REPORT DOCUMENTATION PAGE

The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing the burden, to the Department of Defense, Executive Service Directorate (0704-0188). Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.

PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ORGANIZATION.

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
22-03-2010	Final Technical Report	June 1, 2006-Feb 28, 2010

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
HIGH-PERFORMANCE MACROMOLECULAR MATERIALS	FA9550-06-1-0063
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)	5d. PROJECT NUMBER
M. Gregory Forest	
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT NUMBER
University of North Carolina at Chapel Hill	

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
USAF, AFRL NL	
Office of Scientific Research	
875 N. Randolph St.	11. SPONSOR/MONITOR'S REPORT NUMBER(S)
Room 3112	
Arlington, VA 22203	

12. DISTRIBUTION/AVAILABILITY STATEMENT

DISTRIBUTION A: Approved for Public Release

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The major accomplishments from this contract consist of new theoretical models for nano-rod and nano-platelet hydrodynamics, new algorithms for simulations of benchmark experiments and processing flows, new defect detection and tracking diagnostics, and the applications of each of these developments to understanding of these novel material systems and their flow-processing properties. The publications resulting from this contract can fairly be characterized as the state-of-the-art in the theory, modeling, simulations and behavior of nano-rod and nano-platelet dispersions.

15. SUBJECT TERMS

Nano-composites, theory, modeling, simulations, multi-functional properties

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			M. Gregory Forest
					19b. TELEPHONE NUMBER (Include area code)
					919-962-9606

High Performance Macromolecular Materials

AFOSR FA9550-06-1-0063

June 1, 2006 – February 28, 2010

M. Gregory Forest
Department of Mathematics
Institute for Advanced Materials, Nanoscience & Technology
University of North Carolina at Chapel Hill

Final Report

Activities and Findings

1. Major research accomplishments

The PI and collaborators have successfully accomplished all proposed research projects spanning theory, modeling, algorithms, and computational studies. The projects focus on rigid nano-rod and nano-platelet particles dispersed in solvent, which are prototypes of high-performance synthetic materials for flight applications. Mathematically, we have addressed several fundamental issues, summarized below, followed by a list of peer-reviewed publications which have cited this grant.

The stress-strain map of isotropic and anisotropic viscoelastic media. Under steady and frequency-controlled oscillatory shear strain (respectively, stress) applied at one interface of a layer sample, it is desired to determine: the corresponding shear stress (respectively, strain) at the driven interface; the dynamic moduli which inform the storage and loss properties of the material across several decades of frequency; and how these features change from the linear response regime to onset of, then full-blown, nonlinearity. We have elucidated detailed properties of the stress-strain map for isotropic viscoelastic materials and anisotropic nematic liquid crystalline polymers. We emphasize that the stress-strain map is between a velocity or strain vector field and a stress tensor field, and the well-posed boundary value problems underlying the map are constitutive-law-dependent, and therefore quite different mathematical mappings for general linear and nonlinear isotropic viscoelastic fluids and for nano-particle dispersions. One major finding has been the fundamental role of boundary conditions on dynamic moduli for presumed homogeneous deformations and in the presence of heterogeneity.

Algorithms for the hydrodynamics of nano-rod and nano-platelet dispersions. The flow of nematic polymers in film and mold geometries with physical boundary conditions is a major modeling and computational challenge for several technical reasons. First, one has to couple a Navier-Stokes solver (with extra stress contributions from gradients in the nano-particle orientational distribution) with a model for the orientational distribution of the nano-rod or platelet phase. Our group has developed the *only* algorithm that solves

the full coupling of the Smoluchowski equation for the orientational distribution function with the generalized Navier-Stokes or flow equations. We were the first group to do this for imposed linear flows, then in one-dimensional heterogeneity between two moving parallel plates, and then in two space dimensions. We have also developed algorithms for second-moment tensor closure models of the Smoluchowski equation, which reduces the computational cost and algorithmic complexity by a factor of 15. This is critical for performing parameter studies since a two-space dimensional simulation in the dynamic attractor regime can take several days on a supercomputer.

