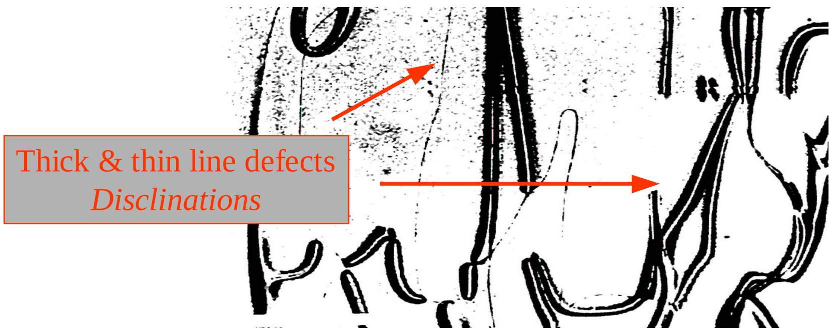
Fiber spinning (pure extensional flow) enhances natural alignment of nematic phase

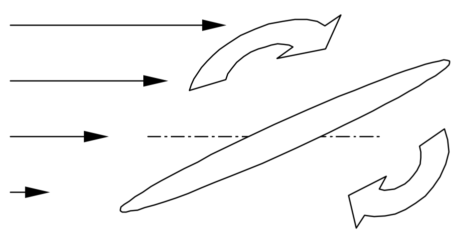
The processing phase for structural material (e.g.injection molding) involves flows with a shear component that disrupts natural alignment in tumbling liquid crystals



Sheared 8CB (Mather et al. '96)

What's so bad of Shear Flow?

What happens to a suspension of rods?



Rotation of single rods because of viscous torque

Brownian motion desynchronizes the rotations of single rods

→ Overall distribution of orientations stationary with the average orientation aligned near the flow direction

What's so bad of Shear Flow?

What happens instead in Nematics?

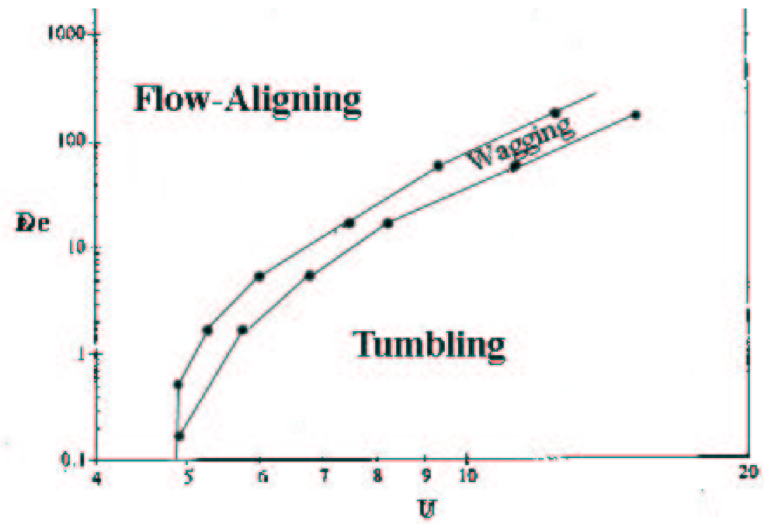
Excluded Volume Interactions correlate the rotation of single rods

