Brian Y. Chen

Curriculum Vitae — April 2017
http://www.cse.lehigh.edu/ ∼chen

A. BIOGRAPHICAL INFORMATION

Business Address:
Packard Laboratory, Room 328
19 Memorial Drive West
Lehigh University
Bethlehem, PA, 18015

Business Contact: chen@cse.lehigh.edu
phone: (610)758-4085
fax: (610)758-4096

Educational History

Ph.D. in Computer Science, Rice University, Houston, TX May 2007
Thesis: "Geometry-Based Methods for Protein Function Annotation"
Advisor: Lydia E. Kavraki

M.S. in Computer Science, Rice University, Houston, TX May 2003
Thesis: "Structural Pattern Matching for the Functional Annotation of Proteins"
Advisor: Lydia E. Kavraki

B.A. in Mathematics and Computer Science, Rutgers University, Piscataway, NJ May 2000

Employment History / Professional Experience

Associate Professor, Dept. of Computer Science and Engineering, July 2016 - current
P.C. Rossin College of Engineering and Applied Science, Lehigh University
Bethlehem, PA

Assistant Professor, Dept. of Computer Science and Engineering, Aug 2010 - June 2016
P.C. Rossin College of Engineering and Applied Science, Lehigh University
Bethlehem, PA

Postdoctoral Research Scientist, Howard Hughes Medical Institute, Dec 2006 - July 2010
Center for Computational Biology and Bioinformatics, Dept. of Biochemistry
and Molecular Biophysics, Columbia University, New York, NY.
Research on the analysis of protein structure features affecting substrate specificity
Supervisor: Barry Honig

Research Assistant, Dept. of Computer Science, Rice University, Houston, TX. Aug 2000 - Dec 2006
Research on Geometry based methods for protein function annotation
Supervisor: Lydia Kavraki

Undergraduate Researcher, NSF Research Experiences for Undergraduates Summers 1999, 2000
DIMACS, Rutgers University, Piscataway, NJ
Research in Graph Theory (1999), and Rehabilitation Robotics (2000).
Supervisors: János Komlós (1999), William Craelius (2000)

Teaching Assistant, Young Scholars Program in Discrete Mathematics Summers 1997, 1998
DIMACS, Rutgers University, Piscataway, NJ
Lectured, graded, and supervised gifted and talented High school students in discrete mathematics and computer science.
Software Developer, Intellipro Inc. Fall 1997
Developed a Java applet for analyzing financial portfolios using quadratic optimization with linear constraints and Markowitz portfolio selection theory.

B. PUBLICATIONS AND CREATIVE ACTIVITIES

Refereed Journal Articles

1. Yijun Zhou, Xiao-Ping Li, Brian Y. Chen, and Nilgun E. Tumer "Ricin uses arginine 235 as an anchor residue to bind to P-proteins of the ribosomal stalk", *Scientific Reports*, 7:42912. doi:10.1038/srep42912 *Impact factor: 5.228*

2. Bridget E. Nolan**, Emily Levenson** and Brian Y. Chen "Influential Mutations in the SMAD4 Trimer Complex Can Be Detected from Disruptions of Electrostatic Complementarity" *Journal of Computational Biology* January 2017, 24(1): 68-78. doi:10.1089/cmb.2016.0162. *Impact factor: 1.564*

3. Ziyi Guo* and Brian Y. Chen "Conformational Sampling Reveals Amino Acids with a Steric Influence on Specificity", *Journal of Computational Biology*, 22(9), pp 861-875, 2016. *Impact factor: 1.564*

4. Brian Y. Chen "VASP-E: Specificity Annotation with a Volumetric Analysis of Electrostatic Isopotentials", *PLoS Computational Biology*, 10(8): e1003792. doi:10.1371/ journal. pcbi. 1003792, 2014. *Impact factor: 4.87*

5. Seth Blumenthal**, Yisheng Tang*, Wenjie Yang*, and Brian Y. Chen "Isolating Influential Regions of Electrostatic Focusing in Protein and DNA Structure", Invited to: *IEEE Transactions on Computational Biology and Bioinformatics*, (in press). *Impact factor: 1.66*

6. Brian G. Godshall**, Yisheng Tang*, Wenjie Yang*, and Brian Y. Chen "An aggregate analysis of many predicted structures to reduce errors in protein structure comparison caused by conformational flexibility", Invited to: *BMC Structural Biology*, (in press). *Impact factor: 2.48*

7. Brian Y. Chen and Soutir Bandyopadhyay. "Modeling Regionalized Volumetric Differences in Protein-Ligand Binding Cavities", Invited to: *Proteome Science*, doi:10.1186/1477-5956-10-S1-S6, 10(Suppl 1):S6, 2012. *Impact factor: 2.33*

8. Brian Y. Chen and Soutir Bandyopadhyay. "A Regionalizable Statistical Model of Intersecting Regions in Protein-Ligand Binding Cavities", Invited to: *Journal of Bioinformatics and Computational Biology*, doi: 10.1142/S0219720012420048, 2012.

