Michela Taufer

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David and Beverly J.C. Mills Career Development Chair
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 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.

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

Jun 2013 – May 2014   Visiting Faculty at the Oak Ridge National Laboratory, Computer Science and Mathematics 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 – Postdoctoral Researcher, Center for Theoretical Biological Physics (CTBP), University of
Dec 2004   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 – Research Student Assistant, Computer Systems Institute, Swiss Federal Institute of Technology
Dec 2002   Zurich (ETH), Switzerland.

Feb 1996 – Visitor Scholar at the Swiss Center for Scientific Computing (SCSC/CSCS), Zurich,
Dec 1996   Switzerland.

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.

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. BDHPC**,** 2015. (In review)
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:

1. B. Zhang(*), T. Estrada, P. Cicotti, P. Balaji, and **M. Taufer**. Enabling Scalable and Accurate Clustering of Distributed Ligand Geometries on Supercomputers. *IEEE Transactions on Cloud Computing (TCC)*, 2015. (In review) *(Corresponding author)*
2. 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 (ParCo)*, 2015. (Accepted) *(Corresponding author)*
3. **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,* July 22, 2015. doi: 10.1177/1094342015594518 *(Corresponding author)*
4. 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.
5. 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. *(Corresponding author)*
6. 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*, January 7, 2014.
7. 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. *(Corresponding author)*

8. 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* 2013, 13(Suppl 1):S3 (8 November 2013) *(Corresponding author with Leung)*

9. **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. *(Corresponding author)*

10. 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, 2012. *(Corresponding author)*

11. 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, 2012.

12. 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. *(Corresponding author with Patel)*

13. 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.

14. 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. *(Corresponding author with Patel)*

15. 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.

16. 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. *(Corresponding author)*

17. **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. *(Corresponding author)*

18. **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, 2009. *(Corresponding author)*

19. **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. *(Corresponding author)*

20. 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. *(Corresponding author)*

21. 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.

22. **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.

23. **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.

24. 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. *(Corresponding author)*

25. 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):

1. 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)*, Melbourne, Australia. December 14 -16, 2015. (*Rate:* 82/230, 35.6%)

2. 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*, Chicago, Illinois, USA. September 8 – 11, 2015. (*Acceptance Rate:* 38/157, 24%)

3. V. Pallipuram, T. Estrada, and **M. Taufer**. A Resource-selection Heuristic for High-performance and Cost-effective Workflow Execution on the Cloud. In *Proceedings of the International Conference on Parallel Processing (ICPP)*, Beijing, China. September 1 – 4, 2015. (*Acceptance Rate:* 99/305, 32.5%)

4. 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)*, Munich, Germany. August 31 – September 4, 2015.

5. 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*. May 2015. (*Award Winners. Acceptance Rate:* 5/15, 33%)

6. 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)*, Reykjavik, Iceland. June 1 – 3, 2015. (*Acceptance Rate:* 26%)

7. 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)*. Hsinchu, Taiwan. December 16 – 19, 2014. (*Acceptance Rate:* 96/322, 29.8%)

8. 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)*, Hong Kong, China. December 2014.

9. 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*. Madrid, Spain. October 22 – 25, 2014.

10. 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*. Madrid, Spain, September 22 – 26, 2014. (*Acceptance Rate:* 29/122, 23.8% - One of four Best Paper Candidates)

11. 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)*, Cairns, Queensland, Australia. June 2014. (*Acceptance Rate:* 197/65, 33%)

12. 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),* Phoenix, Arizona, USA. April 2014. (*Acceptance Rate:* 114/541, 21%)

13. 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), Sydney, Australia. December 2013.

14. 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)*, Sydney, Australia. December 2013.

15. 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),* Beijing, China. October 2013.

16. 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,* Baltimore, Maryland, USA. April 2012.

17. 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,* Salt Lake City, Utah, USA. November 2012. (*Acceptance Rate:* 100/472, 21%)

18. 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)*, Liverpool, England, UK. June 2012. (*Acceptance Rate:* 104/395, ~26.2%)

19. 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,* Baltimore, Maryland, USA. April 2012.

20. 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),* Stockholm, Sweden. December 2011. (*Acceptance Rate:* 54/110, 50%)

21. 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*, Banff, Canada. September 2011. (*Acceptance Rate:* 59/271, 21.7%)

22. 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,* Orlando, Florida, USA. April 2011.

