Suspensions of rigid rods

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Supported by the ACMAC project of European Union FP7

Outline

Derivation and basic properties of models

- viscoelasticity
- stochastic DE's for evolution of microstructure
- kinetic equation for microstructure
- interaction of solvent - suspension

Shear band (or spurt) in shear flows of suspensions.

- shear band solution
- existence theory

Sedimentation under the influence of gravity

- linearized instability
- diffusive scaling - Keller-Segel
- moment closure approximation, flux-limited KS

Viscoelasticity

Additive decomposition of stresses

$$S = \underbrace{\eta\left(\nabla_x u + \nabla_x u^T\right) - pI}_{\text{solvent}} + \underbrace{\sigma}_{\text{polymeric stress}}$$

$$\nabla_x \cdot u = 0$$

$$\rho_f \left[\partial_t u + (u \cdot \nabla_x)\, u\right] = \nabla_x \cdot \Big(\eta(\nabla_x u + \nabla_x u^T) - pI + \sigma\Big) + b$$

Oldroyd models

$$\underbrace{\partial_t \sigma + (u \cdot \nabla)\sigma + \Omega\sigma - \sigma\Omega + \alpha(D\sigma + \sigma D)}_{d_t^\star \sigma} = -\lambda\sigma + 2\mu D$$

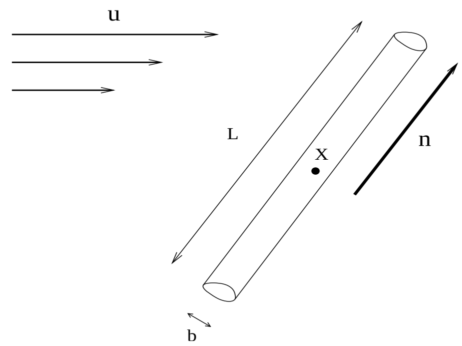
$$\Omega = \tfrac{1}{2}(\nabla u - \nabla u^T)\,,\; D = \tfrac{1}{2}(\nabla u + \nabla u^T)$$

upper convected Maxwell $(\alpha = -1)$

$$\partial_t \sigma + (u \cdot \nabla)\sigma - \nabla u \sigma - \sigma \nabla u^T = -\lambda\sigma + 2\mu D$$

Suspensions of rods

$f = f(t, x, n)$ distribution function of position and orientation of rods



$$dx = u dt + \underbrace{\left(\frac{1}{\zeta_{||}} n \otimes n + \frac{1}{\zeta_\perp} (I - n \otimes n) \right)}_{\frac{1}{\zeta}(n)} G \, dt + \sqrt{2D(n)} \, dW$$

$$dn = P_{n^\perp} (\nabla_x u n) \, dt + \sqrt{2D_r} \, dB$$

$D_r = \frac{k_B T}{\zeta_r}$, $D(n) = k_B T \frac{1}{\zeta}(n)$, $\quad \zeta_\perp = 2\zeta_{||}$

ζ_r rotational friction coefficient, k_B Boltzmann constant, T temperature
W translational Brownian motion, B rotational Brownian motion,
G conservative force, $G = -\nabla_x U$

SDE's model a friction theory

$$m\frac{d^2x}{dt^2} = F_{fr} + G + F_{Br} = -\zeta(\frac{dx}{dt} - u) - \nabla U + \frac{dW}{dt}$$

quasistatic approximation - friction dominates - $m\frac{d^2x}{dt^2} \approx 0$

$$\frac{dx}{dt} = u - \frac{1}{\zeta}\nabla U + \frac{1}{\zeta}\frac{dW}{dt}$$

kinetic equation $f = f(t, x, n)$ Smoluchowski theory of diffusion

$$f = E\Big(\delta(x - x(t))\delta(n - n(t))\Big)$$

$$\partial_t f + \nabla_x \cdot (uf) + \nabla_n \cdot (P_{n^\perp}\nabla_x unf)$$
$$= D_r\Delta_{\vec{n}} f + \nabla_x \cdot D(n)\Big(\nabla_x f + f\nabla_x U\Big).$$