9. Markus Fischer, Qiangfeng C. Zhang, Fabian Dey, Brian Y. Chen, Barry Honig, and Donald Petrey. "MarkUs: a Server to Navigate Sequence - Structure - Function Space", *Nucleic Acids Research*. doi:10.1093/nar/gkr468, pp. 1-5, 2011. *Impact factor: 7.836*

10. C. David Andersson, Brian Y. Chen, Anna Linusson. "Multivariate Assessment of Virtual Screening Experiments", *Journal of Chemometrics*. 24(11-12), pp. 757-67, 2010. *Impact factor: 1.377*

11. Brian Y. Chen and Barry Honig. "VASP: A Volumetric Analysis of Surface Properties Yields Insights into Protein-Ligand Binding Specificity", *PLOS Computational Biology*. 6(8): e1000881. doi:10.1371/journal.pcbi.1000881, 2010. *Impact factor: 5.759*

12. Drew H. Bryant, Mark Moll, Brian Y. Chen, Viacheslav Y. Fofanov, Lydia E. Kavraki. "Analysis of Substructural Variation in Families of Enzymatic Proteins with Applications to Protein Function Prediction", *BMC Bioinformatics*, vol. 11:242, 2010. *Impact factor: 3.44*

13. C. David Andersson, Brian Y. Chen, Anna Linusson. "Mapping of Ligand-Binding Cavities in Proteins", *PROTEINS: Structure, Function, and Bioinformatics*, vol. 78(6), pp. 1408-22, 2010. *Impact factor: 2.813*

14. David M. Kristensen, R. Matthew Ward, A. Martin Lisewski, Serkan Erdin, Brian Y. Chen, Viacheslav Y. Fofanov, Marek Kimmel, Lydia E. Kavraki, Olivier Lichtarge. "Prediction of Enzyme Function Based on 3D Templates of Evolutionarily Important Amino Acids", *BMC Bioinformatics*, vol. 9:17, 2008. *Impact factor: 3.44*

15. Brian Y. Chen, Drew H. Bryant, Viacheslav Y. Fofanov, David M. Kristensen, Amanda E. Cruess, Marek Kimmel, Olivier Lichtarge, Lydia E. Kavraki. "Cavity Scaling: Automated Refinement of cavity aware motifs in protein function prediction", **invited to** *Journal of Bioinformatics and Computational Biology*, vol. 5(2a), pp. 353-382, 2007.

16. Brian Y. Chen, Viacheslav Y. Fofanov, Drew H. Bryant, Bradley D. Dodson, David M. Kristensen, A. Martin Lisewski, Marek Kimmel, Olivier Lichtarge, Lydia E. Kavraki. "The MASH Pipeline for Protein Function Prediction and an Algorithm for the Geometric Refinement of 3D Motifs", **invited to** *Journal of Computational Biology*, vol. 14(6), pp. 791-816, 2007. *Impact factor: 1.694*

17. David M. Kristensen, Brian Y. Chen, Viacheslav Y. Fofanov, R. Matthew Ward, A. Martin Lisewski, Marek Kimmel, Lydia E. Kavraki. "Recurrent Use of Evolutionary Importance for Functional Annotation of Proteins Based on Local Structural Similarity", *Protein Science* vol. 15(6), pp. 1530-6, 2006. *Impact factor: 2.741*

18. Erion Plaku, Kostas E. Bekris, Brian Y. Chen, Andrew M. Ladd, Lydia E. Kavraki. "Sampling-Based Roadmap of Trees for Parallel Motion Planning", *IEEE Transactions on Robotics* vol. 21(4), pp. 587-608, 2005. *Impact factor: 1.763*

Articles in Refereed Conference Proceedings

19. Ziyi Guo* and Brian Y. Chen "A Map of Binding Cavity Conformations Reveals Differences in Binding Specificity", *Proceedings of the IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2016)*, accepted. Washington, DC, November 2015. *Oral presentation, acceptance rate for regular papers: 19%.*

20. Rachel Y. Okun** and Brian Y. Chen "A Statistical Model of Electrostatic Isopotential Variation in Serine Protease Binding Cavities" *Proceedings of the Computational Structural Bioinformatics Workshop (CSBW 2015)*, pp 1246-52. Washington DC, November 2015.

21. Ziyi Guo* and Brian Y. Chen "Predicting Protein-Ligand Binding Specificity Based on Ensemble Clustering" *Proceedings of the Computational Structural Bioinformatics Workshop (CSBW 2015)*, pp 1239-44. Washington DC, November 2015.

22. Ziyi Guo*, Juliana Hong***, Katya Scheinberg and Brian Y. Chen "Superposition of Protein Structures Using Electrostatic Isopotentials", *Proceedings of the IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2015)*, accepted. Washington, DC, November 2015. *Oral presentation, acceptance rate for regular papers: 19%*

23. Ziyi Guo* and Brian Y. Chen "Variational Bayesian Clustering on Protein Cavity Conformations for Detecting Influential Amino Acids", *Proceedings of the Computational Structural Bioinformatics Workshop (CSBW 2014)*, Newport Beach, CA, September 2014. *Oral presentation, acceptance rate: 87.5%*

24. Zachary A. Daniels**, Steven R. Stinson**, Shenchi Tian**, Evan Mulbry**, and Brian Y. Chen. "A gesture-based interface for the exploration and classification of protein binding cavities", invited to *Proceedings of the 2014 workshop on Mobile augmented reality and robotic technology-based systems (MARS 2014)*, pp 47-50. Bretton Woods, NH, June 2014.

25. Ziyi Guo*, Trevor Kuhlengel**, Steven Stinson**, Seth Blumenthal**, Soutir Bandyopadhyay and Brian Y. Chen. "A Flexible Volumetric Comparison of Protein Cavities can Reveal Patterns in Ligand Binding Specificity", *Proceedings of the 5th ACM Conference on Bioinformatics, Computational Biology and Biomedicine*

(BCB 2014), pp 445-454. Newport Beach, PA, September 2014. *Oral presentation, acceptance rate for regular papers: 22.4%*

26. Brian G. Godshall** and Brian Y. Chen. "Improving Accuracy in Binding Site Comparison with Homology Modeling", *Proceedings of the Computational Structural Bioinformatics Workshop (CSBW 2012)*. Philadelphia, PA, Oct 2012. *Oral presentation, acceptance rate for regular papers: 33%*

