Brian Y. Chen

Curriculum Vitae — Public Version — Oct 2022
http://www.cse.lehigh.edu/ ∼chen https://informatics.cas.lehigh.edu/

A. BIOGRAPHICAL INFORMATION

Business Address:
Building C, Room 330
113 Research Drive
Lehigh University
Bethlehem, PA, 18015

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Employment History

Associate Professor with Tenure, Lehigh University, Bethlehem, PA July 2016 - current
P.C. Rossin College of Engineering and Applied Science
Dept. of Computer Science and Engineering
- *Algorithms/AI that examine protein structure and explain binding specificity mechanisms*
- *Algorithms/AI that study the microstructure and interface properties of polycrystalline materials*

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

Education and Training

Postdoctoral Research Scientist, Columbia University, New York, NY. Dec 2006 - July 2010
Howard Hughes Medical Institute,
Center for Computational Biology and Bioinformatics,
Department of Biochemistry and Molecular Biophysics
Identifying steric features of molecular structure that affect ligand binding specificity
Supervisor: Barry Honig

Ph.D. in Computer Science, Rice University, Houston, TX. May 2007
George R. Brown School of Engineering,
Department of Computer Science
Thesis: *Geometry-based Methods for Protein Function Annotation*
Supervisor: Lydia Kavraki

M.S. in Computer Science, Rice University, Houston, TX. May 2003
George R. Brown School of Engineering,
Department of Computer Science
Thesis: *Structural Pattern Matching for the Functional Annotation of Proteins*
Supervisor: Lydia Kavraki

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

B. PUBLICATIONS AND CREATIVE ACTIVITIES

My scientific work has a large part in bioinformatics and a new part in computational materials science. Since 2000, my work in bioinformatics has focused on the computational analysis of molecular structure, most recently on tools that can explain the mechanisms by which proteins select binding partners. Since 2018, I developed a second focus on analyzing the microstructure and interface properties of polycrystalline materials. In both fields, my interests range from fundamental algorithmic and chemical issues to applications in medicine, biotechnology, and defense.

Publishing in my fields. Bioinformatics is a spectrum of computational and biological investigators. Computational researchers are expected to publish in conferences and biological researchers are evaluated by journal publications. To communicate with the field as broadly as possible, I publish in both, choosing only peer reviewed venues. In computational materials science, peer reviewed journals and non-peer reviewed conference proceedings are the norm.

On author order. Throughout both fields, author order on publications begins with workers in descending order of contribution followed by advisors in ascending order of support. Papers without student authors (rare) list the authors in descending order of contribution. The table below clarifies the roles of coauthors as my advisors or advisees under my formal mentorship and/or financial support. Other collaborators are indicated by a lack of designation.

On publication status. Documents listed in B.1, B.2, B.3 and B.3.a are either published or indicated as "in press" (i.e. waiting for publication).

Postdoctoral Advisee	P	Doctoral Advisee	D	Master's Advisee	M
My Postdoctoral Advisor	PA	My Doctoral Advisor	DA	Undergraduate Advisee	U
High School Advisee	H	Equal contribution	†	Lead Faculty Author	**boldface**
* Student effort financially supported by grants for which I am the principal investigator					

B.1. Invited Book Chapters

Summary: *2 book chapters were started and published while at Lehigh University. I was the corresponding author on one chapter, and both were published with Ph.D. students under my direction and financial support.*

1. Ziyi Guo^{D*} and **Brian Y. Chen** "Explaining Small Molecule Binding Specificity with Volumetric Representations of Protein Binding Sites", *Algorithms and Methods in Structural Bioinformatics*, Filip Jagodzinski and Nurit Haspel (Editors), Springer Nature 2022. ISBN: 978-3-031-05913-1. https://doi.org/10.1007/978-3-031-05914-8

2. Ruobing Chen*, Ziyi Guo^{D*}, Brian Y. Chen and **Katya Scheinberg** "Chapter 39: Methodologies and Software for Derivative-free Optimization, Volumetric Alignment of Protein-Binding Cavities", *Optimization Methods in Engineering*, Society for Industrial and Applied Mathematics (SIAM), 2017. ISBN: 978-1-61197-467-6.

B.2. Peer Reviewed Journal Articles

Summary: *22 journal papers were published in total, with 12 as lead or corresponding author. While at Lehigh University, 10 papers were published overall, with 9 papers as lead or corresponding author. 7 papers were published with Lehigh students under my direction, including 2 with Ph.D. advisees, 3 with Master's advisees, and 5 with undergraduate research advisees.*

3. Justin Z. Tam^{D*}, Talulla Palumbo*, Julie M Miwa* and **Brian Y. Chen** "Analysis of Protein-Protein Interactions for Intermolecular Bond Prediction," *MDPI Molecules* 2022, 27(6178). doi.org/10.3390/molecules27196178 *Impact factor: 4.927*

4. Deborah Rupert, Kanan Shah, Brian Y. Chen, Avital Y. O'Glasser, Michael Schiml, Shikha Jain and **Fumiko Chino** "Sex and Location Differences in Verification Status of Physician-Held Social Media Platform Accounts," *JAMA Network Open* 5(8):e2225671. doi:10.1001/jamanetworkopen.2022.25671

5. Georgi D. Georgiev^{U}, Kevin F. Dodd^{M} and **Brian Y. Chen** "Precise Parallel Volumetric Comparison of Molecular Surfaces and Electrostatic Isopotentials", *Algorithms for Molecular Biology*, 2020, 15, 11. https://doi.org/10.1186/s13015-020-00168-z *Impact factor: 2.341*

6. Stephanie Mason^{U}*, Brian Y. Chen and **Filip Jagodzinski** "Exploring Protien Cavities through Rigidity Analysis", *Molecules*, 2018, 23(2), p. 351. doi:10.3390/molecules23020351 *Impact factor: 3.098*

7. 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", *Nature Scientific Reports*, 7:42912, 2017. doi:10.1038/srep42912 *Impact factor: 5.228*

8. Bridget E. Nolan^{U}, Emily Levenson^{U} 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*

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

10. **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*

11. Seth Blumenthal^{U}, Yisheng Tang^{M*}, Wenjie Yang^{M*}, and **Brian Y. Chen** "Isolating Influential Regions of Electrostatic Focusing in Protein and DNA Structure", Invited to: *IEEE Transactions on Computational Biology and Bioinformatics*, 10.5, pp 1188-1198, 2013. *Impact factor: 1.66*

12. Brian G. Godshall^{U}, Yisheng Tang^{M*}, Wenjie Yang^{M*}, 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*, 13.1, 2013. *Impact factor: 2.48*

13. **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*

14. **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*, 2012. doi: 10.1142/S0219720012420048. *Impact factor: .783*

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

16. 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*

17. Brian Y. Chen and **Barry Honig**^{PA}. "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*

18. Drew H. Bryant, Mark Moll, Brian Y. Chen, Viacheslav Y. Fofanov, **Lydia E. Kavraki**^{DA}. "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*

19. 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*

20. David M. Kristensen, R. Matthew Ward, A. Martin Lisewski, Serkan Erdin, Brian Y. Chen, Viacheslav Y. Fofanov, Marek Kimmel, Lydia E. Kavraki^{DA}, **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*

21. Brian Y. Chen, Drew H. Bryant^{U}, Viacheslav Y. Fofanov, David M. Kristensen, Amanda E. Cruess^{U}, Marek Kimmel, Olivier Lichtarge, **Lydia E. Kavraki**^{DA}. "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.