23. 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),* New York, USA. August 2010. (*Acceptance Rate:* 37/136, 28%)

24. 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)*, New York, USA. August 2010. (*Short Paper – Acceptance Rate:* 30/99, 33%)

25. **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),* Atlanta, Georgia, USA. April 2010. (*Acceptance Rate:* 127/527, 24%)

26. 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), Atlanta, Georgia, USA. April 2010. (*Acceptance Rate:* 127/528, 24%)

27. 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),* Honolulu, Hawaii, USA. March 2010. (*Acceptance Rate:* 45%)

28. 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),* Baton Rouge, Louisiana, USA. May 2009. (*Acceptance Rate:* ~30%)

29. 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),* Shanghai, China. May 2009. (*Acceptance Rate*: 57/271, 21%)

30. 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),* New Orleans, Louisiana, USA. April 2009. (*Acceptance Rate:* 30/72, 41.6%)

31. 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),* Ischia, Italy. May 2008. (*Acceptance Rate*: 30/110, 27%)

32. 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,* Orlando, Florida, USA. October 2007.

33. 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),* San Diego, California, USA. June 2007.

34. 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),* Amsterdam, The Netherlands. December 2006. (*Acceptance Rate:* 60/160, 37.5%)

35. **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).* December 2005, Melbourne, Australia. (*Acceptance Rate:* 54/171, 31.6%)

36. 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),* Santa Fe, New Mexico, USA. April 2004. (*Acceptance Rate:* 31.7%).

37. **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),* Hong Kong, China. December 2003. (*Acceptance Rate:* 48/164, 29.3%)

38. 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),* Tokyo, Japan. May 2003. (*Acceptance Rate:* 39/114, 34.2%).

39. 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),* Nice, France. April 2003. (*Acceptance Rate:* 119/407, 29.2%)

40. **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),* Winnipeg, Manitoba, Canada. August 2002.

41. **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),* Berlin, Germany. May 2002. (*Acceptance Rate:* 25.0%)

42. **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),* Fort Lauderdale, Florida, USA. April 2002. (*Acceptance Rate:* 98/258, 38%)

43. **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.

44. 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):

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),* Minneapolis, MN, USA. September 2014. (*Acceptance Rate:* 25/13, 52%)

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)*, 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),* 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),* Boston, Massachusetts, USA. April 2013. (*Acceptance Rate*: 9/17, 52%)

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),* 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)*, Philadelphia, Pennsylvanian, USA. October 2012. (*Acceptance Rate:* 11/33, 33%)

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), 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), Anchorage, Alaska, USA. May 2011. (*Acceptance Rate:* 11/21, 52.3%)

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), 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, 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'09, Rome, Italy. May 2009.

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'08, Miami, Florida, USA. April 2008. (*Acceptance Rate*: 10/25, 40%)

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),* 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, 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, 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, Long Beach, California, USA. March 2007.

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, 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'06, 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, Rhodes Island, Greece. April 2006.

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, 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*,* Denver, Colorado, USA. April 2005. (*Acceptance Rate:* 14/29, 47%)

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'04, 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, 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.

Educational Papers:

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.

Keynotes:

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.

Selected Invited Talks:

Dec 2015   In-Situ Data Analysis of Protein-folding Trajectories. Invited talk at University of Queensland, Brisbane, Australia.

May 2015   Enabling In-situ Analysis of Ligand Geometries in Drug Design Simulations on Supercomputers. Invited talk at the 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. Invited talk at the Novel Tools in Computational Chemistry Coding (NTC3). 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 Almaden, 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.

Selected Conference Talks:

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.

Selected Invited Panel:

Jun 2008	*A Day in the life of a researcher in Graduate School, Academia, and Industry.* 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*. Panel discussion: "The Great Academia/Industry Grid Debate", 4th International Workshop on Grid Computing (Grid 2003), Phoenix, Arizona.

Funding and Awards

Awards in Progress:

NSF CNS#1318417, $814,733 ($427,878 at UD), PI and Project Lead at UD, with Michela Becchi (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 1, 2015 – May 31, 2018
Description: This project tackles numerical errors due to limited arithmetic precision and non-determinism associated with multi-threading; the goal is defining methodologies to enable reproducible accuracy of large ensemble simulations on exascale platforms.