Thermodynamic structure

polymeric stress

$$\sigma = \int_{S^{d-1}} (dn \times n - I) dn$$

free energy

$$A[f] = \int_\Omega \int_{S^{d-1}} f \ln f + U(x) f dn dx$$

satisfies the energy dissipation identity

$$\frac{d}{dt} A[f] + \int_\Omega \int_{S^2} f |\nabla_n \ln f|^2 + \int_\Omega \nabla_x (\ln f + U) \cdot D(n) f \nabla_x (\ln f + U)$$
$$= \int_\Omega G \int_{S^2} f \cdot u + \int_\Omega \nabla_x u : \sigma$$

Interaction solvent - suspension

- solvent $\longrightarrow$ rods   imposed external flow
- rods $\longrightarrow$ solvent   polymeric stress

$$\sigma = \int_{S^{d-1}} \nabla_n \frac{\delta A}{\delta f} \otimes n f \, dn = < \nabla_n \frac{\delta A}{\delta f} \otimes n >$$

Derivation of polymeric stress formula

Consider the case that $\nabla_x u \equiv \kappa = const$

$$dn = P_{n^\perp} \kappa n \, dt + \sqrt{2} dB$$
$$\frac{\partial f}{\partial t} = -\nabla_n \left(P_{n^\perp} \kappa n f \right) + \triangle_n f$$

Free energy $A[f] = \int f \ln f \, dn$

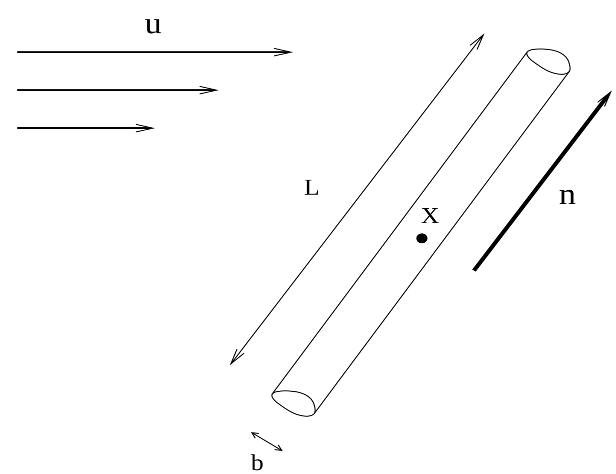


Figure 1: $\nabla_x u = \kappa$

Free energy $\quad A[f] = \int f \ln f \, dn$

Consider a small deformation $\delta\varepsilon = \kappa\delta t$ effected in time $\delta t << 1$
To leading order it deforms the suspension by

$$\delta f = -\nabla_n \big(P_{n^\perp} \kappa n f \big) \, \delta t$$

Require principle of virtual works

$$\delta A = \sigma : \delta\varepsilon = \sigma : \kappa\delta t$$

$$\delta A = \int \frac{\delta A}{\delta f} \delta f \, dn = - \int \frac{\delta A}{\delta f} \cdot \nabla_n \big(P_{n^\perp} \kappa n f \big) \, dn \delta t$$
$$= \Big(\int \nabla_n \frac{\delta A}{\delta f} \otimes n f \, dn \Big) : \kappa\delta t \underbrace{=}_{require} \sigma : \kappa\delta t$$

which yields

$$\sigma = \int_{S^{d-1}} \nabla_n \frac{\delta A}{\delta f} \otimes n f \, dn = < \nabla_n \frac{\delta A}{\delta f} \otimes n >$$

Emerging Thermodynamic structure

$A[f]$ free energy

$$\frac{\partial f}{\partial t} = -\nabla_n\big(P_{n^\perp}\kappa n f\big) + \nabla_n \cdot f \nabla_n \frac{\delta A}{\delta f}$$

multiplier $\frac{\delta A}{\delta f}$ yields

$$\frac{\partial}{\partial t} A[f] + \int_{S^2} f \Big|\frac{\delta A}{\delta f}\Big|^2 \, dn = -\int_{S^2} \nabla_n \frac{\delta A}{\delta f} \cdot \kappa n f \, dn$$
$$= \sigma : \kappa$$

where we use $\sigma = \int_{S^{d-1}} \nabla_n \frac{\delta A}{\delta f} \otimes n f \, dn =< \nabla_n \frac{\delta A}{\delta f} \otimes n >$

