

## Guang Song

### Associate Professor of Computer Science

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### Research Interests

Computational Biology: Protein Structure and Dynamics, Ligand Migration Pathways, Structure-Function Studies of Biophysical Processes, Molecular Dynamics Simulations, Normal Mode Analysis, Coarse-Grained Modeling, Elastic Network Models, Ensemble-based Studies

Other interests: Motion Planning, Robotics, Virtual Reality, Molecular Docking, Quantum Computing

### Education

**Postdoctoral Training in Computational Biology**, Iowa State University 2003-2006

Advisor: Prof. Robert L. Jernigan

**Ph.D. in Computer Science**, Texas A&M University, December 2003

Ph.D. Thesis: A Motion Planning Approach to Protein Folding

Thesis advisor: Prof. Nancy M. Amato

**M.S. in Physics**, Texas A&M University, May 1998 (GPA 4.00/4.00)

**B.S. in Physics**, Jilin University, China, July 1992 (Major GPA 94.5/100)

### Honors and Awards

- NSF CAREER Award, "A computational framework for mapping ligand migration channel networks and predicting molecular control mechanisms", NSF, 2010 - 2016, PI: Guang Song, \$500,000.
- COMPAS Junior Faculty Award, Department of Computer Science, Iowa State University, 2007
- IBM Research PhD Fellowship, 2002 - 2003.
- Excellent Graduate Student Research Award, Computer Science Department, Texas A&M University, 2003.
- Anton Philips Best Student Paper Award Finalist, IEEE International Conference on Robotics and Automation (ICRA), May 2001. Paper Title: "A Motion Planning Approach to Folding: From Paper Craft to Protein Folding" (6 finalists from 678 accepted papers)
- Recipient of the Challenges in Quantum Computing Award, Computer Science Department, Texas A&M University, Fall 2001
- Undergraduate Scholarship for Academic Excellence, Jilin University, 1989 - 1992 (Class rank 1/52)

### Professional Experience

- Associate Professor, Department of Computer Science, Iowa State University, Fall 2012 - present
- Assistant Professor, Department of Computer Science, Iowa State University, Fall 2006 - 2012
- Faculty Member, Bioinformatics and Computational Biology (BCB) Graduate Program, Iowa State University, Fall 2006 - present
- Faculty Member, Laurence H. Baker Center for Bioinformatics and Biological Statistics, Iowa State University, Fall 2006 - present
- Postdoctoral Research Associate, Advisor: Prof. Robert L. Jernigan, Laurence H. Baker Center for Bioinformatics and Biological Statistics, Iowa State University, Fall 2003 - present
- Instructor, Department of Computer Science, Texas A&M University, Spring 2002
  - Taught 5 week graduate class in bioinformatics. Covered an introduction to bioinformatics, protein structure basis, protein structure prediction methods, PRM-based approach to protein folding pathways, molecular dynamics, Monte Carlo simulation, statistical mechanical models, lattice models, folding kinetics
- Research Assistant, Department of Computer Science, Texas A&M University, 1998 - 2002
  - Applied motion planning techniques to study protein folding pathways/kinetics
  - Applied randomized motion planners and haptic device to molecular docking
  - Worked on Randomized Probabilistic Roadmap algorithms for motion planning
  - Researched cooperative human-machine motion planning using PHANToM haptic device
  - Developed motion planning techniques for nonholonomic systems
- Research Assistant, Department of Physics & Cyclotron Institute, Texas A&M University, Summer 1997
  - Used a large simulation program as an event generator, built subroutines to study antikaon production in relativistic nucleus-nucleus collisions
- Teaching Assistant, Department of Physics, Texas A&M University, 1995 - 1998
  - Courses: Undergraduate Mechanics, Electricity & Optics
  - Weekly TA duties: taught recitation (2 hr), lab instruction (4 hr), graded homework and lab reports, held office hours and help desk hours
- Full-time Assistant Researcher, China Institute of Atomic Energy, Beijing, 1992 - 1995
  - Developed computer simulation programs to study physics in relativistic heavy ion collisions

## Professional Activities

Editorial Board,  
Current Proteomics, 2007 - present

Proposal Review Panel: NSF CCF core, 2010

Program Committee Member,

- IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS), 2005, 2006.
- Robotics: Science and Systems (RSS), 2006, 2007, 2009
- IEEE BIBM Workshop on Computational Structural Bioinformatics, 2007-09, 2011, 2013-14
- RSS Workshop on Robotics Methods for Structural and Dynamic Modeling of Molecular Systems, 2014, Berkeley, CA