→The average orientation rotates in the flow
Tumbling behavior

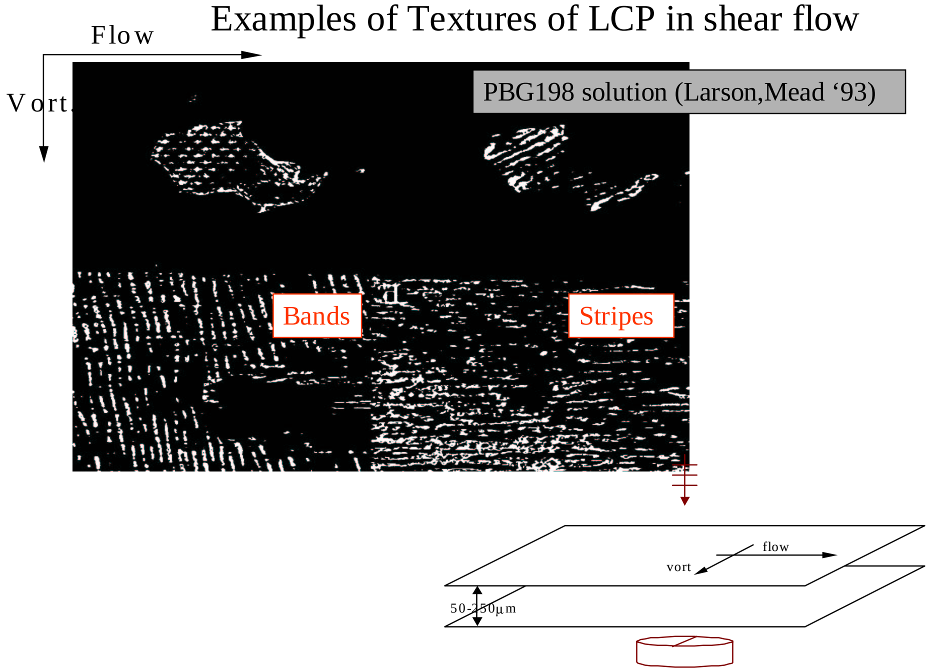
→Instabilities leading to highly non-uniform orientation field (i.e. a texture appears)

→ The high tensile properties are lost

Phase diagram for Monodomain LC

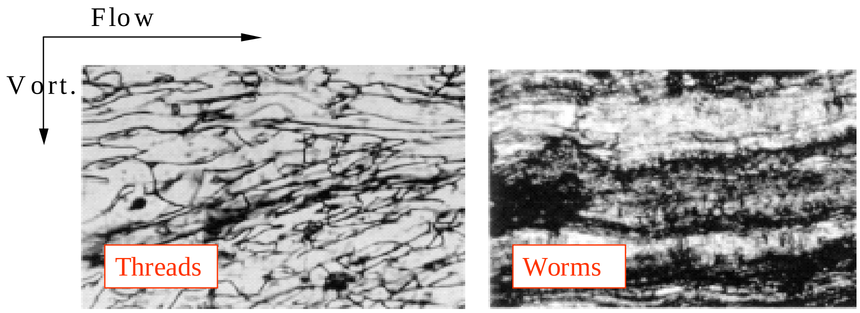


Examples of Textures of LCP in shear flow



Examples of Textures of LCP in shear flow

Vectra (De Neve et al. '93)



The equations of the "Complete Molecular Model"

- Continuity
- Momentum transport with a stress due to the LC:

$$\sigma = \frac{De}{\beta}\mathbf{D}:\mathbf{Q} + \mathbf{S} - U\left[\ (\mathbf{S}\cdot\mathbf{S} - \mathbf{Q}:\mathbf{S}) - \frac{1}{24}\left(\frac{\ell}{L}\right)^2\left(\mathbf{Q}:\nabla^2\mathbf{S} - \mathbf{S}\cdot\nabla^2\mathbf{S} - \frac{\nabla\mathbf{S}\cdot\nabla\mathbf{S} - \nabla\nabla\mathbf{S}:\mathbf{S}}{4}\right)\ \right]$$

- Evolution equation of the orientation (2^{nd} moment of Ψ only)

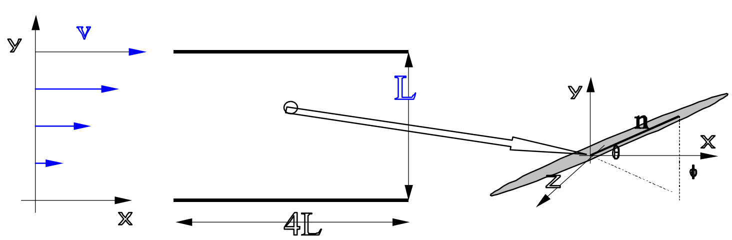
$$\frac{D\mathbf{S}}{Dt} = -2\,\mathbf{D}:\mathbf{Q} - \frac{f}{De}\left(\mathbf{S} - \frac{\mathbf{I}}{3}\right) + \frac{Uf}{De}\left(\mathbf{S}\cdot\mathbf{S} - \mathbf{S}:\mathbf{Q} + \frac{1}{48}\left(\frac{\ell}{L}\right)^2\left(\nabla^2\mathbf{S}\cdot\mathbf{S} + \mathbf{S}\cdot\nabla^2\mathbf{S} - \nabla^2\mathbf{S}:\mathbf{Q}\right)\right)$$

