

Sally R. Ellingson
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Education:

PhD in Genome Science and Technology (GST)
Interdisciplinary Graduate Minor in Computational Science (IGMCS)
University of Tennessee, Knoxville (UTK) and Oak Ridge National Laboratory (ORNL)
May 2014 3.88 GPA

BS in Computer Science
BS in Mathematical Sciences
Florida Institute of Technology, Melbourne, FL
Graduated Summa Cum Laude
May 2009 3.96 GPA

Experience:

University of Kentucky, Lexington, KY 3/2014-present

- Assistant Professor, Division of Biomedical Informatics, UK College of Medicine
- Manager, High Performance Computing Services, Markey Cancer Center, Cancer Research Informatics Shared Resource Facility

Oak Ridge National Laboratory, Oak Ridge, TN 8/2010-2/2014

- Graduate Research Assistant at Center for Molecular Biophysics (CMB) under supervision of Dr. Jerome Baudry.

University of Tennessee, Knoxville, TN 5/2009 – 7/2010

- Graduate Research Assistant: Participate in research rotation projects under the supervision of faculty associated with GST

Florida Institute of Technology, Melbourne, FL 3/2005-5/2009

- Technical Editor for Nonlinear Analysis Journals (Elsevier)
- Train reviewers and editors to use the online editorial system.
- Create web applications with database connectivity for various projects in the Mathematical Sciences department.
- Organize conferences.

- Type research papers/monographs using Latex.

Organizations and Memberships:

- Phi Theta Kappa: Member
- Upsilon Pi Epsilon (UPE): Member and local chapter Vice-President (2007-2008)

Past

- American Chemical Society (ACS): Member
- Association for Computing Machinery (ACM): Member
- International Federation of Nonlinear Analysts (IFNA): Director

Honors, Fellowships, and Awards:

- KL2 Career Development Award sponsored by Center for Clinical and Translational Sciences (CCTS) and College of Medicine, University of Kentucky
- Travel grant to attend SIAM Computational Science and Engineering 2015
- Best Graduate Poster for Translational and Clinical Research at Markey Cancer Center Research Day May 2014
- Conference participation grant through the SC13 Broader Engagement (BE) Program to attend Supercomputing 2013
- Fall 2013 American Chemical Society Chemical Computing Group Research Excellence award
- 2013 Science Alliance graduate student award for outstanding efforts through UTK
- Co-PI High-throughput Docking in Undergraduate Curriculum (Awarded 70,000 CPU hours on Kraken Supercomputer)
- Conference participation grant through the SC12 Broader Engagement (BE) Program to attend Supercomputing 2012
- Neustar scholarship to attend the 2012 Grace Hopper Celebration of Women in Computing (GHC 2012)
- Conference sponsored scholarship to attend National Biomedical Computation Resource Summer Institute 2012.
- EU-US Summer School on HPC Challenges Participation Grant (XSEDE/Prace)
- Advanced track conference participation grant through the SC11 Broader Engagement (BE) Program to attend Supercomputing 2011
- NSF funded scholarship to attend Grace Hopper Celebration of Women in Computing (GHC 2011)
- Research poster accepted in ACM Student Research Competition at GHC 2011
- Invitation to attend Grad Cohort 2011 by Committee on the Status of Women in Computing Research (CRA-W)
- Conference participation grant through the SC10 Broader Engagement (BE) Program to attend Supercomputing 2010
- SCALE-IT (Scalable Computing and Leading Edge Innovative Technologies in Biology) (IGERT/NSF) graduate student training program 2009-2011
- Distinguished Student Scholar Award 2009
- Outstanding Senior Award in Mathematical Sciences 2009

- Outstanding Senior Award in Computer Science 2007
- National Dean's List 2006

Press:

- <https://www.nics.tennessee.edu/ellingson-polypharmacology>
- <http://tntoday.utk.edu/2014/06/24/ut-researchers-use-computers-for-drug-research/>
- NPR interview: <http://www.npr.org/2013/10/28/241371411/science-on-shaky-ground-as-automatic-budget-cutbacks-drag-on>
- <https://www.olcf.ornl.gov/2013/06/04/titan-user-recognized-by-the-american-chemical-society/>
- <http://tntoday.utk.edu/2013/05/10/graduate-student-receives-ac-s-award-drug-discovery-research/>