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: Study aspects of I/O performance and in-situ analysis for applications relevant to the Army.

NSF CCF#1550348, $20,000, single PI
Title: *Student Support: IEEE Cluster 2015-2016 Conferences*
Duration: July 7, 2015 – June 13, 2016
Description: Supporting 20 students from USA institutions to attend the IEEE Cluster 2015 and Cluster 2016 conferences.

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 – December 31, 2015
Description: Investigate distinct—yet complementary—techniques to overcome challenges that can preclude I/O-aware schemes from effectively scheduling massively large-scale systems.

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

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: Supporting 20 students from USA institutions to attend the IEEE Cluster 2014 and Cluster 2015 Conferences.

NSF CNS#1318417, $512,038.00 ($459,000.00 at UD), PI and Project Lead at UD, with Pietro Cicotti (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: Developing transformative analysis methodology to model the properties of large scientific datasets in a distributed manner on petascale and exascale systems.
Supplement:
- NSF REU Supplement, $16,000, single PI, Summer 2014

- NSF REU Supplement, $16,000, single PI, Summer 2015

Awards Completed:

NSF CNS#1217812, $500,000 ($192,487.00 at UD), Collaborating PI at UD, with Arnold L. Rosenberg (PI, Northeastern University) and Rajmohan Rajaraman (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: Developing 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: Studying various data-intensive computing frameworks, including MR-MPI and DataMPI, and investigating their performance characteristics, particularly in the context of processing very large data.

NSF EAR#1027807, $1,841,104 ($101,513 at UD), Collaborating PI at UD, with Jesse F. Lawrence (PI and Project Lead, 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: Provide a Volunteer Computing cyber-infrastructure to process and analyze large new seismic data sets in near-real time and to foster collaboration between 1000's of researchers and interested participants around the world.
Supplement:
- NSF REU Supplement, $7,500, single PI, Fall 2012
- NSF REU Supplement, $6,000, single PI, Fall 2013

AFOSR STTR Program - Highly Scalable Computational-Based Engineering Algorithms for Emerging Parallel Machine Architectures (Topic BT13): $700,000 ($161,101 at UD), PI of sub-contract at UD, 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: Support development of innovative algorithms for scientific computing, modeling, and simulation in a multi-GPU environment. Emphasis is on parallelization of scientific applications across multiple GPUs.

NSF IIS #0968350, $683,199 ($308,719 at UD), PI and Project Lead, with G.M. Zoppetti (Millersville University) and J. Cohoon (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: Support 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 DMS #0800266, $621,193 ($205,561 at UD), Collaborating PI at UD with Ming-Ying Leung (PI at UTEP and Project Lead) and Kyle L. Johnson.
Title: *Collaborative Research: Mathematical Models for RNA*
Duration: June 1, 2008 – May 31, 2014
Description: Develop probabilistic models to study the inversion distribution in RNA sequences and to combine the results with the general theory of excursions to maximize the prediction accuracy using an optimal RNA segment length. My group addresses the computational component with grid computing systems.

NSF CDI #0941318, $ 538,740, co-PI and Project Lead with Sandeep Patel (PI)
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: Design and implement advanced algorithms and middleware packages for polarizable force fields on multi-core and GPU systems, supported by the MapReduce paradigm.

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: Develop accurate and efficient protein-ligand docking applications for hybrid computer systems in HPC, including multi-core 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), PI of sub-contract at UD, 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: Support development of innovative algorithms for scientific computing, modeling, and simulation in a multi-GPU environment. Emphasis is on parallelization of scientific applications across multiple GPUs.

