Defects in nematic polymer hydrodynamics: survey of our work over the past 10 years

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Goals of this lecture

• Survey asymptotic and numerical modeling of non-equilibrium, defect-rich, hydrodynamics of nano-rod dispersions ---potential targets for mathematical analysis

• Focus on dynamical systems behavior---phenomena are robust to details of the models

• Open the door to your questions that our group might be able to model and simulate
How do loads, waves, current pass through, concentrate, .... in such a morphology in a thin film or membrane?

My lecture is going to build up modeling tools to predict what these figures are, how they arise in confined flows (films, cavities), can be thermally quenched, and then we are left to ask what advantage they might have for material properties.
These projects arise from Materials Science Applications that dictate modeling choices

- **Shear processing of nano-rod / nano-platelet dispersions in viscous and polymeric matrices** ---
- **Search for novel material properties for diverse applications (mechanical, conductive, dielectric....)**
- **This compels an assessment of statistical multi-scale properties** of shear-processed nano-rod composite films *from the orientational PDF* w/ P. Mucha, B. Shi, S. Wang, UNC, R. Zhou, ODU, X. Zheng, Kent St.
- Research support from AFOSR, ARO & NSF
Dynamical Systems Perspective

• Nematic polymer monodomains (homogeneous in $x$, “0D”) exhibit diverse "limit cycles" in steady shear conditions. This nonlinear dynamics playground is where I met David Chillingworth and other “bifurcators” (PPM).

• Orientational anchoring at interfaces (spatial BCs) leads to conflicts with interior oscillatory responses, setting the stage for spatial gradients mediated by Frank elasticity, defect generation & hydrodynamic feedback.

• Focus on attractors in 0D, 1D, 2D for kinetic & tensor theory

• What role do defects play: first below the minimum dimension for non-trivial topology, then 2D?
Defects in nematic liquids:
Numerical detection & tracking strategy

Cf. Chaikin & Lubensky

Classical metric: Topological degree from winding number of “the director” in 2d over gradient morphology with a singular core.

For defect detection & tracking, we use an "inside-out" perspective, focusing on defect cores: analytical objects that exist in any space dimension, via zero level sets of scalar metrics.
Orientational space: PDF, 2\textsuperscript{nd} moment tensor, director

**PDF:** \( f(m,x,t) \) orientational probability density function

\[
M = M(f) = \int_{\|m\|=1} mmf(m,x,t)dm
\]

\[
M = d_i n_i^t n_i,
\]

\[
0 \quad d_3 \quad d_2 \quad d_1 \quad 1, \quad d_i = 1
\]

**Second moment tensor**

Positive semi-def, symmetric quadratic form

Admits spectral & geometric representation

\[
M(f) \text{ defines a triaxial ellipsoid}
\]

Ordered and disordered phases are determined by level sets of two scalar defect metrics:

Nematic **director** is uniquely defined iff \( d_1 - d_2 > 0 \) \( \Rightarrow \) prolate M ellipsoid

If \( d_1 \) is not simple, the principal axis spreads to circle or sphere

\[
d_1 - d_3, d_1 - d_2
\]

**Oblate nematic phase** (multiplicity 2)

\( \Rightarrow \) M ellipsoid is an oblate spheroid (platelet)

\[
d_1 - d_3 = 0, (d_1 - d_2 = 0)
\]

**Isotropic phase** (multiplicity 3)

\( \Rightarrow \) M ellipsoid is a sphere

For different purposes, we image PDF, 2\textsuperscript{nd} moment tensor, director
Associate a geometry to each phase for imaging in t & x

We will also superimpose a Color scheme to reinforce
Ordered vs disordered phases

Fig. 1 Sketches of the ellipsoidal geometry defined by the second moment orientation tensor: the triaxial prolate ellipsoid of a nematic phase, with eigenvalues $d_1 > d_2 \geq d_3$, with principal axis $n_1$ of orientation; the sphere of the isotropic phase with $d_1 = d_2 = d_3 = 1/3$; and the oblate spheroid of the disordered phase with $d_1 = d_2 > d_3$. 
Construct a **nested hierarchy of models** in orientation \( \otimes \) flow \( \otimes \) physical space \( \otimes \) time