27. Brian Y. Chen and Debdas Paul*. "A Volumetric Method for Representing and Comparing Regions of Electrostatic Focusing in Molecular Structure", *Proceedings of the 3rd ACM Conference on Bioinformatics, Computational Biology and Biomedicine (BCB 2012)*, pp 242-249. Orlando, FL, October 2012. *Regular paper, oral presentation, acceptance rate for regular papers: 20.7%*

28. Ruobing Chen, Katya Scheinberg, and Brian Y. Chen. "Aligning Ligand Binding Cavities by Optimizing Superposed Volume", *Proceedings of the IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2012)*, pp 606-610. Philadelphia, PA, October 2012. *Full paper presented by Ruobing Chen, acceptance rate for full papers: 20%*

29. Brian Y. Chen and Soutir Bandyopadhyay. "VASP-S: A Volumetric Analysis and Statistical Model for Predicting Steric Influences on Protein-Ligand Binding Specificity", In *Proceedings of the IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2011)*, pp. 22-9. Atlanta, GA, November 2011. *Full paper, oral presentation, acceptance rate for full papers: 19.4%*

30. Brian Y. Chen and Soutir Bandyopadhyay. "A Statistical Model of Overlapping Volume in Ligand Binding Cavities", In *Proceedings of the Computational Structural Bioinformatics Workshop (CSBW 2011), at the IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2011)*, pp. 424-31. Atlanta, GA, November 2011. *Oral presentation, acceptance rate: 61.5%*

31. Viacheslav Y. Fofanov, Brian Y. Chen, Drew H. Bryant, Mark Moll, Olivier Lichtarge, Lydia E. Kavraki, Marek Kimmel. "A Statistical Model to Correct Systematic Bias Introduced by Algorithmic Thresholds in Protein Structural Comparison Algorithms." In *Proceedings of the Computational Structural Bioinformatics Workshop (CSBW 2008), at the IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2008)*. Philadelphia, PA, November 2008.

32. Brian Y. Chen, Drew H. Bryant, Amanda E. Cruess, Joseph H. Bylund, Viacheslav Y. Fofanov, David M. Kristensen, Marek Kimmel, Olivier Lichtarge, Lydia E. Kavraki. "Composite Motifs Integrating Multiple Protein Structures Increase Sensitivity For Function Prediction." In *Proceedings of the 2007 IEEE Computational Systems Bioinformatics Conference (CSB 2007)*. pp. 343-55. San Diego, CA, August 2007. *Full paper presented as poster, acceptance rate for all full papers: 22%*

33. Brian Y. Chen, Drew H. Bryant, Viacheslav Y. Fofanov, David M. Kristensen, Amanda E. Cruess, Marek Kimmel, Olivier Lichtarge, Lydia E. Kavraki. "Cavity-Aware Motifs Reduce False Positives in Protein Function Prediction" In *Proceedings of the 2006 IEEE Computational Systems Bioinformatics Conference (CSB 2006)*. pp 311-23. Stanford, CA, August 2006. *Oral presentation, acceptance rate for full papers: 19.2%*

34. Brian Y. Chen, Viacheslav Y. Fofanov, Drew H. Bryant, Bradley D. Dodson, David M. Kristensen, A. Martin Lisewski, Marek Kimmel, Olivier Lichtarge, Lydia E. Kavraki, "Geometric Sieving: Automated Distributed Optimization of 3D-Motifs for Protein Function Prediction" In *Proceedings of International Conference on Research in Computational Molecular Biology (RECOMB 2006)*. Springer-Verlag, editors Alberto Apostolico, et al., pp. 500-15, Venice, Italy, April 2006. *Oral presentation; acceptance rate: 18%*

35. Brian Y. Chen, Viacheslav Y. Fofanov, David M. Kristensen, Marek Kimmel, Olivier Lichtarge, Lydia E. Kavraki, "Algorithms for Structural Comparison and Statistical Analysis of 3D Protein Motifs" In *Proceedings of the Pacific Symposium on Biocomputing (PSB 2005)*, New Jersey, USA. World Scientific, editors Russ B. Altman et al., pp. 334-45, Big Island, HI, January 2005. *Oral presentation; acceptance rate for full papers: 30%*

36. Kostas E. Bekris, Brian Y. Chen, Andrew M. Ladd, Erion Plaku, Lydia E. Kavraki, "Multiple Query Probabilistic Roadmap Planning Using Single Query Planning Primitives," In *2003 IEEE/RJS International Conference on Intelligent Robots and Systems (IROS 2003)*, pp. 656-661. Las Vegas, NV, 2003. *acceptance rate: 60%*

37. Mert Akinc, Kostas E. Bekris, Brian Y. Chan, Andrew M. Ladd, Erion Plaku, Lydia E. Kavraki, "Probabilistic Roadmaps of Trees for Parallel Computation of Multiple Query Roadmaps." **invited to:** *Eleventh International Symposium of Robotics Research (ISRR 2003)*. Springer-Verlag, Springer Tracts in Advanced Robotics (STAR), editors D. Paolo and R. Chatila, vol. 15, pp. 80-89, Siena, Italy, 2003.

Invited Book Chapters

38. Ziyi Guo* and Brian Y. Chen "Predicting Small Molecule Substrate Specificity for Protein Function Annotation", *Handbook of Computational Molecular Biology*, submitted, 2015.

39. Ruobing Chen, Ziyi Guo*, Brian Y. Chen and Katya Scheinberg. "Methodologies and Software for Derivative-free Optimization", *Optimization Methods in Engineering*, submitted, 2014.

C. HONORS AND AWARDS

1. Lutron Spira Teaching Award, 2014, $2000.

2. Faculty Recognition by Peer Mentors Program, 2014. Two faculty members from each college are selected in recognition of their commitment to educating students with disabilities.

3. P.C. Rossin Assistant Professorship, 2012, $20,000.

4. Sigma Xi, full member, 2011.

5. First Place, W.M. Keck Undergraduate Research Training Program, Research Symposium Poster Contest 2004, with mentees Anand Dharan and Drew Bryant.