Teaching:

- Computational Biology and Bioinformatics (senior level biology class), teaching assistant
- High-Throughput Docking with Conformational Ensembles on Supercomputers (undergraduate biology workshop), curriculum development and lead teacher
- Introduction to Biology for Computational Researchers (graduate level computer science class), guest lecturer
- Structural Basis of Disease (senior level biology class), guest lecturer
- Algorithms in Computational Biology (graduate level computer science class), curriculum development

Conferences and Workshops:

- UT-ORNL-KBRIN Bioinformatics Summit April 2016, Cadiz, KY
- Association for Clinical and Translational Science (ACTS) Translational Science 2016, Washington DC (NIH Mock Study Section)
- Cancer Informatics for Cancer Centers (CI4CC), March 2016, Napa, CA
- Sustainable Research Pathways Fellows: Building Long Term Connections across Diverse Communities With Berkeley Lab's Computing Sciences, December 2015, Lawrence Berkeley National Laboratory (poster blitz and poster session)
- Supercomputing (SC15) November 2015 Austin, TX (Student Volunteer deputy chair, workshop poster and blitz)
- 2015 International Summer School on HPC Challenges in Computational Sciences, Toronto, Canada (returning participant, mentor)
- Markey Cancer Center Research Day May 2015 Lexington, KY (poster session)
- CCTS Spring Conference 2015, Lexington, KY (talk and poster evaluator)
- SIAM Computational Science and Engineering, March 2015, Salt Lake City, UT (organizing committee for Broader Engagement program, poster blitz, poster session, mentoring program)
- Cancer Genome Atlas (TCGA) 4th Annual Scientific Symposium, Washington, DC

- Association for Clinical and Translational Science (ACTS) Translational Science 2015, Washington DC (NIH Mock Study Section)
- Supercomputing (SC14) November 2014 New Orleans, LA (BE Housing Chair, mentoring program)
- Essentials of Next Generation Sequencing summer workshop July 21-25, 2014 at the University of Kentucky
- 3DSIG14 Structural Bioinformatics and Computational Biophysics July 2014 Boston, MA (poster session)
- UT-ORNL-KBRIN Bioinformatics Summit 2014 Cadiz, KY
- Markey Cancer Center Research Day May 2014 Lexington, KY (poster session/award)
- Supercomputing (SC13) November 2013 Denver, CO (Booth talk, Doctoral Showcase, BE Networking poster session, mentoring program)
- American Chemical Society (ACS) National Meeting September 2013 Indianapolis, IN (Chemical Computing Group excellence award poster session)
- Smoky Mountains Computational Sciences and Engineering Conference September 2013 Gatlinburg, TN (poster session)
- Argonne Training Program on Extreme-Scale Computing, July/Aug 2013, St. Charles, IL
- American Chemical Society (ACS) National Meeting April 2013 New Orleans, LA (Poster Session for Technical Program and Sci-Mix)
- Supercomputing (SC12) November 2012 Salt Lake City, UT (Communities Resource Fair)
- Grace Hopper Celebration of Women in Computing (GHC12) October 2012 Baltimore, MD (BOF session)
- Smoky Mountains Computational Sciences and Engineering Conference September 2012 Gatlinburg, TN (poster session)
- The 7th National Biomedical Computation Resource Summer Institute (NBCR-SI) July 30 – August 3, 2012 La Jolla, CA (poster session)
- 2012 European-U.S. Summer School on HPC Challenges in Computational Sciences (sponsored by PRACE and XSEDE) June 2012 Dublin, Ireland (electronic poster session)
- ACM High Performance Distributed Computing (HPDC12) June 2012 Delft, the Netherlands (workshop talk)
- From Computational Biophysics to Systems Biology (CBSB12) June 2012 Knoxville, TN (poster session)
- JICS/GRS Joint Workshop on Large Scale Computer Simulation April 2012 Oak Ridge National Laboratory Oak Ridge, TN (invited talk)
- Supercomputing (SC11) November 2011 Seattle, WA (Communities Resource Fair)
- Grace Hopper Celebration of Women in Computing (GHC11) November 2011 Portland, OR (ACM-SRC poster session)
- Tennessee Celebration of Women in Computing (TNWiC) October 2011 Pikeville, TN (poster session, talk, BOF session)
- Titan Summit August 2011 Oak Ridge National Laboratory
- ACM High Performance Distributed Computing (HPDC11) June 2011 San Jose, CA (workshop talk)
- CRA-W Grad Cohort 2011 Boston, MA (poster session)
- Supercomputing (SC10) November 2010 New Orleans, LA (Communities Resource Fair)

