

# Zhijun Wu

Professor of Mathematics  
Member of Graduate Faculty

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## **Education**

Ph.D., Computational and Applied Mathematics, Rice University, 1991

M.A., Computer Science / Computational Linguistics, Wuhan University, China, 1985

B.Eng., Computer Science, Huazhong University of Sci. and Tech., China, 1982

## **Professional Experience**

Professor, Department of Mathematics, Program on Bioinformatics and Computational Biology, Iowa State University, 2008 --

Associate Professor, Department of Mathematics, Program on Bioinformatics and Computational Biology, Iowa State University, 2000 -- 2008

New Direction Research Professor, Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, Minnesota, September 2007 – June 2008

Visiting Professor, Mathematical Biosciences Institute, Ohio State University, Columbus, Ohio, January 2005 – May 2005

Senior Research Associate, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, Illinois, April 1994 – September 1997

Postdoctoral Associate, Advanced Computing Research Institute, Cornell University, Ithaca, New York, June 1991 – April 1994

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## **Research and Scholarship**

### **Research Interests**

Computational Mathematics: Numerical linear algebra, nonlinear optimization, linear programming, integer and combinatorial optimization, numerical solution of ordinary and partial differential equations, parallel high-performance computing

Computational Biology: Molecular distance geometry, protein structure refinement, simulation of transition of protein conformation, constrained molecular dynamics, potential energy minimization, protein geometry databases, evolutionary game dynamics, inverse evolutionary games

## Publications

Books and Journal Papers:

1. **Zhijun Wu**, Lecture Notes on Computational Structural Biology (book), published by World Scientific Publishing Co., 2008 (250 pages)
2. Min Wang, Yuanyuan Huang, and **Zhijun Wu**, Simulation of Yeast Cooperation in 2D, *Bulletin of Mathematical Biology* 78, 531-555, 2016
3. Yuanyuan Huang, Kejue Jia, Robert Jernigan, and **Zhijun Wu**, A Web Server for Protein Structure Evaluation Using Residue Level Angle Correlation Plots, in *Proceedings of 2015 International Symposium on Bioinformatics Research and Applications*, Springer, 2015
4. Yunayuan Huang, Min Wang, Yiping Hao, Wen Zhou, and **Zhijun Wu**, Optimality and Stability Conditions of Evolutionary Games with Applications in Genetic Selection, *Journal of Mathematical Biosciences and Engineering* 12, 503-523, 2015
5. Junkoo Park, Robert Jernigan, and **Zhijun Wu**, Coarse-Grained NMA vs. Refined GNM for Protein Residue-Level Fluctuations, *Bulletin of Mathematical Biology* 75, 124-160, 2013
6. Peter Vedell and **Zhijun Wu**, A Multiple Shooting Algorithm for Solving the Boundary Value Problems in Molecular Dynamics Simulation, *Numerical Analysis and Modeling* 10, 920-942, 2013
7. Yuanyuan Huang and **Zhijun Wu**, Game Dynamic Model for Yeast Development, *Bulletin of Mathematical Biology* 74, 1469-1484, 2012
8. Yuanyuan Huang, Stephen Bonett, Andrzej Kloczkowski, Robert Jernigan, and **Zhijun Wu**, PRESS – A Software Package for Exploring Protein Residue Level Structural Statistics, *Journal of Bioinformatics and Computational Biology* 10, 2012
9. Zach Voller and **Zhijun Wu**, Distance Geometry Methods for Protein NMR Structure Determination, in *Distance Geometry: Theory, Methods, and Applications*, A. Mucherino, C. Lavor, L. Liberti, N. Maculan, Eds., Springer, 2012
10. Yuanyuan Huang, Stephen Bonett, Andrzej Kloczkowski, Robert Jernigan, and **Zhijun Wu**, Statistical Measures on Protein Residue Level Structural Properties, *Journal of Structural and Functional Genomics* 12, 119-136, 2011
11. Atilla Sit and **Zhijun Wu**, Solving a Generalized Distance Geometry Problem for Protein Structure Determination, *Bulletin of Mathematical Biology* 73, 2809-2836, 2011
12. Xinlong Luo and **Zhijun Wu**, Least-Squares Approximations in Geometric Buildup for Solving Distance Geometry Problems, *Journal of Optimization Theory and Applications* 149, 580-598, 2011
13. Ajith Gunaratne and **Zhijun Wu**, A Penalty-Function Method for Constrained Molecular Dynamics Simulation, *Numerical Analysis and Modeling* 8, 496-517, 2011
14. Zhenzhen Zheng, Xinlong Luo, and **Zhijun Wu**, A Geometric Buildup Algorithm for the Solution of the Sensor Network Localization Problem, *Mathematical Problems in Engineering*, Vol. 2012, Article ID 927031, DOI:10.1155/2012/927031, 2011