NSF MRI #0922657, $451,051, co-PI, with Douglas Doren (PI), Sandeep Patel, Dionisios Vlachos.
Title: *Acquisition of a Facility for Computational Approaches to Molecular-Scale Problems*
Duration: September 15, 2009 - September 14, 2012
Description: Support 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: Seed money 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), PI of sub-contract at UD, 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: Support development of innovative algorithms for scientific computing, modeling, and simulation on a multi-GPU environment. Emphasis is 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 and Project Lead (with C.L. Brooks III, TSRI and D.P. Anderson, 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: Explore of the multi-scale 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: Support for 1 undergraduate student for 10 weeks of research under my supervision. The research targets 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: Support for 2 undergraduate students for 10 weeks of research under my supervision. The research targets 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 and Project Lead, with M.-Y. Leung (co-PI)
Title: *RNA Secondary Structure Prediction Using a Grid of Heterogeneous Computers*
Duration: May 15, 2006 – May 14, 2008
Description: Build an adaptive grid computing system that, at runtime, identifies and exploits 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) and other UTEP faculty
Title: *Performance via Autonomicity, Analysis, Virtualization, and Micro-partitioning, and Research in Life Sciences and Bioinformatics*
Duration: May 2005
Description: Purchase a supercomputer for biology and bioinformatics applications at UTEP.

UTEP Seed Funds, $23,400, co-PI, with P. Solin (PI)
Title: *High-Performance Modular FEM/hp-FEM System (HERMES)*
Duration: Summer 2005

Description: Feasibility study of parallelization of FEM algorithms.

Awards not transferred to UD from UTEP:

NSF DUE #0631168, $275,856, PI and project lead, with P. Teller (co-PI)
Title: *S-STEM - SHiPPER: Spreading High-Performance computing Participation in undergraduate Education and Research*
Duration: October 1, 2006 – January 31, 2011
Description: Create and consolidate a community of UG and graduate students who will pursue 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)
Title: *Computational Prediction of RNA Viral Genome Structures*
Duration: September 1, 2007 – August 31, 2011
Description: Design and implement 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.

Academic Awards:

2015: ACM Distinguished Scientist

2015: Winner of the 8th IEEE International Scalable Computing Challenge - Co-located with the IEEE/ACM CCGrid Conference.

2014: ACM Senior Member

2013: Faculty appointment at ORNL in the Department of Energy (DoE) Higher Education Research Experiences Faculty (HERE Faculty) program

2006: Young Investigator Award, Research and Sponsored Programs (UTEP)

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

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

Selected Research Projects

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

Current Students and Post-doctoral Researchers:

Research Associates and Post-doctoral Researchers:

Travis Johnston, Post-doctoral Researcher

Visitor Scholar:

Tai Gao, NUDT, China.

Graduate Students:

Stephen Herbein, PhD Student

Sean McDaniel, PhD Student

Michael Wyatt, PhD Student

Dylan Chapp, MS Student

Undergraduate Students:

Ryan McKenna

Connor Zanin

Thesis:

PhD Thesis:

Boyu Zhang - *PhD Thesis*, Computer Science, UD, Spring 2015, "Enabling Scalable Data Analysis for Large Computational Structural Biology Datasets on Large Distributed Memory Systems supported by the MapReduce Paradigm." First position: Big Data analyst at Purdue University.

Trilce Estrada – *PhD Thesis*, Computer Science, UD, Spring 2012, "On the Effectiveness of Application-aware Self-management for Scientific Discovery on Volunteer Computing System". First position: assistant professor in Computer Science, University of New Mexico.

Master Thesis:

Abel Licon – *MS Thesis*, Computer Science, UD, Spring 2010, "RNAVLab 2.0: Combining Web Applications, Grid Computing, and Dynamic Programming to Overcome Resource Limitations in RNA Secondary Structure Analysis." First position: Thermo Fisher Scientific, Lafayette, Colorado.

David Flores - *MS Thesis*, Computer Science, UTEP, Spring 2007, co-advised with Dr. Patricia J. Teller (UTEP), "SimBA: A Discrete-event Simulator for Performance Prediction of Volunteer Computing Projects." First position: Ximis, El Paso, Texas.

Richard Zamudio - *MS Thesis*, Computer Science, UTEP, Fall 2006, "TOPAZ: A Firefox Protocol Extension for GridFTP." First position: Rockwell Collins, Iowa. *Outstanding Thesis in Computer Science 2006-2007.*

Senior Thesis:

Ryan McKenna – *Senior UG Thesis*, Computer Science, UD, expected graduation Spring 2016, "Predicting Performance Variability in Parallel File Systems."

Connor Zanin – *Senior UG Thesis*, Computer Science, UD, expected graduation Spring 2016, "Tuning MapReduce with Surrogate-Based Modeling."

