnic Institute	Army HSAP

Graduate Committees (11 committees):

Wei Yang (MS Thesis supervisor:

Wei-Fan Chiang (Thesis supervisor: Ganesh Gopalakrishnan), Ph.D. in Computer Science at U. of Utah, 2016
Fan Yang (Thesis supervisor: Paul Amer), Ph.D. in Computer Science at UD, 2015
Bryan Youse (Thesis supervisor: B. David Saunders), Ph.D. in Computer Science at UD, 2015

Kevin McCormick (Thesis supervisor: Li Liao), Ph.D. in Computer Science at UD, 2013
Daniel Orozco (Thesis supervisor: Guang R. Gao), Ph.D. in Computer Engineering at UD, 2012
Liang Gu (Thesis supervisor: Xiaoming Li), Ph.D. in Computer Engineering at UD, 2011
Kurt Ferreira (Thesis supervisor: Patrick Bridges), Ph.D. in Computer Science at UNM, 2011
Jayaraman Suresh Babu (Thesis supervisor: Patricia J. Teller), M.S. in Computer Science at UTEP, 2006
Maria Gabriela Aguilera (Thesis supervisor: Patricia J. Teller), M.S. in Computer Science at UTEP, 2005
Yash Dayal (Thesis supervisor: Gregory Lush), M.S. in Electrical and Computer Eng. at UTEP, 2005
Javed Bilal Khan (Thesis supervisor: John Chessa), M.S. in Mechanical Engineering at UTEP, 2005

Student Awards:

Department Level (13):
Michael Wyatt: CIS Outstanding Graduate Student Award (UD), 2017
Rachel Kraft: John K. Scoggin Sr. Award, (2017)
Ryan McKenna: CIS Outstanding Senior Student Award (UD), 2016
Stephen Herbein: CIS Outstanding Graduate Student Award (UD), 2016
Boyu Zhang: CIS Lauri Pfeffer Shinn Memorial Award (UD), 2015
Ryan McKenna: CIS Outstanding Junior Student Award (UD), 2015
Stephen Herbein: CIS Outstanding Senior Student Award (UD), 2014
Michael Matheny: CIS Steven Geracimos Memorial Award (UD), 2013
Stephen Herbein: CIS Outstanding Junior Student Award (UD), 2013
Trilce Estrada: CIS Frank A. Pehrson Graduate Student Achievement Award (UD), 2012
Kyle Benson: CIS Outstanding Senior Student Award (UD), 2011
Jason Pack: CIS Steven Geracimos Memorial Award (UD), 2011
Philip Saponaro: CIS Junior Outstanding Student Award (UD), 2009
Trilce Estrada: CIS Lauri Pfeffer Shin Memorial Award (UD), 2009
Richard Zamudio: Outstanding Thesis in the Department of Computer Science (UTEP), 2006

University Level (8):
Rachel Kraft: UD University Graduate Scholar Award, 2016 – 2017
Sean McDaniel: UD University Graduate Scholar Award, 2015 – 2016; 2016 – 2017
Taylor Baldwin: UD University Graduate Scholar Award, 2014 – 2015
Omar Padron: UD University Graduate Scholar Award, 2011 – 2012
Trilce Estrada: UD Graduate Fellow Award, 2010-2011
Philip Saponaro: UD University Graduate Scholar Award, 2010 – 2011
Able Licon: UD University Graduate Scholar Award, 2009 – 2010; 2010 – 2011
Trilce Estrada: Alumni Enrichment Award (UD), 2008

National and International Level (7):

Sean McDaniel: First Place at the ACM Student Poster Competition at SC14
Stephen Herbein: Second Place at the ACM Student Poster Competition at SC13
Matthew Wezowicz: Second Place at the ACM Student Poster Competition at SC12
Philip Saponaro and Omar Padron: Dr. Robert M. Panoff Award at SC09
Abel Licon: Google Hispanic Scholarship Fund (HSF) Scholarship, 2008
David Mireles: Google Hispanic Scholarship Fund (HSF) Scholarship, 2007
Daniel Catarino: Google Hispanic Scholarship Fund (HSF) Scholarship, 2006

