

## PATENTS AND SCIENTIFIC SOFTWARE

- D.J. Jacobs and M.F. Thorpe, *Computer Implemented System for Identifying Rigid and Flexible Regions in Macromolecules*, US patent # 6014449, filed February 20, (1998).
- D.J. Jacobs, L.A. Kuhn and M.F. Thorpe, (and now many others): FIRST, distributed by M.F. Thorpe at ASU, at Web site: <http://firstweb.asu.edu/>

## PUBLICATIONS (# indicates CSUN student, § indicates Research Associate)

### Peer Reviewed: (25 total)

1. D.R. Livesay and D.J. Jacobs, *Conserved quantitative stability/flexibility relationships (QSFR) in an orthologous RNase H pair*. Proteins: Structure, Function, and Bioinformatics, **In Press**
2. D.J. Jacobs and S. Dallakayan<sup>§</sup>, *Elucidating Protein Thermodynamics from the Three Dimensional Structure of the Native State Using Network Rigidity*. Biophysical Journal. 88, 1-13 (2005)
3. D.R. Livesay, S. Dallakayan<sup>§</sup>, G.G. Wood<sup>§</sup> and D.J. Jacobs, *A flexible approach for understanding protein stability*. FEBS Letters, 576, 468-476 (2004)
4. M.S. Lee<sup>#</sup>, G.G. Wood<sup>§</sup> and D.J. Jacobs, *Investigations on the alpha-helix to coil transition in HP-heterogeneous polypeptides using network rigidity*. J. Phys. Cond. Mat. 16, S5035-S5046 (2004)
5. B.M. Hespenheide, D.J. Jacobs and M.F. Thorpe, *Structural rigidity in the capsid assembly of cowpea chlorotic mottle virus*. J. Phys. Cond. Mat. 16, S5055-S5064 (2004)
6. D.J. Jacobs and G.G. Wood<sup>§</sup>, *Understanding the  $\alpha$ -Helix to Coil Transition in Polypeptides Using Network Rigidity: Predicting Heat and Cold Denaturation in Mixed Solvent Conditions*. Biopolymers, 75 1-31 (2004).
7. D.J. Jacobs, S. Dallakayan<sup>§</sup>, G.G. Wood<sup>§</sup> and A. Heckathorne<sup>#</sup>, *Network rigidity at finite temperature: Relationships between thermodynamic stability, the nonadditivity of entropy, and cooperativity in molecular systems*. Phys Rev E 68, 061109 (2003).
8. D.J. Jacobs, A. Rader, L.A. Kuhn and M.F. Thorpe, *Graph Theory Predictions of Protein Flexibility*. Proteins: Structure, Function, and Genetics 44: no. 2, 150-155 (2001). **(Featured on cover page of issue)**
9. M.F. Thorpe, A. Rader, M. Lei, D.J. Jacobs, L.A. Kuhn, *Predicting Flexibility in Proteins using Constraint Theory*. Journal of Molecular Graphics and Modeling 19, 60-69, (2001).
10. M.F. Thorpe, D.J. Jacobs, M.V. Chubynsky and J.C. Phillips, *Self organization in network glasses*. J. Non-Crystalline Solids Volumes 266-269, pages 859-866 (2000).
11. P.M. Duxbury, D.J. Jacobs, M.F. Thorpe and C. Moukarzel, *Floppy Modes and the Free Energy: Rigidity and Connectivity percolation on Bethe Lattices*. Phys. Rev. E 59, 2084-2092 (1999).
12. D.J. Jacobs, *Generic Rigidity in Three-dimensional Bond-bending Networks*. J. Phys. A Math. Gen. 31, 6653-6668 (1998).
13. D.J. Jacobs and M.F. Thorpe, *Comment on "Infinite-Cluster Geometry in Central-Force Networks"*, Phys. Rev. Lett. 80, no. 24, 5452 (1998).
14. D.J. Jacobs and B. Hendrickson, *An Algorithm for Two Dimensional Rigidity Percolation: The Pebble Game*. J. Comput. Phys. 137, 346-365 (1997).
15. D.J. Jacobs and M.F. Thorpe, *Generic Rigidity Percolation: The Pebble Game*. Phys. Rev. E 53, 3682-3693 (1996).
16. D.J. Jacobs and M.F. Thorpe, *Generic Rigidity: The Pebble Game*. Phys. Rev. Lett. 75, 4051-4054 (1995).
17. J.R. Dorfman, M.H. Ernst, R. Nix and D.J. Jacobs, *Mean Field Theory for Lyapunov Exponents and Kolmogorov-Sinai Entropy in Lorentz Lattice Gases*, Phys. Rev. Lett. 74, 4417-4410 (1995).
18. J.R. Dorfman, M.H. Ernst and D.J. Jacobs, *Dynamical Chaos in the Lorentz Lattice Gas*. J. Stat. Phys. 81, 497-513 (1995).
19. S. Mukherjee, D.J. Jacobs and H. Nakanishi, *Diffusion on Loopless Critical Percolation Cluster*. J. Phys. A 28, 291-296 (1995).