Stephen Herbein – *Senior UG Thesis*, Computer Science, UD, graduated in Spring 2014, "Benchmarking and Auto-tuning I/O Intensive Applications at the Extreme Scale." First position: graduate student at U. Delaware.

Philip Saponaro – *Senior UG Thesis*, Computer Science, UD, Spring 2010, "An Efficient Arbitrary Precision Mathematical Library for Accurate and Fast MD Simulations in Single Precision GPUs." First position: graduate student at U. Delaware.

Graduate Committees:

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

Teaching Activities

Courses:

CISC 360 – Computer Architecture (Undergraduate course): Fall 2009, Fall 2008

CISC 361 – Operating Systems (Undergraduate course): Fall 2015, Spring 2015, Spring 2013, Spring 2010

CISC 662 – Computer System: Architecture (Graduate course): Fall 2012, Fall 2011, Fall 2010, Fall 2009, Fall 2008, Fall 2007

CISC 663 - Operating Systems (Graduate course): Spring 2015, Spring 2013, Spring 2012

CISC 849 – High Performance Parallel Algorithms for Computational Science (Graduate course): Spring 2011, Spring 2009

CISC 849 – Analysis of Bio. Simulations (Graduate course): Fall 2008

CISC 879 – Advanced Topics in Architecture and Software Systems: HPC and Data AnALyTICS: Fall 2015, Fall 2014

CS 3320 – Computer Architecture II: Advanced Computer Design and Implementation (Undergraduate course): Spring 2007, Fall 2006, Spring 2006, Fall 2005

CS 3335 – Systems Programming (Undergraduate course): Fall 2006

CS 5334 – Parallel and Concurrent Programming (Graduate course): Spring 2005, Spring 2006,

CS 5341 – Analysis and Modeling of Biological Structures (Graduate course – cross-listed with the Bioinformatics Program and the Chemistry Department): Spring 2007

Professional Services and Activities:

Editor 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.
2014 – present	Associate Editor, Journal of Parallel and Distributed Computing (JPDC), Elsevier.
2014	Associate 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:

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) – elected.
2014 – present	Steering Committee Member for the IEEE International Conference on Cluster Computing (Cluster).

Chair and Co-Chair (Selected Activities):

2016:

Area Chair for the "Performance" Track – International Conference on Parallel Processing (ICPP), March 2016, Philadelphia, PA, USA.

Workshop co-Chair for the 31st ISC High Performance Conference, June 19 – June 23, 2016, Frankfurt, Germany.

Area Chair for the "Multicore and Manycore Parallelism" Track – EuroPar, August 2016, Grenoble, France.

Panel Chair for the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2015. Salt Lake City, UT, USA.

2015:

Workshop Chair for the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2015. Austin, TX, USA.

General co-Chair for the IEEE International Conference on Cluster Computing 2015, September 2015, Chicago, IL, USA.

Technical Program co-Chair for the 24th International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 15-19, 2015, Portland, OR, USA.

2014:

Technical Program co-Chair for the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2014. New Orleans, LA, USA.

Area Chair for the "Cluster Design, Configuration and Administration" Track - IEEE International Conference

on Cluster Computing, September 2014, Madrid, Spain.

2013:

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

2012:

BoF Chair for the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2012, Salt Lake City, UT, USA.

2011:

Deputy BoF Chair for the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2011, Seattle, WA, USA.

2010:

Area Chair for "Distributed Systems and Applications" of the 12th IEEE International Conference on High Performance Computing and Communications (HPCC), September 2010, Melbourne, Australia.

Area co-Chair for 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.

2009:

Program vice-Chair for the topic "Distributed Systems and Applications" Track - 11th IEEE International Conference on High Performance Computing and Communications (HPCC), June 2009, Soul, South Korea.

Program Chair for the 8th IEEE International Workshop on High Performance Computational Biology (HiCOMB), May 2009, Rome, Italy.

2003:

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

Technical Committee of Peer-reviewed Conferences / Workshops / Symposiums / Scholarships:

2016:

Technical Program Committee for the 16th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing *(CCGrid), May 2016,* Cartagena, Colombia.

Technical Program Committee for the 6th International Workshop on Adaptive Self-tuning Computing Systems (ADAPT), January 2016, Prague, Czech Republic.