Reviewer, for journals (*PLOS Computational Biology*; *Proceedings of National Academy of Sciences of USA (PNAS)*; *Bioinformatics*; *Biophysical Journal*; *BMC Structural Biology*; *Physical Biology*; *Proteins: Structure, Function, and Bioinformatics*; *Journal of Computational Chemistry*; *Robotics and Computer-Integrated Manufacturing*; *IEEE Transactions on Robotics*; *IEEE Transactions on Automation Science and Engineering*; *International Journal of Robotics Research*; *IEEE Transactions on Parallel and Distributed Systems*)

Reviewer, for conferences (*Pacific Symposium of Biocomputing (PSB)*; *International Conference on Research in Computational Molecular Biology (RECOMB)*; *IEEE International Conference on Robotics and Automation (ICRA)*; *IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*).

### **Institutional and Departmental Services**

Graduate Admission Committee  
BCB Admission Committee  
BCB Curriculum Committee  
Outreach Committee  
Retention Committee  
Undergraduate Committee  
Library Committee  
Scholarship/Awards Committee

### **Student Advising**

#### **As Major or co-major professor:**

Lin, Tu-Liang (PhD, graduated in 2012, recipient of John V. Atanasoff Award, Department of Computer Science, Iowa State University)

Vammi, Vijay (PhD student, graduated, May 2015)

Na, Hyuntae (PhD student, recipient of Robert Stewart Early Research Award, Department of Computer Science, Iowa State University (2013), recipient of University Research Excellence Award in 2014)

Chen, Liping (MS, graduated, May 2014)

Liu, Xiaoteng (MS, since 2014, graduated, 2015)

Zhang, Ce (MS, since 2014)

Jae-Kyun Song (MS, since August 2015)

Hailu Yang (MS, since Jan 2016)

Cheng, Haitao (Co-major Prof. PhD, graduated)

Kapoor, Abijeet (Co-major Prof., PhD, graduated, 2014)

Mishra, Sambit (co-major professor, 2014)

#### **As Ph.D. Program of Study Committee Member:**

Tian, Jiang (Member. Graduated)

Zhou, Wengang (Member, Graduated)

Jordan-Osorio, Rafael A. (Member, Graduated)

Wu, Feihong (Member. Graduated)

Sit, Atilla (Member. Graduated)

Gao, Yang (Member, Graduated)

Ravindrudu, Rahul (Member. Graduated)

Zimmermann, Michael (Member, graduated)  
Xue, Li (Member, graduated)  
Muppirala, Usha (Member, 2010-2013, graduated)  
Chen, Yingfei (Member, graduated)  
Chakraborty, Debkanta (Member, graduated)  
Andorf, Carson (2011-2013, graduated)  
Nikolova, Olga (2012, graduated)  
Du, Chuanlong (2012 -2014)  
Guo, Feng (2014, graduated)

Watanabe, Muneaki (Member)  
Lin, Hua (2011-2013 MS, 2014-)  
Voller, Zack (2011)  
Chopra, Nikita (2012)  
Sankar, Kannan (2012)  
Jia, Kejue (since 2013)  
Wang, Yuan (since 2013)  
Liu, Jie (2013)  
Nakayama, Brian (March 2014)  
Cho, KyoungTak (2014)  
Huang, Lunan (Physics, 2014)

**As M.S. Program of Study Committees:**

Wang, Feifei (2013, graduated in May 2014)

**Undergraduate advising:**

Hu, Keji (March 2011-Dec 2011)  
Cai, Kenson (high school intern, 2013-2014)

**Publications in Refereed Journals**

Computational Biology:

1. Hyuntae Na, Guang Song, and Daniel ben-Avraham, “Universality of Vibrational Spectra of Globular Proteins”, *Physical Biology*, accepted, 2016
2. Santhosh V. Vammi and Guang Song, “Ensembles of a Small Number of Conformations with Relative Populations”, *Journal of Biomolecular NMR*, 63(4):341-351, 2015.
3. Hyuntae Na, Robert L. Jernigan, and Guang Song, “Bridging between NMA and Elastic Network Models: Preserving All-atom Accuracy in Coarse-grained Models”, *PLoS Comput Biol* 11(10): e1004542, 2015. doi:10.1371/journal.pcbi.1004542
4. Hyuntae Na and Guang Song, “The performance of fine-grained and coarse-grained elastic network models and its dependence on various factors”, *Proteins*, 83(7):1273-1283, 2015
5. Hyuntae Na and Guang Song, “Quantitative Delineation of How Breathing Motions Open Ligand Migration Channels in Myoglobin and Its Mutants”, *Proteins*, 83(4):757-770, 2015