1. suppress flow, physical space, time (I-N diagram)
2. suppress physical space, impose linear flow
3. admit 1 space dimension w/ physical BCs
4. 2 space dims, periodic or physical BCs

In all level models, many choices of **orientational space resolution**: full PDF, \( 2^{nd} \) moment tensor, or director
For imposed planar flows, we can impose "in-plane symmetry" on \( f, M, \) or \( n, \) or not!
"2d or 3d rods"
We also can impose "uniaxiality" on \( f \) or \( M, \) or not!

We have explored all variants of embedded or approximate reduced dynamical systems within higher dim’l systems, finite and infinite, and examined the stability or accuracy wrt each type of reduction.
The Couette cell—model experimental & theoretical system for shear-dominated flow of complex anisotropic fluids compatible with a nested hierarchy of product space models.

\[ v = v_0, \quad Q = Q_0 \quad f = f_0 \]

Molecular inclusions store anisotropy and stresses between moving plates, coupled with hydrodynamic feedback and solid wall confinement.
Model 1: Onsager (1949) equilibrium phase diagram


Prolate uniaxial phase $d_1 > d_2 = d_3$

O(3) degenerate ordered phase

Isotropic phase

Oblate uniaxial phase $d_1 \neq d_2 = 0$

O(3) degenerate ordered phase

Nematic concentration $N$
PDF: spherical harmonic expansions & mesoscopic (2\textsuperscript{nd} moment) projections

Expansion of $f$

$$f(m, t) \approx \sum_{l=0}^{L} \sum_{m=-l}^{l} a_{l,m}(t) Y_l^m(\theta, \phi)$$

Projection onto second moments gives mesoscopic $Q$ tensor

$$Q_{xx} = -\frac{2}{3} \sqrt{\frac{\pi}{5}} a_{2,0} + \sqrt{\frac{8\pi}{15}} \Re(a_{2,2})$$

$$Q_{yy} = -\frac{2}{3} \sqrt{\frac{\pi}{5}} a_{2,0} - \sqrt{\frac{8\pi}{15}} \Re(a_{2,2})$$

$$Q_{xy} = -\sqrt{\frac{8\pi}{15}} \Im(a_{2,2})$$

$$Q_{xz} = -\sqrt{\frac{8\pi}{15}} \Re(a_{2,1})$$

$$Q_{yz} = \sqrt{\frac{8\pi}{15}} \Im(a_{2,1})$$

$Q = M^{-1/3} I$

In any model simulations

Dynamic, 0D, 1D, 2D

Construct $M$, compute

$d_1 \quad d_3 \quad d_1 \quad d_2$

“Cost free” detection of Prolate, Oblate, Isotropic phases. In 2D, print ellipsoid morphology surrounding defect cores after positive test.

$\Re(\cdot)$ and $\Im(\cdot)$ represent real and imaginary part, respectively.
Imaging & “patch scale” of spherical harmonics

\[ f(m, t) \approx \sum_{l=0}^{L} \sum_{m=-l}^{l} a_{l,m}(t) Y_{l}^{m}(m) \]
Imaging of Boltzmann probability distribution on the sphere and your favorite rotation. A big equilibrium set.

The nematic equilibrium distribution, \( f(m) \) of kinetic Doi-Hess PDE, is invariant under rotations. Here we compute \( f(m) \) at a nematic concentration, with peak aligned with “\( z \)” axis. Then we produce another element of the continuous group of equilibria, \( f(Um) \), for \( U \) in \( O(3) \). FWZ, Phys Rev E 02: symmetries of kinetic and mesoscopic theory. This symmetry underlies sheared limit cycles.