15. Di Wu, Steve Smith, Hanna Mahan, Robert Jernigan, and **Zhijun Wu**, Analysis of Protein Dynamics Using Local DME Calculations, *International Journal of Bioinformatics Research and Applications* 7, 146-161, 2011
16. Di Wu and **Zhijun Wu**, Superimposition of Protein Structures with Dynamically Weighted RMSD, *Journal of Molecular Modeling* 16, 611-622, 2010
17. Atilla Sit, **Zhijun Wu**, and Yaxiang Yuan, A Geometric Buildup Algorithm for the Solution of the Distance Geometry Problems with the Least-Squares Approximation, *Bulletin of Mathematical Biology* 71, 1914-1933, 2009
18. Xiaoyong Sun, Di Wu, Robert Jernigan, and **Zhijun Wu**, PRTAD: A Protein Residue Torsion Angle Distribution Database, *International Journal of Data Mining and Bioinformatics* 3, 469-482, 2009
19. Feng Cui, Kriti Mukhopadhyay, Wonbin Young, Robert Jernigan, and **Zhijun Wu**, Improvement of Under-Determined Loop Regions of Human Prion Protein by Database Derived Distance Constraints, *International Journal of Data Mining and Bioinformatics* 3, 454-468, 2009
20. Andrzej Kloczkowski, Robert 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, 2008
21. Rahul Ravindrudu, Di Wu, Ajith Gunaratne, Yaping Feng, and **Zhijun Wu**, A Parallel High-Performance System for Protein Structure Refinement, in *Proceedings of IEEE International Conference on Bioinformatics and Biomedicine*, 25-32, 2008
22. Dan Yang, Tao Jin, Hengfu Zou, and **Zhijun Wu**, Dual Stepsize Explicit Numerical Integration Method and Applications, in the *Proceedings of the IEEE Power Engineering Society General Meeting*, 2008
23. Feng Cui, Robert Jernigan, and **Zhijun Wu**, Knowledge-Based versus Experimentally Acquired Distance and Angle Constraints for NMR Structure Refinement, *Journal of Bioinformatics and Computational Biology* 6, 283-300, 2008
24. Di Wu, **Zhijun Wu**, and Yaxiang Yuan, The Solution of the Distance Geometry Problem for Protein Modeling via Geometric Buildup, *Physical Reviews and Letters* 3, 43-75, 2008
25. **Zhijun Wu** and Yin Zhang, Solving Large Scale Double Digestion Problems for DNA Restriction Mapping by Using Branch and Bound Integer Linear Programming, *International J. of Bioinformatics Research and Applications* 4, 351- 362, 2008
26. Di Wu, **Zhijun Wu**, and Yaxiang Yuan, Rigid vs Unique Determination of Protein Structures with Geometric Buildup, *Optimization Letters* 2, 319-331, 2008
27. Di Wu, Robert Jernigan, and **Zhijun Wu**, Refinement of NMR-Determined Protein Structures with Database Derived Mean Force Potentials, *Proteins: Structure, Function, Bioinformatics* 68, 232-242, 2007
28. Di Wu, Feng Cui, Robert Jernigan, and **Zhijun Wu**, PIDD: A Protein Inter-atomic Distance Distribution Database, *Journal of Nucleic Acid Research* 35, D202-D207, 2007