22. Brian Y. Chen, Viacheslav Y. Fofanov, Drew H. Bryant^{U}, Bradley D. Dodson, David M. Kristensen, A. Martin Lisewski, Marek Kimmel, Olivier Lichtarge, **Lydia E. Kavraki**^{DA}. "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*

23. David M. Kristensen, Brian Y. Chen, Viacheslav Y. Fofanov, R. Matthew Ward, A. Martin Lisewski, Marek Kimmel, **Lydia E. Kavraki**^{DA}. "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*

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

B.3. Peer Reviewed Conference Proceedings

Summary: *30 conference papers were published in total, with 24 as lead or corresponding author. While at Lehigh University, 23 conference papers were published overall, with 20 as lead or corresponding author. 19 papers were published with Lehigh students under my direction, including 11 with Ph.D. advisees, 2 with Master's advisees, 7 with undergraduate research advisees, and 1 with a local high school student.*

25. Pak Yiu Liu, Joanne Yip, Brian Y. Chen, Lifang He, Jason Cheung, Kit Lun Yick and Sun Pui Ng. "Immediate effects of posture correction girdle on adolescents with early scoliosis," In 13th International Conference on Applied Human Factors and Ergonomics (AHFE 2022). New York City, NY, July 2022. *Full paper acceptance rate: 32%* ***AHFE 2022 Best paper award.***

26. Houliang Zhou^{D*}, Yu Zhang, Brian Y. Chen, Shen Li, and Lifang He. "Sparse interpretation of graph convolutional networks for multi-modal diagnosis of Alzheimer's disease," In the 25th International Conference on Medical Image Computing and Computer Assisted Intervention (MICCAI 2022). Singapore, Sept 2022. *Acceptance Rate: 30%*

27. Houliang Zhou^{D*}, Lifang He, Yu Zhang, Li Shen, and **Brian Y. Chen** "Interpretable Graph Convolutional Network of Multi-Modality Brain Imaging for Alzheimer's Disease Diagnosis", *Proceedings of the IEEE International Symposium on Biomedical Imaging (ISBI 2022)*. Kolkata, India, March 2022. *Acceptance Rate: 43.4%*

28. Felix M. Quintana^{U*}, Zhaoming Kong, Lifang He, and **Brian Y. Chen** "DeepVASP-E: A Flexible Analysis of Electrostatic Isopotentials for Finding and Explaining Mechanisms that Control Binding Specificity", *Proceedings of The Pacific Symposium on Biocomputing (PSB 2022)*, World Scientific. Big Island, HI, January 2022. *Acceptance Rate: 30%*

29. Chesphongphach Buranasilp^{U} and **Brian Y. Chen** "A Conical Representation of Hydrogen Bond Geometry for Quantifying Bond Interactions", *Proceedings of the Computational Structural Bioinformatics Workshop (CSBW 2021) at the 2020 IEEE International Conference on Bioinformatics and Biomedicine (BIBM).* Virtual, December 2020. *Acceptance Rate: 79%.* ***Best Paper Award.***

30. Justin Tam^{D*}, Talulla Palumbo*, Julie M. Miwa, and **Brian Y. Chen** "DiffBond: A Method for Predicting Intermolecular Bond Formation", *Proceedings of the Computational Structural Bioinformatics Workshop (CSBW 2021) at the 2020 IEEE International Conference on Bioinformatics and Biomedicine (BIBM).* Virtual, December 2020. *Acceptance Rate: 79%.*

31. Georgi D. Georgiev^{M}, Kevin F. Dodd^{M} and **Brian Y. Chen** "pClay: A Precise Parallel Algorithm for Comparing Molecular Surfaces", *18th International Workshop on Algorithms in Bioinformatics (WABI 2019).* Schloss Dagstuhl-Leibniz-Zentrum fuer Informatik, 2019. *Oral presentation, 2019 Acceptance Rate: 27%*

32. Jinbu Wang^{D*} and **Brian Y. Chen** "On Conformations of peptides bound to class I Major Histocompatibility Complexes", *Proceedings of the CSBW (Computational Structural Biology Workshop) at the 2019 ACM International Conference on Bioinformatics, Computational Biology, and Health Informatics. 2019 Acceptance Rate: 81%*

33. Devan Bicher^{M} and **Brian Y. Chen** "A Volumetric Survey of Cavities and Electrostatic Patterns in Protein-RNA Binding Sites", *Proceedings of the CSBW (Computational Structural Biology Workshop) at the 2019 ACM International Conference on Bioinformatics, Computational Biology, and Health Informatics. 2019 Acceptance Rate: 81%*

34. Jinbu Wang^{D*} and **Brian Y. Chen** "MAPS: Analyzing Peptide Binding Subsites in Major Histocompatibility Complexes", *Proceedings of the CSBW (Computational Structural Biology Workshop) at the 2018 ACM International Conference on Bioinformatics, Computational Biology, and Health Informatics. 2018 Acceptance Rate: 80%*

35. Stephanie Mason^{U*}, Tim Woods, Brian Y. Chen, and **Filip Jagodzinski** "Investigating Rigidity Properties of Protein Cavities", *Proceedings of the CSBW (Computational Structural Biology Workshop) at the 2017 ACM International Conference on Bioinformatics, Computational Biology, and Health Informatics. 2017 Acceptance Rate: 76%*

36. Ziyi Guo^{D*} 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)*. Washington, DC, November 2015. *Oral presentation, acceptance rate for regular papers: 19%*.

37. Rachel Y. Okun^{U*} 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. *2015 Acceptance Rate: 65%*

38. Ziyi Guo^{D*} 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. *2015 Acceptance Rate: 65%*

39. Ziyi Guo^{D*}, Juliana Hong^{H}, 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%*

40. Ziyi Guo^{D*} 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%*

41. Zachary A. Daniels^{U}, Steven R. Stinson^{U}, Shenchi Tian^{U}, Evan Mulbry^{U}, 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.

42. Ziyi Guo^{D*}, Trevor Kuhlengel^{U}, Steven Stinson^{U}, Seth Blumenthal^{U}, 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%*

43. Brian G. Godshall^{U} 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%*

44. **Brian Y. Chen** and Debdas Paul^{D*}. "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%*

45. 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%*

46. **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%*

47. **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%*

48. Viacheslav Y. Fofanov, Brian Y. Chen, Drew H. Bryant^{U}, Mark Moll, Olivier Lichtarge, Lydia E. Kavraki^{DA}, **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.

49. Brian Y. Chen, Drew H. Bryant^{U}, Amanda E. Cruess^{U}, Joseph H. Bylund^{U}, Viacheslav Y. Fofanov, David M. Kristensen, Marek Kimmel, Olivier Lichtarge, **Lydia E. Kavraki**^{DA}. "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%*

50. Brian Y. Chen, Drew H. Bryant^{U}, Viacheslav Y. Fofanov, David M. Kristensen, Amanda E. Cruess^{U}, Marek Kimmel, Olivier Lichtarge, **Lydia E. Kavraki**^{DA}. "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%*

51. Brian Y. Chen, Viacheslav Y. Fofanov, Drew H. Bryant^{U}, Bradley D. Dodson^{U}, David M. Kristensen, A. Martin Lisewski, Marek Kimmel, Olivier Lichtarge, **Lydia E. Kavraki**^{DA}, "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%*

52. Brian Y. Chen, Viacheslav Y. Fofanov, David M. Kristensen, Marek Kimmel, Olivier Lichtarge, **Lydia E. Kavraki**^{DA}, "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%*

53. Kostas E. Bekris, Brian Y. Chen, Andrew M. Ladd, Erion Plaku, **Lydia E. Kavraki**^{DA}, "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%*

54. Mert Akinc, Kostas E. Bekris, Brian Y. Chan, Andrew M. Ladd, Erion Plaku, **Lydia E. Kavraki**^{DA}, "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.

