

Donald J. Jacobs, Ph.D.

University of North Carolina at Charlotte
Department of Physics and Optical Science
9201 University City Blvd.
Charlotte, NC 28223

US Citizen

Tel: (704) 687-8143
Fax: (704) 687-8197
Email: djacobs1@uncc.edu

EDUCATION

- 1985-1992 **Ph.D. Physics**; Purdue University, West Lafayette, Indiana
- Thesis: *Brownian Motion in Disordered Media*
- 1991 **M.S. Physics**; Purdue University, West Lafayette, Indiana
- 1983-1985 **B.S. Physics**; Union College, Schenectady, New York
- Honors Thesis: *Monte Carlo Simulation of Multistate Percolation Models*
- 1981-1983 **A.S. Engineering Science**; Fulton-Montgomery Comm. College, Johnstown, NY

POSITIONS

- 2008-present **Associate Professor of Physics**; University of North Carolina at Charlotte
- Focus Leader for the Center of Biomedical Engineering and Science in the area of Molecular Engineering and Design
 - M.S. Applied Physics Advisor
- 2005-2008 **Assistant Professor of Physics**; University of North Carolina at Charlotte
- Focus Leader for the Center of Biomedical Engineering and Systems in the area of Biomedical Modeling, Imaging and Processing
- 2005-2006 **Associate Professor of Physics**; California State University, Northridge (CSUN)
- While on a one year unpaid leave from CSUN (2005-2006)
- 1999-2005 **Assistant Professor of Physics**; California State University, Northridge (CSUN)
- Biomedical Physics Undergraduate Program Coordinator
 - Developed interdisciplinary Biomedical Physics undergraduate BA-program
- 1999-2001 **Acting president**; MolFlex LLC
- Company discontinued in favor of academic software distribution model
- 1998-1999 **President and Director of Research**; MolFlex LLC
- Co-founder of MolFlex as a spin off company from research on protein flexibility
- 1998-1999 **Assistant Research Professor of Physics**; Michigan State University
- Principal developer of software called FIRST to quantify protein flexibility
- 1994-1998 **Research Associate**; Michigan State University
- Worked on problems in condensed matter, mathematical and computational physics dealing with mechanical properties of covalent bond glass networks
- 1994-1996 **Teaching Instructor (50% time)**; Michigan State University
- Contributed to the CAPA (*Computer Assisted Personalized Assignments*) system
- 1992-1994 **Postdoctoral Fellow**; Inst. of Theoretical Physics, Univ. of Utrecht, The Netherlands
- Worked on problems in fluid dynamics using lattice gas models

HONORS

- 2012 *Scholarly Merit Sabbatical Leave*, fall 2012
2006 *Outstanding Scholarly Merit Sabbatical* granted for fall 2005 (unused)
1993 Attended: Fundamental Problems in Statistical Mechanics VIII, Altenberg Summer School, Germany
1992 *Outstanding Theoretical Physics Thesis*, Edward F. Akeley Memorial Award
1990 David Ross *Research Fellowship* at Purdue University
1989 Attended: Diffusion in Materials, NATO ASI, Aussois, France (March, 1989)
1985 Graduated with distinction, *Magna Cum Laude*, with Honors Research Thesis
1983 Who's Who Among Students in American Junior Colleges

AREAS OF EXPERTISE

Computational Physics, Statistical Physics, Condensed Matter Physics and Biological Physics

SYNERGETIC ACTIVITIES

Founding Member of PsiTopix LLC

Scientific Research Company and Software for Computational Biology Applications

Journal Editor

Entropy

Professional Society Membership

American Physical Society, Biophysical Society, American Chemical Society, Sigma Xi Scientific Research Society

Referee Experience:

Manuscripts: (refereed over 100 manuscripts, since August 1999 as faculty member)

Reviews given for journals ordered from most to least frequent:

Physical Review Letters; Physical Reviews E; Proteins: Structure, Function and Bioinformatics; Biophysics Journal; PLoS Computational Biology; Journal of Physics, Condensed Matter; Journal of the American Chemical Society; Journal of Chemical Physics; Physical Reviews B; The Royal Society; Current Protein and Peptide Science; Journal of Statistical Physics; Journal of Computational Physics; Communications in Computational Physics; Biopolymers; European Physical Journal E; BMC Bioinformatics; Physical Biology, Computer Methods and Programs in Biomedicine; Journal of Photochemistry and Photobiology B, Biology; Journal of Biomolecular Structure and Dynamics; International Journal of Molecular Sciences; Icarus.

Books: (5)

Calculus-based introductory Physics textbook, W.H. Freeman and Company Publishers

Calculus-based introductory Physics textbook, Brooks and Cole publisher

Textbook on Biological Physics, W.H. Freeman and Company Publishers

Graduate textbook on Rigidity, by Simon Guest and Bob Connelly, Cambridge Publisher
Junior level Classical Mechanics, with Jones and Bartlett Publishers

NSF Grant proposals reviewed:

ITR-ASE (1 in 2004), DMR (2 in 2005, 2 in 2007, 1 in 2008, 1 in 2009, 2 in 2010, 1 in 2012), CHE (1 in 2010, 1 in 2011)

NIH Review panels:

June, 2008 BMDA
Oct, 2008 BMDA
June, 2009 BST-Q(01)
July, 2009 ZRG1 BST-M (58) R
Dec, 2011 ZRG1 CB-C (02) (IAR)

Miscellaneous Funding Agencies

2004 (7) GRSP-CRDF Graduate Research Support, Civilian Research & Development Foundation
2006 (1) Biotechnology and Biological Sciences Research Council (Agency of Great Britain)
2008 (7) Bonnie Cone Fellowship, UNC-Charlotte
2009 (8) Bonnie Cone Fellowship, UNC-Charlotte

Postdoctoral Researchers or Research Associates Supervised: (^P implies primary supervisor)

2012 Dr. Tong Li, co-supervisor, Medimunne contract (Jacobs, co-PI)
2009 – 2011 Dr. Chuanbin Du, co-supervisor, NIH R01 GM073082, GM073082-04S2 (Jacobs, PI)
2008 – 2010 Dr. Hui Wang, co-supervisor^P, NIH R01 GM073082, GM073082-04S2, (Jacobs, PI)
2011 Dr. Boris Ni, co-supervisor, NIH R01 GM083600 (Jacobs, co-Inv)
2008 – 2010 Dr. Yuchun Lin, co-supervisor, NIH R01 GM083600 (Jacobs, co-Inv)
2006 – 2009 Dr. Jim Mottonen, co-supervisor^P, NIH R01 GM073082-01S1 (Jacobs, PI)
2006 – 2010 Dr. Oleg Vorov, co-supervisor^P, NIH R01 GM073082 (Jacobs, PI)
2006 – 2008 Dr. Andrei Istomin, co-supervisor, R01 GM073082 (Jacobs, PI)
2002 – 2005 Dr. Gregory G. Wood, supervisor, NIH S06 GM48680-0952 (Jacobs, PI)
2002 – 2005 Dr. Sargis Dallakyan, supervisor, NIH S06 GM48680-0952 (Jacobs, PI)

Officially Assigned Faculty Mentoring: (3)

2011 – ... Dr. Michael Grabchak (Assistant Professor from the Department of Mathematics and Statistics). Mentor program at UNC Charlotte.
2009 – 2010 Dr. Yuri Nesmelov (Department of Physics and Optical Science) NIH-K25 Career Development grant. Mentor for NIH Career Development grant requirements.
2007 – 2009 Dr. Alexander Gordon (Assistant Professor from the Department of Mathematics and Statistics). Mentor program at UNC Charlotte.

SCIENTIFIC SOFTWARE

- 1) **D.J. Jacobs**, L.A. Kuhn and M.F. Thorpe, Software: **FIRST** (*Floppy Inclusion and Rigid Substructure Topography*). Original release of FIRST resulted from work done at MolFlex (NIH-SBIR with D.J. Jacobs PI) and work done at Michigan State University (MSU). Recent versions are distributed by L.A. Kuhn at MSU, and a preferred version by M.F. Thorpe at Arizona State University at Web site: <http://firstweb.asu.edu/>. FIRST is freeware to academics and licensed to commercial users for profit.
- 2) **D.J. Jacobs** and D.R. Livesay, Software: **FAST** (*Flexibility And Stability Test*). This software is currently being developed through NIH-R01 funding (D.J. Jacobs PI). FAST will be used for high throughput applications in computational biology, such as rational protein design. FAST will be made freely available to academics and commercialized through PsiTopix LCC.
- 3) Wei Cai, Andrij Baumketner, Shaozhong Deng and **D.J. Jacobs**, Algorithm development and the implementation of new fast and accurate electrostatics modules that have been incorporated into TINKER, an open source Molecular Dynamics package.

PATENTS

- 1) **D.J. Jacobs** and M.F. Thorpe, *Computer Implemented System for Identifying Rigid and Flexible Regions in Macromolecules*, issued **US Patent No. 6,014,449** (2000). (filed in 1997).
- 2) **D.J. Jacobs**, *Computer Implemented System for Quantifying Stability and Flexibility Relationships in Macromolecules*, issued **U.S. Patent No. 8,244,504** (2012). (filed in 2008)
- 3) **D.J. Jacobs**, *Computer Implemented System for Quantifying ensemble averaged properties of rigidity and flexibility in Macromolecules*. Patent claims pending, law firm: Summa, Allan & Additon, P.A. with UNC Charlotte owner. Application number: **61016551** (2008)
- 4) **D.J. Jacobs** and D.R. Livesay, *Computer Implemented System for Protein Design utilizing Quantitative Stability/Flexibility Relationships to control function*, patent claims pending, law firm: Summa, Allan & Additon, P.A. with UNC Charlotte owner. Application number: **61016848** (2008)

PUBLICATIONS (^c corresponding author, ^p postdoc, ^g graduate student, ^u undergraduate student)

Summary: 79 publications: 58 peer reviewed, 3 invited reviews, 5 book chapters, 13 proceedings, 5 manuscripts in review and 5 manuscripts are in preparation.

In review:

1. Tong Li^p, Deeptak Verma, Malgorzata B. Tracka, Dennis R. Livesay^c and Donald J. Jacobs^c, *Thermodynamic stability and flexibility characteristics of antibody fragment complexes*, submitted to Protein and Peptide Letters.
2. D. Verma, **D.J. Jacobs** and D.R. Livesay^c, *Variations within class-A β -lactamase physiochemical properties reflect evolutionary, but not functional, patterns*, submitted to PloS Computational Biology.
3. S. Barlowe, J. Yang^c, **D. Jacobs**, D. Livesay, J. Alsakran, Y. Zhao, D. Verma and J. Mottonen. *A Visual Analytics Approach for Exploring Protein Flexibility Subspaces*. Submitted to IEEE Pacific-Vis.

4. C. Du^p, H. Wang^p, D.R. Livesay^c and **D.J. Jacobs^c**, *A Three-State Model of Amino Acid Solvation that Accounts for Hydration at Low Temperatures*, submitted to PLoS ONE.
5. L. González^g, H. Wang^p, D.R. Livesay and **D.J. Jacobs^c**, *A virtual pebble game to ensemble average graph rigidity*, submitted to ACM.

