# Research Projects in Applied and Computational Mathematics

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Walker, Davis, Int. Free Bdy., vol. 17, 2015



- Numerical analysis/finite element methods (FEM)
- Liquid crystal modeling and numerics
- Geometric flows, free boundary problems, surface PDEs
- Shape optimization; PDE control of shape
- Mesh generation

### Overview

Liquid crystals are a work-horse technology enabling a variety of electronic displays. They have a host of potential applications in material science, including building new materials with colloidal dispersions controlled through directed self-assembly.







Walker, et. al., in prep., 2016

Research nuggets:

- Created new methods for the Ericksen model of liquid crystals, including colloidal effects and electric fields.
- Can model interesting defect structures, such as the Saturn ring.

Introduction

Liquid Crystals

Geometric Flows, PDEs, and Control

Numerical Analysis and Simulation

Conclusion

## Research Projects in Liquid Crystals



Araki, Tanaka, PRL, vol. 97, 2006



Čopar, Tkalec, Muševič, Žumer, PNAS, vol. 112, 2015

- Optimal control of colloids and (topological) defect structures
- Optimal shape of liquid crystal droplets
- Generalize our Ericksen method to the **full** Q-tensor model
- Coupling liquid crystals to fluid dynamics
- Coupling other physical effects, e.g. electric fields



Čopar, Ravnik, Žumer, Materials, vol. 7, 2014

#### Overview

Geometric flows occur in surface tension/curvature-driven flows in microfluidics (e.g. electro-wetting), soap films and foams, bio-membranes, and shape and topology optimization. Applications include controlling droplets and foams for micro-fluidics and developing new materials.



Walker, M2AN, vol. 48, 2014

Research nuggets:

- Created new models and methods for moving droplets with surface tension, and solidification/melting problems.
- Developed shape optimization tools for fluid pumping, drug delivery, and droplet footprint control.

# Research Projects in Geometric Flows, PDEs, and Control





Laurain, Walker, SIAM J. Control Optim., vol. 53, 2015

- Droplet dynamics and shape control
- Contact line pinning effects
- Shape and topology optimization
- Topology optimization of liquid crystal domains
- Modeling and analysis of liquid crystal nematic shells



#### Overview

Scientific computing is a basic tool for the investigation of scientific phenomena. Numerical analysis provides the mathematical foundation for a variety of "methods" such as finite difference and finite element methods mostly geared toward continuum models.



Walker, et. al., Phys. Fluids, vol. 21, 2009



Walker, SIAM J. Sci. Comp., vol. 35, 2013

Research nuggets:

- New finite element methods, and computational techniques, for problems with complex evolving geometry.
- New methods for electro-wetting (EWOD) and multi-physics problems.
- A new robust method for mesh generation of complex 3-D objects.

# Research Projects in Numerical Analysis and Simulation



Üngör, 2001; Brandts, Korotov, Křížek, 2011

Walker, J. Comp. Phys., vol. 311, 2016

- Self-avoiding curves and surfaces
- Non-obtuse adaptive meshing
- *cut*FEM approach for moving domains and shape optimization
- Phase-field modeling of liquid crystal droplets
- Multi-grid solver for liquid crystal models
- Mesh generation



Burman, Hansbo, et. al., Num. Math., vol. 133, 2016

# More Information

- Website: http://www.math.lsu.edu/~walker/
- FEM package FELICITY: http://www.mathworks.com/matlabcentral/fileexchange/31141felicity
- Liquid crystal *music video*: http://www.math.lsu.edu/~walker/liquid\_crystal.html#LC\_movie

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