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

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

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

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

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

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
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 other Advisory Committees:

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) – elected.
2016 – present	Member of the NSF Advisory Committee for Cyberinfrastructure
2016 – present	Steering Committee Member ISC High Performance Computing
2016 – present	Member of the ACM Senior Member Committee
2015 – present	Member of the Advisory Group on Reproducibility - Advisory to the SC Conference, ACM, and IEEE.
2015 – present	Steering Committee Member for the ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC).
2014 – present	Steering Committee Member for the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC).
2014 – present	Steering Committee Member for the IEEE International Conference on Cluster Computing (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 32nd 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 31st 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 24th 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, 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 12th 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 - 11th IEEE

International Conference on High Performance Computing and Communications (HPCC), June 2009, Soul, South Korea.

23. *Technical Program Chair* of the 8th 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:

2017:

1. *Panel Committee Member* of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2017. Denver, CO, USA.
2. *Technical Program Committee Member* of the 26nd International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2017, Washington DC, USA.
3. *Technical Program Committee Member* of the 32nd ISC High Performance Conference. June 18-22, 2017, Frankfurt, Germany.
4. *Workshop Committee Member of the* International Conference on Computational Science (ICCS). June 12-14, 2017, Zurich, Switzerland.
5. *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:

6. *Technical Program Committee* of the 23rd IEEE International Conference on High Performance Computing, Data and Analytics (HiPC), December 19-22, 2016, Hyderabad, India.
7. *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.
8. *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.
9. *Technical Program Committee Member* of the System Track - IEEE International Conference on Cluster Computing, September 2016, Taipei, Taiwan.
10. *Technical Program Committee Member* ISC High Performance Conference. June 19-23, 2016, Frankfurt, Germany.
11. *Technical Program Committee Member* of the 25nd International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2016, Kyoto, Japan.
12. *Technical Program Committee Member* of the 16th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid), May 2016, Cartagena, Colombia.
13. *Technical Program Committee Member* of the ACM International Conference on Computing Frontiers (CF), May 2016, Como, Italy.
14. *Technical Program Committee Member* of the 6th International Workshop on Adaptive Self-tuning Computing Systems (ADAPT), January 2016, Prague, Czech Republic.

2015:

15. *Technical Program Committee Member* of the 21th IEEE International Conference on Parallel and Distributed Systems (ICPADS), December 2015, Melbourne, Australia.
16. *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.
17. *Technical Program Committee Member* of the IA^3 2015: 5th Workshop on Irregular Applications:

Architectures and Algorithms. November 2015. Austin, TX, USA.

18. *Technical Program Committee Member* of the EduHPC-15: Workshop on Education for High-Performance Computing. November 2015. Austin, TX, USA.
19. *Technical Program Committee Member* of 11nd IEEE International Conference on e-Science and Grid Technologies (eScience), August 2015, Munich, Germany.
20. *Technical Program Committee Member* of the 2014 ACM International Conference on Supercomputing (ICS), June 2015, Long Beach, USA.
21. *Technical Program Committee Member* of the ACM Computing Frontiers (CF), May 2015, Ischia, Italy.
22. *Technical Program Committee Member* of 2015 ACM/IEEE CS George Michael HPC Fellowship.
23. *Technical Program Committee Member* of Workshop and Tutorials at the 2015 Richard Tapia Celebration of Diversity in Computing Conference, Boston, MA, USA.