Kinetic theory
variable: probability distribution function \( f(m, t) \)
Smoluchowski equation: \( \frac{DF}{Dt} = \mathcal{R} \cdot \left[ D_r(m, a)(\mathcal{R}f + \frac{1}{kT} fRV) \right] - \mathcal{R} \cdot [m \times \dot{mf}] \)
Jeffery orbit for the molecule axis \( m \):
\[
\dot{m} = \Omega \cdot m + a[D \cdot m - D : mmm]
\]

Mesoscopic theory
variable: orientation tensor \( Q = \int_{||m||=1} mmf \, dm - \frac{1}{3} I \)
pre-closure equation:
\[
\frac{d}{dt} Q - \Omega \cdot Q + Q \cdot \Omega - a[D \cdot Q + Q \cdot D] = 2\varepsilon D - 2aD : \langle mmmm \rangle
\]
\[-6D^0_r[Q - N(Q + \frac{1}{3}) \cdot Q + NQ : \langle mmmm \rangle] \]

Continuum theory
variable: director \( n \)
L-E model:
\[
0 = n \times \left[ \gamma_1 \left( \frac{dn}{dt} + \Omega \cdot n \right) + \gamma_2 D \cdot n \right]
\]

<table>
<thead>
<tr>
<th>Velocity</th>
<th>( \mathbf{v} )</th>
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<tbody>
<tr>
<td>Vorticity tensor</td>
<td>( \Omega = \frac{1}{2}(\nabla \mathbf{v} - \nabla \mathbf{v}^T) )</td>
</tr>
<tr>
<td>Rate-of-strain tensor</td>
<td>( D = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T) )</td>
</tr>
<tr>
<td>Excluded-volume potential</td>
<td>( V = -\frac{3}{2}NkT \langle \mathbf{mm} \rangle )</td>
</tr>
<tr>
<td>Concentration</td>
<td>( N )</td>
</tr>
<tr>
<td>Molecular shape parameter</td>
<td>( \alpha = \frac{r^2+1}{r^2-1} )</td>
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</tbody>
</table>
**Kayaking Orbit:** selected from orient’l degeneracy in weak shear.

Fokker-Planck limit cycle with 65 spherical harmonic real degrees of freedom

Slide is flow-flow gradient plane, normal to slide is vorticity axis. Even looks like a “circle of Boltzmann-like equilibria”
**Rheological oscillators in steady shear flows:**
the cast of transient nonlinear attractors (limit cycles +
chaotic orbits)

Coarse-imaging based on spectral properties of $M(f)$

<table>
<thead>
<tr>
<th>t-trace of $M$ ellipsoids</th>
<th>t-trace of principal axes</th>
<th>t-trace of $d_1 - d_2, d_1 - d_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kayaking ($K_1$)</td>
<td>Director Orbit</td>
<td>Order Parameter Orbit</td>
</tr>
<tr>
<td>Kayaking ($K_2$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tumbling ($T$)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Rheological oscillators in steady shear
These bulk monodomain responses to imposed pure shear foreshadow onset of gradient morphology since in any spatially confined flow, the local shear rate varies: flow-phase diagrams.
Model 2, 2’ : Monodomain bifurcation diagrams
N=6 slice; attractors vs normalized shear rate (local De)
N.B. “in plane” restriction to circle suppresses key features.

**UPSHOT:** at low-moderate shear rates
- Dynamic response to steady shear
- Multiple limit cycles and steady states exist, stable and unstable, but
- Kayaking is generic at low shear rates
- Flow-alignment is generic at high Pe

Out of plane tensor element shows most stable responses are out of plane!