Peer reviewed: (Published or in press)

6. K. Baker, A. Baumketner, Y. Lin, S. Deng, **D. Jacobs** and W. Cai^c, *ICSM: An order N method for calculating electrostatic interactions added to TINKER*, submitted to Computer Physics Communication (**in press**).
7. W. Song^g, Y. Lin^p, A. Baumketner, S. Deng, W. Cai and **D.J. Jacobs^c**, *Effect of the Reaction Field on Molecular Forces and Torques revealed by an Image-Charge Solvation Model*, Comm. Comp. Phys. 13:129-149 (2013).
8. D.V. Trivedi, C. David^g, **D.J. Jacobs** and C.M. Yengo^c, *Switch II Mutants Reveal Coupling Between the Nucleotide and Actin Binding Regions in Myosin V*, Biophysical Journal, 102(11):2545-2555 (2012).
9. Deeptak Verma, **Donald J. Jacobs^c**, and Dennis R. Livesay^c, *Changes in Lysozyme Flexibility upon Mutation are Frequent, Large and Long-Ranged*, 8:e1002409, PLoS Computational Biology. (2012).
10. L. González^g, H. Wang^p, D.R. Livesay^c and **D.J. Jacobs^c**, *Calculating Ensemble Averaged Descriptions of Protein Rigidity without Sampling*, 7:e29176, PLoS ONE. (2012).
11. L.C. González^g, D.R. Livesay^c, **D.J. Jacobs^c**, *Improving protein flexibility predictions by combining statistical sampling with a mean-field virtual pebble game*. Peer reviewed, ACM Conference on Bioinformatics, Computational Biology and Biomedicine, ISBN: 978-1-4503-0796-3, 294-298 (2011).
12. C. David^g and **D.J. Jacobs^c**, *Characterizing protein motions from structure*, J. Mol. Graph Model, 31:41-56. (2011).
13. S. Barlowe, Y. Liu, J. Yang^c, D. Livesay, D. Jacobs, J. Mottonen^p, D. Verma, *WaveMap: Interactively discovering features from protein flexibility matrices using wavelet-based visual analytics*. Computer Graphics Forum, 30:1001-1010. (2011).
14. **D.J. Jacobs**, D. Trivedi, C. David^g, C.M. Yengo^c, Kinetics and thermodynamics of the rate limiting conformational change in the actomyosin V mechanochemical cycle, J. Mol. Biol. **407**, 716-30 (2011).
15. O.K. Vorov^p, D.R. Livesay^c and **D.J. Jacobs^c**, *Nonadditivity in Conformational Entropy Upon Molecular Rigidification Reveals a Universal Mechanism for Affecting Folding Cooperativity*, Biophys J. **16**, 100 1129-38 (2011).
16. Y. Lin^p A. Baumketner^c, W. Song^g, S. Deng, **D.J. Jacobs**, W. Cai^c, *Ionic solvation studied by image-charge reaction field method*, J. Chem. Phys. **134**, 044105 (2011).
17. G.G. Wood, Drew A. Clinkenbearda, **D.J. Jacobs^c**, *Nonadditivity in the alpha-helix to coil transition*, Biopolymers, **95**, 240–253 (2011).
18. S. Vasilache, N. Mirshahi, S-Y. Ji, J. Mottonen^p, **D. Jacobs** and K. Najarian^c, *A Signal Processing Method to Explore Similarity in Protein Flexibility*, Advances in Bioinformatics, Vol **2010**, 454671, (2010).
19. J.M. Mottonen^p, **D.J. Jacobs^c**, D.R. Livesay^c, *Allosteric Response is Both Conserved and Variable Across Three CheY Orthologs*, Biophysical Journal. **99**, 2245-54 (2010).
20. D. Verma^g, **D.J. Jacobs^c** and D.R. Livesay^c, *Predicting the Melting Point of Human C-Type Lysozyme Mutants*, Current Protein and Peptide Science, **11**, 562-572, (2010).
21. **D.J. Jacobs^c**, *Best probability density Function for Random Sampled Data*, Entropy. **11**:1001-1024 (2009).

22. Y. Lin^p, A. Baumketner^c, S. Deng, Z. Xu, **D. Jacobs**, Wei Cai^c *An image-based reaction field method for electrostatic interactions in molecular dynamics simulations of aqueous solutions*, Journal of Chemical Physics, **131**(15): 154103 (2009).
23. O.K. Vorov^p, D.R. Livesay^c and **D.J. Jacobs**^c, *Helix/coil nucleation: A local response to global demands*, Biophysical Journal, **97**:3000-3009 (2009).
24. Ravi Jasuja^c, Jagadish Ulloor, Christopher M. Yengo, Karen Choong, Andrei Y. Istomin^p, Dennis R. Livesay, **D.J. Jacobs**, Ronald Swerdloff, Jaroslava Mikšovská, Randy W. Larsen, and Shalender Bhasin, *Kinetic and Thermodynamic Characterization of Dihydrotestosterone-Induced Conformational Perturbations in Androgen Receptor Ligand Binding Domain*, Molecular Endo., **23**(8): 1231-1241 (2009)
25. Peihua Qin, Zhenli Xu, Wei Cai^c, **D.J. Jacobs**, *Image charge methods for a three-dielectric-layer hybrid solvation model of biomolecules*. Comm. Comp. Phys., **6**:955-977 (2009).
26. R.A. Karjiban, Mohd Basyaruddin Abdul Rahman^c, M. Basri, A.B. Salleh^g, **D.J. Jacobs**, and H.A. Wahab. *Molecular Dynamics Study of the Structure, Flexibility and Dynamics of Thermostable L1 lipase at High Temperatures*. The Protein journal **28**(1):14-23 (2009).
27. Mohd Basyaruddin Abdul Rahman^c, R.A. Karjiban, A.B. Salleh^g, **D.J. Jacobs**, M. Basri, A.L. Thean Chor, H.A. Wahab, and Raja Noor Zaliha Raja Abd Rahman. *Deciphering the Flexibility and Dynamics of Geobacillus zalihae strain T1 Lipase at High Temperatures by Molecular Dynamics Simulation*. Protein & Peptide Letters, **16**(11) 1360-1370 (2009).
28. J.M. Mottonen^p, Minli Xu, **D.J. Jacobs**^c and D.R. Livesay^c, *Unifying mechanical and thermodynamic descriptions across the thioredoxin protein family*, Proteins, **75**:610-627 (2009).
29. O.K. Vorov^p, D.R. Livesay and **D.J. Jacobs**^c, *Conformational entropy of an ideal cross-linking polymer chain*, Entropy, **10**:285-308 (2008).
30. D.R. Livesay^c, D.H. Huynh^g, S. Dallakyan^p and **D.J. Jacobs**^c, *Hydrogen bond networks determine emergent mechanical and thermodynamic properties across a protein family*, Chemistry Central Journal **2**:17 1-20 (2008).
31. Scott Barlowe, Tianyi Zhang, **D.J. Jacobs** and Jing Yang^c, *Multivariate Visual Explanation for High Dimensional Datasets*, Proc. IEEE VAST'08 symposium; Visual Analytics Science and Technology, 147-154 ISBN: 978-1-4244-2935-6. (2008).
32. Mingxuan Sun, Michael Rose, Shobana K. Ananthanarayanan, **D.J. Jacobs** and Christopher M. Yengo^c, *Characterization of the Pre Force-Generation State in the Actomyosin Cross-bridge Cycle*, Proc. Nat. Acad. Sci. **105**:8631–8636 (2008).
33. A.Y. Istomin^p, M.M. Gromiha, O.K. Vorov^p, **D.J. Jacobs**^c and D.R. Livesay^c, *Insight into Long-Range Nonadditivity within Protein Double-Mutant Cycles*, Proteins: Structure, Function, and Bioinformatics, **70**:915-924 (2008).
34. A.Y. Istomin^{c,p}, D.J. Jacobs and D.R. Livesay, *On the role of structural class of a protein with two-state folding kinetics in determining correlations between its size, topology, and folding rates*, Protein Science, For The Record **16**:2564-69 (2007).
35. Shaozhong Deng^c, Wei Cai and **D.J. Jacobs**, *A comparable study of image approximations to the reaction field*, Computer Physics Communications, **177**:689-699 (2007).
36. Wei Cai^c, Shaozhong Deng and **D.J. Jacobs**, *Extending the Fast Multipole Method to Charges Inside or Outside a Dielectric Sphere*, Journal of Computational Physics, **223**(2):846-864 (2007)
37. D.R. Livesay^c, **D.J. Jacobs**, J. Kanjanapangka, H. Cortez, J. Garcia, P. Kidd, M.P. Marquez, S. Pande, D. Yang, and E. Chea, *Elucidating the conformational dependence of calculated pKa values*. Journal of Chemical Theory and Computation. **2**(4):927-938 (2006)

38. **D.J. Jacobs**^c, D.R. Livesay, J. Hules^g and M.L. Tasayco, *Elucidating quantitative stability-flexibility relationships within thioredoxin and its fragments using a distance constraint model*. Journal of Molecular Biology. **358**, 882-904 (2006)
39. D.R. Livesay and **D.J. Jacobs**^c, *Conserved quantitative stability/flexibility relationships (QSFR) in an orthologous RNase H pair*. Proteins: Structure, Function, and Bioinformatics. **62**, 130-43 (2006)
40. **D.J. Jacobs**^c and S. Dallakayan^p, *Elucidating Protein Thermodynamics from the Three Dimensional Structure of the Native State Using Network Rigidity*. Biophysical Journal. **88**, 1-13 (2005)
41. D.R. Livesay, S. Dallakayan^p, G.G. Wood^p and **D.J. Jacobs**^c, *A flexible approach for understanding protein stability*. FEBS Letters, **576**, 468-76 (2004)
42. M.S. Lee^g, G.G. Wood^p and **D.J. Jacobs**^c, *Investigations on the alpha-helix to coil transition in HP-heterogeneous polypeptides using network rigidity*. Journal Physics, Condensed Matter. **16**, S5035-46 (2004)
43. B.M. Hespeneide, **D.J. Jacobs** and M.F. Thorpe^c, *Structural rigidity in the capsid assembly of cowpea chlorotic mottle virus*. Journal of Physics, Condense Matter. **16**, S5055-64 (2004)
44. **D.J. Jacobs**^c and G.G. Wood^p, *Understanding the α -Helix to Coil Transition in Polypeptides Using Network Rigidity: Predicting Heat and Cold Denaturation in Mixed Solvent Conditions*. Biopolymers. **75**, 1-31 (2004).
45. **D.J. Jacobs**^c, S. Dallakayan^p, G.G. Wood^p and A. Heckathorne^g, *Network rigidity at finite temperature: Relationships between thermodynamic stability, the nonadditivity of entropy, and cooperativity in molecular systems*. Physical Reviews E. **68**, 061109 1-21 (2003)
46. **D.J. Jacobs**, A. Rader, L.A. Kuhn and M.F. Thorpe^c, *Graph Theory Predictions of Protein Flexibility*. Proteins: Structure, Function, and Genetics. **44**, no. 2, 150-65 (2001). **Featured on cover page of monthly issue.**
47. M.F. Thorpe^c, A. Rader, M. Lei, **D.J. Jacobs**, L.A. Kuhn, *Protein Flexibility and Dynamics using Constraint Theory*. Journal of Molecular Graphics and Modeling. **19**, 60-69, (2001)
48. M.F. Thorpe^c, **D.J. Jacobs**, M.V. Chubynsky and J.C. Phillips, *Self organization in network glasses*. Journal of Non-Crystalline Solids. Vols. **266-269**, 859-66 (2000)
49. P.M. Duxbury^c, **D.J. Jacobs**, M.F. Thorpe and C. Moukarzel, *Floppy Modes and the Free Energy: Rigidity and Connectivity percolation on Bethe Lattices*. Physical Reviews E. **59**, 2084-92 (1999)
50. **D.J. Jacobs**^c, *Generic Rigidity in Three-dimensional Bond-bending Networks*. Journal of Physics A, Mathematics and General. **31**, 6653-68 (1998)
51. **D.J. Jacobs** and M.F. Letters Thorpe^c, *Comment on "Infinite-Cluster Geometry in Central-Force Networks"*, Physical Review. **80**, no. 24, 5452 (1998)
52. **D.J. Jacobs**^c and B. Hendrickson^c, *An Algorithm for Two Dimensional Rigidity Percolation: The Pebble Game*. Journal of Computational Physics. **137**, 346-65 (1997)
53. **D.J. Jacobs** and M.F. Thorpe^c, *Generic Rigidity Percolation: The Pebble Game*. Physical Reviews E. **53**, 3682-93 (1996)
54. **D.J. Jacobs** and M.F. Thorpe^c, *Generic Rigidity: The Pebble Game*. Physical Review Letter. **75**, 4051-54 (1995)
55. J.R. Dorfman^c, M.H. Ernst, R. Nix and **D.J. Jacobs**, *Mean Field Theory for Lyapunov Exponents and Kolmogorov-Sinai Entropy in Lorentz Lattice Gases*, Physical Review Letters. **74**, 4417-20 (1995)
56. J.R. Dorfman^c, M.H. Ernst and **D.J. Jacobs**, *Dynamical Chaos in the Lorentz Lattice Gas*. Journal of Statistical Physics. **81**, 497-513 (1995)