2014:

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

2013:

31. *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.
32. *Technical Program Committee Member* of the 13th International Workshop on High Performance Computational Biology (HiCOMB), May 2013, Phoenix, Arizona, USA.
33. *Technical Program Committee Member* of the 6th IEEE/ACM International Conference on Utility and Cloud Computing (UCC), December 2013, Dresden, Germany.
34. *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.
35. *Technical Program Committee Member* of the Workshop on Parallel Computational Biology (PBC), held in conjunction with PPAM 2013, September 8-11, 2013, Warsaw, Poland.
36. *Technical Program Committee Member* of the 1st Workshop on Parallel and Distributed Agent-Based Simulations (PADABS), August 2013, Aachen, Germany.
37. *Technical Program Committee Member* of the 22nd International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2013, New York, NY, USA.
38. *Technical Program Committee Member* of the 12th International Workshop on High Performance Computational Biology (HiCOMB), May 2013, Boston, MA, USA.
39. *Technical Program Committee Member* of the 13th IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid), May 2013, Delft, The Netherlands.

2012:

40. *Technical Program Committee Member* of the International Conference for High Performance

Computing, Networking, Storage, and Analysis (SC), November 2012, Salt Lake City, UT, USA.

41. *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.

42. *Technical Program Committee Member* of the High Performance Computing Conference (HiPC), December 2012, Pune, India.

43. *Technical Program Committee Member* of the 5th IEEE/ACM International Conference on Utility and Cloud Computing (UCC), November 2012, Chicago, IL, USA.

44. *Technical Program Committee Member* of the Grace Hopper Conference (GHC) Panels, Workshops, and Presentations (PWP) Committee, October 2012, Baltimore, MD, USA.

45. *Technical Program Committee Member* of 8nd IEEE International Conference on e-Science and Grid Technologies (eScience), October 2012, Chicago, IL, USA.

46. *Technical Program Committee Member* of Symposium on Application Accelerators in High-Performance Computing (SAAHPC), July 2012, Argonne National Laboratory, IL, USA.

47. *Technical Program Committee Member* of the 21st ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2012, Delft, The Netherlands.

48. *Technical Program Committee Member* of the 12th IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid), May 2012, Ottawa, Canada.

49. *Technical Program Committee Member* of the 2012 ACM International Conference on Computing Frontiers (CF), May 15-17, 2012, Cagliari, Italy.

50. TCPP Travel Award Committee of the 26th IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 21 – 25, 2012, Shanghai, China.

51. *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:

52. *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.

53. *Technical Program Committee Member* of the 13th IEEE International Conference on High Performance Computing and Communications (HPCC) in Biological/Molecular Computing Track, September 2 – 4, 2011, Banff, Alberta, Canada.

54. *Technical Program Committee Member* of the IEEE Cluster 2011 Conference (Cluster), September 26 – 30, 2011, Austin, TX, USA.

55. *Technical Program Committee Member* of the Workshop on Parallel Computational Biology (PBC), held in conjunction with PPAM 2011, September 11-14, 2011, Torun, Poland.

56. *Technical Program Committee Member* of the 11th IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 23 – 26, 2011, Los Angeles, CA, USA.

57. *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.

58. *Technical Program Committee Member* of the 7th International Workshop on High Performance Computational Biology (HiCOMB), May 16, 2011, Anchorage, AK, USA.

59. *Technical Program Committee Member* of the 4th Annual Workshop for General-Purpose Computation on Graphics Processing Units (GPGPU), March 5, 2011, Newport Beach, California, USA.

60. *Technical Program Committee Member* of the 18th Euromicro Conference on Parallel, Distributed and Network-Based Processing (PDP), February 9-11, 2011, Ayia Napa, Cyprus.

2010:

61. *Technical Program Committee Member* of the 2010 IEEE 6th International Conference on e-Science

(eScience), December 7 – 10, 2010, Brisbane, Australia.