Foreshadow Models 3 & 4
In 1D, 2D w/ flow feedback:
- Local De fluctuations → sensitive local selection of orbits
Model 2': Phase diagram of attractors & transitions Shear-concentration phase diagram of **Doi closure model**

Numerical continuation software (AUTO, XPPAUT)

Data compression: attractors + all Bifurcation branches

N.B. Still no proof of kayaking limit cycles!
(except 2d rods)
Model 2: Kinetic monodomain phase diagram

Attractors versus volume fraction (N) and shear rate (De)
Again: sensitivity to local Deborah number

\[ a = 1 \]

- 13 separate regions
- 8 different attractors

<table>
<thead>
<tr>
<th>Region</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Flow-aligned steady</td>
</tr>
<tr>
<td>II</td>
<td>Out-of-plane steady</td>
</tr>
<tr>
<td>IV</td>
<td>Chaos</td>
</tr>
<tr>
<td>V</td>
<td>Tumbling/logrolling</td>
</tr>
<tr>
<td>VI</td>
<td>Tilted kayaking</td>
</tr>
<tr>
<td>IX</td>
<td>Kayaking</td>
</tr>
<tr>
<td>XI</td>
<td>Wagging &amp; logrolling</td>
</tr>
<tr>
<td>XII</td>
<td>Logrolling</td>
</tr>
</tbody>
</table>
Phase transitions between regions: a zoo of bifurcations (why we abandoned SDEs)

<table>
<thead>
<tr>
<th>Boundary (bottom to top)</th>
<th>Bifurcation type</th>
<th>Attractor transition (bottom to top regions)</th>
</tr>
</thead>
<tbody>
<tr>
<td>VI-II</td>
<td>Hopf</td>
<td>$K_2^{+,-}$ to $OS^{+,-}$</td>
</tr>
<tr>
<td>IV-VI</td>
<td>periodic doubling</td>
<td>chaos to $K_2^{+,-}$</td>
</tr>
<tr>
<td>XII-V</td>
<td>periodic doubling</td>
<td>unstable to stable $T$, $LR$ remains</td>
</tr>
<tr>
<td>XII-IX</td>
<td>Hopf</td>
<td>$LR$ to $K_1$</td>
</tr>
<tr>
<td>IX-XIII</td>
<td>periodic doubling</td>
<td>unstable to stable $T$, $K_1$ remains</td>
</tr>
<tr>
<td>XI-VIII</td>
<td>Hopf</td>
<td>$LR$ to $K_1$, $W$ remains</td>
</tr>
<tr>
<td>VIII-VII</td>
<td>transcritical</td>
<td>$TW$ to $K_2$, $K_1$ remains</td>
</tr>
<tr>
<td>VII-VI</td>
<td>saddle-node</td>
<td>$K_1$ disappears, stable $K_2^{+,-}$ remain</td>
</tr>
<tr>
<td>VIII-X</td>
<td>saddle-node</td>
<td>$K_1$ disappears, stable $W$ remains</td>
</tr>
<tr>
<td>X-I</td>
<td>Hopf</td>
<td>$W$ to $FA$</td>
</tr>
<tr>
<td>VII-III</td>
<td>periodic doubling</td>
<td>stable $K_2^{+,-}$ to chaos</td>
</tr>
<tr>
<td>III-IV</td>
<td>saddle-node</td>
<td>$K_1$ disappears, chaos continues</td>
</tr>
</tbody>
</table>

65 dimensional approximation of Doi-Hess dynamical system: 0 space dims!
Heterogeneity + Dynamics  Models 3, 3’ : 1d in space
Confinement BC’ s $\rightarrow$ Gradient Morphology
Are dynamic attractors arrested?  (NO!)

- **Attractor Length Scale Distribution?** What selects scaling behavior of peak (dominant lengthscale of the morphology)? What components of the orientational distribution dominate? What are flow-orientation spatial and temporal correlations?

- Open problems for analysis of attractors. Numerical conjecture coming shortly.

