

## PUBLICATIONS

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### A. Refereed Research articles appeared or accepted

1. “Stability of nonlinearly elastic rods”, Arch. Rat. Mech. Anal. **85** (1984) pp. 311–354
2. (with R.E. Caflisch) “Nonlinear dynamical theory of the elastica”, Proc. Roy. Soc. Edinburgh A **99** (1984) pp. 1–23
3. “Restricted quadratic forms and their application to bifurcation and stability in constrained variational principles”, SIAM J. Math. Anal. **16** (1985) pp. 47–68, Errata **19** (1988) pp. 1256–1257
4. (with G.P. Parry) “A model for twinning”, J. Elasticity **16** (1985) pp. 113–133
5. “Stability and folds”, Arch. Rat. Mech. Anal. **99** (1987) pp. 301–328
6. (with J.B. Keller) “Ropes in equilibrium”, SIAM J. Appl. Math. **47** # 6 (1987) pp. 1185–1200
7. (with J.C. Alexander) “On the maneuvering of vehicles”, SIAM J. Appl. Math. **48** # 1 (1988) pp. 38–52
8. “Restricted quadratic forms, inertia theorems, and the Schur complement”, Linear Algebra and Appl. **108** (1988) pp. 1–36
9. (with J.C. Alexander) “On the kinematics of wheeled mobile robots”, Int. J. Robotics Research, **8** (1989) pp. 15–27
10. “On the Stability of Relative Equilibria”, IMA J. Applied Math., **46** (1991) pp. 71–99
11. (with L-S. Wang and P.K. Krishnaprasad) “Hamiltonian dynamics of a rigid body in a central gravitational field”, Celestial Mechanics and Dynamical Astronomy **50** (1991) pp. 59–96
12. (with R. Malek-Madani) “Steady-state shear-bands in thermoplasticity, Part I: vanishing yield stress”, Int. J. of Solids and Structures, **29** #16 (1992) pp. 2063–2076
13. (with L-S. Wang and P.K. Krishnaprasad) “Steady rigid-body motions in a central gravitational field”, J. of Astronautical Sciences, **40** #4 (1992) pp. 449–478
14. (with J.C. Alexander) “Bounds on the friction-dominated motion of a pushed object”, Int. J. Robotics Research, **12** #3 (1993) pp. 231–248
15. (with D. Jacobson) “On the dynamics of chains”, SIAM J. Applied Math. **52** #6 (1992) pp. 1563–1583
16. (with R.L. Sachs) “On the stability of KdV multi-solitons”, Comm. Pure and Applied Math. **46** (1993) pp. 867–901