57. S. Mukherjee, **D.J. Jacobs** and H. Nakanishi^c, *Diffusion on Loopless Critical Percolation Cluster*. Journal of Physics A, Mathematical and General. **28**, 291-96 (1995)
58. **D.J. Jacobs**, S. Mukherjee and H. Nakanishi^c, *Diffusion on DLA cluster in Two and Three Dimensions*, Journal of Physics A, Mathematical and General. **27**, 4341-48 (1994)
59. **D.J. Jacobs**^c, and A. Masters, *Domain Growth in a One-dimensional Diffusive Lattice Gas with Short Range Attraction*. Physical Reviews E. **49**, 2700-10 (1994)
60. **D.J. Jacobs**^c and H. Nakanishi^c, *A Persistent Random Walk Model for the Frequency-Dependent Electrical Conductivity*. Physica A. **197**, 204-22 (1993)
61. S. Muralidhar, **D.J. Jacobs**, D. Ramkrishna^c and H. Nakanishi^c, *Diffusion on Percolation Clusters: Influence of Cluster Anisotropy*, Physical Reviews A. **43**, 6503-17 (1991)
62. S. Muralidhar, D. Ramkrishna^c, H. Nakanishi^c and **D.J. Jacobs**, *Anomalous Diffusion: A Dynamic Perspective*. Physica A. **167**, 539-53 (1990)
63. **D.J. Jacobs** and H. Nakanishi^c, *Autocorrelation Functions for Discrete Random Walks on Disordered Lattice*, Physical Reviews A. **41**, 706-19 (1990)

Invited Reviews and Commentaries: (3 total)

64. **Invited Review: D.J. Jacobs**^c, *Ensemble-Based methods for Describing Protein Dynamics*, Current Opinion in Pharmacology, D.R. Livesay (Ed.) **10**, 760-769, (2010).
65. **Invited Exposé: D.J. Jacobs**^c and D.R. Livesay, *Protein Analysis: The need for speed*, Research Media Ltd, Anderson S. (Ed.). (2010).
66. **Invited Review: D.J. Jacobs**^c, *Predicting Protein Flexibility and Stability using Network Rigidity: A new Modeling Paradigm*, Recent Research Developments in Biophysics Publisher: Transworld Research Network, Trivandrum, India, 5:71-131 ISBN: 81-7895-215-7 (2006)

Book Chapters: (5 total)

67. Charles C. David^g and **Donald J. Jacobs**. *Principal Component Analysis: A Method for Determining the Essential Dynamics of Proteins*. (accepted for publication) to appear in book on "Protein Dynamics" in **Methods Mol. Biol.**, Ed: Dennis Livesay (2013).
68. **D.J. Jacobs**^c, An Interfacial Thermodynamics Model for Protein Stability, **Biophysics**, Ed: A.N. Misra, Intech publishers, pages 91-132, ISBN 978-953-51-0376-9 (2012)
69. **D.J. Jacobs**^c, D.R. Livesay, J.M. Mottonen^p, O.K. Vorov^p, A.Y. Istomin^p, D. Verma, *Ensemble properties of network rigidity reveal allosteric mechanisms*, **Methods Mol. Biol.**, Ed: Aron Fenton, 796:279-304. (2012).
70. M. Chubynsky, B. Hespeneide, **D.J. Jacobs**, L. Kuhn, M. Lei, S. Menor, A. Rader, M. Thorpe^c, W. Whiteley and M.I. Zavodszky, *Constraint Theory Applied to Proteins*. **Reprinted**. Nanotech. Res. J., Vol. 2, Number 1, pp. 61-72 Nova Science Publishers, Inc. ISSN 1935-2484 (2008).
71. **Invited Article: D.J. Jacobs**^c and M.J. Fairchild^u, *Thermodynamics of a beta-hairpin to coil transition elucidated by Constraint Theory*, **Biopolymer Research Trends** Ed: Pablo C. Sánchez. Nova Publishers, NY ISBN: 1-60021-984-5 45-76 (2007).

Proceedings: (13 total)

72. Mohd Basyaruddin Abdul Rahman, Roghayeh Abedikargiban, Mahiran Basri, Raja Noor Zaliha Abdul Rahman, Abu Bakar Salleh^g, Habibah Abdul Wahab & **Donald Jacobs**. *Thermodynamic Evaluation and*

- Molecular Dynamic Simulation of High Homology Thermostable Lipases; Bacillus stearothermophilus PI, Bacillus stearothermophilus LI and Geobacillus sp.* Enzyme Engineering XIX, Pg 21. UPM (2007).
73. Mohd Basyaruddin Abdul Rahman, Roghayeh Abedikargiban, Mahiran Basri, Raja Noor Zaliha Abdul Rahman, Abu Bakar Salleh[§], Habibah Abdul Wahab and **Donald Jacobs**. *Thermal Unfolding Simulation of Geobacillus zalihaaii sp. Strain T1 lipase at Elevated Temperature* 12th Asian Chemical Congress. Kuala Lumpur, Malaysia (2007)
74. M. Chubynsky, B. Hesperheide, **D.J. Jacobs**, L.A. Kuhn, M. Lei, S. Menor, A.J. Rader, M.F. Thorpe^c, W. Whiteley and M.I. Zavodszky, *Constraint Theory Applied to Proteins*. Proceedings of the Indo-US Biopolymer workshop by Nova Publishers (2006)
75. M.F. Thorpe^c, M. Chubynsky, B. Hesperheide, S. Menor, **D.J. Jacobs**, L.A. Kuhn, M.I. Zavodszky, M. Lei, A.J. Rader and W. Whiteley *Flexibility in Biomolecules, Current Topics in Physics*, Editors R.A.. Barrio and K.K. Kaski, Imperial College Press (London), Chapter 6, 97-112 (2005)
76. **D.J. Jacobs**^c, *Understanding Protein Stability and Flexibility Using Network Rigidity*, Conference Proceedings of the Second International Conference on Multiscale Materials Modeling. Editor: Nasr M. Ghoniem, ISBN 0-9762064-1-2, Printed by Mechanical and Aerospace Engineering Department, UCLA 386-88 (2004)
77. M.F. Thorpe^c, M.V. Chubynsky, **D.J. Jacobs**, J.C. Phillips, *Non-Randomness in Network Glasses and Rigidity*, Glass Physics and Chemistry, Proceedings of the International Conference: Thermodynamics and Chemical Structure of Melts and Glasses. Nauka/Interperiodica International Acad. Pub. Co. **27**, no 2, 160-7 (2001)
78. M.F. Thorpe^c, M.V. Chubynsky, **D.J. Jacobs** and J.C. Phillips, *Rigidity and Flexibility in Network Glasses*. in Panellhnio Sunedrio Fusikhs Stereas Katastasews xv, ed. by Aristeidhz Zdetshz Praktika Patra, 171-81 (2000)
79. M.F. Thorpe^c, M.V. Chubynsky, **D.J. Jacobs** and J.C. Phillips, *The Intermediate Phase in Chalcogenide Glasses in 13th Conference on Glass and Ceramics*, Edited by B. Samuneva, S. Bachvarov, I. Gutzov and Y. Dimitriev, (Publishing House Science Invest) Vol **1**, Glass, 44-54 (1999)
80. **D.J. Jacobs**, L.A. Kuhn and M.F. Thorpe^c, *Flexible and Rigid Regions in Proteins*. Pages 357-84 appearing in book: "Rigidity Theory and Applications", Eds: M.F. Thorpe and P.M. Duxbury, Plenum Publishing, NY (1999)
81. M.F. Thorpe^c, **D.J. Jacobs**, N.V. Chubynsky and A.J. Rader, *Generic Rigidity of Network Glasses*. 239-77 appearing in book: "Rigidity Theory and Applications", Eds: M.F. Thorpe and P.M. Duxbury, Plenum Publishing, NY (1999)
82. M.F. Thorpe^c, **D.J. Jacobs** and B.R. Djordjevic, *The Structure and Rigidity of Network Glasses*. A chapter in "Insulating and Semiconducting Glasses", Editor: Punit Boolchand, World Scientific Publishing Co., Inc. (1998)
83. M.F. Thorpe^c, B.R. Djordjevic and **D.J. Jacobs**, *The Structure and Mechanical Properties of Networks*. In Amorphous Insulators and Semiconductors. Eds: M.F. Thorpe and M.I. Mitkova [NATO ASI Series 3] High Technology - Vol. 23 Kluwer Academic Publishers, 289-328 (1997)
84. M.F. Thorpe^c, **D.J. Jacobs** and B.R. Djordjevic, *Generic Rigidity Percolation*. Condensed Matter Theories, Vol. II Edited by E.V. Ludena, P. Vashishta and R.F. Bishop, Nova Science Publishers, 401-24 (1996)

In preparation: (intended for peer review)

1. Tong Li^p, Deeptak Verma, Malgorzata B. Tracka, Donald J. Jacobs^c and Dennis R. Livesay^c, *Quantitative Stability/Flexibility Relationships reveal non-additive effects between two engineered double mutant scFv antibody fragments*. To be submitted to Proteins.
2. Charles Herring^u, Chris Singer^u, Donald Jacobs^c and Irina Nesmolova^c, The effects of disulfide bonds on the stability and flexibility in Chemokine monomers and homodimers. To be submitted to Protein Science.
3. Tong Li^p, Malgorzata B. Tracka, Dennis R. Livesay^c and Donald J. Jacobs^c, and *Quantitative Stability/Flexibility Relationships reveal maturation mechanisms in antibodies from the germline*. To be submitted to PLoS Computational Biology.
4. Wei Song^g, Aaron Brettin^u and Donald Jacobs^c, *An improved image charge solvation model using finite boundary conditions*. To be submitted to Journal of Chemical Physics.
5. Jenny Farmer^g, and Donald Jacobs^c, *A self-determining data driven method for finding probability density functions from finite sample sets*. To be submitted to Journal of Computational and Graphical Statistics.

PRESENTATIONS

Invited Colloquia or Seminars: (42 total)

Interrelationships Between Protein Stability, Flexibility and Dynamics

- Biochemistry Seminar, Penn State, Hershey Medical School (invited for Dec 17, 2012)
- Biochem & Mol. Biology Seminar, The University of Kansas Medical Center (Sept 14, 2012)
- Pharmacology Chemistry Seminar, The University of Kansas (Sept 13, 2012)

Antibody Fragment Stability: A Focus on Domain-Domain Interactions

- Scientific Discovery seminar, MedImmune, LLC, Gaithersburg, MD. (Aug 23, 2012)

Predicting Protein Flexibility and Stability Using Constraint Theory

- Physics colloquium, Appalachian State University (invited, May 11, 2012)

FAST predictions of protein stability and flexibility (Talk given jointly with Dennis Livesay)

- Scientific Discovery seminar, MedImmune, LLC, Gaithersburg, MD. (November 10, 2010)

From Constraint Theory to FAST Predictions of Protein Thermodynamics

- Physics colloquium, Clemson University (November 19, 2009)

Predicting Protein Flexibility and Stability Using Constraint Theory

- Physics colloquium, The University of Southern Mississippi (April 17, 2009)

FAST track to Quantified Stability/Flexibility Relationships in Proteins

- Bioinformatics seminar, UNC Charlotte (March 21, 2008)

Mind your P's and Q's: A fast algorithm for predicting protein stability

- Computer Science seminar, UNC Charlotte (April 18, 2008)

Understanding Protein Stability, Flexibility and Molecular Cooperativity: Addressing Non-additivity of Entropy in Free Energy Decomposition Schemes

- Condensed Matter Seminar, Department of Physics, Virginia Tech, April 4, 2007.
- Biophysics Seminar, Rensselaer Polytechnic Institute, August 9, 2007
- Physics colloquium, Wake Forest, November 15, 2007.