- SciApps – 10 Challenges and Opportunities for Scientific Applications: learning to sustain the Petaflop with eyes on the Exaflop horizon August 2010 Oak Ridge National Laboratory
- Summer School in Biophysics at ORNL: Computational and Experimental Challenges July 2010 Knoxville, TN
- ACM High Performance Distributed Computing (HPDC10) June 2010 Chicago, IL
- NSF IGERT Project Meeting May 2010 Washington, DC (poster session)
- UT-ORNL-KBRIN Bioinformatics Summit March 2010 Cadiz, KY (poster session)
- Summer School in Biophysics at ORNL: Computational and Experimental Challenges August 2009 Knoxville, TN
- NCUWM: Nebraska Conference for Undergraduate Women in Mathematics February 2008 University of Nebraska
- OurCS: Opportunities for Undergraduate Research in Computer Science October 2007 Carnegie Mellon University. Participated in “A Multi-Robot Choreography: Perception, Cognition, Action, and Coordination” research group, <http://www.cs.cmu.edu/ourcs/presentations/veloso.html>.
- Elsevier Editors’ Conference May 2006 Montreal, Canada

Organized:

- Student Volunteer program at Supercomputing 2015 (Deputy Chair)
- Broader Engagement at SIAM Computational Science and Engineering 2015 (organizing committee)
- Broader Engagement program at Supercomputing 2014 (organizing committee)
- From Computational Biophysics to Systems Biology June 2012 Knoxville, TN (local organizing committee)
- WCNA 2008: Fifth World Congress of Nonlinear Analysts July 2008 Orlando, FL (approx. 1000 in attendance)
- International Conference on Hybrid Systems and Applications May 2006 University of Louisiana, Lafayette (approx. 100 in attendance)

Organized Sessions:

- Poster preparation and presentation tips, Poster Session Activity for Broader Engagement Participants at SIAM CSE 2015
- Are we there yet? Creating an Open Environment for Interdisciplinary Research, Birds of a Feather session at GHC12, October 2012.
- Challenges and Advantages of Interdisciplinary Research, Birds of a Feather Session at Tennessee Celebration of Women in Computing, October 2011.

Posters:

- Sally R. Ellingson. High Performance Computing at the Markey Cancer Center (Sustainable Research Pathways Fellows 2015)
- Sally R. Ellingson. Computational characterization of genomic analysis pipelines. (Woman in HPC workshop at Supercomputing)
- Jinpeng Liu, Tamas Gal, Sally Ellingson, Brent Hallahan, Nathan Vanderford, Michael Sheetz, Vikram Gazula, Dave Fardo, Heidi Weiss, Jinze Liu, Susanne Arnold, Chi Wang.

Exome-Sequencing Pipeline for Genomic Characterization of Lung Cancer in Appalachian Kentucky (Markey Cancer Research Day 2015)