17. (with D.J. Dichmann) “[Conservation laws in the dynamics of rods](#)”, *J. Elasticity* **34** (1994) pp. 83–96
18. (with R. Nair) “[On the forward kinematics of parallel manipulators](#)”, *Int. J. Robotics Research*, **13** #2 (1994) pp. 171–188
19. (with R.L. Pego) “[An unconstrained Hamiltonian formulation for incompressible fluid flow](#)” *Comm. Math. Physics* **170** (1995) pp. 207–217
20. (with M.L. Overton) “[Stability Theory for Dissipatively Perturbed Hamiltonian Systems](#)”, *Comm. Pure and Applied Math.* **XLVIII** (1995) pp. 583–610
21. (with D.J. Dichmann and R.L. Pego) “[Hamiltonian dynamics of an elastica and the stability of solitary waves](#)”, *Arch. Rat. Mech. Anal.* **135** (1996) pp. 357–396
22. (with D.J. Dichmann) “[An Impetus-Striction Simulation of the Dynamics of an Elastica](#)”, *J. Nonlinear Science*, **6** (1996) pp. 271–292
23. (with R.S. Manning and J.D. Kahn) “[A Continuum Model of Sequence-Dependent DNA Structure](#)”, *J. Chemical Physics*, **105** (1996) #13, pp. 5626–5646
24. (with R.S. Manning, R.C. Paffenroth, K.A. Rogers, and J.A. Warner) “[Interactive computation, parameter continuation, and visualization](#)”, *Int. J. Bifurcation and Chaos*, **7** (1997) #8 pp. 1699–1715
25. (with S. Kehrbaum) “[Elastic rods, rigid bodies, quaternions and the last quadrature](#)”, *Phil. Trans. Royal Society of London A*, **355** (1997) pp. 2117–2136
26. (with K. Rogers and R. Manning) “[Isoperimetric conjugate points with application to the stability of DNA minicircles](#)”, *Proc. Royal Society of London A* **454** (1998) pp. 3047–3074
27. (with J. Alexander and B. Michalowski) “[Shortest Distance Paths for Wheeled Mobile Robots](#)”, *IEEE Transactions on Robotics and Automation*, **14** (1998) #5 pp. 657–662
28. (with R.S. Manning) “[Symmetry breaking and the Twisted Elastic Ring](#)”, *Computer Methods in Applied Mechanics and Engineering*, **170** (1999) pp. 313–330
29. (with O. Gonzalez) “[Global Curvature, Thickness and the Ideal Shapes of Knots](#)”, *Proc. National Acad. of Sciences (USA)* **96** (1999) pp. 4769–4773.
30. (with A. Stasiak, J. Dubochet, P. Furrer, and O. Gonzalez), “[DNA : Uncooked, al Dente, or Scotti?](#)”, *Science* **283**, 5408 (1999) p. 1641
31. (with K. A. Hoffman and L. Greenberg) “[The Bordered Operator and the Index of a Constrained Critical Point](#)”, *Math. Nachr.* **219** (2000) pp. 109–124.
32. (with P. Furrer, and R.S. Manning) “[DNA Rings with Multiple Energy Minima](#)”, *Biophysical J.* **79**, #1 (2000).
33. (with O. Gonzalez and R.L. Pego) “[Multi-Multiplier Ambient-Space Formulations of Constrained Dynamical Systems: The Case of Linearized Incompressible Elastodynamics](#)”, *Archive for Rational Mechanics and Analysis* **157**, (2001) pp. 285–323.
34. (with O. Gonzalez), “[Extracting parameters for base-pair level models of DNA from molecular dynamics simulations](#)”, *Theoretical Chemistry Accounts* **106**, (2001) pp. 76–82.
35. (with A. Stasiak), “[Best packing in proteins and DNA](#)”, *Nature* **406**, July (2000) pp. 251–252.
36. (with O. Gonzalez, and J. Smutny), “[Curves, circles, and spheres](#)”, *Contemporary Mathematics* **304** (2002) pp. 195–215.

37. (with O. Gonzalez, F. Schuricht, and H. von der Mosel), “[Global curvature and self-contact of nonlinearly elastic curves and rods](#)”, *Calculus of Variations* **14** (2002) pp. 29-68.
38. (with J.R. Banavar, O. Gonzalez, and A. Maritan), “[Self-interactions of strands and sheets](#)”, *J. Statistical Physics*, **110** (2003) pp. 35-50.
39. (With K.A. Hoffman and R.S. Manning), “[Link, Twist, Energy, and the Stability of DNA Minicircles](#)”, *Biopolymers* **70**, #2 (2003) pp. 145-157.
40. (With O. Gonzalez and A. Graf) “[Dynamics of a rigid body in a Stokes fluid](#)”, *J. Fluid Mech.* **519** (2004) pp. 133-160.
41. (With M. Moakher) “[A double-strand elastic rod theory](#)”, *Archive for Rational Mechanics and Analysis*, **177** (2005) pp. 53-91
42. (With N. Chouaieb) “[Kirchhoff’s Problem of Helical Equilibria of Uniform Rods](#)”, *J. Elasticity*, **77** (2004) 221-247.
43. (With D.L. Beveridge, G. Barreiro, K.S. Byun, D.A. Case, T.E. Cheatham III, S.B. Dixit, E. Giudice, F. Lankas, R. Lavery, R. Osman, E. Seibert, H. Sklenar, G. Stoll, K.M. Thayer, P. Varnai, and M.A. Young) “[Molecular dynamics simulations of the 136 unique tetranucleotide sequences of DNA oligonucleotides. I. Research design and results on d\(CpG\) steps](#)”, *Biophysical J.* **87** (2004) 3799-3813.
44. (With M. Jacob, T. Blu, C. Vaillant, and M. Unser) “[3-D shape estimation of DNA molecules from stereo cryo-electron micro-graphs using a projection-steerable snake](#)”, *IEEE Trans. Image Processing*, **15** # 1 214-227 (2006)
45. (With SB Dixit, DL Beveridge, DA Case, TE Cheatham III, E Giudice, F Lankas, R Lavery, R Osman, H Sklenar, KM Thayer and P Varnai) “[Molecular Dynamics Simulations of the 136 Unique Tetranucleotide Sequences of DNA Oligonucleotides. II. Sequence Context Effects on the Dynamical Structures of the 10 Unique Dinucleotide Steps](#)” *Biophysical Journal* **89** 3721–3740 (2005)
46. (With A. Rosa, F. R. Neumann, S. M. Gasser, A. Stasiak) “[Measuring limits of telomere movement on nuclear envelopes](#)”, *Biophysical Journal Biophysical Letters*, L24-L26 (2005)
47. (With N. Chouaieb and A. Goriely) “[Helices](#)”, *Proc. National Acad. of Sciences (USA)*, **103** # 25 9398-9403 (2006)
48. (With F. Lankas, R. Lavery) “[Kinking occurs during molecular dynamics simulations of small DNA minicircles](#)” *Structure*, **14** (2006), 1527–1534
49. (With A. Amzallag, C. Vaillant, M. Jacob, M. Unser, J. Bednar, J. D. Kahn, J. Dubochet, A. Stasiak) “[3-D reconstruction and comparison of shapes of DNA minicircles observed by cryo-electron microscopy](#)”, *Nucleic Acids Research*, **34**, # 18 (2006) e125
50. (With I. Horenko, E. Dittmer, F. Lankas, P. Metzner, and C. Schuette) “[Macroscopic Dynamics of Complex Metastable Systems: Theory, Algorithms, and Application to B-DNA](#)”, *SIAM J. Dynamical Systems*, **7**, 2 (2008) 532-560
51. (With J.R. Banavar, T.X. Hoang, A. Maritan, C. Poletto, A. Stasiak, and A. Trovato) “[Structural motifs of biomolecules](#)”, *Proc Natl Acad Sci USA*, **104**, # 44 (2007) 17283–17286
52. “[Around the Möbius band](#)”, *Nature Materials*, **6** (2007) 547–548
53. (With R. Lavery, M. Moakher, D. Petkeviciute, K. Zakrzewska) “[Conformational analysis of nucleic acids revisited: Curves+](#)”, *Nucleic Acids Res.* **37** (2009); 5917-5929