Connection to Oldroyd model

$$\frac{\partial f}{\partial t} = -\nabla_n \big(P_{n^\perp} \kappa n f \big) + \triangle_n f$$

$$\sigma = \int (3n \otimes n - I) f dn =< 3n \otimes n - I >, \qquad \sigma^T = \sigma$$

Compute the equation for the polymeric stress

$$\frac{\partial \sigma}{\partial t} = -6\sigma + \frac{1}{2}(\kappa + \kappa^T) + \kappa\sigma + \sigma\kappa^T - 6 < n \otimes n(n \cdot \kappa n) >$$

Doi closure relation $\quad < n \otimes n(n \cdot \kappa n) >=< n \otimes n >< n \cdot \kappa n >$

$$\frac{\partial \sigma}{\partial t} - \kappa\sigma - \sigma\kappa^T = -6\sigma + \frac{1}{2}(\kappa + \kappa^T) - 6tr(\sigma\kappa^T)(\sigma + \frac{1}{3}I)$$

Compare to Oldroyd model

$$\underbrace{\partial_t \sigma + (u \cdot \nabla)\sigma - \nabla u \sigma - \sigma \nabla u^T}_{upper\ convected\ Maxwell} = -\lambda\sigma + \mu(\nabla u + \nabla u^T)$$

Coupled system for solvent - suspension

$$\begin{aligned} \partial_t f + u \cdot \nabla_x f + \nabla_n \cdot (P_{n\perp} \nabla_x u\, n\, f) &= D_r \triangle_n f \\ \sigma &= \int_{S^2} (3\, n \otimes n - \mathrm{id}) f\, dn \end{aligned}$$

$$\begin{aligned} \nabla_x \cdot \big((\nabla_x u + \nabla_x^t u) - p\, \mathrm{id} + \sigma \big) &= 0 \\ \nabla_x \cdot u &= 0 \end{aligned}$$

with

$$f \geq 0 \qquad \int f dn = 1$$

time scales D_r, $\nabla_x u_{ext}$

Deborah number $\quad De = \frac{|\nabla_x u_{ext}|}{D_r}$

Stationary steady states

Seek stationary solutions

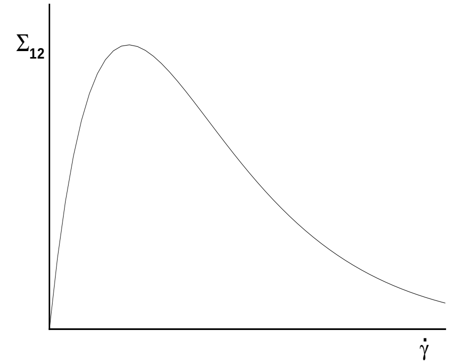
$$u_{ext}(x) = (\nabla u_{ext})x = \kappa x \qquad tr\kappa = 0$$

$$f = f_\kappa(n) \quad \text{solves} \quad \begin{cases} \nabla_n \cdot (P_{n^\perp}\kappa n f) = D_r \triangle_n f \\ \\ f > 0 \quad \int f dn = 1 \end{cases}$$

$$\text{Set} \qquad \Sigma : \kappa \longrightarrow \int_{S^2} (3n \otimes n - I) f_\kappa(n) dn$$