B.3.a Non-Peer Reviewed Conference Proceedings/Abstracts (Materials Science)

Summary: *In computational materials science, conference proceedings are a communications medium that is secondary in significance to peer-reviewed journals. While they are not formally peer reviewed, a selection process is still employed by conference organizers based on scientific interests. In this medium, I contributed to 2 conference proceedings, with 0 as corresponding or primary author, while at Lehigh. 2 were published with students under my direction, including 1 with a Ph.D. advisee, 2 with Master's advisees, and 1 with an undergraduate research advisee.*

55. Christopher J. Marvel, Caroline Riedel, Houliang Zhou^{D*}, Benjamin J. Zalatan^{M*}, Brian Y. Chen, and Martin P. Harmer "Examination of Discontinuous Changes in Grain Boundary Velocity Induced by Grain Boundary Transformations." 47th International Conference and Expo on Advanced Ceramics and Composites (ICACC 2023).

56. Surui Huang^{U*}, Jack Kellerk^{M*}, Brian Y. Chen, Aparna Bharati, Masashi Watanabe, Patrick Cantwell, Christopher J. Marvel and Martin Harmer "Push-Button Microscopy: Automated Instrument Alignment and Reciprocal-space Navigation using PyJEM," Microscopy and Microanalysis 28, S1 (2022). doi:10.1017/S1431927622011771

C. HONORS AND AWARDS

1. Best paper Award at AHFE 2022, with Pak Yiu Liu, Joanne Yip, Lifang He, Jason Cheung, Kit Lun Yick and Sun Pui Ng.

2. Best Paper Award at CSBW 2021, with Chesphongphach Buranasilp, $200.

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

4. 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.

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

6. Sigma Xi, full member, 2011.

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

C.1 Media Coverage

1. "Next-gen tech enables next-level collaboration in materials research." Resolve Magazine, Vol. 2 2022.

2. Kathy Liszewski. "Biocomputing Mining, Modeling and Melding Biological Data: Assessments of protein folding/binding, electrostatics, cell types, and sex-specific genetic differences are speeding drug discovery and advancing precision medicine." Genetic Engineering & Biotechnology News 42.2 (2022): 44-47.

3. "Brian Chen: Solving a Combinatorial Quandary." Resolve Magazine, Vol. 1 2020.

4. "Brian Chen: Molecular matchmaking." Resolve Magazine, Vol. 1 2013.

5. "Brian Chen: Software automates the analysis of protein cavities." Resolve Magazine, Vol. 1 2011.

6. "Katya Scheinberg and Brian Y. Chen: Optimization on steroids." Resolve Magazine, Vol. 1 2012.

D. RESEARCH FUNDING AND TRAINING GRANTS

Summary: As PI or Co-PI, I received 4 federally funded grants, totalling $26,636,630 to Lehigh University. I serve or have served as PI on 3 of these grants, which totaled $1,636,630. These awards have partly supported the stipends, training, research, equipment, travel and publication costs of 6 Ph.D. students, 9 Master's students, and 42 undergraduate research advisees. Agencies receiving my proposals include the National Science Foundation, the National Institutes of Health, and the Army Research Laboratory.

On author order: Below, the PI is distinguished from Co-PIs supporting the proposal. My name is bolded to clarify my contribution. Author order is in order of anticipated contribution to the proposed project.

D.1 Competitively Awarded Extramural Research Grants (Awarded at Lehigh University)

1. Martin Harmer (PI), Helen Chan, **Brian Y. Chen**, Kate Arrington, Masashi Watanbe (Co-PIs). "Lightweight High Entropy Metallic Alloy Discovery (LHEAD)." 2/2022-2/2027 (with annual renewals). Congressional Appropriation to Army Research Laboratory, awarded to Lehigh University (lead institution) and Ohio State University (partner institution). Total funding up to $25,000,000 total, up to $5,000,000 annually, depending on congressional budget process. Agreement number W911NF2220032.

2. **Brian Y. Chen (PI)** and Julia Miwa (Co-PI). "Algorithmic Identification of Binding Specificity Mechanisms in Proteins." 9/2019-8/2023. National Institute of General Medical Sciences, National Institutes of Health. $967,274.00. Award Number: 1R01GM123131-01A1. Administrative Supplement to Support Enhancement of Software Tools for Open Science: $100,356.

3. **Brian 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.

D.2 Non-Competitively Awarded Extramural Research Grants (at Lehigh University)

1. **Brian Y. Chen (PI)**. "Real-time data reduction codesign at the extreme edge for science." 6/2022-5/2023. Fermilab, via. U.S. Department of Energy. $100,000. Award number 688490. Several renewals likely.

D.3 Competitively awarded training grants (Awarded before joining Lehigh in 2010)

1. **Brian Y. Chen**. 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.

D.4 Institutional/Equipment Grants Awarded (Awarded from Lehigh University)

1. **Brian Y. Chen (PI)** and Lifang He and Yu Zhang (Co-PIs). "An Interpretable Deep Learning Framework for Fit-for-Purpose Biomarker Quantification", Lehigh Accelerator Grant, $97,523, 1/11/2021 - 1/11/2023.

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

3. **Brian Y. Chen**, Bryan Hodgson, Henry Korth, Daniel Lopresti, Michael Spear, and John Spletzer (equal contribution). Departmental Proposal. "Computer Science and Engineering Undergraduate Sandbox Lab Upgrade". P.C. Rossin College of Engineering and Applied Science, $66,000, December 2010.

E. EDITOR/EDITORIAL REVIEW BOARD MEMBERSHIPS

1. Associate Editor, International Journal of Data Mining and Bioinformatics, 2012-2020. Editorial Board 2020-present.
2. Guest Editor, Special Issue, Molecules 2018.
3. Guest Editor, Special Issue, Journal of Computational Biology 2016.
4. Guest Editor, Special Issue, Journal of Computational Biology 2015.
5. Guest Editor, Special Issue, BMC Structural Biology 2013.
6. Guest Editor, Special Issue, Journal of Bioinformatics and Computational Biology (JBCB) 2012.