- *Theoretical guidance: asymptotics of slow plate limit (low De) and low Er with steady attractors*
Doi-Marrucci-Greco mesoscopic closure model
1d & 2d coupling of distortional elasticity & flow
Not shown: Kinetic-Navier-Stokes model & Sebastian Heidenreich, S. Hess tensor-flow model

\[ \frac{dv}{dt} = \nabla \cdot \left( -pI + \tau \right) \quad \text{Balance of linear momentum} \]

\[ \tau = \left( \frac{2}{Re} + \mu_3 \right)D + a\alpha F(Q) + \frac{a\alpha}{3Er} \left\{ \Delta Q : Q \left( Q + \frac{I}{3} \right) - \frac{1}{2} (\Delta QQ + Q\Delta Q) - \frac{1}{3} \Delta Q \right\} \]

\[ + \frac{\alpha}{3Er} \left\{ \frac{1}{2} (Q\Delta Q - \Delta QQ) - \frac{1}{4} (\nabla Q : \nabla Q - \nabla \nabla Q : Q) \right\} \quad \text{Stress constitutive equation} \]

\[ + \mu_1 \left\{ \left( Q + \frac{I}{3} \right)D + D \left( Q + \frac{I}{3} \right) \right\} + \mu_2 D : Q \left( Q + \frac{I}{3} \right) \]

\[ \nabla \cdot \nu = 0 \quad \text{Continuity equation} \]

\[ \frac{d}{dt} Q = \Omega Q - Q\Omega + a [DQ + QD] + \frac{2a}{3} D - 2a D : Q \left( Q + \frac{I}{3} \right) \quad \text{Orientation tensor equation} \]

\[ - \frac{1}{\Lambda} \left\{ F(Q) + \frac{1}{3Er} \left[ \Delta Q : Q \left( Q + \frac{I}{3} \right) - \frac{1}{2} (\Delta QQ + Q\Delta Q) - \frac{1}{3} \Delta Q \right] \right\} \]

F(Q) is the variation of the quartic bulk potential that gives I-N equilibrium diagram
Structure scaling laws from asymptotics of tensor-flow models

- Nondimensionalize flow-nematic equations

\[ De = \frac{\text{bulk flow rate}}{\text{nematic relaxation rate}} = \frac{h / v_0}{D_r^0} \]

\[ Er = \frac{8}{N} \left( \frac{h}{L_{\text{elasticity}}} \right)^2 De \]

\[ 2h = \text{gap-width} \]
\[ \pm v_0 = \text{plate-speeds} \]
\[ \psi_0 = \text{orientation anchoring angle} \]

Dual asymptotics of Low De & Er

⇒ Exact solvability & explicit morphology scaling

For Kinetic-Navier-Stokes Simulations, we constrain Boltzmann distribution
Self-consistent flow-orientation steady structures
Then read off scaling behavior

\[
Q = Q^{(0)} + \mathcal{D} \epsilon Q^{(1)} + O(\mathcal{D} \epsilon^2)
\]

\[
Q^{(1)} = \mathcal{E} r (y^2 - 1) Q_1 + \left( \frac{\cosh(B y)}{\cosh(B)} - 1 \right) Q_2 + \left( \frac{\cosh(D y)}{\cosh(D)} - 1 \right) Q_3
\]

where

\[
Q_1 = -\frac{9 s}{2(2 + s)} (1 - \lambda_L \cos 2\psi_0) \begin{pmatrix}
\sin 2\psi_0 & \cos 2\psi_0 & 0 \\
\cos 2\psi_0 & -\sin 2\psi_0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\]

\[
Q_2 = \frac{a(1 - s)^2(1 + 2s)}{36s} \sin 2\psi_0 \begin{pmatrix}
1 - \cos 2\psi_0 & \sin 2\psi_0 & 0 \\
-\sin 2\psi_0 & 1 + \cos 2\psi_0 & 0 \\
0 & 0 & -2
\end{pmatrix}
\]

\[
Q_3 = -\frac{a(4s - 1)}{4 N (3N - 8)s} \sin 2\psi_0 \begin{pmatrix}
1 + 3 \cos 2\psi_0 & \sin 2\psi_0 & 0 \\
\sin 2\psi_0 & 1 - 3 \cos 2\psi_0 & 0 \\
0 & 0 & -2
\end{pmatrix}
\]
Read off **steady structure scaling properties**
Use later as hypothesis for dynamic scaling laws
and to guide numerics beyond asymptotic regime