Technical Program Committee for the ACM International Conference on Computing Frontiers 2016, May 2016, Como, Italy.

2015:

Technical Program Committee for the 21th IEEE International Conference on Parallel and Distributed Systems (ICPADS), December 2015, Melbourne, Australia.

Technical Program Committee for the IA^3 2015: 5th Workshop on Irregular Applications: Architectures and Algorithms. November 2015. Austin, TX, USA.

Technical Program Committee for the EduHPC-15: Workshop on Education for High-Performance Computing. November 2015. Austin, TX, USA.

Technical Program Committee (Data Analytics and Visualization Track) for the IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2015.

Austin, TX, USA.

Technical Program Committee for 11nd IEEE International Conference on e-Science and Grid Technologies (eScience), August 2015, Munich, Germany.

Technical Program Committee for the 2014 ACM International Conference on Supercomputing (ICS), June 2015, Long Beach, USA.

Committee Member of the 2015 ACM/IEEE CS George Michael HPC Fellowship.

Technical Program Committee for the ACM Computing Frontiers (CF), May 2015, Ischia, Italy.

Technical Program Committee for Workshop and Tutorials at the 2015 Richard Tapia Celebration of Diversity in Computing Conference, Boston, MA, USA.

2014:

Technical Program Committee for the 13th IEEE International Conference on Ubiquitous Computing and Communications (IUCC) December 2014, Chengdu, China.

Technical Program Committee for 10nd IEEE International Conference on e-Science and Grid Technologies (eScience), October 2014, Guarujá, San Paulo, Brazil.

Technical Program Committee for the 2nd Workshop on Parallel and Distributed Agent-Based Simulations (PADABS), 25-29 August 2014, Porto, Portugal.

Technical Program Committee for the 2014 ACM International Conference on Supercomputing (ICS), June 2014, Munich, Germany.

Technical Program Committee for the 23nd International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2014, Vancouver, Canada.

Technical Program Committee for the ACM International Conference on Computing Frontiers 2014 (CF), May 2014, Cagliari, Italy.

Technical Program Committee for the 14th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid), May 2014, Chicago, USA.

2013:

Technical Program Committee of the 13th International Workshop on High Performance Computational Biology (HiCOMB), May 2013, Phoenix, Arizona, USA.

Technical Program Committee for the 6th IEEE/ACM International Conference on Utility and Cloud Computing (UCC), December 2013, Dresden, Germany.

Technical Paper Committee for the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2013, Denver, Colorado, USA.

Technical Program Committee for the 2013 IEEE International Conference on Big Data (IEEE Big Data 2013), October 6-9, 2013, Silicon Valley, CA, USA.

Technical Program Committee for the Workshop on Parallel Computational Biology (PBC), held in conjunction with PPAM 2013, September 8-11, 2013, Warsaw, Poland.

Technical Program Committee for the 1st Workshop on Parallel and Distributed Agent-Based Simulations (PADABS), August 2013, Aachen, Germany.

Technical Program Committee of the 22nd International Symposium on High-Performance Parallel and Distributed Computing (HPDC), June 2013, New York, NY, USA.

Technical Program Committee for the 12th International Workshop on High Performance Computational Biology (HiCOMB), May 2013, Boston, MA, USA.

Technical Program Committee for the 13th IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid), May 2013, Delft, The Netherlands.

2012:

Technical Program Committee for the High Performance Computing Conference (HiPC), December 2012, Pune, India.

Doctoral Showcase Committee for the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2012, Salt Lake City, UT, USA.

Technical Paper Committee for the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2012, Salt Lake City, UT, USA.

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

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

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

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

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

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

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

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

Technical Program Committee for the Workshop Innovative Parallel Computing: Foundations and Applications of GPU, Many-core, and Heterogeneous Systems (InPar), May 2012, San Jose, CA, USA.

2011:

Technical Paper Committee for the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), November 2011, Seattle, WA, USA.

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

Technical Program Committee for the IEEE Cluster 2011 Conference (Cluster), September 26 – 30, 2011, Austin, TX, USA.

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

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

Technical Program Committee for the 2011 Symposium on Application Accelerators in High Performance Computing (SAAHPC), July 19 – 20, 2011, University of Tennessee Conference Center, TN, USA.