- Sally R. Ellingson, Chi Wang, & Radhakrishnan Nagarajan. Convex-hull voting method on a large data set (SIAM CSE and Markey Cancer Center Research Day 2015)
- Tamas S. Gal, Sally R. Ellingson, Chi Wang, Jinpeng Liu, Stuart G. Jarrett, and John A. D’Orazio. Using large public data repositories to discover novel genetic mutations with prospective links to melanoma (KBRIN Bioinformatics Summit, Paris, TN and Markey Cancer Research Day 2015)
- Sally R. Ellingson, Yinglong Miao, Jeremy C. Smith, & Jerome Baudry. The Role Of Protein Dynamics In Computational Docking: Identifying Novel Binding Sites In The Cancer Drug Target Tyrosine-Protein Kinase Src (Markey Cancer Center Research Day and 3Dsig 2014)
- Sally R. Ellingson and Jerome Baudry. High-throughput Docking in Undergraduate Curriculum (Broader Engagement and HPC Educators Networking SC13 Denver, CO)
- Sally R. Ellingson, Jeremy C. Smith, and Jerome Baudry. Multi-Receptor High-Throughput Virtual Docking on Supercomputers with VinaMPI (2013 Smoky Mtn. Computational Sciences and Engineering Gatlinburg, TN and ACS National Meeting 2013 Indianapolis, IN)
- Sally R. Ellingson, Jeremy C. Smith, and Jerome Baudry. Acceleration of High-Throughput Molecular Docking for Novel Drug Discovery on Supercomputers (ACS National Meeting 2013 New Orleans, LA)
- Sally R. Ellingson, Jeremy C. Smith, and Jerome Baudry. Towards High-Throughput Virtual Docking with Multiple Receptor Conformations on High-Performance Computers (2012 Smoky Mtn. Computational Sciences and Engineering Gatlinburg, TN and Communities Resource Fair SC12 Salt Lake City, UT)
- Sally R. Ellingson and Jerome Baudry. High-throughput Virtual Molecular Docking on High-Performance Computers (CBSB12 Knoxville, TN and NBCR-SI 2012 La Jolla, CA).
- Sally R. Ellingson. High-Throughput Virtual Molecular Docking within the MapReduce Framework of Hadoop (ACM-SRC session at GHC11 Portland, OR and Communities Resource Fair SC11 Seattle, WA)
- Sally R. Ellingson and Jerome Baudry. Screening for potential novel drugs with the power of cloud computing (CRA-W Grad Cohort Boston, MA 2011 and Tennessee Celebration of Women in Computing 2011)
- Sally R. Ellingson and Jerome Baudry. Drug Discovery in a Cloud (Supercomputing New Orleans 2010 “Curriculum Resource Fair and Student Research Projects”).
- Sally Ellingson, Justin Vaughn, Albrecht von Arnim. Determining conserved peptide uORFs by evolutionary signature (GST Orientation Summer 2010).
- Justin N. Vaughn, Sally R. Ellingson, Bijoyita Roy, Byung-Hoon Kim, and Albrecht G. von Arnim. The evolution and mechanics of uORF-mediated translation repression in plants (Gordon Research Conference on Post-Transcriptional Regulation 2010).
- Jin Ha Hwang, Sally R. Ellingson, Won Gyu Choi, and Daniel M. Roberts. Functional analysis of NH₃ and H₂O transport of soybean nodulin 26 and regulation under conditions of flooding and hypoxia (The 21st North American Symbiotic Nitrogen Fixation Conference University of Missouri-Columbia 2010).

- Sally Ellingson, Joe Hughes, Dylan Storey, Rick Weber and Nathan VerBerkmoes. Development of Tools for the Automated Analysis of Spectra Generated by Tandem Mass Spec (Bioinformatics Summit 2010).
- Sally R Ellingson, Charles A Phillips, Randy Glenn, Douglas Swanson, Thomas Ha, Daniel Goldowitz and Michael A Langston. Serendipitous discoveries in microarray analysis (GST Spring Retreat 2010, Bioinformatics Summit 2010, and NSF IGERT Project Meeting 2010).

Talks:

- Computational Prediction of Adverse Drug Reactions at Systems Biology and Omics Integration seminar series at University of Kentucky, March 2016
- Detecting genomic structural variations using NGS data at Systems Biology and Omics Integration seminar series at University of Kentucky, August 2015
- Big Data Analytics: Parallelization of Algorithms for Precision Medicine at CCTS Spring Conference March 2015, Lexington, KY
- Scientific Workflow Solutions: Facilitating Bioinformatics Research at Systems Biology and Omics Integration seminar series at University of Kentucky, April 2014
- Adventures in Computational Biology at Markey Cancer Center, University of Kentucky, December 2013 (invited seminar)
- Leveraging the Power of the Fastest Supercomputers to Advance Drug Discovery at University of Tennessee Exhibitor Booth Supercomputing 2013
- Multi-Receptor High-Throughput Virtual Docking on Supercomputers with VinaMPI at Supercomputing 2013 Doctoral Showcase
- The future of drug discovery: Supercomputers as virtual laboratories at Using Bioinformatics Data and Tools to Engage Students in Problem Solving: A Curriculum Development Workshop at NIMBioS, Knoxville, TN (invited talk)
- Accelerating Virtual High-Throughput Ligand Docking: Screening One Million Compounds Using a Petascale Supercomputer at *HPDC12* workshop on Emerging Computational Methods in the Life Sciences
- Discovering Next Generation Pharmaceuticals: Acceleration of Virtual High-Throughput Molecular Docking at NSF IGERT Project Meeting 2012 (presented by Dr. Cynthia Peterson, PI SCALE-IT)
- Virtual high-throughput molecular docking at JICS/GRS Joint Workshop on Large Scale Computer Simulation April 2012
- Running Parallel Tracks: Family and Grad School at Tennessee Celebration of Women in Computing 2011
- High-Throughput Virtual Molecular Docking: Hadoop Implementation of AutoDock4 on a Private Cloud at *HPDC11* workshop on Emerging Computational Methods in the Life Sciences
- Using Digital Technologies in Research and Education at NSF IGERT Project Meeting 2010
- Homology modeling and molecular dynamics using MOE of Nodulin-like intrinsic protein 6 (NIP6;1) at GST colloquium Spring 2010

Publications:

- Xiaofei Zhang and Sally Ellingson. Computationally characterizing genomic pipelines and benchmarking results using GATK best practices on the high performance computing cluster at the University of Kentucky. Workshop on Biomedical and Bioinformatics Challenges for Computer Science (BBC2016) (submitted)
- Sally Ellingson and David Fardo. Automated quality control for genome wide association studies. Workshop on Biomedical and Bioinformatics Challenges for Computer Science (BBC2016) (submitted)
- Sarah E. Monsell, Charles Mock, David W. Fardo, Sarah Bertelsen, Nigel J. Cairns, Catherine M. Roe, Sally Ellingson, John C. Morris, Alison M. Goate, Walter A. Kukull. Genetic comparison of symptomatic and asymptomatic persons with Alzheimer disease neuropathology. *Neurology*. (submitted)
- Tamas S Gal, Sally R Ellingson, Chi Wang, Jinpeng Liu, Stuart G Jarrett and John A D'Orazio. Using large public data repositories to discover novel genetic mutations with prospective links to melanoma. *BMC Bioinformatics* 2015, 16(Suppl 15):P3 doi:10.1186/1471-2105-16-S15-P3 (abstract)
- Sally R. Ellingson, Chi Wang, and Radhakrishnan Nagarajan. Convex-hull voting method on a large data set. *BMC Bioinformatics* 2015, 16(Suppl 15):P2 doi:10.1186/1471-2105-16-S15-P2 (abstract).
- Peter T. Nelson, Wang-Xia Wang, Amanda B. Partch, Sarah E. Monsell, Otto Valladares, Sally R. Ellingson, Bernard R. Wilfred, Adam C. Naj, Li-San Wang, Walter A. Kukull, David W. Fardo. Reassessment of risk genotypes (GRN, TMEM106B, and ABCC9 variants) associated with hippocampal sclerosis of aging pathology. *Journal of Neuropathology and Experimental Neurology*, January 2015, Volume 74, Issue 1, p 75-84. doi: 10.1097/NEN.0000000000000151.
- Sally Ellingson, Yinglong Miao, Jerome Baudry, Jeremy Smith. Multi-Conformer Ensemble Docking to Difficult Protein Targets. *J. Physical Chemistry Part B. J. Phys. Chem. B*, 2015, 119 (3), pp 1026–1034. DOI: 10.1021/jp506511p
- *Sally R. Ellingson, Jeremy C. Smith, and Jerome Baudry. Polypharmacology and supercomputer-based docking: opportunities and challenges. *Molecular Simulations*. Volume 40, Issue 10-11, 2014. Special Issue: Recent Advances in Molecular Biology (***Co-Corresponding Author**)
- Sally R. Ellingson, Sivanesan Dakshanamurthy, Milton Brown, Jeremy C. Smith, and Jerome Baudry. (2014), Accelerating virtual high-throughput ligand docking: current technology and case study on a petascale supercomputer. *Concurrency Computat.: Pract. Exper.*, 26: 1268–1277. doi: 10.1002/cpe.3070
- Sally R. Ellingson, Jeremy C. Smith, and Jerome Baudry. VinaMPI: Facilitating Multiple Receptor High-Throughput Virtual Docking on High Performance (2013) Computers. *J. Comp. Chem*. Volume 34, Issue 25, pages 2212–2221, DOI: 10.1002/jcc.23367.
- Nicholas Be, James Thissen, Shea Gardner, Kevin McLoughlin, Viacheslav Fofanov, Heather Koshinsky, Sally Ellingson, Thomas Brettin, Paul Jackson, and Crystal Jaing. (2013) Detection of Bacillus anthracis DNA in Complex Soil and Air Samples Using Next-Generation Sequencing. *PLoS ONE* 8(9): e73455. doi:10.1371/journal.pone.0073455
- Sally R. Ellingson, Sivanesan Dakshanamurthy, Milton Brown, Jeremy C. Smith, and Jerome Baudry. 2012. Accelerating virtual high-throughput ligand docking: screening one million compounds using a petascale supercomputer. In *Proceedings of the 3rd*