- Recover Marrucci scaling law, $Er^{-1/2}$, of continuum theory in plate boundary layers dominated by scalar order parameters
- Non-uniform structure spans the entire shear gap, dominated by director distortions, $Er^{-1}$ mean scaling law
- Predict strong sensitivity to plate anchoring conditions
Spherical harmonic expansion for orientational configuration space

- Galerkin expansion

\[ f(m, x, t) = \sum_{l=0}^{L} \sum_{m=-l}^{l} a_{l,m}(x, t)Y_{l}^{m}(m) \]

spherical harmonic basis functions:

\[ Y_{l}^{m}(m) = P_{l}^{m}(\cos \theta)e^{im\phi} \]

- Amplitude functions:

\[ a_{l}^{m}(x, t) = \int_{\|m\|=1} f(m, x, t)(Y_{l}^{m}(m))^{*} dm \]

Smoluchowski equation is transformed to a system of PDEs for heterogeneous simulations, ODEs for monodomains
1D attractor phase diagram: steady – unsteady morphology transitions

Impose linear shear & in-plane orientational PDFs to reduce cost

<table>
<thead>
<tr>
<th>De \ Er</th>
<th>5</th>
<th>10</th>
<th>15</th>
<th>50</th>
<th>180</th>
<th>500</th>
<th>2000</th>
<th>5000</th>
<th>(\infty)</th>
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</table>

Table 1: In-plane structure attractors and phase transitions for 3 decades of Deborah number \((De)\) and Ericksen number \((Er)\). ES and VS stand for elastic (E) and viscous (V) dominated steady (S) states. T or W indicates a transient structure in which the peak orientation axis at each height between the plates either oscillates with finite amplitude (wagging) or rotates continuously (tumbling).

“Tumbling-Wagging” attractors are most interesting ones to explore for stability to hydrodynamic feedback. Next.
Models 3, 3’ cont’d: 1d heterogeneity + flow

Focus on Defect-Mediated Phenomena

• Numerics of 3 different models & codes: JNNFM 2010, GF-Hess-Heidenreich-Yang-Zhou

• 1\textsuperscript{st}: Tune parameters to induce strong shear-banding coincident w/ pulsating oblate defect layers.

• 2\textsuperscript{nd}: Pass to high $Er$ limit to explore scaling behavior associated w/ a sea of oblate defects

• High $Er$ limit is an intriguing challenge
Use **level sets of oblate defect metric** to detect something interesting, then explore in greater detail.

Order parameter $s$ for the TW attractor for $Er = 500$, $De = 4$. The defect cores are the spots where $s$ drops precipitously toward 0. Top: parallel anchoring. Bottom: normal
- 1-d heterogeneous film flows, stable to 2-d perturbations !!!!
- 3 models & codes ➞ pulsating oblate defect, jet & T-W transition layer

Phase incoherence of Tumbling & Wagging orbits Spawns oblate phase

Nonlinear shear generation Pulsating jet layer forms coincident with oblate defect domain

Velocity jet shear

$d_1-d_2 \approx 0.03$
Move to more realistic parameters $De = 5$, $Er = 50,000$

Local Deborah number
Recall bifurcation diagram of local Monodomain orbits vs $De$!!!!

Oblate defect metric shows defect density & size of oblate domains … movies show dynamics

N.B. Still below minimum dimension for topological defects!!!!!
High Ericksen number limit phenomena  $\text{Er}=50,000 \quad \text{De}=5$

Oblate defect metric:
Non-topological defects form, propagate, interact and melt correlated with local phase incoherence of the major axis of orientation

$$d_1 - d_2$$

Primary velocity – nonlinear shear

Local Deborah number fluctuates across the gap
Time series of flow-orientation scalars at 4 nearby gap heights

Local De at 4 neighboring sites

Velocity fluctuations at 4 nearby gap heights

Strong flow-defect spatio-temporal Correlations!

Strong T-W transition & defect correlations!