D. RESEARCH FUNDING AND TRAINING GRANTS

Competitively awarded research grants

1. B.Y. Chen (PI) and Katya Scheinberg (Co-PI) "AF: Small: Volumetric Alignment of Protein Cavities for the Analysis of Ligand Binding Specificity". 1/2014-12/2016. Algorithmic Foundations Program, Division of Computer and Communication Foundations, National Science Foundation. $445,000.00. Award Number: 1320137. Supplemented three times with REU funding: 6/16/2015, $8,000, 2/19/2014, $8,000, 3/24/17, $8,000.

Competitively awarded training grants

1. Predoctoral Fellowship supported by The WM Keck Center for Computational and Structural Biology via funding from the National Library of Medicine, an institute of the National Institutes of Health. Calendar year 2004, competitively renewed 2005, 2006. Total Award: $93,988.00.

Institutional/Equipment Grants

1. "Atom Independent Alignment for the Volumetric Comparison of Protein Binding Pockets by Optimization", Internal Lehigh Faculty Innovation Grant (FIG), $24,480, 2011-2012, Katya Scheinberg (PI) and Brian Y. Chen (Co-PI).

2. Co-PI: "Computer Science and Engineering Undergraduate Sandbox Lab Upgrade". Submitted to P.C. Rossin College of Engineering and Applied Science, $66,000, December 2010, Collaborators: B. Chen, B. Hodgson, H. Korth, D. Lopresti, M. Spear, and J. Spletzer.

E. EDITOR/EDITORIAL REVIEW BOARD MEMBERSHIPS

1. Associate Editor, International Journal of Data Mining and Bioinformatics.
2. Guest Editor, Special Issue, Journal of Computational Biology 2016.
3. Guest Editor, Special Issue, Journal of Computational Biology 2015.
4. Guest Editor, Special Issue, BMC Structural Biology 2013.
5. Guest Editor, Special Issue, Journal of Bioinformatics and Computational Biology (JBCB) 2012.

F. SCHOLARLY PRESENTATIONS

Invited presentations

1. "Algorithms for discovering mutations that alter binding specificity." American Chemical Society, National Meeting, August 20-24 2017, Washington, DC.
2. "Computational detection of steric and electrostatic influences on protein binding specificity." American Chemical Society, Northeast Regional Meeting, October 5-8, 2016, Binghamton, NY.
3. "A system for the volumetric analysis of protein structure", Department of Computer Science, Rutgers University, Piscataway, NJ, Spring 2014.
4. "Volumetric and Electrostatic Dissection of Protein-Ligand and Protein-Protein Interactions", Department of Biomedical Engineering, Rutgers University, Piscataway, NJ, Spring 2014.
5. "Automatically Detecting Influences on Protein Binding Specificity", Center for Bioinformatics and Computational Biology, University of Delaware, Newark, DE, November 26, 2012.
6. "Deconstructing the Molecular World", Genomic Informatics Center, Hankyong National University, Korea, May 15, 2012.
7. "Geometric and Statistical Techniques for Predicting Structural Influences on Protein-Ligand Binding Specificity", Departmental Colloquium, Dept. of Computer Science, Texas A&M, College Station, TX, March 5, 2012.
8. "Comparing Solid Representations of Protein Cavities to Reveal Influences on Protein-Ligand Binding Specificity", Minisymposium on Geometry in Macromolecular Modeling, SIAM Conference on Geometric and Physical Modeling, Orlando, FL, October 25, 2011.
9. "An Algorithm for Discovering Steric Influences on Protein-Ligand Binding Specificity", Departmental Colloquium, Dept. of Computer Science, George Mason University, Fairfax, VA, October 11, 2011.
10. "A Quantitative Universe", Sigma Xi Lecture Series, Lehigh University Chapter, Bethlehem, PA, January 21, 2011.
11. "Volume-based Analysis of Protein Cavties", Dept. of Computer Science, Rice University, Houston, TX, October 25, 2010.
12. "Volumetric Dissection of Protein Functional Sites", Departmental Colloquium, Dept. of Computer Science, Hunter College of The City University of New York, New York, NY, Apr 9, 2010.
13. "Volumetric Dissection of Protein Functional Sites", Institute Colloquium, Toyota Technological Institute, Chicago, IL, Apr 1, 2010.
14. "Geometric Analyses of Protein Structure, Function and Specificity", Departmental Colloquium, Dept. of Computer Science, University of Massachusetts Boston, Boston, MA, Mar 11, 2009.
15. "Geometric Refinement of Active Site Motifs for Improved Annotation of Protein Function", 2006 NLM Informatics Training Meeting, Vanderbilt University, Nashville, TN. June 27-28, 2006.

16. "Geometric Pattern Matching for Biological Problems", John P. McGovern Town Meeting on Biocomputing and Imaging, Texas Medical Center, Houston, TX. March 2, 2005.