Predicting Protein Stability and Flexibility

- Department of Physics and Optical Science, UNC Charlotte. March 7, 2005.
- Biophysics Seminar, Physical Optics Corporation, Los Angeles, June 29, 2005

Predicting Protein Stability from a Free Energy Decomposition

- Physics and Astronomy Colloquium, CSUN Nov 12, 2003.
- Biophysics Seminar, Physics Department, Arizona State University. March 4, 2004.
- Computer Science Seminar, Rensselaer Polytechnic Institute. April 16, 2004.
- Seminar, IRG Materials Research Lab UCSB, April 28, 2004.
- Seminar, RISE-program, CSUN. June 28, 2004.

Understanding Protein Flexibility, Stability and Folding from a Mechanical Point of View

- Physics and Astronomy Colloquium, CSUN. Feb 13, 2002.
- Condensed Matter Seminar, Physics and Astronomy, UCLA. April 26, 2002.
- Chemistry Department Colloquium, California State Polytechnic Univ., Pomona. May 7, 2002.
- Chemical Engineering Department, Colorado State University. June 28, 2002.
- Biophysics Seminar, Physics and Astronomy Department, Michigan State Univ., Aug 9 2002.
- Seminar Series, Chemistry Department, University of California, Irvine. Sept 6, 2002.
- Seminar Series, Department of Mechanical Engineering, Yale University, Dec 18, 2002

Conformational Flexibility in Protein Structure: Can it be Used Like a Fingerprint?

- NASA-JPL PAIR program at CSUN. Oct 2, 2001.

Characterizing Conformational Flexibility in Proteins

- Department of Chemical Engineering, Colorado State University. June 13, 2001.
- Seminar, RISE-program, CSUN. June 29, 2001.

Characterizing Conformational Flexibility in Proteins with a FlexPrint: Working Toward a Fingerprinting System

- Graduate Student Seminar: Methods in Computational Biology Group, UCLA. July 11, 2000.

Generic Rigidity in 2 and 3 Dimensions and Applications to Network Glasses and Protein Structure

- Mathematical Physics Institute at CSUN. Sept 27, 1999.

Generic Rigidity: A “Civil Engineering” Approach to Microscopic Structure in Network Glasses and Macromolecules

- Condensed Matter Seminar, Florida Atlantic University, Boca Raton, FL. April, 1997.

Generic Rigidity, the Pebble Game and its Applications to Amorphous Materials

- Condensed Matter Seminar, Michigan State University, East Lansing, MI, Feb, 1996.
- Solid State Physics Seminar, Purdue University, West Lafayette, IN. April, 1996.

Generic Rigidity, the Pebble Game and its Applications to Percolation Theory

- Combinatorics & Graph Theory Seminar, Michigan State Univ., East Lansing, MI. Feb, 1996.

Floppy modes and rigidity in 2d random networks

- Condensed Matter Seminar, Michigan State Univ., East Lansing, MI. Feb, 1995.

Dynamical Chaos in the Lorentz Lattice Gas

- Condensed Matter Physics Seminar, Univ. of West Virginia, Morgantown, WV. July, 1994.
- Condensed Matter Physics Seminar, Michigan State Univ., East Lansing, MI. July, 1994.
- Condensed Matter Physics Seminar, Purdue University, West Lafayette, IN. July, 1994.

Domain Growth in a One-dimensional Diffusive Lattice Gas With Short Range Attraction

- Solid State Physics Seminar, Purdue University, West Lafayette, IN. August 1993.

Velocity correlation functions for Brownian motion in disordered media

- IMB Scientific Center, Palo Alto CA. March 1990.

Invited Talks at Conferences/Meetings: (19 total)

- (19) **D.J. Jacobs**, *Free Energy Driven Geometrical Simulation of Protein Dynamics*, Cambridge Healthtech Institute, Structure based Drug Design. Boston, MA, June 6-8 (2012).
- (18) **D.J. Jacobs**, *FAST Prediction of Protein Thermodynamics*, Cambridge Healthtech Institute, Structure based Drug Design. Boston, MA, June 8-10 (2011).
- (17) **D.J. Jacobs**, *Overview of a new Image-Charge Solvation Model (ICSM) for electrostatic interactions*, Modeling Electrostatics in Molecular Biology, Clemson, SC. (2011).
- (16) **D.R. Livesay**, H. Wang and **D.J. Jacobs**, *FAST predictions of protein stability and flexibility*, Division of Small Chemical Businesses, American Chemical Society meeting, Boston, 2010.
- (15) **D.J. Jacobs**, *FAST Prediction of Protein Thermodynamics*, PepCon-2010. Beijing International Convention Center, Beijing, China, March 21-23 (2010)
- (14) **D.J. Jacobs**, *Quantifying stability and flexibility in proteins using constraint theory*, Biopolymer Gordon conference. Salve Regina University, Newport RI, June 8-13 (2008)
- (13) **D.J. Jacobs**, *Protein Stability Modeled by Constraint Theory*. Interdisciplinary Workshop on Geometric Simulation Techniques in Bio-macromolecules, Tempe, AZ (May 11-15, 2008)
- (12) **D.J. Jacobs**, **Series of 4 Lectures: (i) Modeling Protein Conformational Flexibility Using Network Rigidity, (ii) Modeling Thermodynamic Stability in Polypeptides and Proteins with Non-additive Free Energy Decomposition, (iii) Predicting Protein Stability, Flexibility and Molecular Cooperativity, (iv) New Method of Images to Calculate Electrostatic Reaction Field Energies, TSL Expository Lecture Series V. Theme: Computational Aspects of Physical Sciences**, Universiti Putra Malaysia, (Dec 12-15, 2006)
- (11) **D.J. Jacobs**, *The Role of Mechanics in Understanding Protein Stability, Flexibility and function*. 7th World Congress on Computational Mechanics, in the Molecular & Cell Biology Symposium, Los Angeles, CA (July 16-22, 2006)
- (10) **D.J. Jacobs**, *The ins and outs of the FIRST pebble game*. Workshop on Rigidity, Flexibility and Motion in Biomolecules, Tempe, AZ (May 15-18, 2006)
- (9) **D.J. Jacobs**, *Predicting Protein Stability Using Network Rigidity at Finite Temperatures*. Second International Conference on Multiscale Materials Modeling (MMM-II), in focus session "Multiscale Modeling of Biomaterials" at UCLA, Los Angeles, CA (October 11-15, 2004)

- (8) **D.J. Jacobs**, *Protein Stability and Flexibility: Application to Network Rigidity*. Modeling Protein Flexibility and Motions Workshop at Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Banff Canada (July 17-22, 2004)
- (7) **D.J. Jacobs**, *Network Rigidity at Finite Temperatures and Free Energy Landscapes*. American Mathematical Society, Geometry of Protein Modeling, Lawrenceville, NJ (April, 2004)
- (6) **D.J. Jacobs**, *Predicting Protein Stability from a Free Energy Decomposition*. Mathematics and Computer Science Workshop: The Geometry of Modeling Proteins, Bellairs Research Institute of McGill University, Holetown, Barbados, West Indies (January 16-23, 2004)
- (5) **D.J. Jacobs**, *Generic rigidity of glasses and proteins*. Society for Interdisciplinary and Applied Mathematics (SIAM) annual conference in focus session: Mapping Materials Problems to Graph Algorithms, Atlanta GA (May 1999)
- (4) **D.J. Jacobs**, *Graph rigidity: Applications to material science and proteins*. Canadian Mathematical Society, Kingston, Ontario Canada (Dec 1998)
- (3) **D.J. Jacobs**, *Real-time protein domain evaluator and design tool*. Discrete Mathematics and Theoretical Computer Science (DIMACS) – Combinatorial Clustering & Multi-Domain Protein Structure Analysis, Rutgers University, Piscataway, NJ (June 1998)
- (2) **D.J. Jacobs**, *Identifying floppy and rigid regions in proteins*. Fundamental Materials Research Series: Workshop on Rigidity Theory and Applications, Traverse City, MI (June 1998)
- (1) **D.J. Jacobs**, *Generic Rigidity: The Pebble Game*. American Physical Society (APS) in focus session on network glasses, St. Louis MO (March 1996)

Contributed Talks/Posters at Meetings: (95 total)

Notation: Presentations since August 1999 when started as Assistant Professor:

The presenter is underlined, ^p Postdoc, ^g Graduate student, ^u Undergraduate student

- (95) Wei Song^g and **D.J. Jacobs**, *Image charge optimization for the reaction field by matching to an electrostatic force tensor*, American Physical Society, 78th Annual Meeting of the Southeastern Section of the APS, October 19-22, 2011
- (94) Charles David^g and **D.J. Jacobs**, *A Model Comparison for Characterizing Protein Motions from Structure*, American Physical Society, 78th Annual Meeting of the Southeastern Section of the APS, October 19-22, 2011
- (93) C. Du^p, H. Wang^p, D. Livesay and **D. Jacobs**, *Adaptive Sparse Grid Methods for High-Dimensional Functions*, 117th annual meeting of American Mathematical Society, New Orleans, Louisiana, January 2011.
- (92) D. Verma, **D.J. Jacobs** and D.R. Livesay, *Elucidating the Effects of Mutation upon c-type Lysozyme Through Quantitative Stability/Flexibility Relationships*, 55th Biophysical Society Annual Meeting, Baltimore, MD, March 2011.
- (91) Charles David^g and **D.J. Jacobs**, *A model comparison for characterizing protein motions from structure*, 55th Biophysical Soc. Annual Meeting, Baltimore, MD, March 2011.
- (90) Wei Song^g, Yuchun Lin^p, Andrij Baumketner, Wei Cai and **D.J. Jacobs**, *Optimized Image Charges for Reaction Field Calculations*, 55th Biophysical Society Annual Meeting, Baltimore, MD, March 2011.

- (89) D. Trivedi, Charles David^g, Jörg Rösgen, **D.J. Jacobs** and C.M. Yengo, *The switch II region is critical for the formation of the open cleft weak binding conformation in myosin V*, 55th Biophysical Society Annual Meeting, Baltimore, MD, March 2011.
- (88) **D.J. Jacobs**, D. Trivedi, Charles. David^g and M. Yengo, *Kinetics and thermodynamics of the rate limiting conformational change in the myosin V chemomechanical cycle*, 55th Biophysical Society Annual Meeting, Baltimore, MD, March 2011.
- (87) C. Du^p, H. Wang^p, D. Livesay and **D. Jacobs**, *Adaptive Sparse Grid Method for Represent-ation of the Free Energy Landscape of Proteins*, SIAM Life Science, Pittsburg, July 2010.
- (86) H. Wang^p, C. Du^p, D.R. Livesay and **D.J. Jacobs**, *FAST prediction of protein thermo-dynamics*, Structure-based drug design, Cambridge Health Institute, Boston, June 2010.
- (85) H. Wang^p, C. Du, D.R. Livesay and **D.J. Jacobs**, *FAST prediction of protein thermodynamics*, 54th Biophysical Society annual Meeting, San Francisco, CA (Feb 20-24, 2010)
- (84) D. Verma, **D.J. Jacobs**, Jun-Tao Guo and D.R. Livesay, *Towards comprehensive analysis of protein family quantitative stability/flexibility relationships*, 54th Biophysical Society annual Meeting, San Francisco, CA (Feb 20-24, 2010)
- (83) W. Song^g, P. Qin, Y. Lin^p, A. Baumketner, Wei Cai and **D.J. Jacobs**, *Testing a hybrid solvation model with a transition layer via Molecular Dynamics Simulation*, 54th BPS Meeting, San Francisco, CA (Feb 20-24, 2010)
- (82) C. David^g, C.M. Yengo and **D.J. Jacobs**, *Critical assessment of the statistical significance of simulated motions in Myosin V*, 54th BPS Meeting, San Francisco, CA (Feb 20-24, 2010)
- (81) O.K. Vorov^p, D.R. Livesay, **D.J. Jacobs**, *The competition between degree of freedom excess vs. deficit results in a unified model of protein folding cooperativity*, Protein Folding Gordon Conference, Four Points Sheraton, Ventura, CA (Jan 10-15, 2010).
- (80) Yuchun Lin^p, A. Baumketner, S. Deng, Z. Xu, **D.J. Jacobs** and W. Cai, *An Image-based reaction field method for electrostatic interactions in molecular dynamics simulations of aqueous solutions*, 238th ACS National Meeting, Washington, DC, August 16-20, 2009)
- (79) D.R. Livesay, J.M. Mottonen^p, and D.J. Jacobs, *How conserved are quantitative stability-flexibility relationships across protein families?*, Protein Dynamics, Allostery and Function. Keystone, Colorado USA (June 5-10, 2009)
- (78) J.M. Mottonen^p, D.R. Livesay and D.J. Jacobs. *Allosteric Mechanisms Probed Through Alterations in Network Rigidity*, Protein Dynamics, Allostery and Function. Keystone, Colorado USA (June 5-10, 2009)
- (77) **Platform talk:** J.M. Mottonen^p, **D.J. Jacobs** and D.R. Livesay, *Assessing mechanical and thermodynamic response upon allosteric perturbation*, 53rd Annual BPS Meeting, Boston, MA (March 2009)
- (76) D. Trivedi, C. David, M. Rose, **D.J. Jacobs** and C.M. Yengo, *Temperature Dependent Energy Transfer Measurements Reveal Flexibility in the Upper 50 kDa Domain of Myosin V*, 53rd Annual BPS Meeting. Boston MA (March 2009)
- (75) D. Verma, **D.J. Jacobs** and D.R. Livesay, *Predicting protein mutant stability with a combined experimental and theoretical approach*, 53rd Annual BPS Meeting, Boston, MA (March 2009)
- (74) H. Wang^p, M. Farchild^g, D.R. Livesay and **D.J. Jacobs**, *Molecular partition functions for amino acids and beyond*, 53rd Annual BPS Meeting, Boston, MA (March 2009)
- (73) P. Qin, Z. Xu, W. Cai and **D.J. Jacobs**, *Image Charge Methods for a Hybrid Solvation Model with Transition Layer*, 53rd Annual BPS Meeting, Boston, MA (March 2009)