Defect detection and tracking diagnostics during flow and quench simulations. Our group has completely changed the methods for defect detection and tracking. In particular, we have shown that the local disordered phases that exist in the classical Onsager equilibrium phase diagram, the isotropic and oblate nematic phases, are ubiquitous in dynamic attractors in one and two space dimensions. Furthermore, in two space dimensions, these locally disordered phases exist in the cores of topological defects. Since these local defects are characterized by an eigenvalue degeneracy of the second moment of the orientational distribution, it is essentially cost-free to monitor for their respective degeneracies. Once a defect is detected, it is cost-free to dynamically track and to image using level sets of their respective local metrics. To see the surrounding topological defect morphology, we then simply print snapshots based on the geometry of the second-moment of the orientational distribution. These tools thereby replace costly and time-consuming defect metrics in two and three space dimensions, and furthermore reveal the critical role of local disordered phases in one space dimension. We have shown that dynamic shear banding is characterized by local oblate defects which appear and disappear between each band; these defects also have been identified as the source of the smallest lengthscales of morphology in the dynamic attractors which are always present at realistic flow processing parameter regimes.

Data-mining of network properties of the flow-generated nano-particle ensemble. In our previous work, also supported by AFOSR, we derived homogenization formulas and predicted the volume-averaged effective properties of nano-rods dispersed in a traditional material. These gains were shown to be well below the observed benchmark properties, which led us to build new methods for the nano-particle network properties based on our flow-generated databases for the orientational probability distribution functions of the nano-rod particle phase. We developed methods to statistically populate flow-generated nano-rod dispersions, and then build cluster distributions consisting of each cluster of percolating paths among the particles. When a cluster spans physical boundaries of the sample, then the dispersion exhibits percolation, which dominates transport properties of the bulk material. We developed percolation phase diagrams versus particle volume fraction and imposed bulk shear rate. The extension of these tools to heterogeneous nano-particle networks is a current activity by Forest and collaborators, which relies upon all of the tools built over the course of this award. Thus we anticipate a strong legacy of the results obtained under the auspices of AFOSR.

2. Outreach activities undertaken by the project.

- The PI has maintained relationships and collaborations with scientists at the Air Force Research Laboratory at Wright Patterson AFB, and with Dr. Richard Vaia in particular.
- The PI served on the Scientific Advisory Board of the Clemson Advanced Fibers and Films Center.
- The PI is co-Director of the UNC Institute for Advanced Materials, Nanoscience & Technology.
- The PI organized or lectured in minisymposia at national meetings of the American Mathematical Society, SIAM, the Society of Rheology, the American Physical Society, and the American Chemical Society.

The following presentations were given by the PI during the funding period.

- 2006, The Virtual Lung Project at the University of North Carolina, International Conference on Applied Mathematics and Interdisciplinary Studies, Nankai University, Tianjin, China, June 12.
- 2006, Coupled Smoluchowski and Navier-Stokes simulations for rigid-rod macromolecular dispersions in parallel plate geometries, Workshop on Multiscale Modeling of Complex Fluids, Peking University, Beijing, China, June 15.
- 2006, Nematic polymer flows, International Conference on Recent Advances in Scientific Computation, Beijing Normal University, Beijing, China, June 17.
- 2006, Hydrodynamics of nano-composite materials, Jiaotong University, Xi'an, China, June 19.
- 2006, Hydrodynamics of nano-rod composites, Workshop on Partial Differential Equations and Applied Analysis, Fudan University, Shanghai, China, June 23.
- 2006, Mathematical Modeling, Analysis, and Scientific Computation of Complex Fluids, Introductory lecture of a Minisymposium so titled at the SIAM Annual Meeting, Boston, MA, July 11.
- 2006, Linear viscoelastic properties of nematic polymers, Society of Engineering Sciences, State College, PA, August 15
- 2006, Autoregressive (direct) and maximum likelihood (inverse) methods for microrheology simulations and experiments, Society of Rheology Annual Meeting, Portland, ME, October 8-12.
- 2007, Nano-rod composites: a flow strategy to control anisotropic percolation, Minisymposium on Mathematics & Materials Science, American Mathematical Society National Meeting, New Orleans, LA, January 5.
- 2007, The Virtual Lung Project at UNC: what's math got to do with it?, Duke Analysis and Applied Mathematics Seminar, January 22
- 2007, Nano-materials: what's really different?, Dean's Distinguished Lecture Series, Old Dominion University, February 7
- 2007, The Virtual Lung Project at UNC, Mathematics and Statistics Department Colloquium, Old Dominion University, February 8