Refereed presentations

1. "A Flexible Volumetric Comparison of Protein Cavities can Reveal Patterns in Ligand Binding Specificity", ACM Conference on Bioinformatics, Computational Biology and Biomedicine (BCB 2014), Newport Beach, CA, September, 2014.
2. "A Volumetric Method for Representing and Comparing Regions of Electrostatic Focusing in Molecular Structure", ACM Conference on Bioinformatics, Computational Biology and Biomedicine (BCB 2012), Orlando, FL, October 7, 2012.
3. "Improving Accuracy in Binding Site Comparison with Homology Modeling", Computational Structural Bioinformatics Workshop (CSBW 2012), Philadelphia, PA, October 5, 2012.
4. "VASP-S: A Volumetric Analysis and Statistical Model for Predicting Steric Influences on Protein-Ligand Binding Specificity", IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2011), Atlanta, GA, November 12, 2011.
5. "A Statistical Model of Overlapping Volume in Ligand Binding Cavities", Computational Structural Bioinformatics Workshop (CSBW 2011), Atlanta, GA, November 11, 2011.
6. "Composite Motifs Integrating Multiple Protein Structures Increase Sensitivity for Function Prediction", 2007 IEEE Computational Systems Bioinformatics Conference (CSB 2007), UC San Diego, San Diego, CA. August 13-17, 2007.
7. "Cavity-Aware Motifs Reduce False Positives in Protein Function Prediction", 2006 IEEE Computational Systems Bioinformatics Conference (CSB 2006), Stanford University, Palo Alto, CA. August 14-18, 2006.
8. "Geometric Sieving: Automated Distributed Optimization of 3D-Motifs for Protein Function Prediction", International Conference on Research in Computational Molecular Biology (RECOMB 2006), April 4, 2006.
9. "Optimizing 3D-Motifs for Protein Function Prediction", Houston Society for Engineering in Medicine and Biology (HSEMB 2006), February 9, 2006.
10. "Geometric and Statistical Analysis of 3D Protein Substructures using Match Augmentation", DIMACS Workshop on Information Processing by Protein Structures, June 23, 2005.
11. "Algorithms for Structural Comparison and Statistical Analysis of 3D Protein Motifs", Pacific Symposium for Biocomputing (PSB 2005), January 5, 2005.
12. "Structural Pattern Matching for Functional Annotation of Proteins", Houston Society for Engineering in Medicine and Biology (HSEMB 2003), April 3, 2003.

Chaired sessions

1. Session Chair, Computational Structural Bioinformatics Workshop (CSBW) 2014, 2013, 2012, 2011.
2. Session Chair, ACM Conference on Bioinformatics, Computational Biology and Biomedicine (BCB) Newport Beach, September 20, 2014.
3. Session Chair, ACM Conference on Bioinformatics, Computational Biology and Biomedicine (BCB) Orlando, FL, October 7, 2012.
4. Session Chair, IEEE International Conference on Bioinformatics and Biomedicine (BIBM) Philadelphia, PA, October 4, 2012.
5. Session Chair, Lehigh High Performance Computing Symposium 2013, 2012, 2011. Invited, hosted, and introduced 12 external speakers over three years.

G. TEACHING AND RESEARCH ADVISING

Courses Taught

Summary: 24 courses (graduate and undergraduate) for 847 students completed at Lehigh. Teaching effectiveness averaged 4.16/5.00, course quality averaged 4.24/5.00, and student learning averaged 4.44. College-wide, teaching effectiveness averaged 4.20, course quality averaged 4.22, and student learning averaged 4.22 over the same period.

1. Fall 2016: **Structural Bioinformatics (BioE/CSE 307/407)** three lectures per week, 10 enrolled in the course. *Students evaluated teaching effectiveness as 4.13/5.0 versus a college average of 4.18. Students evaluated course quality as 4.13/5.0 versus a college average of 4.22. Students evaluated overall learning as 4.13/5.0 versus a college average of 4.2.*

2. Fall 2016: **Foundations of Programming (CSE 2)** Two lectures and one laboratory session per week, 65 enrolled in my section of the course. *Students evaluated teaching effectiveness as 4.37/5.0 versus a college average of 4.18. Students evaluated course quality as 4.38/5.0 versus a college average of 4.22. Students evaluated overall learning as 4.5/5.0 versus a college average of 4.2.*

3. Spring 2016: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)** three lectures per week, 10 enrolled in the course. *Students evaluated teaching effectiveness as 4.43/5.0 versus a college average of 4.25. Students evaluated course quality as 4.43/5.0 versus a college average of 4.28. Students evaluated overall learning as 4.43/5.0 versus a college average of 4.27.*

4. Spring 2016: **Foundations of Programming (CSE 2)** Two lectures and one laboratory session per week, 61 enrolled in my 2 sections of the course. *Students evaluated teaching effectiveness as 4.21/5.0 versus a college average of 4.25. Students evaluated course quality as 4.19/5.0 versus a college average of 4.28. Students evaluated overall learning as 4.54/5.0 versus a college average of 4.27.*

5. Fall 2015: **Structural Bioinformatics (BioE/CSE 307/407)** three lectures per week, 4 enrolled in the course. *Students evaluated teaching effectiveness as 5.0/5.0 versus a college average of 4.18. Students evaluated course quality as 5.0/5.0 versus a college average of 4.22. Students evaluated overall learning as 5.0/5.0 versus a college average of 4.22.*

6. Fall 2015: **Foundations of Programming (CSE 2)** Two lectures and one laboratory session per week, 83 enrolled in my 2 sections of the course. *Students evaluated teaching effectiveness as 4.28/5.0 versus a college average of 4.18. Students evaluated course quality as 4.375/5.0 versus a college average of 4.22. Students evaluated overall learning as 4.56/5.0 versus a college average of 4.22.*

7. Spring 2015: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)** three lectures per week, 10 enrolled in the course. *Students evaluated teaching effectiveness as 4.8/5.0 versus a college average of 4.23. Students evaluated course quality as 4.8/5.0 versus a college average of 4.26. Students evaluated overall learning as 4.8/5.0 versus a college average of 4.28.*

8. Spring 2015: **Foundations of Programming (CSE 2)** Two lectures and one laboratory session per week, 116 enrolled in my 3 sections of the course. *Students evaluated teaching effectiveness as 3.91/5.0 versus a college average of 4.23. Students evaluated course quality as 3.93/5.0 versus a college average of 4.26. Students evaluated overall learning as 4.49/5.0 versus a college average of 4.28.*