- Closure relating Q(4^{th} moment of Ψ) to S

THE FLOW BEHAVIOR OF LCPs BASED ON A GENERALIZED DOI MODEL WITH DISTORTIONAL ELASTICITY

Sgalari G., Feng J., Leal G.

Journal of Non-Newtonian Fluid Mechanics, 41 (2002)

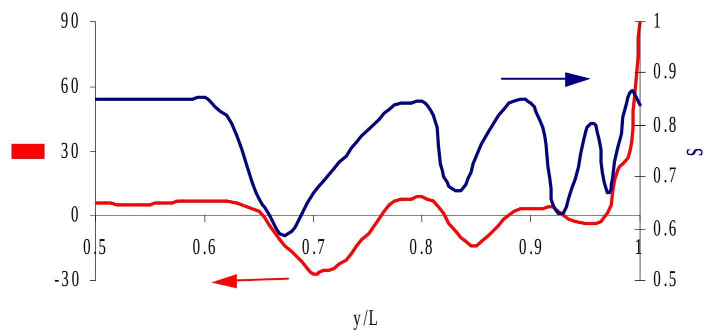


2D Geometry (flow, shear-gradient plane)
2D Velocity field, 3D Orientation field

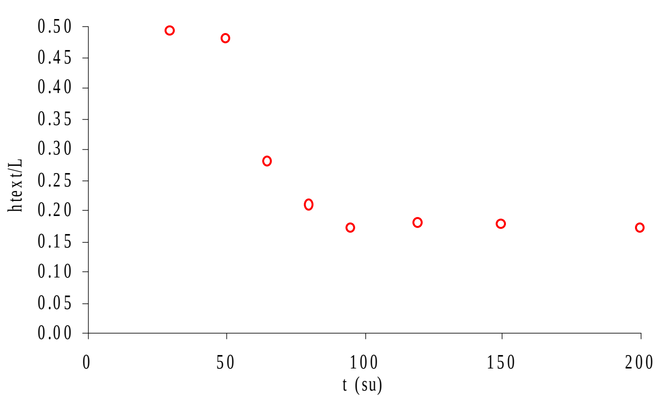
Finite Element Code

What our simulations are able to predict:

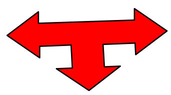
1. A texture develops across the gap



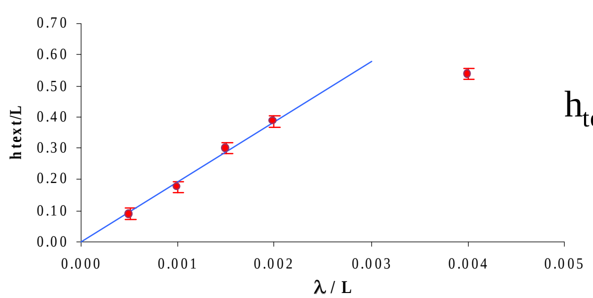
2. The characteristic length scale of this texture saturates in time
3. Tumbling is correspondingly suppressed



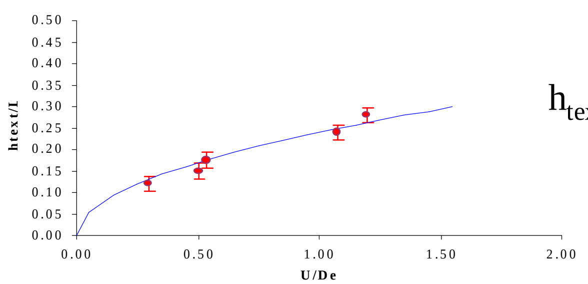
Steady-state Texture scale

- Marrucci scaling ('85)
  Distortional (Frank) Elasticity ↔ Viscous torques
- A molecular Marrucci-like scaling
  Distortional Elast.  Molecular Elast.
  Viscous forces