F. SCHOLARLY PRESENTATIONS

F.1 Invited presentations

1. Keynote. Title TBD. Computational Structural Bioinformatics Workshop, Dec 6-7 2022, Las Vegas, NV.
2. "Algorithms for discovering mutations that alter binding specificity." American Chemical Society, National Meeting, August 20-24 2017, Washington, DC.
3. "Computational detection of steric and electrostatic influences on protein binding specificity." American Chemical Society, Northeast Regional Meeting, October 5-8, 2016, Binghamton, NY.
4. "A system for the volumetric analysis of protein structure", Department of Computer Science, Rutgers University, Piscataway, NJ, Spring 2014.
5. "Volumetric and Electrostatic Dissection of Protein-Ligand and Protein-Protein Interactions", Department of Biomedical Engineering, Rutgers University, Piscataway, NJ, Spring 2014.
6. "Automatically Detecting Influences on Protein Binding Specificity", Center for Bioinformatics and Computational Biology, University of Delaware, Newark, DE, November 26, 2012.
7. "Deconstructing the Molecular World", Genomic Informatics Center, Hankyong National University, Korea, May 15, 2012.
8. "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.
9. "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.
10. "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.
11. "A Quantitative Universe", Sigma Xi Lecture Series, Lehigh University Chapter, Bethlehem, PA, January 21, 2011.
12. "Volume-based Analysis of Protein Cavties", Dept. of Computer Science, Rice University, Houston, TX, October 25, 2010.
13. "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.
14. "Volumetric Dissection of Protein Functional Sites", Institute Colloquium, Toyota Technological Institute, Chicago, IL, Apr 1, 2010.

15. "Geometric Analyses of Protein Structure, Function and Specificity", Departmental Colloquium, Dept. of Computer Science, University of Massachusetts Boston, Boston, MA, Mar 11, 2009.

16. "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.

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

F.2 Refereed presentations

1. "DeepVASP-E: A Flexible Analysis of Electrostatic Isopotentials for Finding and Explaining Mechanisms that Control Binding Specificity." Pacific Symposium on Biocomputing, Jan 3-7, 2022, Big Island, Hawaii.

2. "pClay: A Precise Parallel Algorithm for Comparing Molecular Surfaces", 2019 International Workshop on Algorithms in Bioinformatics (WABI 2019), Niagara Falls, NY, September, 2019.

3. "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.

4. "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.

5. "Improving Accuracy in Binding Site Comparison with Homology Modeling", Computational Structural Bioinformatics Workshop (CSBW 2012), Philadelphia, PA, October 5, 2012.

6. "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.

7. "A Statistical Model of Overlapping Volume in Ligand Binding Cavities", Computational Structural Bioinformatics Workshop (CSBW 2011), Atlanta, GA, November 11, 2011.

8. "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.

9. "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.

10. "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.

11. "Optimizing 3D-Motifs for Protein Function Prediction", Houston Society for Engineering in Medicine and Biology (HSEMB 2006), February 9, 2006.

12. "Geometric and Statistical Analysis of 3D Protein Substructures using Match Augmentation", DIMACS Workshop on Information Processing by Protein Structures, June 23, 2005.

13. "Algorithms for Structural Comparison and Statistical Analysis of 3D Protein Motifs", Pacific Symposium for Biocomputing (PSB 2005), January 5, 2005.

14. "Structural Pattern Matching for Functional Annotation of Proteins", Houston Society for Engineering in Medicine and Biology (HSEMB 2003), April 3, 2003.

F.3 Chaired Conference Sessions

1. Session Chair, 2019 Workshop on Algorithms in Bioinformatics (WABI 2019), Niagara Falls, NY, September 2019.

2. Session Chair, Computational Structural Bioinformatics Workshop (CSBW) 2014, 2013, 2012, 2011, various locaitons.

3. Session Chair, ACM Conference on Bioinformatics, Computational Biology and Biomedicine (BCB) Newport Beach, September 20, 2014.

4. Session Chair, ACM Conference on Bioinformatics, Computational Biology and Biomedicine (BCB) Orlando, FL, October 7, 2012.

5. Session Chair, IEEE International Conference on Bioinformatics and Biomedicine (BIBM) Philadelphia, PA, October 4, 2012.

6. Session Chair, Lehigh High Performance Computing Symposium 2013, 2012, 2011. Invited, hosted, and introduced 12 external speakers over three years.

G. TEACHING AND ADVISING

Summary: *Over 12 years at Lehigh University, I have taught 40 regular courses, producing grades for 1548 students. 7 courses were newly developed or fully redesigned. My lab created research training opportunities for 7 Ph.D. students, 6 master's students, 41 undergraduate students, and 2 high school students through research experiences in bioinformatics and computational materials science.*

G.1 Overview of Courses Taught as Instructor of Record

Over 23 semesters of teaching, 40 regular courses were taught in 50 sections. 13 cross-listed courses supported three departments (Computer Science and Engineering, BioEngineering, and Biological Sciences) and two programs (Biocomputational Engineering and Bioengineering). Over this period, Lehigh employed two course evaluation systems:

Evaluations through Spring 2018. Course evaluation scores from Fall 2010 until Spring 2018 are summarized in table 1 below. These data describe 15 semesters where 1004 students were taught in 27 courses, divided into 37 sections. Courses were evaluated by students at the end of the semester, via optional questionnaire, according to three standard questions relating to teaching effectiveness, course quality, and student learning. Evaluation scores, which are decimals between 0.0 (poor) and 5.0 (excellent), are averaged per-course to avoid under-weighting smaller senior and graduate level courses. Leading scores in each category are bolded and shown in comparison to departmental and college (RCEAS) averages for courses taught in the same semester.

Table 1. Summary of 27 courses taught Fall 2010 – Spring 2018. (1004 students)

	Teaching Effectiveness	Course Quality	Student Learning
Personal	**4.27 / 5.00**	**4.29 / 5.00**	**4.45 / 5.00**
CSE (Dept.)	4.16 / 5.00	4.18 / 5.00	4.22 / 5.00
RCEAS (College)	4.19 / 5.00	4.20 / 5.00	4.21 / 5.00

Evaluations beginning Fall 2018. In Fall 2018, Lehigh transitioned to course evaluation questions relating to six criteria, shown in the headings of table 2 below. These data describe 9 semesters where 544 students were taught in 13 courses divided into 13 sections. Courses were evaluated by students at the end of the semester, via optional questionnaire. Evaluation scores, which are decimals between 0.0 (poor) and 5.0 (excellent) are averaged per-course to avoid under-weighting smaller senior and graduate level courses. Leading scores in each category are bolded and shown in comparison to departmental and college (RCEAS) averages for courses taught in the same semester.

Table 2. Summary of 12 courses taught from Fall 2018 until the present. (544 students)

	Organization	Effectiveness	Responsiveness	Feedback	Assignments	Knowledge
Personal	4.11 / 5.00	3.99 / 5.00	4.21 / 5.00	4.09 / 5.00	4.35 / 5.00	4.43 / 5.00
CSE (Dept.)	**4.38 / 5.00**	**4.19 / 5.00**	**4.47 / 5.00**	**4.25 / 5.00**	**4.39 / 5.00**	**4.56 / 5.00**
RCEAS (College)	4.32 / 5.00	**4.19 / 5.00**	4.38 / 5.00	4.21 / 5.00	4.30 / 5.00	4.45 / 5.00

Courses that are not evaluated or have yet to be evaluated are not incorporated into the summary tables above. However, in the text above, these courses are still included when counting the number of courses, students and semesters taught, because these counts still quantify effort expended in teaching even if the course is not evaluated. Due to the global pandemic in 2019, Lehigh University omitted evaluations from Spring 2020 for promotion and tenure considerations. Evaluations from that semester are thus omitted in table 2 and the listing below.