9. Fall 2014: **Structural Bioinformatics (CSE 307/407)** three lectures per week, 9 enrolled in the course. *Students evaluated teaching effectiveness as 4.00/5.0 versus a college average of 4.07. Students evaluated course quality as 4.00/5.0 versus a college average of 4.15. Students evaluated overall learning as 3.78/5.0 versus a college average of 4.15.*

10. Fall 2014: **Foundations of Programming (CSE 2)** Two lectures and one laboratory session per week, 162 enrolled in my 3 sections the course. *Students evaluated teaching effectiveness as 3.53/5.0 versus a college average of 4.07. Students evaluated course quality as 3.92/5.0 versus a college average of 4.15. Students evaluated overall learning as 4.46/5.0 versus a college average of 4.15.*

11. Spring 2014: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)** three lectures per week, 11 enrolled in the course. *Students evaluated teaching effectiveness as 4.82/5.0 versus a college average of 4.26. Students evaluated course quality as 4.82/5.0 versus a college average of 4.26. Students evaluated overall learning as 4.64/5.0 versus a college average of 4.26.*

12. Spring 2014: **Foundations of Programming (CSE 2)** Two lectures and one laboratory session per week, 149 enrolled in my 2 sections the course. *Students evaluated teaching effectiveness as 4.01/5.0 versus a college average of 4.26. Students evaluated course quality as 4.12/5.0 versus a college average of 4.26. Students evaluated overall learning as 4.31/5.0 versus a college average of 4.26.*

13. Fall 2013: **Foundations of Programming (CSE 2)** Two lectures and one laboratory session per week, 147 students enrolled in my 2 sections of the course. *Students evaluated teaching effectiveness as 3.89/5.0 versus a college average of 4.17. Students evaluated course quality as 4.03/5.0 versus a college average of 4.18. Students evaluated overall learning as 4.27/5.0 versus a college average of 4.17.*

14. Fall 2013: **Structural Bioinformatics (CSE 307/407)**. Tri-weekly lectures, 18 students enrolled in my course. *Students evaluated teaching effectiveness as 4.73/5.0 versus a college average of 4.17. Students evaluated course quality as 4.73/5.0 versus a college average of 4.18. Students evaluated overall learning as 4.67/5.0 versus a college average of 4.17.*

15. Fall 2013: **Bioinformatics in 21st Century. (BioS/CSE 090)**. Weekly lectures, 11 students enrolled in my course. *Students evaluated teaching effectiveness as 4.71/5.0 versus a college average of 4.17. Students evaluated course quality as 4.43/5.0 versus a college average of 4.18. Students evaluated overall learning as 4.14/5.0 versus a college average of 4.17.*

16. Spring 2013: **Foundations of Programming (CSE 2)** Two lectures and one laboratory session per week, 106 students enrolled in my 2 sections of the course. *Students evaluated teaching effectiveness as 4.38/5.0 versus a college average of 4.31. Students evaluated course quality as 4.54/5.0 versus a college average of 4.32. Students evaluated overall learning as 4.43/5.0 versus a college average of 4.28.*

17. Spring 2013: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)**. Bi-weekly lectures, 10 students enrolled in the course. *Students evaluated teaching effectiveness as 4.6/5.0 versus a college average of 4.31. Students evaluated course quality as 4.5/5.0 versus a college average of 4.22. Students evaluated overall learning as 4.6/5.0 versus a college average of 4.28.*

18. Fall 2012: **Foundations of Programming (CSE 2)** Two lectures and one laboratory session per week, 58 students enrolled in my section of the course. *Students evaluated teaching effectiveness as 4.63/5.0 versus a college average of 4.25. Students evaluated course quality as 4.62/5.0 versus a college average of 4.26. Students evaluated overall learning as 4.62/5.0 versus a college average of 4.21.*

19. Fall 2012: **Structural Bioinformatics (CSE 397/497)**. Bi-weekly lectures, 11 students. *Students evaluated teaching effectiveness as 4.46/5.0 versus a college average of 4.25. Students evaluated course quality as 4.36/5.0 versus a college average of 4.26. Students evaluated overall learning as 4.18/5.0 versus a college average of 4.21.*

20. Spring 2012: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)**. Bi-weekly lectures, 5 students enrolled in my section of the course. *Students evaluated teaching effectiveness as 4.5/5.0 versus a college average of 4.34. Students evaluated course quality as 4.5/5.0 versus a college average of 4.35. Students evaluated overall learning as 4.5/5.0 versus a college average of 4.32.*

21. Fall 2011: **Bioinformatics in 21st Century. (BioS/CSE 090)**. Weekly lectures, 18 students. *Students evaluated teaching effectiveness as 4.38/5.0, versus a college average of 4.17. Students evaluated course quality as 4.19/5.0 versus a college average of 4.19. Students evaluated overall learning as 4.0/5.0 versus a college average of 4.17.*

22. Fall 2011: **Structural Bioinformatics (CSE 397/497).** Bi-weekly lectures, 9 students. *Students evaluated teaching effectiveness as 4.63/5.0 versus a college average of 4.17. Students evaluated course quality as 4.75/5.0 versus a college average of 4.19. Students evaluated overall learning as 4.5/5.0 versus a college average of 4.17.*

23. Spring 2011: **Bioinformatics: Issues and Algorithms (CSE 308/408)**. Bi-weekly lectures, 10 students. *Students evaluated teaching effectiveness as 4.88/5.0 versus a college average of 4.28. Students evaluated course quality as 5.00/5.0 versus a college average of 4.29. Students evaluated overall learning as 4.63/5.0 versus a college average of 4.23.*

24. Fall 2010: **Structural Bioinformatics (CSE 350/450).** Bi-weekly lectures, 3 students. *Students evaluated teaching effectiveness as 4.50/5.0 versus a college average of 4.17. Students evaluated course quality as 4.00/5.0 versus a college average of 4.20. Students evaluated overall learning as 4.5/5.0 versus a college average of 4.19.*

Advising, Research Direction: Doctoral Students, Lehigh University

1. Debdas Paul, Fall 2011-Spring 2012, "Electrostatic Focusing and Protein Binding Specificity".
2. Ziyi Guo, Fall 2012-ongoing, "Mitigating Conformational Flexibility in Protein Structure Comparison".
3. Jinbu Wang, Fall 2014-ongoing, "Structural Immunoinformatics".