6. Hyuntae Na and Guang Song, "Conventional NMA As a Better Standard for Evaluating Elastic Network Models", *Proteins*, 83(2):259-267, 2015
7. Hyuntae Na and Guang Song, "A Natural Unification of GNM and ANM and the role of inter-residue forces", *Physical Biology*, 11(3):036002, 2014
8. Hyuntae Na and Guang Song, "Bridging between NMA and Elastic Network Models", *Proteins*, 2014, 82(9):2157-68, 2014.
9. Santhosh V. Vammi, Tu-Liang Lin, and Guang Song, "Enhancing the Quality of Protein Conformation Ensembles With Relative Populations", *Journal of Biomolecular NMR*, 58(3):209-25, 2014.
10. Tu-Liang Lin and Guang Song, "Efficient Mapping of Ligand Migration Channel Networks in Dynamic Proteins", *Proteins*, 79:2475-90, 2011.
11. Tu-Liang Lin and Guang Song, "Generalized Spring Tensor Models for Protein Fluctuation Dynamics and Conformation Changes," *BMC Structural Biology*, 2010, Suppl 1:S3. Selected papers from 2009 IEEE BIBM Workshop on Computational Structural Bioinformatics.
12. Lei Yang, Guang Song, and Robert L. Jernigan, "Protein Elastic Network Models and the Ranges of Cooperativity", *Proc. Natl. Acad. Sci. USA*, 106:12347-52, 2009.
13. Andrzej Kloczkowski, Robert L. Jernigan, Zhijun Wu, Guang Song, Lei Yang, Andrzej Kolinski and Piotr Pokarowski, "Distance Matrix-Based Approach to Protein Structure Prediction", *Journal of Structural and Functional Genomics*, 10:67-81, 2009
14. Lei Yang, Guang Song, and Robert L. Jernigan, "Comparison of Experimental and Computed Protein Anisotropic Temperature Factors," *Proteins*, 76:164-175, 2009.
15. Lei Yang, Guang Song, Alicia Carriquiry and Robert L. Jernigan, "Close Correspondence between the Essential Protein Motions from Principal Component Analysis of Multiple HIV-1 Protease Structures and Elastic Network Modes," *Structure*, 16(2):321-30, 2008
16. Guang Song and Robert L. Jernigan, "vGNM: a Better Model for Understanding the Dynamics of Proteins in Crystals" *Journal of Molecular Biology*, 369(3):880-93, 2007.
17. Lei Yang, Guang Song, and Robert L. Jernigan, "How Well Can We Understand Large-Scale Protein Motions Using Normal Modes of Elastic Network Models?" *Biophysical Journal*, 93(3):920-9, 2007.
18. Guang Song and Robert L. Jernigan, "An Enhanced Elastic Network Model to Represent the Motions of Domain-Swapped Proteins," *Proteins*, 63(1):197-209, 2006.
19. Shawna Thomas, Guang Song, and Nancy M. Amato, "Protein folding by motion planning," *Physical Biology*, 2(4):S148-55, 2005.
20. Xinyu Tang, Bonnie Kirkpatrick, Shawna Thomas, Guang Song, and Nancy M. Amato, "Using Motion Planning to Study RNA Folding Kinetics," *Journal of Computational Biology*, 12(6):862-81, 2005.
21. Guang Song and Nancy M. Amato, "A Motion Planning Approach to Folding: From Paper Craft to Protein Folding," *IEEE Transactions on Robotics and Automation*, 20(1):60-71, 2004.
22. Nancy M. Amato, Ken A. Dill, and Guang Song, "Using Motion Planning to Map Protein Folding Landscapes and Analyze Folding Kinetics of Known Native Structures," *Journal of*

Computational Biology, 10(3-4):239-256, 2003. Featuring selected papers from RECOMB 2002.

23. Nancy M. Amato and Guang Song, "Using Motion Planning to Study Protein Folding Pathways," *Journal of Computational Biology*, 9(2):149-168, 2002. Featuring selected papers from RECOMB 2001.