$$h_{text} \propto \ell \left(\frac{U}{De} \right)^{\frac{1}{2}}$$

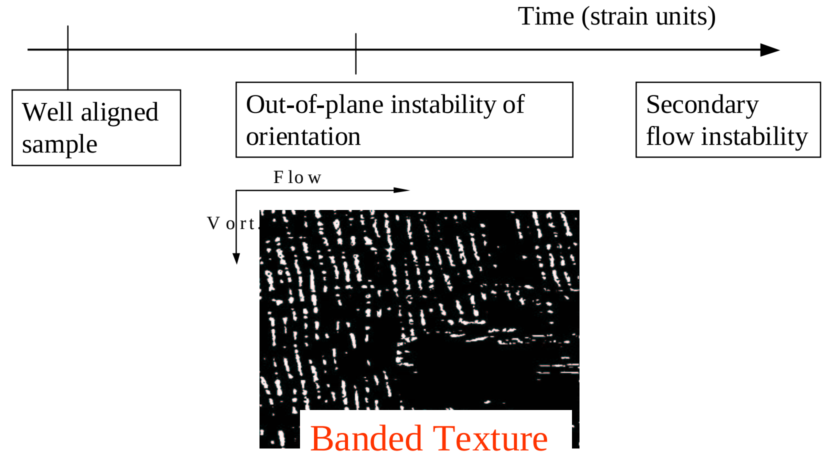


h_{text} vs. λ



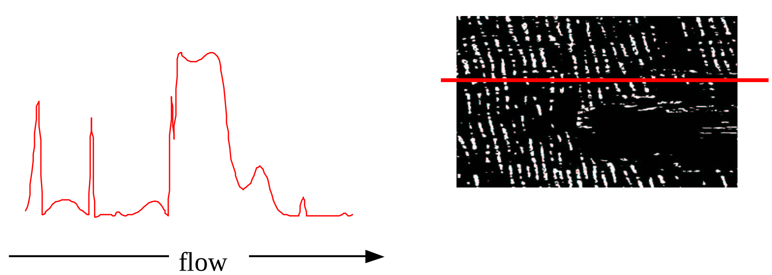
h_{text} vs $(U/De)^{1/2}$

Can we predict with this model the evolution of real systems?



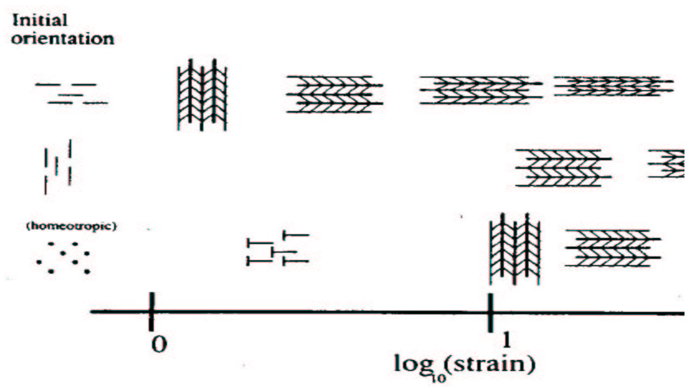
Profiles of Transmitted Light Intensity only "measure" available of orientation field

4. The director is unstable to out-of-plane tipping
5. The tipping is not uniform along the flow direction and a texture along the flow develops as a result of this



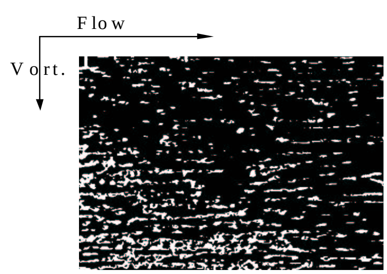
6. Analysis of Fourier spectrum indicates a characteristic length scale: λ ~.8L (Yan,Labes '95 λ ~.5L)

7. The banded texture does not develop for initial orientation along the vorticity direction
8. The time scale for the development of the texture is different for initial orientation along the flow or along the shear-gradient directions



Can we predict with this model the evolution of real systems?