54. (With D. Demurtas, A. Amzallag, E.J. Rawdon, J. Dubochet, A. Stasiak) “[Bending modes of DNA directly addressed by cryo-electron microscopy of DNA minicircles](#)”, *Nucleic Acids Research*, **37**, 9 (2009) 2882-2893
55. (With F. Lankas, O. Gonzalez, L. M. Heffler, G. Stoll, M. Moakher) “[On the parameterization of rigid base and basepair models of DNA from molecular dynamics simulations](#)”, *Phys. Chem. Chem. Phys.* **11** (2009) 10565-10588
56. (With R. Lavery, K. Zakrzewska, D. Beveridge, T. C. Bishop, D. A. Case, T. Cheatham III, S. Dixit, B. Jayaram, F. Lankas, Ch. Lughton, A. Michon, R. Osman, M. Orozco, A. Perez, T. Singh, N. Spackova, J. Sponer) “[A systematic molecular dynamics study of nearest neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA](#)”, *Nucleic Acids Research* (2009) 1–15
57. (With V.M. Panaretos, D. Kraus) “[Second-Order Comparison of Gaussian Random Curves and the Geometry of DNA Minicircles](#)”, *J. of the American Statistical Association*, **105**, 490 (2010) 670-682
58. (With J. Walter, O. Gonzalez) “[On the stochastic modeling of rigid body systems with application to polymer dynamics](#)”, *SIAM Multiscale Modeling and Simulation* **8**, 3 (2010) 1018–1053
59. (with L. Cotta-Ramusino) “[Looping probabilities of elastic chains: A path integral approach](#)”, *Physical Review E* **82**, (2010) 051924 1-15
60. (With J. Walter, C. Hartmann) “[Ambient space formulations and statistical mechanics of holonomically constrained Langevin systems](#), *Eur. Phys. J. Special Topics* **200** (2011) 153-181
61. (With O. Gonzalez, D. Petkeviciute) “[A sequence-dependent rigid-base model of DNA](#)”, *J. of Chemical Physics* **138**, no. 5 (2013), 055122 1-28
62. (With B. Durickovic and A. Goriely) “[Twist and Stretch of Helices Explained via the Kirchhoff-Love Rod Model of Elastic Filaments](#)”, *Physical Review Letters* **111**, 108103 (2013)

