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Multiscale Mathematics for Nano-Particle-Endowed
Active Membranes and Films

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Final Report

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AFOSR Final Report

AFOSR Award: FA9550-12-1-0178
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PI: Qi Wang, University of South Carolina
Co-PIs: Xiaofeng Yang, University of South Carolina
&

M. Greg Forest and Peter Mucha, University of North Carolina at Chapel Hill

In this project, we conducted a systematic investigation on active liquid crystal flows and flowing polymer nano-composites including studies of nonlinear phenomenon in active magnetic microbead rheology, detailed analyses and simulations of active liquid crystal models in thin films, free surface geometries, and the channel geometry, applications of active liquid crystal models to complex biological systems, numerical algorithm development for multiphase fluid flows, network analysis and simulations of nanocomposite systems. In the study of active liquid crystals, we explored spatial-temporal structures using the two-scale kinetic model by mapping out the dynamics in the phase space consisting of the active parameter and the strength of active particle-particle interaction. In the meantime, we used a reduced order, continuum active polar liquid crystal model to study the robustness of the structures and their genesis in relation to the inherent instability in the active liquid crystal model. Detailed studies are conducted with respect to channel flows and free surface filament flows which have direct relevance to various engineering and biological applications. Network models are brought in to analyze nanocomposites transport properties and network properties of various complex networks.

New numerical algorithms are developed for a host of multiphase phase field based hydrodynamic models, in which a new method called Energy Quadraticization or EQ was invented to systematically linearize transport equations derived from the generalized Onsager principle. These new methods are then applied to efficiently integrate the governing system of equation for the active matter systems are continuously improved.

We present experimental data and numerical modeling of a nonlinear phenomenon in active magnetic microbead rheology that appears to be common to entangled polymer solutions (EPS). Dynamic experiments in a modest range of magnetic forces show (1) a short-lived high viscosity plateau, followed by (2) a bead acceleration phase with a sharp drop in apparent viscosity, and (3) a terminal steady state that we show resides on the shear-thinning slope of the steady-state flow curve from cone and plate data. This latter feature implies a new protocol to access the nonlinear steady state flow curve for biological EPS available only in microliter-scale volumes. We use the moment closure form of the Rolie–Poly kinetic model for EPS hydrodynamics, together with a decoupling approximation that obviates the need for a full three-dimensional (3D) flow solver, to qualitatively reproduce this dynamic experimental sequence. We thereby explain the phenomenon in terms of entangled polymer physics, and show how the nonlinear event

(acceleration and termination on the shear-thinning response curve) is tunable by the interplay between molecular-scale mechanisms (relaxation via reptation and chain retraction) and magnetic force controls. The experimental conditions mimic movement of cilia tips, bacteria, and sperm in mucus barriers, implying a physiological relevance of the phenomenon and compelling further quantitative kinetic-flow 3D numerical modeling.

We have developed a set of kinetic models and simulation tools to study anisotropic nano-particle dispersions and active particle dispersions to generate spatial-temporal structures that the ensemble can exhibit. Using the kinetic models, we have investigated the spatial-temporal structure of the model solutions. In the end, we have obtained the phase diagram for the solutions in the important model parameters. Using a coarse-grain model for active polar liquid crystals, we analytically and numerically explored the spatial-temporal patterns in active particle systems and studied the solution instability in details in channel flows and free surface liquid filaments. In particular, we investigated the capillary instability of a falling active liquid crystal filament and discovered a stunning set of instabilities due to the activities of the liquid crystal molecules or active nanoparticles. We anticipate that this will lead to new applications of active particle dispersions in material processing and interpretation for capillary dynamics in biological systems.

After quenching/annealing, we adopt the statistics in the probability density function to analyze the materials properties, primarily electric properties, using network models and assessment tools developed for community networks. The work performed builds on kinetic models and corresponding solution algorithms for processing conditions of nano-particle-endowed films, coatings and membranes. Drawing from databases generated by these codes, we are actively investigating network-mediated properties that are not well-modeled by homogenization theory. We have explored DC resistive electrical response of connected nanorod composites at particle volume fractions above the percolation threshold. These calculations are performed in the high aspect ratio conductivity limit, wherein only currents along particulates are considered. As an extension of the above investigation, and as a means towards understanding the general behaviors observed there, we have also considered similar effects and observations obtained in the classic “random resistor” setting of bond percolation on 3D cubic lattices. We have also investigated dielectric properties at particle volume fractions below the percolation threshold. In these calculations, the associated network is an all-to-all capacitance network.