Advising, Research Direction: Masters Students, Lehigh University

1. Devan Bicher, CSE major, Fall 2013-ongoing, "Predicting Resistance in HIV Proteases".
2. Yisheng Tang, CSE major, Fall 2012-Summer 2013, "Statistical Modeling of Structural Variations in Protein Binding Sites".
3. Wenjie Yang, CSE major, Fall 2012-Summer 2013, "Surveys of Protein Cavities".
4. Kevin Dodd, CSE major, Fall 2013-Summer 2015, "Parallel Exact Constructive Solid Geometry on Molecular Surfaces".

Advising, Research Direction: Undergraduates Supervised, Lehigh University

1. Davis Rempe, Summer 2016, REU student "Multimarker Object Detection in Augmented Reality". **Student later admitted to Stanford PhD program**
2. Josiah Smith, Summer 2016, REU student "Multimarker Object Detection in Augmented Reality".
3. Georgi Georgiev, Summer 2015-ongoing, CSB major, "Parallelizing Constructive Solid Geometry Algorithms with Threading Building Blocks".
4. Jacob Parker, Fall 2013-Spring 2014, IDEAS major, "Applying Structural Bioinformatics to Materials Science".
5. Rachel Okun, Summer 2015-Spring 2016, IBE major, "Parameterized statistical models of electrostatic variation".
6. Chanh Nguyen, Fall 2013-ongoing, CSE major, "Javascript Visualization of Structural Bioinformatics Software Outputs".
7. Sara Grogan, Spring 2015-Spring 2016, BioE major, independent Study, "Electrostatic Analysis of Rescue Mutants in P53."
8. Emma Bird, Spring 2015-Spring 2015, BioE major, independent Study, "Selecting nucletides that control binding preferences in DNA."
9. Emily Levenson, Fall 2014-Spring 2016, BioE major, independent Study, "The Role of Electrostatics in SMAD4 trimer specificity."
10. Eric Metcalf, Fall 2013-Spring 2015, CSE major, independent Study, "Statistical Analysis of Protein Electrostatics."
11. Jonah Kohen, Spring 2013-Spring 2015, CompE major, independent Study, "Structural Analysis of Rescue Mutants in P53". **Now pursuing a masters at Stanford University**

12. Megan Lynch, Spring 2013-Summer 2015, BioE major, independent Study, "Analysis of specificity in the Major Histocompatibility Complex". **Student later admitted to University of Maryland PhD program in Genomics**

13. Kevin Dodd, Spring 2013-Fall 2013, Math major, independent Study, "Exact Solid Representations of Molecular Surfaces".

14. Devan Bicher, Summer 2012-Summer 2013, BioE major, BioE independent study, "Predicting Resistance in HIV Proteases", now a masters student in Lehigh CSE.

15. Bridget Nolan, Spring 2012-Spring 2015, BioE major, independent study, "Electrostatic influences on Protein-Protein Interfaces". **Now employed at Regeneron pharmaceuticals**

16. Kevin Lee, Spring 2012-Summer 2013, BioE major, independent study, "Structural Analysis of Major Histocompatibility Complexes", **Now pursuing a masters at Columbia University**

17. Steven Stinson, Fall 2011-Spring 2014, CSE major, independent study, "Structural Analysis of Major Histocompatibility Complexes". **Selected for poster presentations at the 2013 David and Lorraine Freed Undergraduate Research Symposium and the 2013 Academic Symposium. Student now a developer at Microsoft**

18. Trevor Kuhlengel, Spring-Summer 2012, CSE major, independent study, "Molecular Dynamics Simulation for Protein Structure Comparison", **now a research assistant at Pennsylvania State Medical Center.**

19. Brian G. Godshall, CSB major, Fall 2011-Spring 2012, independent study, "Modeling the impact of conformational variation in protein structure comparison", **winner, NSF Graduate Research Fellowship**, **Student won an NSF Graduate Research Fellowship based on this work**

20. Sean O'Keefe, BioE major, Summer 2011, summer research, "Volumetric Analysis of Protein Cavities".

21. David A. Stolfo, CSE major, Spring 2011, independent study, "Multitouch Interfaces for Structural Bioinformatics".

22. Seth N. Blumenthal, CSE major, Fall 2010-Fall 2012, independent study, multiple topics, now a software developer at Klish Group. **Selected for poster presentations at the 2012 David and Lorraine Freed Undergraduate Research Symposium**

Advising, Research Direction: Undergraduates Supervised, Rice University

1. Drew H. Bryant, summer 2004-fall 2006, completed a Ph.D. at Rice University, Dept. Computer Science, now a software developer at Google.

2. Joseph H. Bylund, summer 2005-spring 2006, now a Ph.D. student at Columbia University.

3. Anne E. Christian, summer 2002-spring 2004, now a consultant with Bain Management Consulting.

4. Amanda E. Cruess, summer 2005, now a developer at National Instruments.

5. Anand P. Dharan, summer 2004, currently an engagement manager at McKinsey and Company.

6. Brad D. Dodson, summer 2005, now a software developer at Microsoft.

7. Jessica Y. Wu, summer 2005, now a Ph.D. student at the Massachusetts Institute of Technology.

Advising, Undergraduate Senior Projects Supervised, Lehigh University

1. Jomille Averion and Charles Wallace, fall 2016, "An algorithm for aligning bone fragments by maximal volume overlap"

2. Steven Stinson and Zachary Daniels, fall 2013, "A Gesture-based Interface for Interacting with Protein Cavities."

3. Frank J. Kriete and David A. Stolfo, fall 2010, "vaspMT: A Multitouch Interface for Protein Geometry Analysis," **Peer's choice winner of CSE Senior Project Poster Session**.