## B. Conference Proceedings

1. “[Stability of the elastica](#)”, in “*Systems of Nonlinear Partial Differential Equations*” Proc. of NATO London Math. Soc. Advanced Study Institute, ed. J.M. Ball, Reidel, (1983) pp. 311–322
2. (with S. Kehrbaum) “[Effective properties of elastic rods with high intrinsic twist](#)”, Proceedings of the 16th IMACS World Congress, Lausanne (2000).
3. (with S. Rey), “[Buckling of an Elastic Rod with High Intrinsic Twist](#)”, Proceedings of the 16th IMACS World Congress, Lausanne (2000).
4. (with R. Paffenroth, D.Vrajitoru, T. Stone), “[DataViewer: A Scene Graph Based Visualization Tool](#)”, extended abstract , The 20th Eurographics UK Conference , IEEE Computer Society Publications, pp. 147-148, and full version, The 5th IASTED Conference on Computer Graphics and Imaging (CGIM 2002), ACTA Press, pp. 200-205.

## C. Book Chapters

1. “[A model for disclinations in nematic liquid crystals](#)”, in “*Theory and Applications of Liquid Crystals*”, *IMA Volumes in Mathematics and Its Applications*, **5**, Springer-Verlag (1987) pp. 255–269
2. (with J.C. Alexander) “[On the kinematics of wheeled mobile robots](#)”, in “*Autonomous Robot Vehicles*” ed. I.J. Cox and G.T. Wilfong, Springer-Verlag (1990) pp. 5–24 (Reprint of A.9 above)

3. (with R.L. Sachs) “[Constrained Variational Principles and Stability in Hamiltonian Systems](#)”, in “*Hamiltonian Dynamical Systems*”, *The IMA Volumes in Mathematics and Its Applications*, **63** (1995) Eds. H.S. Dumas, K.R. Meyer and D.S. Schmidt. pp. 231–264
4. (with D.J. Dichmann and Y. Li) “[Hamiltonian formulations and symmetries in rod mechanics](#)”, in “*Mathematical Approaches to Biomolecular Structure and Dynamics*”, *The IMA Volumes in Mathematics and Its Applications*, **82** (1996) Eds. J.P. Mesirov, K. Schulten, & D.W. Sumners. pp. 71–113
5. (with S. Kehrbaum) “[Elastic rods, rigid bodies, quaternions and the last quadrature](#)” in “*Localization and Solitary Waves in Solid Mechanics*” ed. A.R. Champneys, G.W. Hunt, J.M.T. Thompson, *Advanced Series in Nonlinear Dynamics* **V. 12**, World Scientific (1999) pp. 181–200 (Reprint of A.25 above)
6. (with D.J. Dichmann) “[An Impetus-Striction Simulation of the Dynamics of an Elastica](#)” in “*Mechanics: From Theory to Computation, Essays in Honor of Juan-Carlos Simo*”, papers invited by the Journal of Nonlinear Science Editors, Springer (2000) pp. 217–238 (Reprint of A.22 above)
7. “[Bifurcation Theory, Symmetry Breaking and Homogenization in Continuum Mechanics Descriptions of DNA](#)”, in “*A Celebration of Mathematical Modeling: The Joseph B. Keller Anniversary Volume*,” Eds. D. Givoli, M.J. Grote, G. Papanicolaou, Kluwer Academic Publishers, (2004)
8. (with M. Carlen, B. Laurie, and J. Smutny) “[Biarcs, Global Radius of Curvature, and the Computation of Ideal Knot Shapes](#)”, in “*Physical and Numerical Models in Knot Theory and Their Application to the Life Sciences*”, Eds. J. Calvo, K. Millett, E. Rawdon, and A. Stasiak, World Scientific (2005)
9. (With V.M. Panaretos, D. Kraus) “[Second-Order Inference for Functional Data with Application to DNA Minicircles](#)”, in *Recent Advances in Functional Data Analysis and Related Topics* (2011), 245-250

## D. Computer Code

1. (with C.K. Mesztenyi) [MC<sup>2</sup>](#) (an acronym for Multiplier and Constraint Continuation). An interactive 3D graphics and numerical continuation package for the construction of multi-parameter bifurcation diagrams associated with constrained variational principles.
2. (with R.C. Paffenroth and other group members) [DataViewer](#), a high-level portable library for accessing OpenGL graphics from high performance computational packages
3. (with R.C. Paffenroth and other group members) [VBM](#), an object oriented package allowing easy interactive steering of distributed parameter-continuation computations using many different computational engines. Interactive control exploits advanced visualization techniques applied to both bifurcation manifolds and solutions at fixed parameter values.

## E. Thesis

“Analysis of nonlinear differential equations governing the equilibria of an elastic rod and their stability”, University of Oxford, 1981