Striped Texture



Well aligned sample

Out-of-plane instability of orientation

Secondary flow instability
Roll cells structure

Progressive refinement of texture

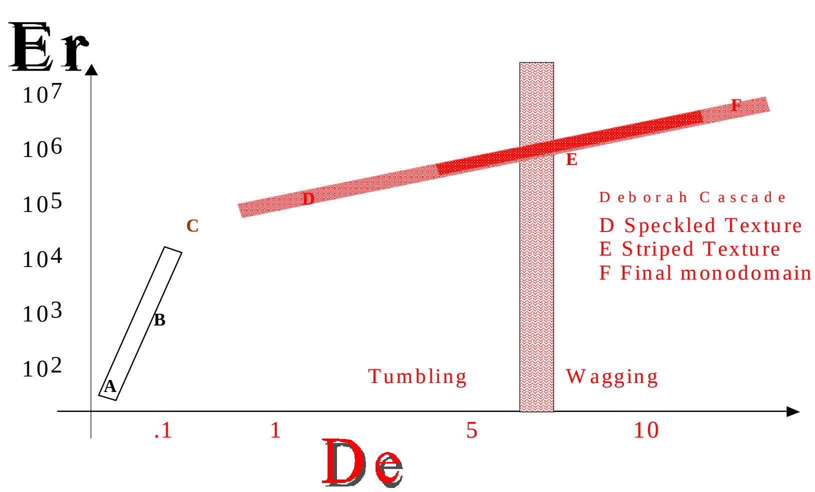
Time (strain units)

Prediction of Strong non-homogeneities of director
Coreless ("thick") defects in the center of the roll-cells

Problems:

1. Experiments say defects form between rolls
2. Experiments show also formation of "thin" defects
3. Processing conditions are for much higher shear rates, i.e. in the Deborah number cascade*

Need to use our Molecular Model!

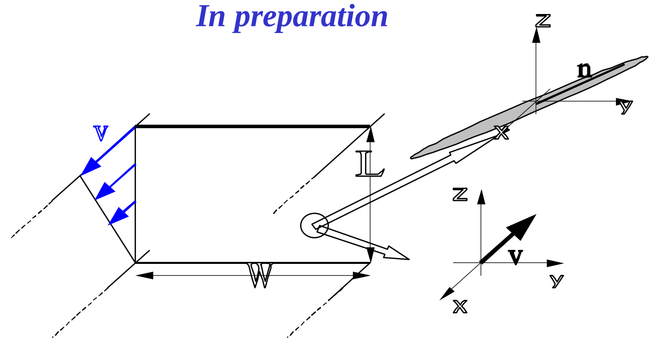


1. Understand the relative role of the various forces
2. Predict qualitatively the Deborah cascade
3. Confirm LEF calculations

THE DEBORAH NUMBER CASCADE FOR SHEARED LIQUID CRYSTALLINE POLYMERS: STRIPED TEXTURE, ROLL CELLS AND DIRECTOR TURBULENCE

Sgalari G., Klein D.H., Leal G.

In preparation



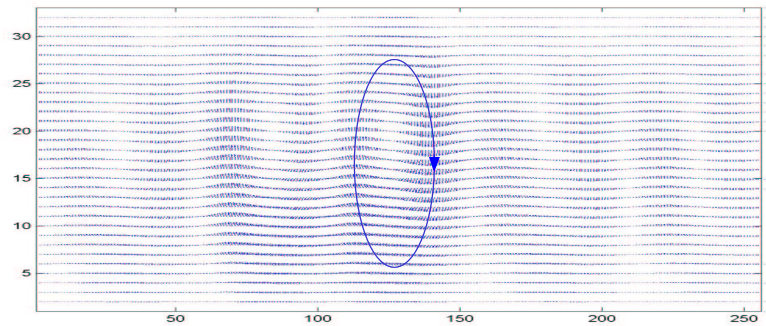
2D Geometry (vorticity, shear-gradient plane)
3D Orientation and velocity fields