- 2007, Direct and Inverse Algorithms for Stochastic Models of Microrheology, Computational and Engineering Sciences Meeting, Costa Mesa, CA, Symposium on Complex Fluids, February 20
- 2007, High Performance Macromolecular Materials, Seminar Series on Complex Fluids, Department of Mathematics and Center for Computational and Applied Mathematics, Purdue University, March 23.
- 2007, A Theory-Modeling-Simulation Strategy for the Polymer Nano-Composite Pipeline, Distinguished Lecture Series of the Industrial Mathematics Institute & NanoCenter, University of South Carolina, April 10.
- 2007, Flow processing of nematic polymer materials, Materials Science and Soft Matter Colloquium, ETH-Zurich, May 2.
- 2007, Rigid-rod macromolecular dispersions: 30 years after the Hess 1976 classic, Festkolloquium in honor of the retirement of Professor Siegfried Hess, Technical University, Berlin, Germany, May 4.
- 2007, Active and passive microrheology, Applications of Analysis in Mathematical Biology, in honor of Michael Reed, Duke University, May 22.
- 2007, The polymer nano-composite pipeline: processing to performance, Dielectric Polymer Nanocomposite Workshop, Wright-Patterson AFB,Wright Brothers Institute, Dayton, OH, June 1.
- 2007, Linear to Nonlinear Transitions in Microrheology: Extensions of the Ferry Shear Wave Experiment, Society of Rheology Annual Meeting, Salt Lake City, UT, October 9.
- 2008, Heterogeneity in Biological Media, SAMSI Transition Workshop of 2007-2008 Program on Random Media, May 1.
- 2008, Tensorial defect diagnostics in hydrodynamics of sheared nematic polymers, SIAM Meeting on Mathematics and Materials, May 11.
- 2008, Stress propagation in sheared biological layers, American Institute of Mathematical Sciences International Conference, Session on Nonlinear Wave Progagation, Arlington, TX, May 18.
- 2008, The Coupling of Viscoelastic Stresses and Biochemistry in the Lung, SIAM Annual Meeting, Mini-Symposium on Multiscale & Multiphysics Modeling and Computation, San Diego, CA, July 9.
- 2008, Predictive Tools for Processing to Performance of Nano-Rod and Nano-Platelet Composites, AFOSR Physical Applied Mathematics Program Review, Dayton, OH, July 30.
- 2008, Shear flows of nano-rod dispersions: what can Brownian do for you? Naval Postgraduate School, Department of Applied Mathematics Colloquium, Aug 7.
- 2008, Stress communication (with ion & nucleotide biochemistry & hydration) in biological layers, Intl. Congress of Rheology, Session on Biological Materials, August 7.
- 2009, The interplay between hydrodynamic feedback and defects in sheared nematic liquids, Workshop on Complex Fluids, Modeling and Numerics, Ecole des Ponts, Paris, France, Jan 5.
- 2009, The Virtual Lung Project at UNC, Courant Institute of Mathematical Sciences, NYU, Fluid Mechanics Seminar, February 18.
- 2009, Coupling of Biochemistry and Stresses: A Mechanism for Lung Airway

Water Volume Regulation, SIAM Annual Computational Sciences & Engineering Meeting, Miami, FL, March 5

- 2009, Transport in Viscoelastic Media, The 6th IMACS International conference on Nonlinear Evolution Equations and Wave Phenomena: Computation and Theory, Athens, GA, March 25
- 2009, The Virtual Lung Project at UNC, SIAM Southeastern Sectional Meeting, Plenary Lecture, April 5
- 2009, The Virtual Lung Project at UNC, Colloquium in honor of Steve Rosencrans, Department of Mathematics, Tulane University, May 6
- 2009, Uniquely biological challenges for rheology, Plenary lecture, Institute for Mathematics and Its Applications, Workshop on Rheological Measurements and Constitutive Modeling, University of Minnesota, Minneapolis, MN, September 17
- 2009, Anomalous diffusion of tracers in polymeric liquids, Society of Rheology Annual Meeting, Microrheometry and Microfluidics Session, Madison, WI, October 19
- 2010, The Virtual Lung Project at UNC, University of California at San Diego, Mathematics, February 18

Publications citing this grant (from 2006 through the present)