29. Di Wu and **Zhijun Wu**, An Updated Geometric Buildup Algorithm for Solving the Molecular Distance Geometry Problem with Sparse Distance Data, *Journal of Global Optimization* 37, 661-673, 2007
30. **Zhijun Wu**, Linear Algebraic Computing in Biomolecular Modeling (book chapter), in *Encyclopedia of Linear Algebra*, Leslie Hogben, ed., Chapman/Hall CRC Press, 60.1-60.15, 2006
31. Feng Cui, Robert Jernigan, and **Zhijun Wu**, Refinement of NMR-Determined Protein Structures with Database Derived Distance Constraints, *Journal of Bioinformatics and Computational Biology* 3, 1315-1330, 2005
32. Feng Cui, Tauqir Bibi, and **Zhijun Wu**, A Matlab Toolbox for Macromolecular Modeling, in *Advances in Bioinformatics and Its Applications*, Mathew He, Giri, Narasimhan, and Sergei Petoukhov, eds., 319-328, 2004
33. Jeong-Mi Yoon, Yash Gad, and **Zhijun Wu**, Mathematical Modeling of Protein Structure with Distance Geometry, in *Numerical Linear Algebra and Optimization*, Y. Yuan, ed., Scientific Press, 68-80, 2003
34. Qunfeng Dong and **Zhijun Wu**, A Geometric Buildup Algorithm for Solving the Molecular Distance Geometry Problem with Sparse Distance Data, *Journal of Global Optimization* 26, 321-333, 2003
35. John Dennis and **Zhijun Wu**, Parallel Continuous Optimization (book chapter), in *Sourcebook for Parallel Computing*, Jack Dongarra, Ian Foster, Geoffrey Fox, Ken Kennedy, Linda Torczon, and Andy White, eds., Morgan Kaufmann, 640-670, 2002
36. Qunfeng Dong and **Zhijun Wu**, A Linear-Time Algorithm for Solving the Molecular Distance Geometry Problem with Exact Inter-Atomic Distances, *Journal of Global Optimization* 22, 365-375, 2002
37. **Zhijun Wu**, George Phillips, Richard Tapia, and Yin Zhang, A Fast Newton's Algorithm for Entropy Maximization in Phase Determination, *SIAM Review* 43, 623-642, 2001
38. **Zhijun Wu**, George Phillips, Richard Tapia, and Yin Zhang, A Fast Newton's Method for Entropy Maximization in Statistical Phase Estimation, *ACTA Crystallographica A* 57, 681-685, 2001
39. Jorge Moré and **Zhijun Wu**, Distance Geometry Optimization for Protein Structures, *Journal of Global Optimization* 15, 219-234, 1999
40. John Feo, Simon Kahan, and **Zhijun Wu**, Crash Analysis on the Tera Multi-threaded Architectures, *IEEE Journal on Computational Science and Engineering*, October-December, 53-59, 1998
41. Jorge Moré and **Zhijun Wu**, Global Continuation for Distance Geometry Problems, *SIAM Journal on Optimization* 7, 814-836, 1997
42. Jorge Moré and **Zhijun Wu**, Issues in Large Scale Global Molecular Optimization, in *IMA Series on Mathematics and Its Applications*, Vol. 94, *Large Scale Optimization with Applications*, L. Biegler, T. Coleman, A. Conn and F. Santosa, eds., Springer-Verlag, 99-122, 1997
43. Jorge Moré and **Zhijun Wu**, Epsilon-Optimal Solutions to Distance Geometry Problems via Global Continuation, in *Global Minimization of Non-convex Energy Functions: Molecular Conformation and*

Protein Folding, P. M. Pardalos, D. Shalloway, and G. Xue, eds., American Mathematical Society, 151-168, 1996

44. Jorge Moré and **Zhijun Wu**, Smoothing Techniques for Macromolecular Global Optimization, in Nonlinear Optimization and Applications, G. Di Pillo and F. Gianessi, eds., Plenum Press, 297-312, 1996

45. **Zhijun Wu**, The Effective Energy Transformation Scheme as a Special Continuation Approach to Global Optimization with Application to Molecular Conformation, SIAM Journal on Optimization 6, 748-768, 1996

46. Thomas Coleman and **Zhijun Wu**, Parallel Continuation-Based Global Optimization for Molecular Conformation and Protein Folding, Journal of Global Optimization 8, 49-65, 1996

47. Robert Bixby, John Dennis, and **Zhijun Wu**, Solving Nonlinear Integer Programs with a Sub-gradient Approach on Parallel Computers, in Applications on Advanced Architecture Computers, Greg Astfalk, ed., SIAM, 277-286, 1996

48. Thomas Coleman, David Shalloway, and **Zhijun Wu**, A Parallel Buildup Algorithm for Global Energy Minimization of Molecular Clusters Using Effective Energy Simulated Annealing, Journal of Global Optimization 4, 171-185, 1994

49. Thomas Coleman, David Shalloway, and **Zhijun Wu**, Isotropic Effective Energy Simulated Annealing Searches for Low Energy Molecular Cluster States, Journal of Computational Optimization and Applications 2, 145-170, 1993

*Technical Reports:*

50. Le Thi Hoai An, Pham Dihn Tao, and **Zhijun Wu**, Solving the Molecular Distance Geometry Problem as a Bound-Constrained Minimization Problem, Technical Report, Laboratoire LMI, Département Génie Mathématiques, Institut National Des Sciences Appliquées De Rouen, France, 2002