New and efficient numerical algorithms for multiphase fluid flows formulated using phase field are developed to decouple the momentum transport equation from the phase transport equations making the numerical computational tool more robust and modular. Some of these numerical schemes are applied to study cellular aggregate fusions and liquid jet dynamics of liquid crystal polymers.

We also applied the active liquid crystal models and the numerical technology to develop a set of new models and simulation tools for cell motion in mitosis and migration on patterned substrate. These models are being used in collaboration with applied physicists

and material scientists to study the interaction between the cell and the substrate material in order to design novel cell-sensing and guiding materials.

5 PhD students have been partially supported by this award during their graduate studies. They have graduated and move on to either continue their postdoc training or working in universities and industries.

The team has been very productive during the last four years. Papers published and submitted in the period are listed below:

Publications:

1. Chen Chen and Qi Wang, "3-D Pattern Formation in Biofilms," *Contemporary Mathematics* (586), 2013, 105-116.
2. Yi Sun and Qi Wang, "Modeling and Simulations of Multicellular Aggregate Self-assembly in Biofabrication Using Kinetic Monte Carlo Methods," *Soft Matter*, 2013, 9, 2172-2186.
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7. J. Cribb, P.A. Vasquez, P. Moore, S. Norris, S. Shah, R. Superfine, M.G. Forest. Nonlinear signatures of entangled polymer solutions in active microbead rheology, *J. Rheology*, 57, 1247-1265 (2013)
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9. F. Shi, P.J. Mucha, S. Wang, R. Zhou, M.G. Forest. Network-based assessments of percolation-induced current distributions in sheared rod macromolecular dispersions, *SIAM Multiscale Modeling and Simulation*, 12(1), 249-264 (2014)
10. F. Shi, P. Mucha. Nonaxisymmetric high-aspect-ratio ellipsoids under shear: Lowest-order correction for finite aspect ratios, *PHYSICAL REVIEW E* 90, 013005 (2014)
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12. M. G. Forest, Panon Phuworawong, Qi Wang, and Ruhai Zhou, "Rheology of active polar and apolar liquid crystalline suspensions," *Philosophical Transactions of Royal Society A*, 2014, 372:20130362.