Advising, Other than Research Direction, Undergraduates, Lehigh University

1. 5 undergraduate CSE majors in the classes of 2016-7.
2. 6 undergraduate CSE majors in the class of 2014.
3. 1 undergraduate CSE major in the class of 2015.

H. SERVICE

University Service

University Level Service

1. Lehigh High Performance Computing Symposium, General Chair (2012), Co-Chair (2013) Personally coordinated logistical, promotional, financial, and speaker planning for Lehigh's annual HPC Symposium, with 75+ attendees.
2. Staff Search committee for HPC Support Specialist Fall 2011. Assisted in screening, interviewing, and selecting applications for an LTS position in High Performance Computing.
3. Lehigh High Performance Computing Steering Committee, Member, Fall 2010-ongoing. Ongoing member of User Policy and Storage Policy Subcommittees.
4. Presenter, Bits, Bytes, and Volts Specialty Tour, for potential undergraduate applicants, 11/8/2012, 4/21/2011, 11/4/2010.

Service to Interdisciplinary Programs

1. Guest lectures for BioS 10 on 9/10/2014/, 11/22/2013, 11/16/2012, 11/21/2011, 10/10/2010, taught by Vassie Ware, Dept. of Biological Sciences. Titled: "Structural Bioinformatics".
2. Guest lectures for BioE 02 on 4/18/2011, 4/9/2012 taught by Svetlana Tatic-Lucic, Dept. of Chemical Engineering. Titled: "Of Informatics and Biology".
3. Guest lecture, "Informatics for Biology" to Biosystems Dynamics Summer Institute, Lehigh University, June 9, 2011.
4. Guest lecture, "Structural Bioinformatics in Modern Biology" to BioE 020 on 4/19/2012 and 2/3/2011, taught by Lori Herz, Dept. of Chemical Engineering.

Service to Department of Computer Science and Engineering

1. Colloquium Chair, 2012-2016. Hosted William Craelius (2015), Lydia Kavraki (2012), Amarda Shehu (2011), Willy Wriggers (2015).
2. Lehigh ACM club Co-Advisor, 2012-2014.
3. Facilities Committee, Fall 2010-ongoing. Assisted in the development and implementation of two internal funding proposals instructional labs.
4. Guest lectures for CSE 411 (fall 2012, 2013) titled: "Numerical Precision".
5. Guest lectures for CSE 497/406 (fall 2010-2013) titled: "Structural Bioinformatics".
6. Guest lectures for CSE 411 (fall 2015, 2016) titled: "Ethics and Academic Integrity".
7. Presenter, Candidates Day, for students considering Computer Science and Engineering majors, 2011, 2012, 2013, 2014.
8. Graduate Admissions Committee, academic year 2010-2011. Assisted in the evaluation of M.S. and Ph.D. applications for Fall 2011.

Service to Other Departments

1. Member, Industrial and Systems Engineering Faculty Search Committee (AY 2012, 2013) I am assisting members of the ISE Dept. in identifying, interviewing, and selecting a tenure-track faculty candidate.
2. Member, Neuroscience Faculty Search Committee (AY 2011). I assisted members of the Dept. of Biological Sciences in identifying, interviewing, and selecting faculty members Julie Haas and Julie Miwa.
3. Member, Civil Infrastructure Systems Faculty Search Committee (AY 2011). I assisted members of the Dept. of Civil and Environmental Engineering Department in interviewing faculty members for a tenure track position.

Professional (External) Service

Organizing Committee Memberships

1. General Co-Chair, Computational Structural Bioinformatics Workshop (CSBW 2011-2016, annually). Coordinated the peer review of workshop papers, organized workshop logistics, scheduling and communications.
2. Co-Chair, IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2012). Promotion, selection, and management of 12 workshops at the core of IEEE's flagship bioinformatics conference. (400+ attendees)
3. Co-Chair, IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2015). Promotion, selection, and management of 25 workshops at the core of IEEE's flagship bioinformatics conference. (400+ attendees)

Program Committee Memberships

1. Asia Pacific Bioinformatics Conference (APBC) 2014-ongoing.
2. International Conference on Intelligent Systems for Molecular Biology (ISMB) 2013-ongoing.
3. International Conference on Research in Computational Molecular Biology (RECOMB) 2013-ongoing.
4. ACM Conference on Bioinformatics, Computational Biology and Biomedicine (BCB) 2012-2014.
5. IEEE International Conference on Bioinformatics and Biomedicine (BIBM) 2012-ongoing.
6. Computational Structural Bioinformatics Workshop (CSBW) 2011-ongoing.

Peer Reviewer

1. PLoS Computational Biology (2012-ongoing)
2. BMC Bioinformatics (2011-ongoing)
3. IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB) (2006-ongoing)
4. International Journal of Data Mining and Bioinformatics (IJDMB) (2012)
5. International Journal of Computational Biology and Drug Design (IJCBDD) (2012-ongoing)
6. Computer Aided Design (2011-ongoing)
7. Journal of Bioinformatics and Computational Biology (JBCB) (2007-ongoing)
8. International Conference on Intelligent Systems for Molecular Biology (ISMB) (Posters) (2009, 2010)
9. European Conference on Computational Biology (ECCB) (Posters) (2009)

Professional Society Memberships

1. Association for Computing Machinery, member (2012-).
2. Institute of Electrical and Electronic Engineers, member (2010-).
3. International Society for Computational Biology, member (2006-).
4. Life Sciences Society, member (2006-).