- Flow solver developed in collaboration with Prof.Meiburg
  a. Vorticity formulation (instead of pressure formulation)
  b. 1 Grid for all variables
  c. Spectral method in y
  d. 6^{th}-order Compact Finite difference in z
- 2^{nd} order Finite difference formulation of Configuration equation from molecular model
- Implicit time stepping with iterative explicit inner loop solution and SOR

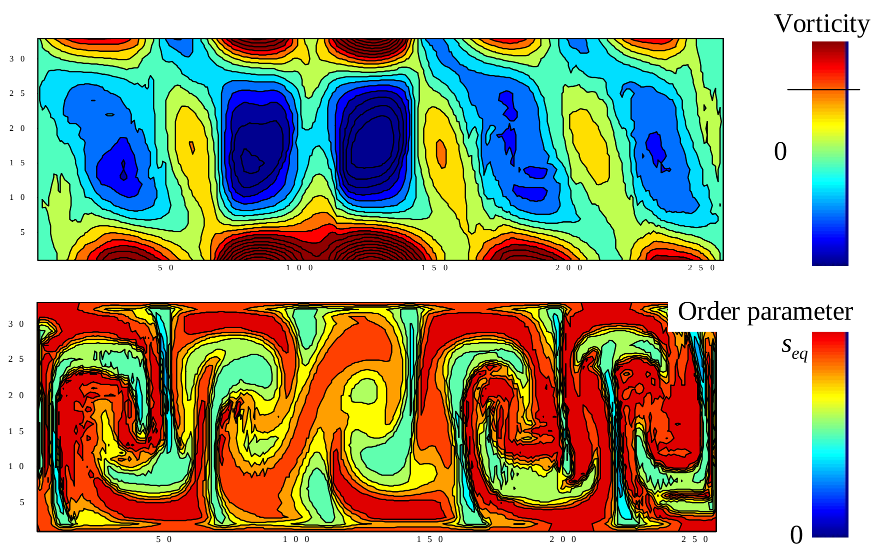
  (Under comparison with explicit Runge-Kutta time stepping and spatial high-order compact finite difference)

What our simulations are able to predict:

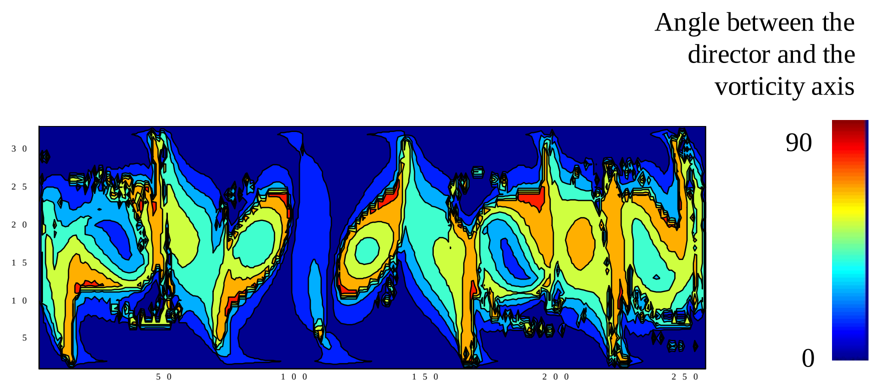
1. Roll Cells of secondary flow form and diffuse