- (72) **D.J. Jacobs**, D.R. Livesay and O.K. Vorov, *Protein Thermodynamics from Maxwell Constraint Counting*, American Physical Society, March meeting, Pittsburgh, PA (March, 2009)
- (71) O.K. Vorov^p, D.R. Livesay and **D.J. Jacobs**, *Rigidity effects and mechanical unfolding of a beta hairpin*, American Physical Society, March meeting, Pittsburgh, PA (March, 2009)
- (70) H. Wang^p, M. Fairchild^g, D.R. Livesay and **D.J. Jacobs**, *Amino Acid Free Energy Decomposition*, American Physical Society, March meeting, Pittsburgh, PA (March, 2009)
- (69) Scott Barlowe, Tianyi Zhang, **D.J. Jacobs** and Jing Yang, *Multivariate Visual Explanation for High Dimensional Datasets*, IEEE VAST'08 symposium, Columbus OH (October, 2008).
- (68) O. Vorov^p, D.R. Livesay, **D.J. Jacobs**, *Solvable model of mechanical unfolding of biopolymers*, Biopolymer Gordon conference. Salve Regina University, Newport RI, June 8-13 (2008)
- (67) Oleg Vorov^p, D.R. Livesay and **D.J. Jacobs**, *Solvable model of mechanical unfolding of proteins*, Annual American Physical Society March meeting, New Orleans (March 10-14, 2008)
- (66) **D.J. Jacobs**, D.R. Livesay and Oleg Vorov^p, *Correlation functions of flexible macro-molecules*, American Physical Society March meeting, New Orleans (March 10-14, 2008)
- (65) **Platform Talk: D.J. Jacobs**, M.B. Rose, S.R. Adams, R.Y. Tsien and Christopher M. Yengo, *Role of the Upper 50 kDa Domain in Coupling the Actin- and Nucleotide-Binding Regions of Myosin*, 52st Biophysical Society Annual Meeting, Long-Beach, CA (Feb 2-6, 2008)
- (64) Shira Stav^u and **D.J. Jacobs**, *Solving the Linearized Position-Boltzmann Equation for a dielectric sphere using image point multipoles*, 52st Biophysical Society Annual Meeting, Long-Beach, CA (Feb 2-6, 2008)
- (63) Gregory G. Wood, Drew A. Clinkenbeard and **D.J. Jacobs**, *Computational Study on the Helix Propensity of Amino Acids*, 52st Biophysical Society Annual Meeting, Long-Beach, CA (Feb 2-6, 2008)
- (62) Michael J. Fairchild^g, Oleg K. Vorov^p, Jenny Farmer^u, D.R. Livesay and **D.J. Jacobs**, *All atom free energy decomposition for amino acids*, 52st Biophysical Society Annual Meeting, Long-Beach, CA (Feb 2-6, 2008)
- (61) Andrei Y. Istomin^p, **D.J. Jacobs** and D.R. Livesay, *Calculation of Protein Thermodynamics via Distance Constraints: Refined Account of Hydration Effects*, 52st Biophysical Society Annual Meeting, Long-Beach, CA (Feb 2-6, 2008)
- (60) James M. Mottonen^p, D.R. Livesay and **D.J. Jacobs**, *Flexibility and Rigidity Predictions across a Protein Family: Application of the DCM to Oxidized and Reduced Thioredoxins*, Biomolecular Interactions and Methods Gordon Conference, Four Points Sheraton, Ventura, CA (Jan 13-18, 2008).
- (59) A.Y. Istomin^p, **D.J. Jacobs** and D.R. Livesay, *Modeling protein thermodynamic ensemble via distance constraints: Improved account of hydrogen bonding to solvent*, Protein Folding Gordon Conference, Four Points Sheraton, Ventura, CA (Jan 6-11, 2008).
- (58) D.R. Livesay, Dang H. Huynh^g, Sargis Dallakyan^p and **D.J. Jacobs**, *A unified mechanical and thermodynamic analysis of bacterial periplasmic binding protein homologs reveals substantial diversity across the family*, Protein Folding Gordon Conference, Ventura, CA (Jan 6-11, 2008).
- (57) **D.J. Jacobs**, *Protein thermodynamics modeled by self-consistent constraint theory*, Protein Folding Gordon Conference, Four Points Sheraton, Ventura, CA (Jan 6-11, 2008).
- (56) Mingxuan Sun, Michael Rose, Shobana Ananthanarayanan, Roger Y. Tsien, Stephen R. Adams, **D.J. Jacobs**, and Christopher M. Yengo, *A Novel Pre Force-Generation State in the Actomyosin Cross-bridge Cycle*, American Heart Association, Orlando FL (Nov 4-7, 2007).

- (55) James M. Mottonen^p, D.R. Livesay and **D.J. Jacobs**, *Quantitative Stability/Flexibility Relationships Across a Protein Family*, Proteins Gordon Conference, Holderness School, Holderness, NH (June 17-22, 2007).
- (54) A.Y. Istomin^p, **D.J. Jacobs** and D.R. Livesay, *Correlations between size, topology, and folding rate of a protein with two-state kinetics: The role of structural class*, Proteins Gordon Conference, Holderness School, Holderness, NH (June 17-22, 2007).
- (53) O.K. Vorov^p, **D.J. Jacobs** and D.R. Livesay, *Thermodynamics of the Beta-hairpin to Coil Transition using a Distance Constraint Model*, 2007 Annual American Physical Society Meeting, Denver CO (March 5-9, 2007)
- (52) Shira Stav^u, Wei Cai, Shaozhong Deng and **D.J. Jacobs**, *Reaction Field Calculations Using Efficient Image Charge Method*, 51st Biophysical Society Annual Meeting, Baltimore, MD (March 3-7, 2007)
- (51) Mike Fairchild^u and **D.J. Jacobs**, *Thermodynamics of a beta-hairpin to coil transition elucidated by an exact solution using a minimal distance constraint model*, 51st Biophysical Society Annual Meeting, Baltimore, MD (March 3-7, 2007)
- (50) Mike Rose, Whitney Hubbard^u, Mingxuan Sun, Roger Y. Tsien, Stephen R. Adams, Christopher M. Yengo and **D.J. Jacobs**, *Searching for Conformational Pathways in Myosin V*, 51st Biophysical Society Annual Meeting, Baltimore, MD (March 3-7, 2007)
- (49) Andrei Y. Istomin^p, **D.J. Jacobs**, M. Michael Gromiha, Dennis R. Livesay, *Is Non-additivity within double mutant cycles related to protein structure rigidity?* 51st Biophysical Society Annual Meeting, Baltimore, MD (March 3-7, 2007)
- (48) O.K. Vorov^p, D.R. Livesay and **D.J. Jacobs**, *Thermodynamics of the Beta-hairpin to Coil Transition Revealed by a Distance Constraint Model*, 20th Annual Gibbs Conference on Biothermodynamics, Carbondale IL (Oct 7-10, 2006)
- (47) D.R. Livesay, **D.J. Jacobs** and M.L. Tasayco, *Quantifying Stability/Flexibility Relationships in Proteins*, 20th Annual Gibbs Conference on Biothermodynamics, Carbondale IL (Oct 7-10, 2006)
- (46) **D.J. Jacobs**, D.R. Livesay and M.L. Tasayco, *Relating Thermodynamic Stability to Mechanical Flexibility in Proteins*, Biopolymer Research Conference, Salve Regina University, Newport RI (June 11-16, 2006)
- (45) **Platform talk: D.J. Jacobs**, D.R. Livesay, J. Hules[§] and M.L. Tasayco, *Elucidating quantitative stability/flexibility relationships within thioredoxin and its fragments using a distance constraint model*, 50th Biophysical Society (BPS) annual meeting, Salt Lake City, Utah (Feb 18-22, 2006)
- (44) D.R. Livesay and **D.J. Jacobs**, *Conserved quantified stability/flexibility relationships (QSFR) in an Orthologous RNase H pair*, Proteins Gordon Research Conference, Plymouth, NH (June, 2005)
- (43) **D. J. Jacobs**, J. Hules[§], S. Green[§] and D. R. Livesay, *Quantifying Stability-Flexibility Relationships in Proteins*, American Physical Society (APS) March Meeting, LA CA (March 21-25, 2005)
- (42) **D.J. Jacobs**, S. Dallakyan^p, G. Wood^p and Dennis R. Livesay, *The Mechanics of Protein Stability and Flexibility*, 49th Biophysical Society (BPS) annual meeting, Long Beach, CA (Feb 12-16, 2005)
- (41) Dundar Karabay[§], Sargis Dallakyan^p and **D.J. Jacobs** *Thermodynamic Properties of Protein Backbone Hydrogen Bonds Predicted by a Quantum Mechanical Model*, 49th Biophysical Society (BPS) annual meeting, Long Beach, CA (Feb 12-16, 2005)
- (40) Moon S. Lee[§], Gregory Wood^p and **D.J. Jacobs**, *Bioinformatic and Statistical Analysis of Thermodynamic Stability of Alpha-Helix to Coil Transition in Polypeptides*, 49th Biophysical Society Annual Meeting, Long Beach, CA (Feb 12-16, 2005)
- (39) Sargis Dallakyan^p, **D.J. Jacobs** and Dang. Huynh[§], *Quantifying Thermodynamic Stability and Flexibility in Bacterial Periplasmic Binding Proteins*, 49th Biophysical Society Annual Meeting, Long Beach, CA (Feb 12-16, 2005)