G.2 Reverse Chronological Listing of Courses Taught

1. Fall 2022: **Computer Graphics (CSE 313/498)** two meetings per week, 33 enrolled in the course. *Ongoing.*

2. Spring 2022: **Structural Bioinformatics (BioE/CSE 307/407)** three meetings per week, 19 enrolled in the course. *Students evaluated course organization as 4.57/5.0 versus a college average of 4.5, teaching method effectiveness as 4.71/5.0 versus a college average of 4.28, instructor responsiveness as 4.57/5.0 versus a college average of 4.51, instructor feedback as 4.71/5.0 versus a college average of 4.34, assignment quality as 4.43/5.0 versus a college average of 4.42, and knowledge enhancement as 4.86/5.0 out of a college average of 4.58.*

3. Fall 2021: **Introduction to Programming A (CSE 3)** three meetings per week, 55 enrolled in the course. *Students evaluated course organization as 4.15/5.0 versus a college average of 4.35, teaching method effectiveness as 4.13/5.0 versus a college average of 4.15, instructor responsiveness as 4.15/5.0 versus a college average of 4.37, instructor feedback as 3.8/5.0 versus a college average of 4.15, assignment quality as 4.45/5.0 versus a college average of 4.29, and knowledge enhancement as 4.56/5.0 out of a college average of 4.47.*

4. Spring 2021: **Computer Graphics (CSE 313)** three meetings per week, 36 enrolled in the course. *Students evaluated course organization as 4.25/5.0 versus a college average of 4.37, teaching method effectiveness as 4.38/5.0 versus a college average of 4.24, instructor responsiveness as 4.63/5.0 versus a college average of 4.44, instructor feedback as 4.13/5.0 versus a college average of 4.24, assignment quality as 4.63/5.0 versus a college average of 4.36, and knowledge enhancement as 4.69/5.0 out of a college average of 4.5.*

5. Spring 2021: **Introduction to Programming B (CSE 4)** three meetings per week, 27 enrolled in the course. **New course developed in this semester.** *Students evaluated course organization as 3.89/5.0 versus a college average of 4.37, teaching method effectiveness as 3.89/5.0 versus a college average of 4.24, instructor responsiveness as 4.67/5.0 versus a college average of 4.44, instructor feedback as 4.29/5.0 versus a college average of 4.24, assignment quality as 4.78/5.0 versus a college average of 4.36, and knowledge enhancement as 4.78/5.0 out of a college average of 4.5.*

6. Spring 2021: **Introduction to Programming A (CSE 3)** three meetings per week, 38 enrolled in the course. ***In Spring 2021, I stepped in to support the department and college by offering this course when the planned instructor unexpectedly departed.*** *I taught the full semester as an overload of my normal duties while coping with the additional challenges created by the global pandemic. Recognizing the immense challenges and personal stress induced by this unplanned burden, a departmental and college level agreement was made that my teaching evaluations would not be considered for this class. As a result, course evaluations are omitted here.*

7. Spring 2020: **Fundamentals of Programming (CSE 2)** three meetings per week, 61 enrolled in the course. ***Due to the global pandemic****, Lehigh University omitted evaluations from Spring 2020 for promotion and tenure considerations. Evaluation scores are thus omitted here. In spite of the pandemic, this course achieved typical student outcomes, to the credit of all involved.*

8. Fall 2020: **Introduction to Programming A (CSE 3)** three meetings per week, 51 enrolled in the course. **New course developed in this semester.** *Students evaluated course organization as 4.05/5.0 versus a college average*

of 4.31, teaching method effectiveness as 3.38/5.0 versus a college average of 4.16, instructor responsiveness as 3.71/5.0 versus a college average of 4.38, instructor feedback as 4.05/5.0 versus a college average of 4.16, assignment quality as 4.33/5.0 versus a college average of 4.3, and knowledge enhancement as 4.71/5.0 out of a college average of 4.48.

9. Fall 2019: **Fundamentals of Programming (CSE 2)** three meetings per week, 70 enrolled in the course. *Students evaluated course organization as 3.93/5.0 versus a college average of 4.26, teaching method effectiveness as 3.77/5.0 versus a college average of 4.16, instructor responsiveness as 3.71/5.0 versus a college average of 4.38, instructor feedback as 3.55/5.0 versus a college average of 4.16, assignment quality as 4.05/5.0 versus a college average of 4.26, and knowledge enhancement as 4.44/5.0 out of a college average of 4.42.*

10. Fall 2019: **Structural Bioinformatics (BioE/CSE 307/407)** three meetings per week, 10 enrolled in the various sections of the course. *Students evaluated course organization as 3.5/5.0 versus a college average of 4.26, teaching method effectiveness as 3.0/5.0 versus a college average of 4.16, instructor responsiveness as 4.5/5.0 versus a college average of 4.38, instructor feedback as 4.5/5.0 versus a college average of 4.16, assignment quality as 3.5/5.0 versus a college average of 4.26, and knowledge enhancement as 3.0/5.0 out of a college average of 4.42.*

11. Spring 2019: **Fundamentals of Programming (CSE 2)** three meetings per week, 58 enrolled in the course. *Students evaluated course organization as 4.31/5.0 versus a college average of 4.34, teaching method effectiveness as 4.13/5.0 versus a college average of 4.17, instructor responsiveness as 3.75/5.0 versus a college average of 4.40, instructor feedback as 3.50/5.0 versus a college average of 4.25, assignment quality as 4.25/5.0 versus a college average of 4.35, and knowledge enhancement as 4.50/5.0 out of a college average of 4.46.*

12. Fall 2018: **Computer Graphics (CSE 313/413)** three meetings per week, 26 enrolled in the course. **Course redeveloped in this semester.** *Students evaluated course organization as 4.13/5.0 versus a college average of 4.33, teaching effectiveness as 4.50/5.0 versus a college average of 4.14, instructor responsiveness as 4.50/5.0 versus a college average of 4.32, instructor feedback as 4.64/5.0 versus a college average of 4.20, assignment quality as 4.63/5.0 versus a college average of 4.28, and knowledge enhancement as 4.75/5.0 out of a college average of 4.41.*

13. Fall 2018: **Fundamentals of Programming (CSE 2)** three meetings per week, 60 enrolled in the course. *Students evaluated course organization as 4.34/5.0 versus a college average of 4.33, teaching effectiveness as 4.00/5.0 versus a college average of 4.14, instructor responsiveness as 3.90/5.0 versus a college average of 4.32, instructor feedback as 3.69/5.0 versus a college average of 4.20, assignment quality as 4.48/5.0 versus a college average of 4.28, and knowledge enhancement as 4.55/5.0 out of a college average of 4.41.*

14. Spring 2018: **Fundamentals of Programming (CSE 2)** three meetings per week, 76 enrolled in the course. *Students evaluated teaching effectiveness as 4.35/5.0 versus a college average of 4.06. Students evaluated course quality as 4.24/5.0 versus a college average of 4.08. Students evaluated overall learning as 4.61/5.0 versus a college average of 4.14.*

15. Fall 2017: **Fundamentals of Programming (CSE 2)** three meetings per week, 72 enrolled in the course. *Students evaluated teaching effectiveness as 3.71/5.0 versus a college average of 4.04. Students evaluated course quality as 3.67/5.0 versus a college average of 4.06. Students evaluated overall learning as 4.20/5.0 versus a college average of 4.10.*

16. Fall 2017: **Structural Bioinformatics (BioE/CSE 307/407)** three meetings per week, 9 enrolled in the course. *Students evaluated teaching effectiveness as 4.43/5.0 versus a college average of 4.04. Students evaluated course quality as 4.71/5.0 versus a college average of 4.06. Students evaluated overall learning as 4.43/5.0 versus a college average of 4.10.*