Proposition

$$\kappa_s = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \dot\gamma \kappa_s \longrightarrow \Sigma_{12}(\dot\gamma \kappa_s)$$



$$\Sigma_{12}(\dot\gamma \kappa_s) \to 0 \quad \dot\gamma \to \infty$$

Corollary For $D_r << 1$ there exist stationary solutions with a jump of $\nabla_x u$

$$u(x) = \begin{cases} \dot\gamma_- \kappa_s x & x_2 < 0 \\ \dot\gamma_+ \kappa_s x & x_2 > 0 \end{cases} \quad f(x,n) = \begin{cases} f_{\dot\gamma_- \kappa_s}(n) & x_2 < 0 \\ f_{\dot\gamma_+ \kappa_s}(n) & x_2 > 0 \end{cases}$$

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Shear bands for Johnson-Segalman and/or Oldroyd models were studied in late 80's.
They were associated to spurt phenomena and shown to be due to nonmonotonicity of steady response for the stress vs. strain rate curve

Hunter-Slemrod , D. Malkus-Nohel-Plohr , Nohel-Pego-AT

Material instability in complex fluids (shear induced transitions from isotropic to nematic states) was experimentally observed and computationally studied in 90's.

Review article J. Goddard, Ann. Rev. Fluid Mech. '03

Shear bands - Spurt

Corollary For $D_r << 1$ there exist stationary solutions with a jump of $\nabla_x u$

$$u(x) = \begin{cases} \dot\gamma_- \kappa_s x & x_2 < 0 \\ \dot\gamma_+ \kappa_s x & x_2 > 0 \end{cases} \qquad f(x,n) = \begin{cases} f_{\dot\gamma_- \kappa_s}(n) & x_2 < 0 \\ f_{\dot\gamma_+ \kappa_s}(n) & x_2 > 0 \end{cases}$$

At the same time the blow-up of the gradient occurs in infinite time

Thm Let $f_{eq}(n)$, $u_{ext}(x) = \kappa_0 x$, $tr\kappa_0 = 0$ and consider data f_0, u_0 with

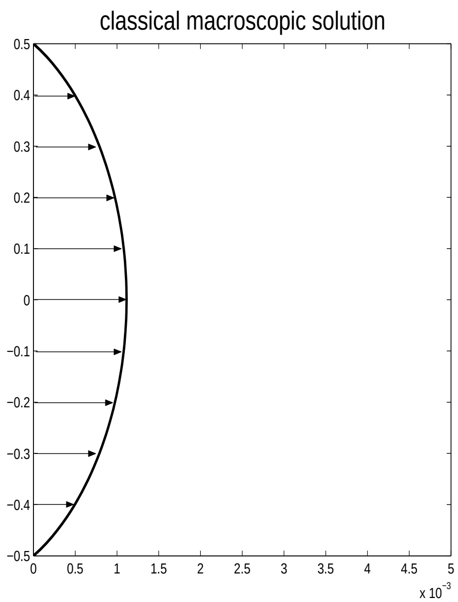
$$E(0) = \int_{\mathbb{R}^3} \int_{S^2} \left(\ln \frac{f_0}{f_{eq}} \right) f_0 dndx < \infty$$

then

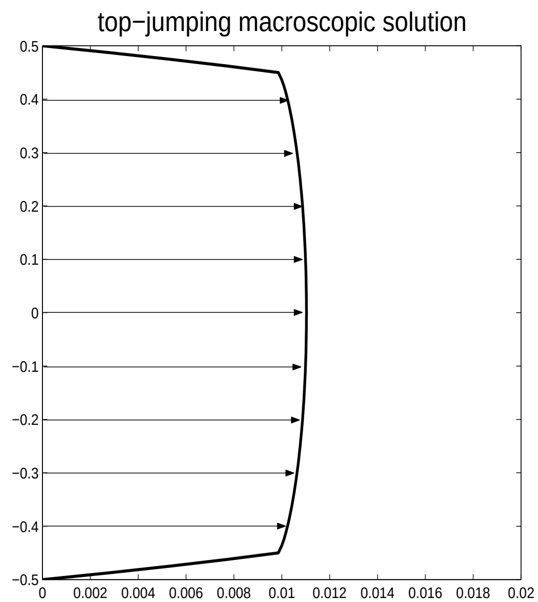
$$\sup_x |\nabla_x u(x,t) - \nabla_x u_{ext}| \leq K e^{e^{at}}$$