20. D.J. Jacobs, S. Mukherjee and H. Nakanishi, Diffusion on DLA cluster in Two and Three Dimensions, J. Phys. A 27, 4341-4348 (1994).
21. D.J. Jacobs, and A. Masters, *Domain Growth in a One-dimensional Diffusive Lattice Gas with Short Range Attraction*. Phys. Rev. E 49, 2700-2710 (1994).
22. D.J. Jacobs and H. Nakanishi, *A Persistent Random Walk Model for the Frequency-Dependent Electrical Conductivity*. Physica A 197, 204-222 (1993).
23. S. Muralidhar, D.J. Jacobs, D. Ramkrishna and H. Nakanishi, *Diffusion on Percolation Clusters: Influence of Cluster Anisotropy*, Phys. Rev. A 43, 6503-6517 (1991).
24. S. Muralidhar, D. Ramkrishna, H. Nakanishi and D.J. Jacobs, *Anomalous Diffusion: A Dynamic Perspective*. Physica A 167, 539-553 (1990).
25. D.J. Jacobs and H. Nakanishi, *Autocorrelation Functions for Discrete Random Walks on Disordered Lattice*, Phys. Rev. A 41, 706-719 (1990).

**In preparation:**

1. J. Hules<sup>#</sup>, D.R. Livesay, M.L. Tasayco and D.J. Jacobs, *Elucidating Quantitative Flexibility/Stability Relationships within Thioredoxin and its Fragments Using a Distance Constraint Model*, **to be submitted** to Protein Science.
2. D. H. Huynh<sup>#</sup>, S. Dallakyan<sup>§</sup> and D.J. Jacobs, *Connection Between Thermodynamics and Flexibility in Bacterial Periplasmic Binding Proteins*. In Preparation, **to be submitted** to Journal of Molecular Biology.

**Proceedings and Chapters in Books:** (11 total)

1. M. Chubynsky, B. Hesperheide, D.J. Jacobs, L.A. Kuhn, M. Lei, S. Menor, A.J. Rader, M.F. Thorpe, W. Whiteley and M.I. Zavodszky, *Constraint Theory Applied to Proteins*. **To be published** in the proceedings of the Indo-US Biopolymer workshop by Nova Publishers (2004).
2. M.F. Thorpe, Mykyta Chubynsky, Brandon Hesperheide, Scott Menor, Donald J. Jacobs, L.leslie A. Kuhn, Maria I. Zavodszky, Ming Lei, A.J. Rader and Walter Whiteley *Flexibility in Biomolecules*, **Current Topics in Physics**, Editors R.A.. Barrio and K.K. Kaski, Imperial College Press (London, 2005), Chapter 6, 97-112
3. D.J. Jacobs, *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 386-388 (2004)
4. M.F. Thorpe, 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, 160-167 (2001).
5. M.F. Thorpe, 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, 171-181 (2000).
6. M.F. Thorpe, M.V. Chubynsky, D.J. Jacobs and J.C. Phillips, *The Intermediate Phase in Chalcogenide Glasses in 13<sup>th</sup> 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).
7. D.J. Jacobs, L.A. Kuhn and M.F. Thorpe, *Flexible and Rigid Regions in Proteins*. 357-384 "Rigidity Theory and Applications", Eds: M.F. Thorpe and P.M. Duxbury, Plenum Publishing , NY (1999).
8. M.F. Thorpe, D.J. Jacobs, N.V. Chubynsky and A.J. Rader, *Generic Rigidity of Network Glasses*. 239-277 "Rigidity Theory and Applications", Eds: M.F. Thorpe and P.M. Duxbury, Plenum Publishing , NY (1999).
9. M.F. Thorpe, 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).
10. M.F. Thorpe, 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).
11. M.F. Thorpe, 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, 401-424 (1996)