    Spring 2017: *I did not teach in this semester in order to support my family during the birth of a child.*

17. Fall 2016: **Structural Bioinformatics (BioE/CSE 307/407)** three meetings 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.*

18. Fall 2016: **Fundamentals of Programming (CSE 2)** Two meetings 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.*

19. Spring 2016: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)** three meetings 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.*

20. Spring 2016: **Fundamentals of Programming (CSE 2)** Two meetings 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.*

21. Fall 2015: **Structural Bioinformatics (BioE/CSE 307/407)** three meetings 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.*

22. Fall 2015: **Fundamentals of Programming (CSE 2)** Two meetings 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.*

23. Spring 2015: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)** three meetings 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.*

24. Spring 2015: **Fundamentals of Programming (CSE 2)** Two meetings 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.*

25. Fall 2014: **Structural Bioinformatics (CSE 307/407)** three meetings 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.*

26. Fall 2014: **Fundamentals of Programming (CSE 2)** Two meetings 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.*

27. Spring 2014: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)** three meetings 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.*

28. Spring 2014: **Foundations of Programming (CSE 2)** Two meetings 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.*

29. Fall 2013: **Fundamentals of Programming (CSE 2)** Two meetings 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.*

30. Fall 2013: **Structural Bioinformatics (CSE 307/407)**. Tri-weekly meetings, 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.*

31. Fall 2013: **Bioinformatics in 21st Century. (BioS/CSE 090)**. Weekly meetings, 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.*

32. Spring 2013: **Fundamentals of Programming (CSE 2)** Two meetings 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.*

33. Spring 2013: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)**. Bi-weekly meetings, 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.*

34. Fall 2012: **Fundamentals of Programming (CSE 2)** Two meetings and one laboratory session per week, 58 students enrolled in my section of the course. **New course developed in this semester.** *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.*

35. Fall 2012: **Structural Bioinformatics (CSE 397/497)**. Bi-weekly meetings, 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.*

36. Spring 2012: **Bioinformatics: Issues and Algorithms (BioE/CSE 308/408)**. Bi-weekly meetings, 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.*

37. Fall 2011: **Bioinformatics in 21st Century. (BioS/CSE 090)**. Weekly meetings, 18 students. **New course developed in this semester.** *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.*

38. Fall 2011: **Structural Bioinformatics (CSE 397/497).** Bi-weekly meetings, 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.*

39. Spring 2011: **Bioinformatics: Issues and Algorithms (CSE 308/408)**. Bi-weekly meetings, 10 students. **Course redeveloped in this semester.** *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.*

40. Fall 2010: **Structural Bioinformatics (CSE 350/450).** Bi-weekly meetings, 3 students. **New course developed this semester.** *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.*

G.3 Curriculum Development

Summary: Developing or redeveloping a course is a tremendous undertaking. The efforts involved include, *at a minimum*, the creation or full replacement of all lecture slides, lecture notes, lecture videos, supporting materials, assignments, assignment rubrics, exams, exam rubrics projects, project grading rubrics, and the selection of class software and textbooks. In some cases, teaching assistant and grader staffing plans, staffing proposals, staff budgets, self-computing spreadsheets, ABET certification documents, academic integrity testing protocols, cloud storage organizational systems, proctoring instructions, may also need to be created.

Development or redevelopment efforts are orders of magnitude more substantial then the effort involved in reteaching a course in a future semester after development has been performed. When reteaching, I only create new assignments, projects and exams for core courses (freshman to junior level), or I refine the projects assigned in advanced courses (senior and graduate level), for integrity reasons.

During my career at Lehigh, seven courses were either newly developed or redesigned.

1. **CSE 4: Introduction to Programming B**. *New Course Development*, 2021. A new second-semester undergraduate course focused on making basic concepts in Java accessible for as many people as possible. Topics were selected specifically to synchronize with existing higher-level curricula after alignment with Advanced Placement Exam topic areas. As an experiment, the class was created with twice as much experiential time in the computer lab than its predecessor, CSE 2, so twice as much lab material was created for the class. Beyond the minimum materials involved in developing a new class, a scalable staffing plan and budget was created to handle dynamic pandemic-era class sizes, a new attendance system was created to engage students in virtual learning, and a new system for recording and posting lectures was developed.

2. **CSE 3: Introduction to Programming A**. *New Course Development*, 2020. A new first-semester undergraduate course focused on making basic concepts in Java accessible for as many people as possible. Curriculum modified for complementarity to Advanced Placement Exam structure, to better support incoming students at a range of qualifications. As an experiment, the class was created with twice as much experiential time in the computer lab than its predecessor, CSE 2, so twice as much lab material was created for the class. Beyond the minimum materials involved in developing a new class, a scalable staffing plan and budget was created to handle dynamic pandemic-era class sizes, a new attendance system was created to engage students in virtual learning, and a new system for recording and posting lectures was developed.

3. **CSE 313/413: Computer Graphics**. *Course Re-Designed*, 2018. An completely refreshed undergraduate and graduate course on computer graphics to reflect modern graphics techniques and technologies. The pre-existing conventional C-based OpenGL course was transformed into a javascript webGL-based course, enabling cross platform software development system was created to maximize inclusivity to the diversity of student computing hardware (laptops, phones, tablets, desktop computers). Novel assignments were created to drill students in the use of more sophisticated data structures, in linear algebra concepts, and mature software development practices.

4. **CSE 2: Fundamentals of Programming**. *New Course Development* with Brian Davison, 2012. A new undergraduate course focused on making basic concepts in Java accessible for as many people as possible. *Course Reorganized, 2013*. Grader, TA, and adjunct roles were redesigned to enhance scalability to many more students. *Course Instrumented, 2018*. Survey and assignment structures were redesigned to support educational research.

5. **CSE/BioE 308/408: Bioinformatics: Issues and Algorithms**. *Course Re-Designed*, 2011. A undergraduate and graduate course focused originally on the classic algorithms of genomics was redesigned based on research papers and knowledge of the wider field of bioinformatics. Cross-listed in both computer science and bioengineering curricula. Course features experiential and interdisciplinary projects for students with no programming background, and for others with no biological background, enabling students to experience firsthand the challenges of interdisciplinary communication.

6. **CSE/BioS 90: Bioinformatics in the 21^{st} Century**. *New Course Development*, 2011. A new undergraduate course for freshmen intended to illustrate concepts and new technologies in bioinformatics to students without any significant background. Cross-listed in both computer science and biological sciences curricula.

7. **CSE/BioE 307/407: Structural Bioinformatics**. *New Course Development*, 2010. A new undergraduate and graduate course based entirely on research papers and knowledge of the field. Full coverage of the diversity

of topics in computational structural biology, not found in any existing course or textbook, to my knowledge. A significant project component, *redesigned 2012*, gets students involved in novel research in the field. Cross-listed in both computer science and bioengineering curricula.