#### Virtual Reality and Haptic Input:

24. O. Burchan Bayazit, Guang Song, Nancy M. Amato, "Enhancing Randomized Motion Planners: Exploring with Haptic Hints," *Autonomous Robots*, 10(2):163-174, 2001. Special issue on Personal Robotics.

#### Quantum Computing:

25. Guang Song and Andreas Klappenecker, "Optimal Realizations of Simplified Toffoli Gates," *Journal of Quantum Information and Computation*, 4(5):361-372, 2004.
26. Guang Song and Andreas Klappenecker, "Optimal Realizations of Controlled Unitary Gates," *Journal of Quantum Information and Computation*, 3(2):139-155, 2003.

#### Physics:

27. Guang Song, Bao-An Li, Che-Ming Ko, "Antikaon Production and Medium Effects in Heavy-Ion Collisions at AGS," *Nuclear Physics A*, 646(4):481-499, 1999.
28. Zhongqi Wang, Benhao Sa, Guang Song, Xiaoze Zhang, Zhongdao Lu, Yuming Zheng, "Rescattering Effect of Pion on K/PI Ratio in Relativistic Nucleus-Nucleus Collisions," *Nuclear Physics A*, 566:495-498, 1994.
29. Zhongqi Wang, Benhao Sa, Xiaoze Zhang, Guang Song, Zhongdao Lu, Yuming Zheng, "Systematic Behavior of K/PI Ratio in Relativistic Nucleus-Nucleus Collisions," *Physical Review C*, 48(6):2995-2999, 1993.
30. Zhongqi Wang, Benhao Sa, Xiaoze Zhang, Zhongdao Lu, Guang Song, Yuming Zheng, "Rapidity, Transverse Mass Distribution and Nuclear Stopping in 14.6GeV/c Si+Au Reactions," *Chinese Physics Letters*, 10:468, 1993.

#### **Publications in Refereed Conference Proceedings**

##### Computational Biology:

31. Hyuntae Na and Guang Song, "Quantitative Delineation of How Protein Breathing Motions Open Ligand Migration Channels", in *Proceedings of 2014 RSS (Robotics: Science and Systems) Workshop on Robotics Methods for Structural and Dynamic Modeling of Molecular Systems*, 7 pages, 2014, Berkeley, CA (<https://cs.unm.edu/amprg/rss14workshop/PAPERS/Na.pdf>)
32. Hyuntae Na and Guang Song, "Ellipsoid-Weighted Protein Conformation Alignment", *Proceedings of the 9<sup>th</sup> International Symposium on Bioinformatics Research and Application (ISBRA)*, Charlotte, NC, USA, May 2013. *Lecture Notes in Computer Science* 7875:273-285, 2013
33. Tu-Liang Lin, Shantosh K. Vammi, and Guang Song, "Evaluate the Quality of Conformation Sampling Methods Using Experimental Residual Dipolar Coupling Data", in *Proceedings of 2011 ACM Conference on Bioinformatics, Computational Biology, and Biomedicine (ACM-BCB)*, Chicago, Illinois.

34. Tu-Liang Lin and Guang Song, "Generalized Spring Tensor Models for Protein Fluctuation Dynamics and Conformation Changes," in Proceedings of the 2009 IEEE BIBM Workshop on Computational Structural Bioinformatics, pp. 136-143, November 2009, Washington DC, USA.
35. Tu-Liang Lin and Guang Song, "Predicting Allosteric Communication Pathways Using Motion Correlation Network," in Proceedings of the 7th Asia Pacific Bioinformatics Conference(APBC), pp. 588-598, Beijing, China, January 2009.
36. Lei Yang, Guang Song, and Robert L. Jernigan, "Comparison of Experimental and Computed Protein Anisotropic Temperature Factors," in Proceedings of the 2007 IEEE BIBM Workshop on Computational Structural Bioinformatics, pp. 89-96, November 2007, Silicon Valley, USA.
37. Xinyu Tang, Bonnie Kirkpatrick, Shawna Thomas, Guang Song, and Nancy M. Amato, "Using Motion Planning to Study RNA Folding Kinetics," in Proceedings of the 8th ACM International Conference on Computational Molecular Biology (RECOMB), pp. 252-261, March 2004, San Diego, California.
38. Guang Song, Shawna L. Thomas, Ken A. Dill, J. Martin Scholtz and Nancy M. Amato, "A Path Planning-based Study of Protein Folding with a Case Study of Hairpin Formation in Protein G and L," in Proceedings of the 2003 Pacific Symposium on Biocomputing (PSB), pp. 240-251, January 2003, Hawaii, U.S.A.
39. Nancy M. Amato, Ken A. Dill, and Guang Song, "Using Motion Planning to Map Protein Folding Landscapes and Analyze Folding Kinetics of Known Native Structures," in Proceedings of the 6th ACM International Conference on Computational Molecular Biology (RECOMB), pp. 2-11, April 2002, Washington D.C., U.S.A.
40. Guang Song and Nancy M. Amato, "A Motion Planning Approach to Folding: From Paper Craft to Protein Folding," in Proceedings of the 2001 IEEE International Conference on Robotics and Automation (ICRA), pp. 948-953, May 2001, Seoul, Korea. **One of six finalists selected from 678 accepted papers for Best Student Paper Award.**
41. Guang Song and Nancy M. Amato, "Using Motion Planning to Study Protein Folding Pathways," in Proceedings the 5th ACM International Conference on Computational Molecular Biology (RECOMB), pp. 287-296, April 2001, Montreal, Canada.