international workshop on Emerging computational methods for the life sciences (ECMLS '12). ACM, New York, NY, USA, 33-38.
<http://doi.acm.org/10.1145/2483954.2483961>

- Sally R. Ellingson and Jerome Baudry. High-Throughput Virtual Molecular Docking with AutoDockCloud. *Concurrency and Computation: Practice and Experience*. DOI: 10.1002/cpe.2926.
- Justin N. Vaughn, Sally R. Ellingson, and Albrecht G. von Arnim. Known and novel post-transcriptional regulatory sequences are conserved across highly diverged plant lineages. *RNA*. March 2012 18: 368-384; Published in Advance January 11, 2012, doi:10.1261/rna.031179.111.
- Sally R. Ellingson and Jerome Baudry. High-Throughput Virtual Molecular Docking: Hadoop Implementation of AutoDock4 on a Private Cloud. In Proceedings of the second international workshop on Emerging computational methods for the life sciences (ECMLS '11). ACM, New York, NY, USA, 33-38. DOI=10.1145/1996023.1996028 <http://doi.acm.org/10.1145/1996023.1996028>.
- Jin Ha Hwang, Sally R. Ellingson, Daniel M. Roberts. Ammonia Permeability of the Soybean Nodulin 26 Channel *FEBS Letters* 22 October 2010 (Vol. 584, Issue 20, Pages 4339-4343, DOI: 10.1016/j.febslet.2010.09.033).
- Ellingson et al.: Development of tools for the automated analysis of spectra generated by tandem mass spectrometry. *BMC Bioinformatics* 2010 11(Suppl 4):P27. (abstract)
- Ellingson et al.: Serendipitous discoveries in microarray analysis. *BMC Bioinformatics* 2010 11(Suppl 4):P24. (abstract)

Reviewer:

- Parallel Computing (reviewer)
- Concurrency and Computation: Practice and Experience (reviewer)
- Interdisciplinary Sciences: Computational Life Sciences (reviewer)
- Computers in Biology and Medicine (co-reviewer)
- NCWIT Award for Aspirations in Computing (application reviewer)

Service:

- 3rd and 4th Grade Science Lab volunteer teacher at Farragut Intermediate School
- Volunteer Wiki note taker at GHC12
- Help host and guide high school students at Supercomputing 2010, New Orleans.
- Graduate student panel for 2010 summer Research Experience for Undergraduates, National Institute for Mathematical and Biological Synthesis (NIMBioS) Knoxville, TN.
- Student mentor for incoming GST students
- Student host for perspective students during GST Spring Retreat
- Computer Science Help Desk, freshman CS tutoring, and female CS outreach for Upsilon Pi Epsilon (UPE)
- Volunteer tutoring in Calculus, Statistics, Pre-Calculus, and College Algebra