1. Alignment and rheo-oscillator criteria for sheared nematic polymer films in the monolayer limit, (with J. Lee, R. Zhou), Discrete and Continuous Dynamical Systems, Vol. 6, 339-356 (2006).
2. Anchoring distortions coupled with plane Couette & Poiseuille flows of nematic polymers in viscous solvents: morphology in molecular orientation, stress & flow, (with H. Zhou), Discrete & Continuous Dyn. Systems, Vol. 6, 407-425 (2006).
3. On weak plane Couette and Poiseuille flows of rigid rod and platelet ensembles, (with Z. Cui, Q. Wang, H. Zhou), SIAM J. Applied Math, Vol. 66(4), 1227-1260 (2006).
4. A classical problem revisited: Rheology of nematic polymer monodomains in small amplitude oscillatory shear, (with E. Choate), Rheologica Acta, Vol. 46(1), 83-94 (2006).
5. Monodomain dynamics for rigid rod & platelet suspensions in strongly coupled coplanar linear flow and magnetic fields, II: Kinetic theory, (with S. Sircar, Q. Wang, R. Zhou), Phys. Fluids, Vol. 18, 103102:1-14 (2006).
6. Nematic polymer mechanics: flow-induced anisotropy, (with X. Zheng, R. Lipton, R. Zhou), Continuum Mechanics & Thermodynamics, Vol.18, 377-394 (2007).
7. Monodomain dynamics for rigid rod & platelet suspensions in strongly coupled coplanar linear flow and magnetic fields, (with Q. Wang, R. Zhou), J. Rheology, Vol. 51(1), 1-21 (2007).
8. On the correspondence between creeping flows of viscous and viscoelastic fluids, (with I. Klapper, K. Xu), J. Non-Newtonian Fluid Mech., Vol. 145, 148–170,

(2007).

9. Characterization of stable kinetic equilibria of rigid, dipolar rod ensembles for coupled dipole-dipole and excluded-volume potentials, (with H. Zhou, H. Wang, Q. Wang), Nonlinearity, Vol. 20, 277-297 (2007).

10. Nematic liquids in weak capillary Poiseuille flow: structure scaling laws and effective conductivity implications, (with H. Zhou), Int. J. Numerical Analysis & Modeling, Vol. 4 (3), 460-477 (2007).

11. Nano-rod suspension flows: a 2D Smoluchowski-Navier-Stokes solver, (with R. Zhou, Q. Wang), Int. J. Numerical Analysis & Modeling, Vol. 4(3), 478-488 (2007).

12. Anchoring-induced structure transitions of flowing nematic polymers in plane Couette cells, (with H. Zhou, Q. Wang), Discrete and Continuous Dynamical Systems B, Vol. 8(3), 707-733 (2007).

13. A strategy for dimensional percolation in sheared nano-rod dispersions, (with X. Zheng, R. Vaia, M. Arlen), Advanced Materials, Vol. 19 (22), 4038-4043 (2007).

14. Microscopic-macroscopic simulations of rigid-rod polymer hydrodynamics: heterogeneity & rheochaos, (with R. Zhou, Q. Wang), SIAM Multiscale Modeling & Simulation, Vol. 6(3), 858-878 (2007).

15. Effects of strong anchoring on the dynamic moduli of heterogeneous nematic polymers, (with E. Choate, Z. Cui), Rheol. Acta, Vol. 47, 223–236 (2008).

16. Dipole-induced first-order phase transitions of nano-rod monolayers, (with J. Lee, Q. Wang, R. Zhou), Physics Letters A, Vol. 372, 3484–3487 (2008).

17. Dimensional robustness & instability of sheared, semi-dilute, nano-rod dispersions, (with X. Yang, Z. Cui, J. Shen, Q. Wang), SIAM Multiscale Modeling and Simulation, Vol. 7(2) (2008).

18. Extensions of the Ferry shear wave model for active linear and nonlinear microrheology, (with S. Mitran, B. Lindley, L. Yao, D. Hill), J. Non-Newtonian Fluid Mechanics, Vol. 154, 120-135 (2008).

19. Direct and Inverse Modeling for Stochastic Data in Microbead Rheology, (with C. Hohenegger), Proceedings in Applied Mathematics and Mechanics (PAMM), **Special Issue:** Sixth International Congress on Industrial Applied Mathematics (ICIAM07) and GAMM Annual Meeting, Zürich 2007, Published Online: Oct 30 (2008).

20. Robustness of pulsating jet-like layers in sheared nano-rod dispersions, (with S. Heidenreich, S. Hess, X. Yang, R. Zhou), J. Non-Newtonian Fluid Mechanics, Vol. 155(3), 130-145 (2008).