In-plane projection of major director

Oblate defect metric at 4 sites
High Ericksen number limit: Compute scaling of the dominant lengthscale of morphology from the peak of a time-averaged lengthscale distribution function. Constantin said you folks can possibly derive bounds on this object!

\[ (ds/dy)^{-1} \]

\[ Er = (5000, 10000, 20000, 50000) \]

\[ L = \frac{1}{\max|ds/dy|}, \quad L = 0.9957Er^{-0.4338} \]

\[ L = 0.4Er^{-0.49} \]

Irreversible Thermodynamics model from Hess-Heidenreich

Smoluchowski-Navier-Stokes model

Clearly, this metric reflects oblate defect layers. Strong evidence for the Marrucci scaling prediction.
2d morphology: minimum dimension for topology

topological vs local defect metrics

Vorticity alignment BCs promote cellular secondary flows

Resolve: all 3 flow variables + full orientational space

periodicity in vorticity (z) direction -- JOR ‘09

then

2d driven cavity (physical BCs in x & y) -- Soft Matter ‘09
Take stock before 2D structure simulations

1. **Topological defects arise from double projection:**
   - Configuration space: PDF $\Rightarrow$ 2$^{\text{nd}}$ moment $\Rightarrow$ principal axis
   - Physical space: project principal axis onto 2d physical space

2. Kinetic and 2$^{\text{nd}}$-moment model solutions are smooth “up” in the full configuration space. Defect cores in 2d or 3d are regularized by principal value (scalar order parameter) degeneracies. Cf. Schopohl & Sluckin 87

3. Order parameter degeneracies determine non-topological defects, where the principal axis spreads to a circle (oblate defect phase) or a sphere (isotropic defect phase). These defect metrics are local, analytical conditions in configuration space, independent of physical space dimension, inexpensive!

The core of defects in 2d and 3d, or non-topological defects in 0d, 1d, have local diagnostics in any space dimension: utilize these algebraic metrics for “blind” detection & tracking.

After a positive test in 2d or 3d, then we measure topology.
• 2-d Stable Steady Roll Cells: For $De=1.5$, $Er=50$ & vorticity anchoring; Larson & Mead experiments

Leal, Klein, Garcia-Cervera, Ceniceros
2d & 3d results on Larson-Mead expts

Secondary flow
Generation of cells
Weak relative to $\alpha$
Strong shear ($V_x$) which is nearly linear

Director-dominated weak distortions associated with steady roll cells

Prolate everywhere
Very little defocusing
No defects of any kind

$d_1$ – $d_2$ color scale applied to ellipsoids:
Detection and tracking w/ level sets of the oblate defect metric

- **Roll Cell instability**: For $De=3.5$, $Er=50$  2 stationary cells destabilize, 4 cells form

- Oblate phase stripes
- Twin topological defects are at the tips of the cores (+1, -1/2) “updraft” (-1, +1/2) “downdraft”

- Order parameter defect stripes pinch-off

- Order parameter defects and topological defects(+- 1,+-1/2) arise close to the boundary
Defect core: oblate phase

Vorticity alignment at plates

Blow-up of one defect domain:
Oblate core with two topological defects of degree $+1, -1/2$

This defect forms in updraft between 2 roll cells
Other type forms in downdrafts
2D shear cell simulation in unstable roll cell regime
Dirichlet BC at top/bottom wall, Periodicity transverse

t=10
Velocity Streamlines: startup of driven cavity

Colors = level sets of oblate defect metric
Dark blue is zero level set

Field of M tensor ellipsoids
Painted with oblate defect metric

Red ovals +1/2  Blue rectangles -1/2
Continuous process: defect domains shed, propagate, collide, annihilate.....

Longtime behavior: stationary + transient oblate defect domains w/ +/- ½ charge
Driven cavity simulation: near startup
Defect shedding, propagation
Ok, that’s all for today from me.

Most “results” shown here have no proofs.

Other recent results of our group on phase field modeling of shear rupture of LCP droplets suspended in viscous fluids, anchoring-induced selection of global defect structures; active nano-rod hydrodynamics; active nematic gel modeling of the cell cortex. I will be happy to discuss those projects while I’m here.