51. **Zhijun Wu** and Yin Zhang, SMV – An Object-Oriented Sparse Matrix-Vector Computation Class Library – A Programming Manual, Technical Report, TR00-20, Department of Computational and Applied Mathematics, Rice University, 2000

52. **Zhijun Wu**, George Phillips, Richard Tapia, and Yin Zhang, The Bayesian Statistical Approach to the Phase Problem in Protein X-ray Crystallography, Technical Report, TR99-13, Department of Computational and Applied Mathematics, Rice University, 1999

53. Ali Bouaricha, Jorge Moré, and **Zhijun Wu**, Newton's Method for Large Scale Optimization, Technical Report MCS-P635-0197, Mathematics and Computer Science Division, Argonne National Laboratory, 1997

54. Jorge Moré, Brian Walenz, and **Zhijun Wu**, Configuration of Large, Confined Ionic Systems by Potential Energy Minimization, Technical Report, Mathematics and Computer Science Division, Argonne National Laboratory, 1996

55. Thomas Coleman and **Zhijun Wu**, A Parallel Row Distributed Linear Algebra System -- PRDLA Users' Guide, Technical Report, Advanced Computing Research Institute, Cornell University, 1992

*Papers submitted and in Preparation:*

56. Yiping Hao, Wen Zhou, and **Zhijun Wu**, Computation of Nash Equilibria of Evolutionary Games, submitted, 2015
57. Min Wang, Wen Zhou, and **Zhijun Wu**, Optimality and Stability Analysis of Equilibrium States of Biological Populations on Social Networks, submitted, 2015
58. Min Wang and **Zhijun Wu**, Convergence Analysis of Replicator Equations with Diffusion, submitted 2015
59. Yiping Hao and **Zhijun Wu**, Sparse and Dense Solutions of Evolutionary Games, in preparation, 2015
60. Ozgur Aydogmus, Wen Zhou, and **Zhijun Wu**, Simulation of Spatial Games with Gaussian Structures, in preparation, 2015

### *Software Developed*

1. TEDA – A Matlab Toolbox for Evolutionary Dynamics Analysis, Department of Mathematics and Graduate Program on Bioinformatics and Computational Biology, Iowa State University, 2015, Yiping Hao, Wen Zhou, and **Zhijun Wu**
2. PRESS-PLOT – A Web-Server for Protein Residue Level Structural Evaluation Using Virtual Angle Correlation Plots, Department of Mathematics and Graduate Program on Bioinformatics and Computational Biology, Iowa State University, 2013, Yuanyuan Huang, Kejue Jia, and **Zhijun Wu**
3. PRESS – A Software Package for Computing Protein Residue Level Structural Statistics, Department of Mathematics and Graduate Program on Bioinformatics and Computational Biology, Iowa State University, 2011, Yuanyuan Huang, Stephen Bonett, and **Zhijun Wu**
4. PRTAD – A Protein Residue Torsion Angle Distribution Database, Department of Mathematics and Graduate Program on Bioinformatics and Computational Biology, Iowa State University, 2007, Xiaoyong Sun, Di Wu, Robert Jernigan, and **Zhijun Wu**
5. PIDD – A Protein Inter-Atomic Distance Distribution Database, Department of Mathematics and Graduate Program on Bioinformatics and Computational Biology, Iowa State University, 2005, Di Wu, Robert Jernigan, and **Zhijun Wu**
6. MTMM – A Matlab Toolbox for Macromolecular Modeling, Department of Mathematics, Iowa State University, 2003, Tauqir Bibi, Feng Cui, and **Zhijun Wu**
7. SMV – An Object-Oriented Sparse Matrix-Vector Computation Class Library, Department of Computational and Applied Mathematics, Rice University, 2000, **Zhijun Wu** and Yin Zhang
8. DGSOL – A Parallel Molecular Distance Geometry Optimization Package, Mathematics and Computer Science Division, Argonne National Laboratory, 1997, Jorge Moré and **Zhijun Wu**
9. PRDLA – A Parallel Row Distributed Linear Algebra System, Cornell Theory Center, Cornell University, 1992, Thomas Coleman and **Zhijun Wu**