G.4 Advising, Research Direction: Doctoral Students, Lehigh University

1. Houliang Zhou, Fall 2021-Spring 2026 (Expected), on Computational Materials Science, co-advised and co-supported by Prof. Lifang He in the Dept. of Computer Science and Engineering.
2. Yangying Liu, Fall 2021-Spring 2026 (Expected), on Structural Bioinformatics.
3. Justin Tam, Fall 2020-Spring 2025 (Expected), on Structural Bioinformatics.
4. Shuyu Qin, Fall 2019-Spring 2024 (Expected), on Computational Materials Science, co-advised and co-supported by Prof. Joshua Agar in the Dept. of Materials Science and Engineering (now of Drexel University).
5. Jinbu Wang, Fall 2014-Spring 2020, on Structural Bioinformatics.
6. Ziyi Guo, Fall 2012-Summer 2017, Thesis titled "Leveraging Structural Flexibility to Predict Protein Function". **Now a researcher at Baidu Search Science.**
7. Debdas Paul, Fall 2011-Spring 2012, on Electrostatic Focusing and Protein Binding Specificity.

G.5 Advising, Research Direction: Masters Students, Lehigh University

1. Grant Armstrong, CSE major, Summer 2022-ongoing, on large scale analysis of the impact of Hydrogen bonds on protein-protein recognition.
2. Ben Zalatan, CSE major, Summer 2022-ongoing, on the prediction of abnormal grains in polycrystalline microstructures.
3. Omar Ahmed, CSE major, Spring 2019-Spring 2020, on geometric Analysis of Hydrogen bond Formation Trends. **Joined Johns Hopkins Ph.D. program in Computer Science.**
4. Chanh Nguyen, CSE major, Fall 2018-Spring 2019, on AI methods for classifying in protein specificity. **Now a Machine Learning Engineer at Lawrence Livermore National Laboratory.**
5. Georgi Georgiev, CSE major, Fall 2018-Spring 2019, Thesis titled "Algorithms in protein cavity classification". **Joined Stonybrook University Ph.D. program in Computer Science.**
6. Devan Bicher, CSE major, Fall 2013-Spring 2015, Thesis titled "A Volumetric Survey of Focusing and Electrostatic Contributions to Protein RNA Interfaces". **Now a Software Engineer at Memorial Sloan Kettering Cancer Center.**
7. Kevin Dodd, CSE major, Fall 2013-Summer 2016, on parallel exact constructive solid geometry on molecular surfaces.
8. Wenjie Yang, CSE major, Fall 2012-Summer 2013, on Surveys of Protein Cavities.
9. Yisheng Tang, CSE major, Fall 2012-Summer 2013, on statistical modeling of structural variations in protein binding sites. **Now a Senior Software Engineer at Compass.**

G.6 Advising, Research Direction: Undergraduate Students, Lehigh University

1. Felix M. Quintana, "3D convolutional neural networks for classifying protein binding sites." Fall 2019-Summer 2022. **Joined Rice University Ph.D. program in Computer Science.**
2. Ben Zalatan, "Volumetric visualization of metallic grain boundaries." Summer 2021-Ongoing. **Joined Lehigh University Ph.D. program in Computer Science.**

3. Surui Huang, "Design of an automated control system for STEM image acquisition and control." Summer 2021-Ongoing. **Joined Lehigh University predoctoral program in Materials Science while maintaining research activity.**

4. Joss Duff, "Design of an automated control system for STEM image acquisition and control." Summer 2021-Fall 2021.

5. Maximillian Machado, "Graph-based analysis of simulated metallic alloys." Summer 2021-Summer 2022.

6. Jack Kellerk, "Segmentation of kikuchi lines in CBED images for zone axis navigation." Summer 2021-Summer 2022. **Joined high frequency trading group at J.P. Morgan Chase & Co.**

7. Chesphongphach Buranasilp, "3D volumetric representations of hydrogen bond limits." Fall 2020-Summer 2022.
Joined University of California San Diego masters program in Computer Science.

8. Agustin Mendoza, "A web-based interface for remote microscope control." Summer 2020.

9. Allison Codi, Michelle Zhang, "AI methods for treating adolescent scoliosis." Fall 2019-Spring 2020.

10. Bethany Chen, Dylan Schaschl, "A large scale validation of volumetric methods for predicting electrostatic influences on protein-protein binding specificity." Spring 2019. **Bethany later joined JPMorgan Chase & Co.**

11. Poplar Yang, "Detecting influential mutations in immune checkpoints." Spring 2019.

12. Travis Barnes, Anna Thomas, Jack Kellerck, Desai Xie, Xuewei Wang, Eddie Sohn, Agustin Mendoza *Nanohuman Interface Summer Fellows*, "An AI-driven universal remote interface for Electron Microscopy." Summer 2019-Spring 2020. **Joined University of Michigan Ann Arbor PhD program in Mathematics.**

13. Desai Xie, "Deep Neural Networks for Protein Structure Comparison." Fall 2018-Spring 2019.
Joined Stonybrook University PhD program in Computer Science.

14. Stephanie Mason, "Exploring Protein Cavities through Rigidity Analysis." Summer 2018.

15. Davis Rempe, Summer 2016, REU student "Multimarker Object Detection in Augmented Reality".
Joined Stanford University PhD program in Computer Science.

16. Josiah Smith, Summer 2016, REU student "Multimarker Object Detection in Augmented Reality".

17. Georgi Georgiev, Summer 2015-ongoing, CSB major, "Parallelizing Constructive Solid Geometry Algorithms with Threading Building Blocks". **Joined Stonybrook University PhD program in Computer Science.**

18. Jacob Parker, Fall 2013-Spring 2014, IDEAS major, "Applying Structural Bioinformatics to Materials Science".

19. Rachel Okun, Summer 2015-Spring 2016, IBE major, "Parameterized statistical models of electrostatic variation". **Joined CourseHero.**

20. Chanh Nguyen, Fall 2013-ongoing, CSE major, "Javascript Visualization of Structural Bioinformatics Software Outputs".

21. Sara Grogan, Spring 2015-Spring 2016, BioE major, independent Study, "Electrostatic Analysis of Rescue Mutants in P53."

22. Emma Bird, Spring 2015-Spring 2015, BioE major, independent Study, "Selecting nucletides that control binding preferences in DNA."

23. Emily Levenson, Fall 2014-Spring 2016, BioE major, independent Study, "The Role of Electrostatics in SMAD4 trimer specificity."

24. Eric Metcalf, Fall 2013-Spring 2015, CSE major, independent Study, "Statistical Analysis of Protein Electrostatics." **Joined Brown University PhD program in Computer Science.**

25. Jonah Kohen, Spring 2013-Spring 2015, CompE major, independent Study, "Structural Analysis of Rescue Mutants in P53". **Joined Masters program in Computer Science at Stanford University**

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

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

28. Devan Bicher, Summer 2012-Summer 2013, BioE major, BioE independent study, "Predicting Resistance in HIV Proteases". **Joined Lehigh University Masters program in Computer Science.**

29. Bridget Nolan, Spring 2012-Spring 2015, BioE major, independent study, "Electrostatic influences on Protein-Protein Interfaces". **Joined Regeneron pharmaceuticals.**

30. Kevin Lee, Spring 2012-Summer 2013, BioE major, independent study, "Structural Analysis of Major Histocompatibility Complexes", **Joined masters program at Columbia University**

31. 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 later joined Microsoft**

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

33. 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 and later joined the PhD program in Computer Science at the University of Arizona**

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

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

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

G.7 Advising, Research Direction: High School Students Supervised

1. Udit Garg, Parkland High School, 2018-2019 "Structural Analysis of the CTLA4-CD80 and CTLA4-CD86 Interfaces." **Winner of the Merck Science Achievement Award, at Delaware Valley Science Competition, Spring 2019. Later accepted undergraduate admission to University of Pennsylvania.**

2. Juliana Hong, Liberty High School, 2014 "Molecular Superposition via mathematical optimization". **Co-author of "Superposition of Protein Structures Using Electrostatic Isopotentials", BIBM 2015. Later accepted undergraduate admission to Cornell University.**

G.8 Advising, Research Direction: Undergraduates Supervised, Rice University

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

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

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

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

5. Anand P. Dharan, summer 2004, later an engagement manager at McKinsey and Company.
6. Brad D. Dodson, summer 2005, later a software developer at Microsoft.
7. Jessica Y. Wu, summer 2005, later a Ph.D. student at the Massachusetts Institute of Technology.