62. *Technical Program Committee Member* of the International Conference of Computer Design (ICCD), October 3-6, 2010, Amsterdam, The Netherlands.
63. *Technical Program Committee Member* of the 22nd International Symposium on Computer Architecture and High-Performance Computing (SBAC-PAD), October 2010, Petropolis, Brazil.
64. *Technical Program Committee Member* of the Workshop on Parallel Programming and Applications on Accelerator Clusters (PPAAC), September 2010, Heraklion, Greece.
65. *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.
66. *Technical Program Committee Member* of the 2010 ACM International Symposium on High Performance Distributed Computing (HPDC), June 2010, Chicago, IL, USA.
67. *Technical Program Committee Member* of the ACM Computing Frontiers Conference (CF), May 2010, Bertinoro, Italy.
68. *Technical Program Committee Member* of the 10th IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 2010, Melbourne, Australia.
69. *Technical Program Committee Member* of the Second Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2010, Melbourne, Australia.
70. *Technical Program Committee Member* of the 18th Euromicro Conference on Parallel, Distributed and Network-Based Processing (PDP), February 2010, Pisa, Italy.

2009:

71. *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.
72. *Technical Program Committee Member* of the International Conference of Computer Design (ICCD), November 4 – 7, 2009, Lake Tahoe, CA, USA.
73. *Scholarship Committee Member* of the Grace Hopper Celebration of Women in Computing 2009, October 2009, Tucson, AZ, USA.
74. *Technical Program Committee Member* of the 2009 IEEE International Conference on Cluster Computing (Cluster), August 29 – September 4, 2009, New Orleans, LA, USA.
75. *Technical Program Committee Member* of the 12th IEEE International Conference on Computational Science and Engineering (CSE), August 29 – 31, 2009, Vancouver, Canada.
76. *Technical Program Committee Member* of 9th IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 2009, Shanghai, China.
77. *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.
78. *Technical Program Committee Member* of the Second Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2009, Rome, Italy.
79. *Technical Program Committee Member* of the 2009 Richard Tapia Celebration of Diversity in Computing Conference, April 2009, Portland, OR, USA.
80. *Technical Program Committee Member* of the 17th Euromicro Conference on Parallel, Distributed and Network-Based Processing (PDP), February 2009, Bauhaus-University Weimar in Thuringia, Germany.

2008:

81. *Technical Program Committee Member* of the Intl. Conference on Advanced Computing and Communications, December 2008, Chennai, India.
82. *Technical Program Committee Member* of the Computational Structural Bioinformatics Workshop 2008 November 2008, Philadelphia, PA, USA.
83. *Technical Program Committee Member* of the International Conference for High Performance

Computing, Networking, Storage, and Analysis (SC). November 2008, Austin, TX, USA.

84. *Technical Program Committee Member* of the Grace Hopper Celebration of Women in Computing 2008, October 2008, Denver CO, USA.
85. *Technical Program Committee Member* of the IEEE Intl. Conference on Computer Design (ICCD), October 2008, Lake Tahoe, CA, USA.
86. *Technical Program Committee Member* of the 10th IEEE International Conference on High Performance Computing and Communications (HPCC), September 2008, DaLian, China.
87. *Technical Program Committee Member* of the International Conference on Computational Science (ICCS), June 2008, Krakow, Poland.
88. *Technical Program Committee Member* of the ACM Computing Frontiers (CF), May 2008, Ischia, Italy.
89. *Technical Program Committee Member* of the Global and Peer-to-Peer Computing (GP2PC), May 2008, Lyon, France.
90. *Technical Program Committee Member* of the 7th International Workshop on High Performance Computational Biology (HiCOMB), May 2008, Miami, FL, USA.
91. *Technical Program Committee Member* of the 9th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC), May 2008, Miami, FL, USA.
92. *Technical Program Committee Member* of the 2nd Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2008, Miami, Florida, USA.
93. *Technical Program Committee Member* of the 22nd IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2008, Miami, FL, USA.
94. *Technical Program Committee Member* of the Euromicro Conference on Parallel, Distributed and Network based Processing (PDP) February 2008, Toulouse, France.