### *PhD Students Directed*

1. Feng Cui, PhD in Bioinformatics; graduated in summer 2005 and joined the NIH National Cancer Institute as a research fellow. Thesis Topics: Distance Based Protein Structure Determination and Refinement.
2. Ajith Gunaratne, PhD in Applied Math; graduated in summer 2006 and joined the faculty in Department of Mathematics, Florida A & M University. Thesis Topics: A Penalty Function Method for Constrained Molecular Dynamics.
3. Di Wu, PhD in Applied Math & Bioinformatics; graduated in summer 2006 and joined the faculty in Department of Mathematics, Western Kentucky University. Thesis Topics: Distance Based Protein Modeling.
4. Peter Vedell, PhD in Applied Math & Bioinformatics; graduated in spring 2007 and joined the Jackson Lab as a postdoctoral associate. Thesis Topics: Multiple Shooting Approaches to Boundary-Value Problems in Molecular Dynamics Simulation.
5. Rahul Ravindrudu, PhD in Computer Science; graduated in fall 2008 and joined the Proteomics Research Company as a research scientist. Thesis Topics: A Parallel High-Performance System for Protein Structure Refinement.
6. Atilla Sit, PhD in Applied Math; graduated in summer 2010 and joined the Wisconsin Institute of Discovery, U Wisconsin at Madison as a postdoctoral associate. Thesis Topics: Geometric Approaches to Protein Modeling.
7. Jun-Koo Park, PhD in Applied Math, graduated in summer 2012. Thesis Topics: Coarse-Grained Normal Mode Analysis for Protein Structural Fluctuations.
8. Ozgur Aydogmus, PhD in Applied Math, graduated in summer 2013. Thesis Topics: Evolutionary Game Dynamics, Inverse Problems.
9. Yuanyuan Huang, PhD in Bioinformatics, graduated in summer 2013. Thesis Topics: Protein Structural Analysis, Evolutionary Game Dynamics.
10. Yiping Hao, PhD in Applied Math, graduated in summer 2013. Thesis Topics: Evolutionary Game Dynamics and Applications in Plant Development.
11. Min Wang, PhD in Applied Math, graduated in summer 2015. Thesis Topics: Evolutionary Game Dynamics and Applications.

### **Recent Invited Lectures**

1. Optimality and Stability of Equilibrium States of Social Network Games, International Workshop on Discrete Mathematics and Optimization, Fuzhou, China, June 2016
2. Simulation of Evolution of Social Cooperation of Microorganism, Institute of Systems Science, Chinese Academy of Sciences, Beijing, China, July 2016
3. Equilibrium States of Network Structured Populations, AMS Eastern Sectional Meeting, Georgetown University, Washington DC, March 2015

4. Evolution of Social Cliques, MBI Workshop on Evolutionary Game Theory and Applications, Columbus, Ohio, May 2015
5. Optimality and Stability of Symmetric Evolutionary Games, International Symposium on Mathematical Programming, Pittsburgh, Pennsylvania, July 2015
6. Optimality and Stability of Symmetric Evolutionary Games, Department of Mathematics, Peking University, Beijing, China, June 2014
7. Evolution of Social Cliques, Institute of Computational Mathematics, Chinese Academy of Sciences, Beijing, China, July 2014
8. Game Theory, Optimization, and Evolution, Institute of Computational Mathematics, Chinese Academy of Sciences, Beijing, July 2012
9. Protein Structural Analysis and Computation, Workshop on Protein Folding and Dynamics, Telluride, Colorado, June 2012
10. Determination of Protein Structural Fluctuations with Geometrical and Physical Constraints, Protein and RNA Structure Prediction Conference, Xcaret, Mexico, December 2011
11. Toward Bioinformatics Approach to Protein Structure and Dynamics, Wisconsin Institute of Discovery, University of Wisconsin at Madison, October 2011
12. Optimization and Game Theory Models for Evolution, 2011 International Congress on Industrial and Applied Mathematics, Vancouver, Canada, July 2011
13. Statistical Measures on Residue-Level Protein Structural Properties, Workshop on Modeling and Computation of Macromolecular Structure and Dynamics, Mathematical Biosciences Institute, Ohio State University, Columbus, Ohio, May 2011
14. Direct Geometric Methods for Sensor Network Localization, School of Information and Communication Engineering, Beijing University of Posts and Telecommunication, Beijing, China, December 2010
15. A Subspace Optimization Approach to the Distance Geometry Problem, 2009 Math Programming International Conference, Chicago, Illinois, August 2009

#### **Awards / Honors**

- Visiting Professorship, Mathematical Biosciences Institute, Ohio State University, 2005
- Graduate Advising Excellence Award, Department of Mathematics, Iowa State University, 2006
- New Direction Research Professorship, Institute for Math Applications, University of Minnesota, 2007
- Member, SIGMA XI Society, Iowa State University Chapter, 2012