13. Xiaogang Yang and Qi Wang, Capillary Instability of an Active Liquid Crystal Jet, *Soft Matter*, 10, 2014, 6758-6776.
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19. Guanghua Ji, M. G. Forest, and Qi Wang, Structure Formation in Sheared Polymer-Rod Nanocomposites, *DCDS-S*, 8(2), 2015, 341-379.
20. M. G. Forest, Qi Wang, and Ruhai Zhou, Kinetic attractor phase diagrams of active nematic suspensions: the dilute regime, *Soft Matter*, 2015, 11, 6393 – 6402.
21. Hua Jiang, Hao Yang, Jun Zeng, Zhiyuan Zhou, Jin Peng, Qi Wang, Analytic Oncology, *Electron J Metab Nutr Cancer*, Jun. 2015, Vol. 2, No. 2, 26-30.
22. Chen Chen, Dacheng Ren, Mingming Ren and Qi Wang, “3-D Spatial-Temporal Structures of Biofilms in A Water Channel,” *Mathematical Methods in Applied Sciences*, 38 (18), 2015, 4461-4478.
23. J. Zhao, Q. Wang and X. Yang, Numerical Approximations for a Phase Field Dendritic Crystal Growth Model Based on the Invariant Energy Quadratization approach, to appear, *Inter. J. Num. Meth. Engr.*, 2016.
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34. Jia Zhao and Qi Wang, “Modeling and Simulations of Cytokinesis of Eukaryotic Cells,” *International Journal for Numerical Methods in Biomedical Engineering*, 2016, DOI: 10.1002/cnm.2774.
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36. Kapustina, M., Tsygankov, J., Zhao, J., Yang, X., Chen, A., Roach, N., Wessler, T., Elston, T.C., Wang, Q., Jacobson, K., Forest, G., “Modeling the excess cell surface stored in a complex morphology of bleb-like protrusions”. *Plos Computational Biology*, March 25, 2016 <http://dx.doi.org/10.1371/journal.pcbi.1004841>
37. Jia Zhao, Xiaofeng Yang, Jun Li and Qi Wang, “Energy stable numerical schemes for a hydrodynamic model of nematic liquid crystals.” *Siam J. Sci. Comp.*, in press, 2016.
38. Ya Shen, Jia Zhao, César de la Fuente-Núñez, Zhejun Wang, Robert E. W. Hancock, Clive R. Roberts, Jingzhi Ma, Jun Li, Markus Haapasalo and Qi Wang, “Development and Experimental Validation of a Model for Oral Multispecies Biofilm Recovery after Chlorhexidine Treatment”, *Scientific Reports*, 6, 2016, 27537.
39. Yuezheng Gong, Xinfeng Liu, and Qi Wang, “Fully Discretized Energy Stable Schemes for Hydrodynamic Models of Two-phase Viscous Fluid Flows”, *Journal of Scientific Computing*, in press 2016.
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41. Jia Zhao and Qi Wang, A hydrodynamic model for biofilms accounting for persisters and susceptibles, *Mathematics of Biosciences*, 2016.
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PhD graduates of Qi Wang, Forest and Mucha supported in part by this contract:

1. Jia Zhao, University of South Carolina, 2012-2016, PhD May 2015, University of South Carolina, June 2015-July 2016, University of North Carolina at Chapel

- Hill, July 2016-present
2. Norazaliza Mond Gamil, PhD May 2015, Universiti Malaysia Pahang, 2015-present
 3. Chen Chen, PhD August 2012, Citibank, 2013-present
 4. Feng (Bill) Shi, PhD May 2013, University of Chicago, Computation Institute, June 2013 - present
 5. Simi Wang, PhD May 2014, Amazon, May 2014 - present

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Abstract

In this project, we conducted a systematic investigation on active liquid crystal flows and flowing polymer nano-composites including studies of nonlinear phenomenon in active magnetic microbead rheology, detailed analyses and simulations of active liquid crystal models in thin films, free surface geometries, and the channel geometry, applications of active liquid crystal models to complex biological systems, numerical algorithm development for multiphase fluid flows, network analysis and simulations of nanocomposite systems. We explored spatial-temporal structures using the two-scale kinetic model by mapping out the dynamics in the phase space consisting of the active parameter and the strength of active particle-particle interaction. In addition, we used a continuum active polar liquid crystal model to study the robustness of the structures and their genesis in relation to the inherent instability in the active liquid crystal model in various geometries. Network models are brought in to analyze nanocomposites transport properties and network properties of various complex networks. A series of numerical algorithms for multiphase complex fluid models are developed using a new method that we invented call energy quadratization (EQ) technique. With the new EQ technique, we designed energy stable schemes for several important model systems of multiphase viscous fluid mixtures, liquid crystal drops, active matter drops, active cells, etc, making the

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Archival Publications (published) during reporting period:

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 21. Hua Jiang, Hao Yang, Jun Zeng, Zhiyuan Zhou, Jin Peng, Qi Wang, Analytic Oncology, Electron J Metab Nutr Cancer , Jun. 2015 , Vol. 2 , No. 2, 26-30.
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2. New discoveries, inventions, or patent disclosures:

Do you have any discoveries, inventions, or patent disclosures to report for this period?

No

Please describe and include any notable dates

Do you plan to pursue a claim for personal or organizational intellectual property?

Changes in research objectives (if any):

Change in AFOSR Program Manager, if any:

Extensions granted or milestones slipped, if any:

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, \$K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

Report Document

Report Document - Text Analysis

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Appendix Documents

2. Thank You

E-mail user

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