2007:

95. Technical Poster Committee Member of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2007, Reno, NV, USA.
96. *Technical Program Committee Member* of the First Computational Structural Bioinformatics Workshop, November 2007, San Jose, CA, USA.
97. *Technical Poster Committee Member* of the 2007 Richard Tapia Celebration of Diversity in Computing Conference, October 2007, Orlando, FL, USA.
98. *Scholarship Committee Member* of the Grace Hopper Celebration of Women in Computing 2007, October 2007, Orlando, FL, USA.
99. *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.
100. *Technical Program Committee Member* of the International Conference on Computational Science 2007 (ICCS), May 2007, Beijing, China.
101. *Technical Program Committee Member* of the 6th International Workshop on Global and Peer-to-Peer Computing (GP2P), May 2007, Rio de Janeiro, Brazil.
102. *Technical Program Committee Member* of 26th IEEE International Performance Computing and Communications Conference (IPCCC), April 2007 - New Orleans, LA, USA.
103. *Technical Program Committee Member* of the First Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), March 2007, Long Beach, CA, USA.

2006:

104. *Technical Program Committee Member* of the 4th IEEE International Symposium on Parallel and Distributed Processing and Applications (ISPA), December 2006, Sorrento, Italy.
105. *Technical Program Committee Member* of the 2nd IEEE International Conference on e-Science and Grid Technologies (eScience), December 2006, Amsterdam, The Netherlands.
106. *Technical Program Committee Member* of the 5th International Workshop on Global and Peer-to-Peer Computing (GP2P), May 2006, Singapore.

107. *Technical Program Committee Member* of the 20th IEEE International Parallel and Distributed Processing Symposium (IPDPS), April 2006, Rhodes, Greece.
108. *Technical Program Committee Member* of the 5th IEEE International Workshop on High Performance Computational Biology (HiCOMB), April 2006, Rhodes, Greece.

2005:

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

Conference Reviewer:

2009   GPGPU'09

2008   PADS'08, LCPC'08

2007   PARA'07, SC'07

2006   HPDC'06, Cluster'06, MCWC'06

2005   SC'05, ICS'05

2004   Cluster'04, HPDC'04

2003   CCGrid'03, SC'03, Cluster'03

Journal and Book Referee:

Since 2005, I 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)

Services to the University, College, and Department (Selected):

At UD:

2016 – present   Chair, Publicity/Awards/Development Activity Committee (CIS Department)

2016 – present   Faculty Secretary, College of Engineering (CoE)

2016 – present   Member, Adhoc College of Engineering Committee on Server Room Relocation (CoE)

2015 – present   Acting Director, Center for Bioinformatics & Computational Biology (CBCB), Delaware Biotechnology Institute (DBI)

2015 – present   Member, Faculty Recruitment Committee (ECE Department)

2014 – present	Member, Bioinformatics Steering Committee (Bioinformatics Program)
2014 – present	Advisor, Bioinformatics Student Association (Bioinformatics Program)
2007 – present	Coordinator, CIS/ECE booth at the Supercomputing Conference (CIS Department)
2015	Member, Undergraduate Committee (CIS Department)
2014 – 2015	Chair, Distinguished Speaker Series Committee (CIS Department)
2014	Chair, Faculty Recruitment Committee (CIS Department)
2012 – 2013	Member, Biomedical Engineering Graduate Committee (BME Program)
2012 – 2013	Chair, Distinguished Speaker Series Committee (CIS Department)
2010	Organizer, CIS Research Day (CIS Department)
2009 – 2013	Member, Bioinformatics Program Committee (University Committee)
2009 – 2011	Member, Research Computing Task Force (University Committee)
2009 – 2010	Member, Graduate Recruiting Committee (CIS Department)
2008 – 2009	Member, Graduate Committee (CIS Department)
2007 – 2009	Advisor, Student ACM Chapter (CIS Department)
2007 – 2008	Member, Graduate Recruiting Committee (CIS Department)

At UTEP:

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

Professional Affiliations:

- ACM, ACM SIGHPC, ACM Computing Reviews
- IEEE
- SIAM