#### Virtual Reality and Haptic Input:

42. O. Burchan Bayazit, Guang Song, and Nancy M. Amato, "Ligand Binding with OBPRM and User Input," in Proceedings of the 2001 IEEE International Conference on Robotics and Automation (ICRA), pp. 954-959, May 2001, Seoul, Korea.
43. O. Burchan Bayazit, Guang Song, Nancy M. Amato, "Enhancing Randomized Motion Planners: Exploring with Haptic Hints," in Proceedings of the 2000 IEEE International Conference on Robotics and Automation (ICRA), pp. 529-536, April 2000, San Francisco, California.

#### Motion Planning Techniques and Applications:

44. Guang Song, Shawna L. Thomas, and Nancy M. Amato, "A General Framework for PRM Motion Planning," in Proceedings of the 2003 IEEE International Conference on Robotics and Automation (ICRA), pp. 4445-50, September 2003, Taiwan.

45. Guang Song and Nancy M. Amato, "Randomized Motion Planning for Car-like Robots with C-PRM," in Proceedings of the 2001 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS), pp. 37-42, November 2001, Hawaii, U.S.A.
46. Guang Song, Shawna Miller, Nancy M. Amato, "Customizing PRM Roadmaps at Query Time," in Proceedings of the 2001 IEEE International Conference on Robotics and Automation (ICRA), pp. 1500-1505, May 2001, Seoul, Korea.

### **Book Chapters**

47. Hyuntae Na, Tu-Liang Lin, and Guang Song, "Generalized Spring Tensor Models for Protein Fluctuation Dynamics and Conformation Changes," in Ke-li Han, Xin Zhang, and Ming-jun Yang, editors, Protein Conformation Dynamics, Advances in Experimental Medicine and Biology, Volume 805, pages 107-135, Springer, 2014.
48. Robert L. Jernigan, Lei Yang, Ozge Kurkcuoglu, Guang Song, and Pemra Doruker, "Elastic Network Models of Coarse-Grained Proteins Are Effective for Studying the Structural Control Exerted over Their Dynamics," in Gregory A. Voth, editor, Coarse-Graining of Condensed Phase and Biomolecular Systems, pp. 237-254, Chapman and Hall/CRC Press, Taylor and Francis Group, 2008
49. O. Burchan Bayazit, Guang Song, Nancy M. Amato, "Ligand Binding with OBPRM and Haptic User Input: Enhancing Automatic Motion Planning with Virtual Touch," Currents in Computational Molecular Biology, N. El-Mabrouk, T. Lengauer and D. Sankoff (eds.), Les Publications CRM, Montreal, Canada, 2001, pp. 81-82. Book includes short papers from the 5th ACM International Conference on Computational Molecular Biology (RECOMB), April 2001, Montreal, Canada.

### **Publications in Non-Refereed Conference Proceedings**

50. Nancy M. Amato, O. Burchan Bayazit, Guang Song, "Providing Haptic 'Hints' to Automatic Motion Planners," in Proceedings of the 4th PHANTOM User's Group Workshop (PUG), October 1999.
51. Guang Song, "Parton Cascade Model," in Proceedings of Modeling Relativistic Heavy Ions Collisions Workshop, China Center of Advanced Science and Technology, 1994, Beijing, China.

### **Conference Posters**

52. Nancy M. Amato and Guang Song, "A Motion Planning Approach to Protein Folding," Poster, the 8th International Conference on Intelligent System for Molecular Biology (ISMB), August 2000, La Jolla, California.