- (38) **D.J. Jacobs**, Sargis Dallakyan^p, Gregory Wood^p and Dennis R. Livesay. *Protein Thermodynamics from the 3D topological structure of the Native State*, 17th Annual CSU Biotechnology Symposium LA, CA. (Jan 14-15, 2005)
- (37) Moon Lee^g, G. Wood^p and **D.J. Jacobs**, *Identifying Thermodynamic Stability Characteristics in Heterogeneous Polypeptides that Undergo the Alpha-Helix to Coil Transition*, 17th Annual CSU Biotechnology Symposium (LA, CA Jan 14-15, 2005)
- (36) Dundar Karabay^g, S. Dallakyan^p and **D.J. Jacobs**, *Calculating Thermodynamic Properties of Protein Backbone Hydrogen Bonds Predicted by a Quantum Mechanical Model*, 17th Annual CSU Biotechnology Symposium (LA, CA Jan 14-15, 2005)
- (35) Jeremy Hules^g, D.R. Livesay and **D.J. Jacobs**, *Quantitative Stability and Flexibility Relationships within Thioredoxin*, 17th Annual CSU Biotechnology Symposium (LA, CA Jan 14-15, 2005)
- (34) **D.J. Jacobs**, Sargis Dallakyan^p, Gregory Wood^p and Dennis R. Livesay. *Protein Thermodynamics from the 3D topological structure of the Native State*, 18th Symposium of the Protein Society, San Diego, CA. (Aug. 14-18, 2004)
- (33) **D.J. Jacobs**, Sargis Dallakyan^p, Gregory Wood^p and Dennis R. Livesay. *Protein Thermodynamics from the 3D topological structure of the Native State*, Biopolymers Gordon Research Conference, Salve Regina University, Newport, RI (June 13-18, 2004)
- (32) Dundar Karabay^g, Sargis Dallakyan^p and **D.J. Jacobs**. *Enthalpies and entropies for hydrogen bonds in proteins from quantum mechanics*, 48th Biophysical Society (BPS) annual meeting, Baltimore, MD (Feb 14-18, 2004)
- (31) **D.J. Jacobs**, Sargis Dallakyan^p, Gregory Wood^p and Dennis R. Livesay. *Protein Thermodynamics from the 3D topological structure of the Native State*, 48th Biophysical Society (BPS) annual meeting, Baltimore, MD (Feb 14-18, 2004)
- (30) Gregory Wood^p, Sargis Dallakyan^p and **D.J. Jacobs**. *Protein Thermodynamics from the 3D Topological Structure of the Native State*, American Physical Society (APS) annual March meeting, Montreal, Quebec Canada (March 22-26, 2004)
- (29) G.G. Wood^p, A. Heckathorne^g and **D.J. Jacobs**. *Network Rigidity Calculations of Cold Denaturation*, American Physical Society (APS) annual March meeting, Montreal Quebec, Canada (March 22-26, 2004)
- (28) M.V. Chubynsky, M.F. Thorpe, **D.J. Jacobs**, W. Whiteley, *Rigidity of central-force elastic networks in three dimensions*, American Physical Society (APS) annual March meeting, Austin, TX (March 3-7, 2003)
- (27) Alicia Heckathorne^g, Gregory Wood^p and **D.J. Jacobs**, *Understanding folding and stability from a mechanical point of view: The alpha-helix to coil transition revisited*, 47th Biophysical Society (BPS) annual meeting, San Antonio, Texas (March 1-5, 2003)
- (26) Alicia Heckathorne^g and **D.J. Jacobs**, *The Alpha Helix to Coil Transition Revisited*, Biopolymers Gordon Research Conference, Salve Regina University, Newport RI, (June 16-21, 2002)
- (25) Dang H. Huynh^g, Jaime D. Osorio, Laura I. Gomez^u, Arnulfo Martinez^u, **D. J. Jacobs**, *Comparison of Conformational Flexibility in Four Homologous Periplasmic Binding Proteins*, 46th Biophysical Society (BPS) annual meeting. San Francisco, CA (Feb 23-27, 2002)
- (24) (*award winning poster*) Dang Huynh^g, J.D. Osorio^u, Laura I. Gomez^u, Arnulfo Martinez^u and **D.J. Jacobs**, *Comparison of Conformational Flexibility in Four Homologous Periplasmic Binding Proteins*, SACNAS (Society for Advancement of Chicanos and Native Americans in Science) National Conference, Phoenix AZ (Sept. 27-30, 2001)

- (23) **D.J. Jacobs** and Jeremy Hules^g, *Characterization of Conformational Flexibility in Hinge-Binding Proteins: Hierarchical Flexibility Maps in Terms of Dihedral Angle Internal Coordinates*, Protein Flexibility and Folding Workshop. Traverse City, MI (Aug, 2000)
- (22) **D. J. Jacobs**, *Characterizing the Degree of Flexibility in Proteins*, Quantitative Challenges in the Post-Genomic Sequence Era Symposium. San Diego, CA (Jan, 2000)

Additional Contributions at Meetings: (Selected presentations prior to Assistant Professor)

- (21) **D.J. Jacobs**, L.A. Kuhn, and M.F. Thorpe, *Flexibility and rigidity in protein structures*, American Physical Society (APS) **Special Centennial Meeting**, Atlanta GA (March, 1999)
- (20) **D.J. Jacobs**, L.A. Kuhn and M.F. Thorpe, *Predicting conformational flexibility in protein structure*, American Physical Society (APS), Ohio Section, Flint MI (May, 1999)
- (19) **D.J. Jacobs**, M.F. Thorpe and L.A. Kuhn, *Identifying Floppy and Rigid Regions in Proteins*, American Physical Society, annual March meeting, Los Angeles, CA (March, 1998)
- (18) (*award winning poster*) **D.J. Jacobs** and M.F. Thorpe, *Rigidity in Network Glasses and Proteins*, Fundamental Materials Research Symposium, East Lansing, MI (April, 1998)
- (17) **D.J. Jacobs** and M.F. Thorpe, *Rigidity in Network Glasses and Proteins*, Midwest Solid State Theory Symposium, Argonne National Lab, IL. (Oct, 1997)
- (16) **D.J. Jacobs**, *Floppy Modes and the Nature of the Rigidity Transition*, 77th Statistical Mechanics meeting at Rutgers, Piscataway, NJ (May, 1997)
- (15) **D.J. Jacobs** and M.F. Thorpe, *The Rigidity Transition in Two and Three Dimensions*, American Physical Society (APS) annual March meeting, Kansas City, KA (March, 1997)
- (14) **D.J. Jacobs** and M.F. Thorpe, *The Rigidity Transition in Two and Three Dimensions*. Midwest Solid State Theory Symposium, University of Illinois at Urbana-Champaign, IL (October, 1996)
- (13) M.F. Thorpe, **D.J. Jacobs** & A.R. Day, *Generic rigidity percolation in two dimensions*. American Physical Society (APS) annual March meeting, St. Louis, MO (March, 1996)
- (12) **D.J. Jacobs**, B.R. Djordjevic and M.F. Thorpe, *Exact Counting of Floppy Modes Using Graph Theory in Two Dimensional Network Glasses*, American Physical Society (APS) annual March meeting, San Jose, CA (March, 1995)
- (11) **D.J. Jacobs**, *Domain Growth in a One-dimensional Diffusive Lattice Gas with Short Range Attraction*, American Physical Society, March meeting, Pittsburgh, PA (March, 1994)
- (10) **D.J. Jacobs** and Andrew Masters, *Domain growth in one-dimensional geometries*. FOM statistical physics meeting, Lunteren, The Netherlands (Jan, 1994)
- (9) Sonali Mukherjee, **D.J. Jacobs** and Hisao Nakanishi, *Breakdown of the Scaling Relation $d_s = 2d_f/d_w$ in DLA*. 70th Statistical Mechanics Meeting at Rutgers, NJ (Dec, 1993)
- (8) **D.J. Jacobs**, *Phase Separation in a 1-d Diffusive Lattice Gas with Short Range Attraction*, 69th Statistical Mechanics Meeting at Rutgers, Piscataway, NJ (May, 1993)
- (7) **D.J. Jacobs** and Hisao Nakanishi, *Persistent random walks in static disordered media*. FOM Statistical Physics meeting, Lunteren, The Netherlands (Jan, 1993)
- (6) **D.J. Jacobs** and Hisao Nakanishi, *Persistent random walks in static disordered media*. American Physical Society, Indianapolis, IN. (March, 1992)
- (5) **D.J. Jacobs** and Hisao Nakanishi, *Persistent random walks in disordered media*. 19th Midwest Solid State Theory Symposium, Mich. State Univ., East Lansing MI (Oct, 1991)
- (4) **D.J. Jacobs**, Muralidhar, Ramkrishna and Hisao Nakanishi, *Anisotropic diffusion on percolation clusters*. American Physical Society, Annual March Meeting, Cincinnati, OH (March, 1991)

- (3) **D.J. Jacobs**, Muralidhar, Ramkrishna and Hisao Nakanishi, *Anisotropic diffusion on percolation clusters*. 18th Midwest Solid State Theory Symposium, Northwestern University, Evanston, IL (Oct, 1990)
- (2) **D.J. Jacobs** and Hisao Nakanishi, *Long time tails, anomalous diffusion and periodicity for the autocorrelations of diffusion in disordered media*. American Physical Society, Annual March meeting Anaheim, CA (March, 1990)
- (1) **D.J. Jacobs** and Hisao Nakanishi, *Correlation functions and the diffusion coefficient for random hopping models*. NATO ASI Diffusion in Materials, Aussois, France (March, 1989)

FUNDING HISTORY

A total of \$4,925,168 (direct and indirect) worth of funding has been obtained over my career to date. Of which **\$2,228,557** (direct and indirect) has been to support my lab.

External Support: Pending

Quantified Stability/Flexibility Relationships within Antibody Fragment.
\$20,790 specifically to extend postdoc from February 2013 to April 2013.
Medimunne Inc. (contract at full overhead rate)
Role: co-PI.

External Support

Antibody fragment stability: A focus on domain-domain interactions.
\$99,495 specifically to support 1 postdoc from February 2012 to February 2013.
Medimunne Inc. (contract at full overhead rate)
Role: co-PI.

High Performance Computing in Computational Biology
\$497,908 requested for one-time purchase of state-of-art computer.
NIH Shared Instrumentation Grant Program (S10).
Livesay, DR (PI) Department of Bioinformatics and Genomics
Role: Major user as either Principal or Co-Investigator on three different NIH awards.

ARRA Administrative Supplement to Parent Grant GM073082
\$102,124 over 8 months, from February 2010 to October 2010.

NIH NIGMS

Jacobs, Principal investigator

Energy Transduction in Myosin
\$385,000 over 2 years, from January 2009 to December 2011
NIH-R21 HL093531
Yengo, M.C. PI
Role: Co-Investigator

Numerical Methods for Fast and Accurate Calculation of Electrostatic Interactions in Biomolecular Simulations
\$1,440,000 over 4 years, from July 1, 2007 to June 30, 2011
NSF/NIH joint DMS/NIGMS Mathematical Biology Initiative

Awarded through NIH NIGMS R01 funding mechanism
Wei Cai (PI) Department of Mathematics and Statistics, UNC Charlotte
Shaoyong Deng (co-PI), Department of Mathematics and Statistics, UNC Charlotte
Andrij Baumketner (co-PI), Department of Physics and Optical Science, UNC Charlotte
Role: Co-PI

Predicting protein stability and flexibility

\$1,284,144 over 4 years, from March 2006 to Feb 2010 and a no cost extension to Feb 2011
NIH-R01 GM073082

Jacobs, D.J. (PI)

Role: Principal investigator

CRI Duke Postdoctoral Matching (~\$50,000 over 2 yrs) Spring 2008 to Spring 2010

Successful for two years 50/50 matching on grant R01 GM073082 (Jacobs, PI)

Successful for two years 50/50 matching on grant R01 GM08300 (Cai, PI)

Internal UNC Charlotte Support

- ✓ *Quantitative stability/flexibility relationships in the GABA transport protein.*

\$12,000 from May 2012 to Aug 14, 2013.