G.9 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**.

H. SERVICE

I.1 Service at Lehigh University

I.1.a University-level Service Activities

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

I.1.b Service to the P.C. Rossin College of Engineering and Applied Sciences

1. Member, RCEAS Academic Policy Committee, Fall 2018 - Spring 2022.

I.1.c Service to Interdisciplinary Programs

1. CSE Liaison, Biocomputational Engineering Major curriculum development committee, Spring 2018-ongoing.
2. 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".
3. Guest lectures for BioE 02 on 4/18/2011, 4/9/2012, 3/4/2019 taught by Svetlana Tatic-Lucic, Dept. of Chemical Engineering. Titled: "Of Informatics and Biology".
4. Guest lecture, "Informatics for Biology" to Biosystems Dynamics Summer Institute, Lehigh University, June 9, 2011.
5. 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.

I.1.d Service to the Department of Computer Science and Engineering

1. Chair, Graduate Recruiting and Admissions, Computer Science and Engineering, Fall 2020 - ongoing.

2. Member, Tenure Track Faculty Search Committee, Computer Science and Engineering, AY 2021.
3. Member, Ad Hoc Committee on Teaching Load and Planning, Computer Science and Engineering, AY 2020.
4. Member, Tenure Track Faculty Search Committee, Computer Science and Engineering, AY 2019.
5. Member, Curriculum Committee, Computer Science and Engineering, AY 2019.
6. Member, Tenure Track Faculty Search Committee, Computer Science and Engineering, AY 2018.
7. Member, Curriculum Committee, Computer Science and Engineering, AY 2018.
8. Member, Tenure Track Faculty Search Committee, Computer Science and Engineering, AY 2016.
9. Member, CoreCS Tenure Track Faculty Search Committee, Computer Science and Engineering, AY 2015.
10. Chair, Building C Rules and Procedures (R&P) Development Committee, 2016.
11. Member, Tenure Track Faculty Search Committee, Computer Science and Engineering, AY 2014.
12. Colloquium Chair, 2012-2016. Hosted William Craelius (2015), Lydia Kavraki (2012), Amarda Shehu (2011), Willy Wriggers (2015).
13. Lehigh ACM club Co-Advisor, 2012-2014.
14. Facilities Committee, Fall 2010-Spring2018. Assisted in the development and implementation of two internal funding proposals instructional labs.
15. Guest lectures for CSE 411 (fall 2012 onwards, annually) titled: "Numerical Precision".
16. Guest lectures for CSE 497/406 (fall 2010 onwards, annually) titled: "Structural Bioinformatics".
17. Guest lectures for CSE 406 (fall 2015, 2016) titled: "Ethics and Academic Integrity".
18. Presenter, Candidates Day, for students considering Computer Science and Engineering majors, 2011, 2012, 2013, 2014.
19. Graduate Admissions Committee, academic year 2010-2011. Assisted in the evaluation of M.S. and Ph.D. applications for Fall 2011.
20. Host for visitor Lydia Kavraki, Noah Harding Professor of Computer Science and Bioengineering at Rice University, March 20, 2012, to department colloquium.
21. Host for visitor Amarda Shehu, Assistant Professor of Computer Science at George Mason University, at department colloquium 3/16/2011.

I.1.e Service to Other Departments

1. Member, Tenure Track faculty search committee, BioEngineering, AY 2019.
2. Member, Industrial and Systems Engineering Tenure Track Faculty Search Committee, AY 2013.
3. Member, Industrial and Systems Engineering Tenure Track Faculty Search Committee, AY 2013.
4. Member, Neuroscience Faculty Tenure Track 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.
5. Member, Civil Infrastructure Systems Faculty Tenure Track 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.

I.2. Professional Service

I.2.a Offices and Committee Memberships in Professional Organizations

1. IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2022).
   - **Vice Chair:** Oversaw the review of 150 papers by 346 reviewers across a wide range of subfields in bioinformatics for IEEE's flagship bioinformatics conference.
   - **Workshop Co-Chair:** Promotion, selection, and management of 25 workshops at the core of IEEE's flagship bioinformatics conference (2015, 450+ Attendees).
   - **Workshop Co-Chair:** Promotion, selection, and management of 25 workshops at the core of IEEE's flagship bioinformatics conference (2012, 400+ Attendees).
2. Computational Structural Bioinformatics Workshop (CSBW).
   - **Steering Committee Member:** Promotion of and visioning for the premier algorithms-focused workshop in structural bioinformatics (2015-ongoing).
   - **Co-Chair:** Coordinated the peer review of papers, organized workshop logistics, scheduling and communications (2011-2015).

I.2.b Service on Grant Review Panels for Federal Agencies

1. NSF Directorate for Computer and Information Science and Engineering (CISE)
2. NSF Directorate for Biological Sciences (BIO)

I.2.c Service to International Conferences in my Research Field (Program Committee)

Note: While initially I was reviewing manuscripts for every conference each year, I have slowly reduced this activity to focus on organizational work. I am still active in several program committees each year, but I do not review manuscripts for every conference every year.

1. Intelligent Systems for Molecular Biology (ISMB) 2013-ongoing (not all years).
2. Research in Computational Molecular Biology (RECOMB) 2013-ongoing (not all years).
3. Computational Structural Bioinformatics Workshop (CSBW) 2011-ongoing.
4. IEEE International Conference on Bioinformatics and Biomedicine (BIBM) 2012-ongoing (not all years).
5. ACM Conf. on Bioinformatics, Computational Biology and Biomedicine (BCB) 2012-ongoing (not all years).
6. Asia Pacific Bioinformatics Conference (APBC) 2014-2020.
7. European Conference on Computational Biology (ECCB)

I.2.d Service to Journals in my Research Field (Manuscript Review)

1. PLoS Computational Biology
2. BMC Bioinformatics
3. IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB)
4. International Journal of Data Mining and Bioinformatics (IJDMB)
5. International Journal of Computational Biology and Drug Design (IJCBDD)
6. International Conference on Bioinformatics (INCOB)

7. International Work-Conference on Bioinformatics and Biomedical Engineering
8. Computer Aided Design
9. Journal of Bioinformatics and Computational Biology (JBCB)
10. MDPI Molecules
11. MDPI Biomolecules

I.2.e Professional Society Memberships

1. International Society for Computational Biology, member (2006-).
2. Association for Computing Machinery, member (2010-).
3. Institute of Electrical and Electronic Engineers, member (2010-).
4. Life Sciences Society, member (2006-2010).
5. Sigma Xi, member (2010-2011).