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

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

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

2010:

Technical Program Committee for the 2010 IEEE 6th International Conference on e-Science (eScience), December 7 – 10, 2010, Brisbane, Australia.

Technical Program Committee for the International Conference of Computer Design (ICCD), October 3-6, 2010, Amsterdam, The Netherlands.

Technical Program Committee for the 22nd International Symposium on Computer Architecture and High-Performance Computing (SBAC-PAD), October 2010, Petropolis, Brazil.

Technical Program Committee for the Workshop on Parallel Programming and Applications on Accelerator Clusters (PPAAC), September 2010, Heraklion, Greece.

Technical Program Committee for the 2010 Symposium on Application Accelerators in High Performance Computing (SAAHPC), July 13 – 15, 2010, University of Tennessee Conference Center, TN, USA.

Technical Program Committee for the 2010 ACM International Symposium on High Performance Distributed Computing (HPDC), June 2010, Chicago, IL, USA.

Technical Program Committee for the ACM Computing Frontiers Conference (CF), May 2010, Bertinoro, Italy.

Technical Program Committee for the 10th IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 2010, Melbourne, Australia.

Technical Program Committee for the Second Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2010, Melbourne, Australia.

Technical Program Committee for the 18th Euromicro Conference on Parallel, Distributed and Network-Based Processing (PDP), February 2010, Pisa, Italy.

2009:

Technical Program Committee for the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2009, Portland, OR, USA.

Technical Program Committee for the International Conference of Computer Design (ICCD), November 4 – 7, 2009, Lake Tahoe, CA, USA.

Scholarship Committee for the Grace Hopper Celebration of Women in Computing 2009, October 2009, Tucson, AZ, USA.

Technical Poster Committee for the 2009 IEEE International Conference on Cluster Computing (Cluster), August 29 – September 4, 2009, New Orleans, LA, USA.

Technical Program Committee for the 12th IEEE International Conference on Computational Science and Engineering (CSE), August 29 – 31, 2009, Vancouver, Canada.

Technical Program Committee for 9th IEEE International Symposium on Cluster Computing and Grid (CCGrid), May 2009, Shanghai, China.

Technical Program Committee for the Workshop on Using Emerging Parallel Architectures for Computational Science, held in conjunction with the ICCS 2009, May 2009, Baton Rouge, LA, USA.

Technical Program Committee for the Second Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2009, Rome, Italy.

Technical Program Committee for the 2009 Richard Tapia Celebration of Diversity in Computing Conference, April 2009, Portland, OR, USA.

Technical Program Committee for the 17th Euromicro Conference on Parallel, Distributed and Network-Based Processing (PDP), February 2009, Bauhaus-University Weimar in Thuringia, Germany.

2008:

Technical Program Committee for the Intl. Conference on Advanced Computing and Communications, December 2008, Chennai, India.

Technical Program Committee for the Computational Structural Bioinformatics Workshop 2008 November 2008, Philadelphia, PA, USA.

Technical Poster Committee for the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2008, Austin, TX, USA.

Scholarship Committee for the Grace Hopper Celebration of Women in Computing 2008, October 2008, Denver CO, USA.

Technical Program Committee for the IEEE Intl. Conference on Computer Design (ICCD), October 2008, Lake Tahoe, CA, USA.

Technical Program Committee for the 10th IEEE International Conference on High Performance Computing and Communications (HPCC), September 2008, DaLian, China.

Technical Program Committee for the International Conference on Computational Science (ICCS), June 2008, Krakow, Poland.

Technical Program Committee for the ACM Computing Frontiers (CF), May 2008, Ischia, Italy.

Technical Program Committee for the Global and Peer-to-Peer Computing (GP2PC), May 2008, Lyon, France.

Technical Program Committee for the 7th International Workshop on High Performance Computational Biology (HiCOMB), May 2008, Miami, FL, USA.

Technical Program Committee for the 9th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC), May 2008, Miami, FL, USA.

Technical Program Committee for the 2nd Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), May 2008, Miami, Florida, USA.

Technical Program Committee for the 22nd IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2008, Miami, FL, USA.

Technical Program Committee for the Euromicro Conference on Parallel, Distributed and Network based Processing (PDP) February 2008, Toulouse, France.

2007:

Technical Poster Committee for the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC). November 2007, Reno, NV, USA.