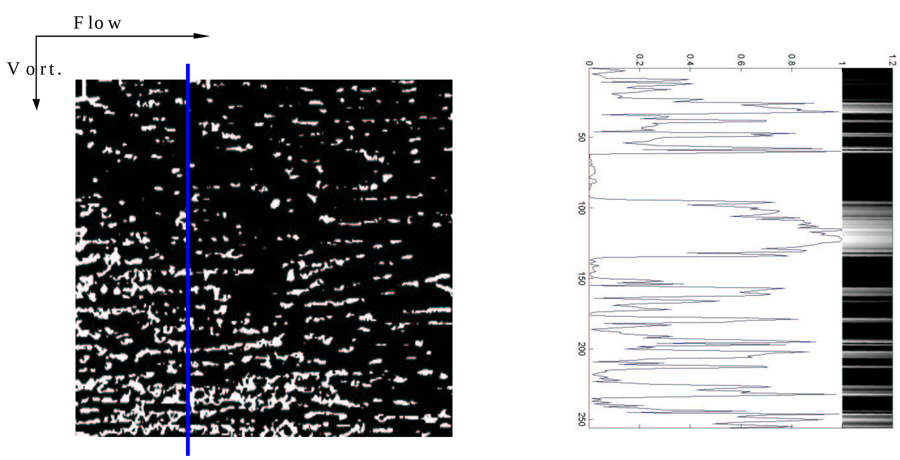


2. The rolls structure gives rise to corresponding region of reduced order paramater

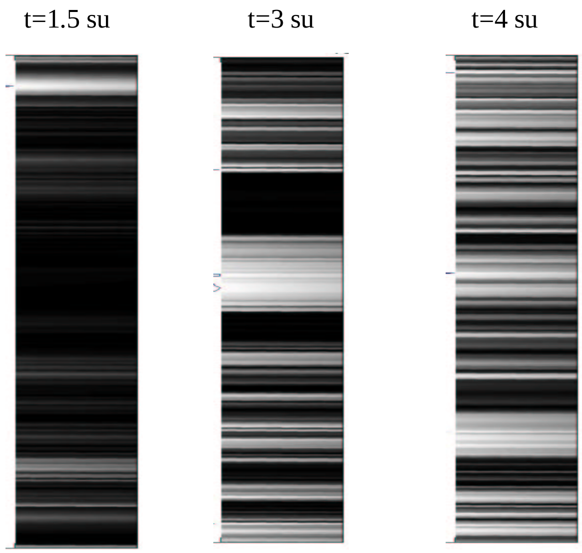


…and to regions where the director has escaped toward the flow direction





3. A texture along the vorticity direction develops

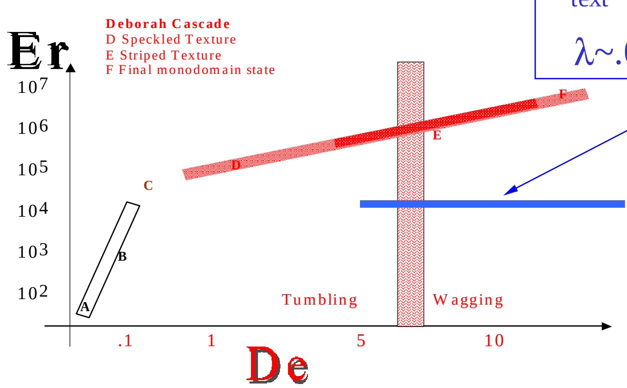


4. The texture is progressively refining

5. At low De number the system refines to a completely isotropic domain
6. At high De number the system reaches a state where the characteristic length scale of the texture seems to saturate

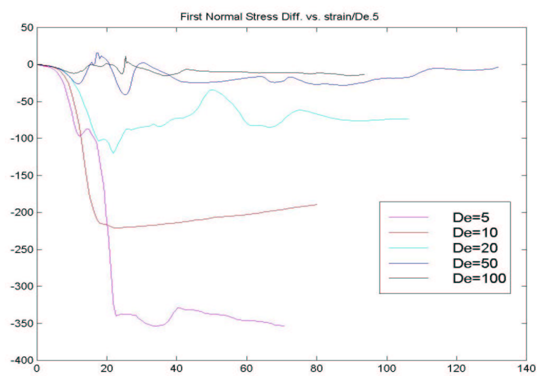
$l_{text} \propto \lambda = (De/Er\ U)^{1/2}$

$\lambda \sim .03 \quad \Delta x_{mesh} \sim .03$



5. The evolution of texture is strongly dependent on the type of BC imposed, i.e. flow vs. vorticity. Still unclear how to quantify and to interpret these differences in time history
6. The characteristic time for the evolution of texture depends on De, approximately ~strain/$De^{.5}$. Physical relevance?

9. The evolution of wall shear stress and first normal stress difference exhibits damped oscillations reflecting the progressive texture refinement



We are on a promising way but there is still need of quantitative comparison with detailed experimental observations!!!

For us: Need to perform fully 3D calculations and use finer meshes

For “the experimentalists”: Need to give us local data of orientation (not only average birefrengence)