21. Oscillating hydrodynamical jets in steady shear of nano-rod dispersions, (with S. Heidenreich, S. Hess, S. H. L. Klapp, X. Yang, R. Zhou, Q. Wang), Proceedings of XVth International Congress on Rheology, Springer, August, 2008, AIP Conference Proceedings, Materials Physics & Applications Series, Vol. 1027 (2008).

22. Effects of tilted director angle anchoring conditions on the dynamic moduli of heterogeneous nematic polymers, (with E. Choate, Z. Cui, L. Ju), Proceedings of XVth International Congress on Rheology, Springer, August, 2008, AIP Conference Proceedings, Materials Physics & Applications Series, Vol. 1027 (2008).

23. Modeling aspects of two-bead microrheology, (with C. Hohenegger), Proceedings of XVth International Congress on Rheology, Springer, August, 2008, AIP Conference Proceedings, Materials Physics & Applications Series, Vol. 1027 (2008).

24. Two-point microrheology: modeling protocols, (with C. Hohenegger), Phys. Rev. E, Vol. 78, 031501 (2008).

25. Stress communication and filtering of viscoelastic layers in oscillatory shear, (with E. Howell, B. Smith, G. Rubinstein, B. Lindley, D. Hill, R. Superfine, S. Mitran), J. Non-Newtonian Fluid Mechanics, Vol. 156, 112-120 (2009).

26. Sheared nematic liquid crystal polymer monolayers, (with H. Wang, H. Zhou), Discrete & Continuous Dynamical Systems B, Vol. 11(2), 497-517 (2009).

27. Time-domain methods for passive microrheology and anomalous diffusive transport in soft matter, (with J. Fricks, L. Yao, T. Elston), SIAM J. Appl. Math., Vol. 69(5), 1277-1308 (2009).

28. A simple model for non-topological defects in sheared nematic polymer monodomains, (with E. Choate, L. Yao, X. Zheng, R. Zhou), Journal of Computational and Theoretical Nanosciences, to appear (2009).

29. Dynamic defect morphology and hydrodynamics of sheared nematic polymers in two space dimensions, (with X. Yang, Q. Wang, W. Mullins), J. Rheology, to appear (2009).

30. Quench sensitivity of defects and shear banding in nematic polymer film flows, (with X. Yang, W. Mullins, Q. Wang), J. Non-Newtonian Fluid Mechanics, Vol.159 (1-3), 115-129 (2009).

31. Transient anomalous diffusion of tracer particles in soft matter, (with S. McKinley, L.Yao), J. Rheology, Vol. 53(6), 1487-1506 (2009).

32. A simple model for non-topological defects in sheared nematic polymer monodomains, (with E. Choate, L. Yao, X. Zheng, R. Zhou), Journal of Computational and Theoretical Nanosciences, Vol. 7, 787-794 (2010); special issue on Nematic Liquid Crystalline Polymers and Nanocomposites, edited by Forest, Zhou & Wang.

33. Mathematical studies and simulations of nematic liquid crystalline polymers and nanocomposites (A review), (with H. Zhou, H. Wang), J. Comput. Theor. Nanosci. Vol. 7, 645-660 (2010); special issue on Nematic Liquid Crystalline Polymers and Nanocomposites, edited by Forest, Zhou & Wang.

34. 2D Lid-driven cavity flow of nematic polymers: an unsteady sea of defects, (with X. Yang, Q. Wang, W. Mullins), Soft Matter **DOI**:10.1039/b908502e (2010).

35. A 2-D kinetic theory for monodomain flows of polymer-rod nanocomposites, (with L. Liao, Q. Wang), Communications in Computational Physics, Vol. 7, No. 2, pp. 250-282, February 2010.

36. Effects of strong anchoring on the dynamic moduli of heterogeneous nematic polymers II: Oblique anchoring angles, (with E. Choate, L. Ju), Rheologica Acta, **DOI**:10.1007/s00397-009-0397-1 (2010).

37. Dynamic texture scaling of sheared nematic polymers in the large Ericksen number limit, (with S. Heidenreich, S. Hess, R. Zhou, X. Yang), J. Non-Newtonian Fluid Mechanics, accepted March15, 2010, to appear.

Prepared and submitted by PI Forest, March 22, 2010.