Technical Program Committee for the First Computational Structural Bioinformatics Workshop, November 2007, San Jose, CA, USA.

Technical Poster Committee for the 2007 Richard Tapia Celebration of Diversity in Computing Conference, October 2007, Orlando, FL, USA.

Scholarship Committee for the Grace Hopper Celebration of Women in Computing 2007, October 2007,

Orlando, FL, USA.

Technical Program Committee for the 5th IEEE International Symposium on Parallel and Distributed Processing and Applications (ISPA), August-September, 2007, Niagara Falls, Ontario, Canada.

Technical Program Committee for the International Conference on Computational Science 2007 (ICCS), May 2007, Beijing, China.

Technical Program Committee for the 6th International Workshop on Global and Peer-to-Peer Computing (GP2P), May 2007, Rio de Janeiro, Brazil.

Technical Program Committee for 26th IEEE International Performance Computing and Communications Conference (IPCCC), April 2007 - New Orleans, LA, USA.

Technical Program Committee for the First Workshop on Large-Scale, Volatile Desktop Grids (PCGrid), March 2007, Long Beach, CA, USA.

2006:

Technical Program Committee for the 4th IEEE International Symposium on Parallel and Distributed Processing and Applications (ISPA), December 2006, Sorrento, Italy.

Technical Program Committee for the 2nd IEEE International Conference on e-Science and Grid Technologies (eScience), December 2006, Amsterdam, The Netherlands.

Technical Program Committee for the 5th International Workshop on Global and Peer-to-Peer Computing (GP2P), May 2006, Singapore.

Technical Program Committee for the 20th IEEE International Parallel and Distributed Processing Symposium (IPDPS), April 2006, Rhodes, Greece.

Technical Program Committee for the 5th IEEE International Workshop on High Performance Computational Biology (HiCOMB), April 2006, Rhodes, Greece.

2005:

Technical Program Committee for the 1st IEEE International Conference on e-Science and Grid Technologies (eScience), December 2005, Melbourne, Australia.

Technical Program Committee for the 2005 IEEE International Conference on Cluster Computing (Cluster), September 2005, Boston, MA, USA.

Technical Program Committee for the 2005 International Conference on High Performance Computing and Communications (HPCC), September 2005, Sorrento, Italy.

Technical Program Committee for 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.

Selected Services to the University, College, and Department:

At UD:

2015 - 2016	Acting Director at Center for Bioinformatics & Computational Biology (CBCB)
2015 – present	Member of Faculty Recruitment Committee (ECE Department)
2015 – present	Acting Director at Center for Bioinformatics & Computational Biology (CBCB), Delaware Biotechnology Institute (DBI), Newark, DE, USA
2014 – present	Member of the Bioinformatics Steering Committee (Bioinformatics Program)
2014 – present	Faculty advisor of the Bioinformatics Student Association (Bioinformatics Program)
2007 – present	CIS coordinator of the CIS/ECE booth at the Supercomputing Conference (CIS Department)
2015	Member of the Undergraduate Committee (CIS Department)
2014 – 2015	Chair of Distinguished Speaker Series Committee (CIS Department)
2014	Chair of Faculty Recruitment Committee (CIS Department)
2012 – 2013	Member of the Biomedical Engineering Graduate Committee (BME Program)
2012 – 2013	Chair of Distinguished Speaker Series Committee (CIS Department)
2010	Leading Organizer of the CIS Research Day
2009 – 2013	Member of the Bioinformatics Program Committee (University Committee)
2009 – 2011	Member of the Research Computing Task Force (University Committee)
2009 – 2010	Member of the Graduate Recruiting Committee (CIS Department)
2008 – 2009	Member of the Graduate Committee (CIS Department)
2007 – 2009	Advisor for the student organization ACM Chapter (CIS Department)
2007 – 2008	Member of the Graduate Recruiting Committee (CIS Department)

At UTEP:

2006 – 2007	Member of the Bioinformatics Research Committee and Bioinformatics Colloquium Committee (University Committee)
2005 – 2007	Member of the High-End Computing Along the Rio Grande Consortium
2005 – 2007	Member of the Computer System Curriculum Committee and the Facilities Committee

2006   Member of the NSF-CSEMS Scholarship Committee at the University of Texas at El Paso, 2006

Professional Affiliations:

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