Faculty Research Grant

Dennis Livesay (PI) Bioinformatics and Genomics, UNC Charlotte

Role: Co-PI

- ✓ *Using Information Visualization to Identify Sequence Pattern Signatures for Alpha Helix Stability within Model HP-Polypeptides*

\$12,000 over 18 months, from July 1, 2006 to Dec 31, 2007

Faculty Research Grant

Yang, J. (PI) Computer Science Department, UNC Charlotte

Role: Co-PI

External UNC Charlotte Support

- ✓ **Supplement to:** *Predicting protein stability and flexibility*

Subproject title: *Investigations of Underlying Mechanisms of Allostery in Proteins*

\$282,943 over 2 ½ years, from Sept. 1, 2006 to Feb 28, 2009

NIH-R01 GM073082-01A1s1

Role: Principal investigator

- ✓ *Elucidating protein flexibility and dynamics using distance constraint model for “in silico” protein design*

~ \$20,000 for two years from Dec 31, 2006 to Dec 31, 2008

Malaysia, Fundamental Research Grant, Protein Chemistry and Theoretical Biophysics

Prof. Basyaruddin Bin Abdul Rahman (PI), University Putra Malaysia

Role 1: co-PI involving a shared Ph.D. student: Ms. Rosa Abedi (Advisor Prof. Rahman)

Role 2: Thesis committee member for Ms. Rosa Abedi

- ✓ *Investigations of conformational changes in myosin*

\$3,500 for summer 2006, Undergraduate stipend for Ms. Whitney Hubbard

UNC General Administration Undergraduate Research Opportunity Expansion

Jacobs, D.J. (PI) Student stipend for Ms. Whitney Hubbard:
Role: Principal investigator, and undergraduate mentor

- ✓ **Travel supplement** for *Investigations of conformational changes in myosin*
\$1,000 for Ms. Whitney Hubbard to travel to the Biophysical Society Meeting
UNC General Administration Undergraduate Research Opportunity Expansion
Role: Principal investigator, and undergraduate research mentor

Internal CSUN Support (each grant provided 3 units of teaching release time, equivalent to **\$5,000**)

- ✓ *Investigation of conformational flexibility in protein structure*
Fall 2000; Source: University Wide Probationary Faculty Competition
Role: Principal investigator
- ✓ *Monte Carlo simulation of protein fold dynamics using a skeletal model*
Fall 2000; Source: University Wide Research, Scholarship and Creative Activity Competition.
Role: Principal investigator
- ✓ *Characterizing Conformational Flexibility in Dihydroflavone Reductase using a 1 nanosecond MD simulation*
Spring 2001; Source: College of Science and Mathematics Research Competition.
Role: Principal investigator
- ✓ *Does Network Rigidity Explain the Cooperative Hydrogen Bond Interactions within Proteins?*
Fall 2001; Source: University Wide Research, Scholarship and Creative Activity Competition.
Role: Principal investigator
- ✓ *An Exact Model Solution for the alpha-helix to Coil Transition: Investigation of Cooperative Hydrogen Bond Interactions Mediated Via Network Rigidity*
Fall 2001; Source: College of Science and Mathematics Research Competition.
- ✓ *Investigation of the Alpha-Helix to Coil Transition in Heterogeneous Peptides*
Spring 2002; Source: University wide Probationary Faculty Competition.

External CSUN Support

- ✓ *Dihedral-angle characterization of conformational flexibility in protein structure*
\$370,328 from October 2002 to June 2005
NIH S06 GM48680-0952; Zavala, M.E. (Adm. Director)
Jacobs, D.J. (PI)
Role: Principal Investigator
- ✓ *Bioinformatic study correlating protein flexibility with function*
\$100,000 from January 2003 to December 2004
CSUPERB-Joint Venture Matching Grant (\$25,000)
Cengent Therapeutics in-kind industrial match (\$75,000)
Jacobs, D.J. (PI)
Role: Principal investigator
- ✓ *Dihedral Angle Characterization of Conformational Flexibility in Hinge-bending Proteins Deduced from Hydrogen Bond Interactions*
\$31,218 from 2000 to 2004

Research Corporation, CC5141

Jacobs, D.J. (PI)

Role: Principal investigator

- ✓ *Development of a Coherent Biomedical Physics Program*

\$72,880 from 2000-2002

State of California Strategic work-force initiative, (Blanco, Jacobs, Lee)

University Wide Competition for Lottery Funds

Role: Principal Program Developer

External Support (prior to arriving at CSUN)

- ✓ *Real-time Protein Domain and Flexibility Identification*

\$100,000 from September 1998 to August 1999

NIH-SBIR R43 GM58337-01

Jacobs, D.J. Director of Research at MolFlex, LLC a Biotechnology Software Company

Role: Principal investigator

- ✓ *Floppy Modes in Glasses: The Pebble Game*

\$169,000 from July 1996 to June 1999

NSF-DMR 96-32182

Thorpe, M.F. (PI)

Role: Key personnel (largely wrote this proposal)

TEACHING

Ph.D. Thesis graduate students: (4)

Wei Song (Expected graduation, spring 2013. Field: Computer Science. University: UNCC)

Thesis: *Modeling, simulation and analysis of the electrostatic force reaction field from solvent*

Charles David (Graduated, summer 2012. Field: Bioinformatics. University: UNCC)

Thesis: *Essential dynamics of proteins using geometrical simulation and subspace analysis*

Luis Gonzalez (Graduated, summer 2011. Field: Computer Science. University: UNCC)

Thesis: *A virtual pebble game to ensemble average graph rigidity*

Rosa Abedi (Graduated, Summer 2008. Field: Chemistry. University: Universiti Putra Malaysia)

Thesis: *Thermal Unfolding Study of Thermoalkalophilic Lipases at High Temperatures*

Remark: Thesis advisor: Prof. Haji Mohd Basyaruddin. As part of an international collaboration, I served as Rosa's secondary Ph.D. thesis advisor.

M.S. Thesis graduate students: (7)

Jenny Farmer (Expected Graduation, spring 2014. Field: Applied Physics. University: UNCC)

Thesis: *Distribution functions from small random samples using a novel maximum entropy method*

Moon Lee (Graduated, spring 2005. Field: Physics. University: CSUN)

Thesis: *Investigations on thermodynamic characteristics of helix-coil transition in HP-heterogeneous polypeptides using network rigidity*

Shelley Green (Left Graduate School on good standing due to personal reasons. University: CSUN)

Thesis: *Investigating Protein Flexibility using a Temperature Dependent Elastic Network*

Dundar Karabay (Graduated, spring 2005. Field: Physics. University: CSUN)

Thesis: *Calculating Thermodynamic Properties of Protein Backbone Hydrogen Bonds Predicted by a Quantum Mechanical Model*

Jeremy Hules (Graduated, spring 2005. Field: Physics. University: CSUN)

Thesis: *Quantitative Flexibility and Stability Relationships Within the Protein Thioredoxin*

Alicia Heckathorne (Graduated, spring 2002. Field: Physics. University: CSUN)

Thesis: *A New Approach to the Alpha Helix Coil Transition Using Network Rigidity*

Dang Huynh (Graduated, spring 2002. Field: Biology. University: CSUN)

Thesis: *Comparison of Conformational Flexibility in Proteins Exhibiting Hinge-Bending Motions*

Project based M.S. graduate students: (4)

Charles David (Graduated, summer 2007. Field: Applied Physics. University: UNCC)

Project: *Quaternions and the rotation of rigid bodies*

Carlos Soria (Graduated, unknown to me. Field: Physics. University: CSUN)

Project: *Dynamics of coupled rigid bodies through hinge motions*

Vahan Minassian (Graduated, unknown to me. Field: Physics. University: CSUN)

Project: *Dynamics of simple two-dimensional networks under fixed constraint topology*

Tirso Silva (Graduated, spring 2002. Field: Physics. University: CSUN)

Project: *Application of the Conjugate Gradient Method to minimize energy in elastic networks*

Honors Thesis Undergraduate Research: (5)

Raymond More (Expected Graduation, spring 2014. Field: Physics. University: UNCC)

Thesis: *Uncovering atomic correlations from trajectories describing protein dynamics*

Aron Brettin (Expected Graduation, spring 2013. Field: Physics. University: UNCC)

Thesis: *Study of ion-ion interactions in aqueous solutions*

Chris Singer (Expected Graduation, spring 2013. Field: Physics. University: UNCC)

Thesis: *Study of dynamics in the chemokine family of proteins*

Shira Stav (Graduated spring 2008. Field: Physics and Mathematics. University: UNCC)

Thesis: *Calculating the reaction field for charges inside a sphere embedded in a dielectric continuum*

Michael Fairchild (Graduated, spring 2007. Field: Physics and Mathematics. University: UNCC)

Thesis: *Thermodynamics of the β -Hairpin to Coil Transition*

Research Experience for Undergraduates (NSF REU program): (2)

John Grinstead (REU summer 1998. Field: Physics. University: Michigan State University)

Project: *Analysis of rigidity in secondary protein structures using constraint counting*

Keith Johnson (REU summer 1995. Field: Mathematics. University: Michigan State University)

Project: *Comparison of Maxwell constraint counting with the Pebble Game in 2D generic networks*

Summer Undergraduate Research (UNC General Administration Opportunity): (1)

Whitney Hubbard (Graduated, unknown to me. Field: Mechanical Engineering. University: UNCC)
Project: *Investigations of conformational changes in myosin*

Research credit research experience at CSUN (term papers required): (6)

Laura Gomez, Chad Yamasaki, Rolando Maldonado, Arnulfo Martinez, Jamie Osorio, Trang Tong.

Undergraduate Independent Studies (required component in Biomedical Physics program): (5)

Mahnaz Asghaei, Berrie Goldman, Aaron Halverson, Chekuri Sahithi, Mychica Simmons.

Graduate Student Independent Studies given: (3)

Charles David (6000 level Classical Mechanics. University: UNCC)

Duong Luong (5000 level Statistical Mechanics and Thermal Physics. University: UNCC)

Ammar Durghalli (600 level Biophysics. University: CSUN)

Committee member for Ph.D. Thesis Defense: (6) (^{C,N} denotes either core or neutral member)

^CBrett Peters (Defense: Expected spring 2014. Field: Mechanical Engineering. Advisor: Mesbah Uddin)

^CKyle Kreth (Defense: Expected spring 2013. Field: Bioinformatics. Advisor: Anthony Fodor)

^CDeeptak Verma (Defense: Expected fall 2012. Field: Bioinformatics. Advisor: Dennis Livesay)

^CScott Barlowe (Defense: Oct 2011. Field: Computer Science. Advisor: Jing Yang)

^NRoya Hakimzadeh (Defense: March 2010. Field: Electrical Engineering. Advisor: Miri Mehdi)

^CJudy Moore (Defense: Oct 2009. Field: Biology. Advisor: Chris Yengo)

^CSeungmoo Yang (Defense: March 2009. Field: Optics. Advisor: Vasily Astratov)

Committee member for Masters Thesis Defense: (6) (^{C,N} denotes either core or neutral member)

^CRichard Dudley (Defense: June 2012. Field: Applied Physics. Advisor: Mike Fiddy)

^CKenneth Allen (Defense: April 2012. Field: Applied Physics. Advisor: Vasily Astratov)

^NJon Maner (Defense: Jul 2011. Field: Chemistry. Advisor: Dan Rabinovich)

^CBen Faulk (Defense: Nov 2009. Field: Applied Physics. Advisor: Ana Joffre)

^NShaun Shelton (Defense: Jul 2007. Field: Chemistry. Advisor: Brian Cooper)

^NRania Dumarieh (Defense: April 2006. Field: Chemistry. Advisor: Brian Cooper)

COURSES TAUGHT (FORMAT = (teaching units, course, description))

UNC Charlotte: (Since August 2005)

1. (3) PHYS 6251 Graduate level: Statistical Mechanics
2. (3) PHYS 5242 Graduate level: Quantum Mechanics II
3. (3) PHYS 4242 Senior level: Quantum Mechanics II
4. (3) PHYS 4241 Senior level: Quantum Mechanics I
5. (3) PHYS 3121 Junior level: Newtonian Mechanics
6. (3) PHYS 4222 Junior/Senior level: Lagrangian and Hamiltonian Mechanics
7. (3) PHYS 3151 Junior/Senior level: Thermal and Statistical Mechanics
8. (3) PHYS 6121 Graduate level: Classical Dynamics (Given as Independent study)

CSUN: (Since August 1999)

9. (2) PHYS 100A Algebra-based Intro Physics (Mechanics, Sound, Thermodynamics)
10. (2) PHYS 100AL Corresponding Lab to PHYS 100A

11. (3) PHYS 100B Algebra-based Intro Physics (Electromagnetism, Electricity, Optics, Nuclear)
 12. (3) PHYS 220A Calculus-based Introductory Course for Engineers and Scientist (Mechanics)
 13. (3) BMPH 304 Junior-level: Physical modeling applied to the human body
 14. (3) PHYS 389 Junior-level: Applied mathematics course for Physicists
 15. (4) PHYS 405 Special topics course pertaining to Biological Physics (macro and micro)
 16. (4) BMPH 405 Senior-level: Biophysics, molecular thermodynamic principles and applications
 17. (4) BMPH 406 Senior-level: Biophysics, statistical mechanics with advanced applications
 18. (4) PHYS 431 Senior-level: Thermal and Statistical Physics
 19. (2) PHYS 496 Senior-level: Advanced physics research-computational lab
 20. (3) PHYS 630 Graduate-level: Core Course in Statistical Physics
 21. (3) PHYS 650 Graduate-level: Core Course in Quantum Mechanics
-

Courses developed in biomedical physics and biophysics at CSUN

1. (3) BMPH 304 Junior level: Physics of the Body
2. (2) BMPH 360 Junior level: Measurements in Biomedical Physics (advised in content)
3. (4) BMPH 405 Senior level: Biomedical Physics I
4. (4) BMPH 406 Senior level: Biomedical Physics II
5. (3) PHYS 595MB Senior/Graduate level: Molecular Biophysics

Post Ph.D. and Pre-faculty teaching experience:

Michigan State University: (1994 to 1996 I was teaching 50% and doing research 50%)

Courses taught: I gave guest lectures for large-class (200 students) algebra-based introductory physics courses and one small-class (40 students) liberal arts physics course designed for non-science majors. I was responsible for providing informal off-the-cuff open-time problem solving sessions that was done in a round-table discussion forum. I worked these open help rooms simultaneously among many MSU faculty members and graduate students. In all these courses, this special format for the open-time recitations was tied to a new CAPA system that was being developed at MSU.

CAPA: About 50% of my teaching responsibilities were in designing questions for the new CAPA (*Computer Assisted Personalized Assignments*) system. The CAPA system exists today, and it has the feature that every student in the class gets a personalized homework assignment. This prevents simple cheating by copying answers. Instead it stimulates learning by encouraging students to discuss methods of solutions. For the computer to do this, someone (like me) had to formulate the questions and program the questions with certain given information using random variables over physically reasonable ranges. I was involved in the initial development stages. Today, CAPA is commercially available.

Mentored Student Presentations: (Student events, underlined name indicates presenter)

UNC Charlotte:

(to be added: at least 10 more CBES student posters plus 1 Undergraduate Research Scholar, poster 2012)

(18) Talk: Shira Stav (**2nd place award**)

Solving the Linearized Poisson-Boltzmann Equation for a dielectric sphere using image point multipoles
15th Annual Undergraduate Research Conference (April 18, 2008)

- (17) Talk: Shira Stav (**1st place award**)
Reaction Field Calculations Using an Efficient Image Charge Method
14th Annual Undergraduate Research Conference (April 20, 2007)
- (16) Talk: Michael Fairchild (**1st place award**)
Thermodynamics of the β -Hairpin to Coil Transition
14th Annual Undergraduate Research Conference (April 20, 2007)
- (15) Poster: Shira Stav
New Electrostatic Calculations for Biological Systems: Bringing Mathematics to Life
Raleigh --- **State Senate** UNC Undergraduate Research Presentations (April 17, 2007)
- (14) Poster: Michael Fairchild
Using Theoretical Physics to Help Understand Protein Thermodynamics
Raleigh --- **State Senate** UNC Undergraduate Research Presentations (April 17, 2007)

CSUN:

- (13) Talk: Shelley Green
Quantifying Stability-Flexibility Relationships in Proteins: Web Interface
Sigma Xi 2005 Graduate Student Research Symposium (April, 2005)
- (12) Talk: Jeremy Hules (**3rd place award**)
Quantitative Stability and Flexibility Relationships within the Protein Thioredoxin
Sigma Xi 2005 Graduate Student Research Symposium (April, 2005)
- (11) Talk: Moon Suk Lee
Thermodynamic Stability of Alpha-helix to Coil Transition in HP-polypeptides
Sigma Xi 2005 Graduate Student Research Symposium (April, 2005)
- (10) Talk: Dundar Karabay
Empirical Model for Molecular Atomic Partial Charges
Sigma Xi 2005 Graduate Student Research Symposium (April, 2005)
- (9) Talk: Moon S. Lee
Identifying Thermodynamic Stability Characteristics in Heterogeneous Polypeptides Using a Minimal HP-model that Undergo the Alpha-Helix to Coil Transition
Graduate Level, 9th Annual Student Research Symposium (Nov, 2004)
- (8) Talk: Dundar Karabay
Calculating Thermodynamic Properties of Protein Backbone Hydrogen Bonds Predicted by a Quantum Mechanical Model
Graduate Level, 9th Annual Student Research Symposium (Nov, 2004)
- (7) Talk: Dundar Karabay
Hydrogen Bond Thermodynamic Properties from a Simple Quantum Mechanical Model
Sigma Xi 2004 Graduate Student Research Symposium (April, 2004)
- (6) Talk: Dang Huynh (**1st place**)
Comparison of Conformational Flexibility of Four Homologous Periplasmic Binding Proteins
Graduate Level, Statewide 2002 CSU Student Research Symposium (April, 2002)
- (5) Talk: Dang Huynh (**1st place**)
Comparison of Conformational Flexibility of Four Homologous Periplasmic Binding Proteins
Sigma Xi 2002 Graduate Student Research Symposium (April, 2002)
- (4) Talk: Alicia Heckathorne
Understanding the Alpha Helix Coil Transition Using Network Rigidity
Sigma Xi 2002 Graduate Student Research Symposium (April, 2002)

- (3) Poster: D. Huynh, J. Osorio, L. Gomez and A. Martinez
Comparison of Conformational Flexibility of four Homologous Periplasmic Binding Proteins
Graduate Level, 6th Annual Student Research Symposium (Nov, 2001)
- (2) Talk: Dang Huynh (**1st place**)
Comparison of Conformational Flexibility of Four Homologous Periplasmic Binding Proteins
Graduate Level, 6th Annual Student Research Symposium (Nov, 2001)
- (1) Talk: Jeremy Hules
Characterizing Flexibility in Proteins
Undergraduate Level, 5th Annual Student Research Symposium (Nov, 2000)

UNIVERSITY SERVICE

UNC Charlotte: (Since August 2005, # indicates chair of committee)

- Nov 2005 Guest speaker for career/research opportunities in Physics for PHYS 1000.
- Nov 2005 On Campus Explore UNC Charlotte Physics Student Recruitment
- Dec 2005 Participated in Graduation Ceremonies
- 2005 – 2006 Dept. Faculty Search Committee (Corwin, Jacobs, Moyer, Suleski[#])
- 2005 – 2007 Dept. Graduate Curriculum Committee (Davies, Gbur, Jacobs, Tyson[#])
- 2005 – ... **Focus Leader** on Molecular Engineering and Design (MED) for the *Center for Biomedical Engineering and Science* (CBES). (Robin Coger, Matt Davies, Don Jacobs, Charles Lee, Pat Moyer, Rick Peindl, Nigel Zheng).
- 2005 – 2007 Arranged **Six** special Biophysics related Seminars
- 2006 – 2007 **Chaired** Dept. Faculty Search Committee (Baumketner, Corwin, Fried, Jacobs[#], Raja)
- 2006 – 2007 **Chaired** Dept. Biophysics Program sub-committee (Baumketner, Fried, Jacobs[#])
- 2006 Graduate seminar series talk: *Overview of Biomedical Activities at UNC Charlotte*
- 2007 – 2008 Dept. Chair Search Committee (Pat Moyer[#], Eric Johnson, Susan Trammell, Lawrence Mays and Alan Dow).
- 2007 – 2008 **Chair** department task force on the development of a BA Biomedical Physics program and Applied Physics Ph.D. program (Baumketner, Fried, Jacobs[#], Jofre).
- 2007 – 2008 Undergraduate Curriculum Committee of Physics and Optical Science (Elisabeth Benchich, Mike Corwin, Don Jacobs, Eric Johnson, and Susan Trammell[#].)
- 2007 – 2008 Planning Committee for Applied Physics Ph.D. program in conjunction with the Graduate Curriculum Committee. (Davies, Jacobs, Suleski, Tyson[#])
- 2007 – 2008 College of Arts and Science (COAS) Diversity Task Force
- 2008 – 2009 CMC-UNC-Charlotte Nano-medicine Collaborative Advisory Steering Committee
- Sept 2008 Guest speaker for career/research opportunities in Physics for PHYS 1000.
- 2008 – 2009 Dept. Chair Search Committee (Corwin[#], Davies, Fried, Jacobs, Trammell, Mays and Dow).
- 2008 – 2009 **Chaired** Dept. Faculty Search Committee for Assistant Prof. Biophysics/Soft matter, (Fiddy, Her, Jacobs[#], Jofre, Moyer)
- Nov 2009 Guest speaker for career/research opportunities in Physics for PHYS 1000.
- 2009 – 2010 RPT committee. (Davies, Jacobs, Suleski, Trammell[#])
- 2010 – 2011 RPT committee. (Aktas, Jacobs, Suleski, Trammell[#], Tyson)
- 2010 – 2011 **Chaired** Dept. Chair Search Committee (Baumketer, Gbur, Jacobs[#], Mullany, Allan)
- 2011 – 2012 RPT committee. (Fiddy, Jacobs[#], Moyer, Trammell).
- 2011 – ... M.S. Applied Physics Program Coordinator/Advisor.

CSUN: (Between 8/1999 and 6/2005)

Department Activities and Committees: (# indicates chair)

- 1999-2002 Physics and Astronomy Faculty Research Seminar Series (speaker)
- 1999-2003 Colloquium Organizer (3 semesters)
- 2000-2001 Budget Committee Member (Cadavid, Doty[#], Jacobs)
- 2000-2001 Chair's Advisory Committee Member (Cadavid, Doty[#], Jacobs)
- 2000-2001 Biomedical Physics program Development ad hoc committee (Blanco, Jacobs[#], Lee)
- Fall 2001 Ad hoc Department Faculty Retreat Committee (Blanco[#], Cadavid, Jacobs)
- 2001-2002 Department Curriculum Committee (Cadavid, Jacobs, Lim[#])
- 2002-2003 Department Curriculum Committee (Jacobs[#], Lim, Walton)
- 2001-2005 Biomedical Physics Coordinator
- 2002-2005 Society of Physics Students Advisor
- 2003-2005 Department Curriculum Committee (Jacobs, Park, Ranganathan[#])

College of Science and Mathematics Committees:

- 1999-2001 Commencement Committee
- 2001-2002 Computer Resource Committee (representing Department of Physics and Astronomy)
- 2001-2005 Interdisciplinary Mathematical Research and Education Center
- 2001-2005 Center for Supramolecular Studies
- 2002-2005 College Curriculum Committee

University Activities and Committees:

- Spring 2000 CSUN Faculty Retreat
- Spring 2000 Science Olympiad for middle school children
- Spring 2000 University Creative Activities Fair
- Fall 2001 Steering committee for the California Science Project Site at CSUN
- 2001-2002 Sigma Xi Research Society Nomination committee
- Fall 2003 Judge in Science, 8th Annual Student Research Symposium
- 2002-2004 Faculty Senator representing the College of Science and Mathematics

Community service as faculty

- Spring 2001 **TV Presentation:** D. J. Jacobs, *Analysis of Carey Hart's 360 degree mid-air vertical rotation on a motorcycle*, Appeared on TV: "Ripley's Believe It or Not".
- 2001, 2002 Volunteer at CSUN-LAB School Fall October Fest Fund-Raiser
- Spring 2004 Judge in Natural Science and Mathematics division for the graduate level 2004 Statewide CSU Student Research Symposium
- Fall 2003 Science workshop at Chime Elementary School ("What is Friction?")
- Spring 2004 Science workshop at Chime Elementary School ("Fun with Simple Machines")