Numerical Simulations - Spurt

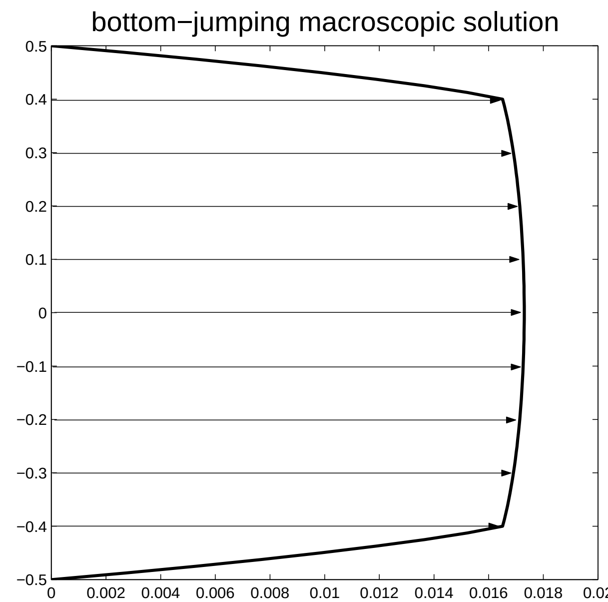
Numerical simulation of suspension of rigid rods in shear flow between two parallel walls. Small rotational diffusion D_r.



(a) smooth profile



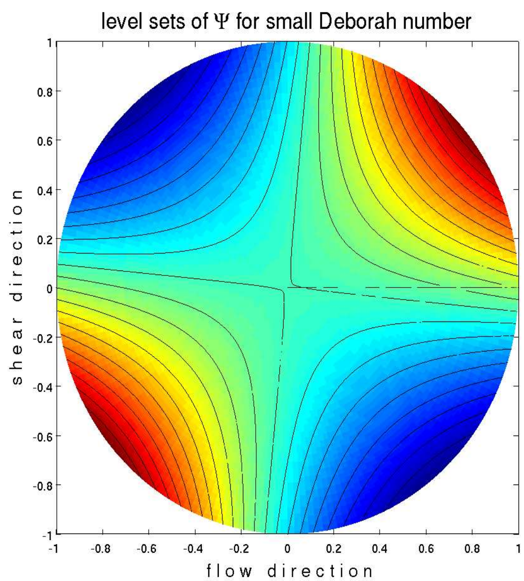
(b) shear band



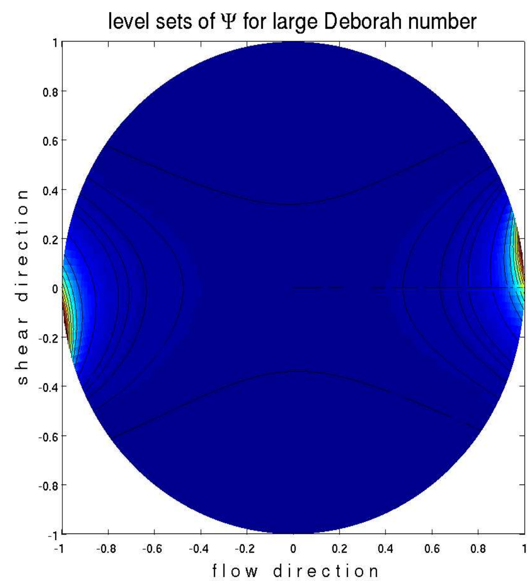
(c) shear band

In (a) $F_{ext} = .68$. In (b) $F_{ext} = .8$. In (c) $F_{ext} = .8$.

Angular distribution of particle density at positions near the center of the channel (graph (d)) and near the wall (graph (e))



(d) angular distribution near center of channel



(e) angular distribution at wall

Sedimentation

- Particles in slow flows move with the same order of magnitude velocity independently of their shape
- To separate them (or to understand locomotion) one needs to consider issues of collective behavior

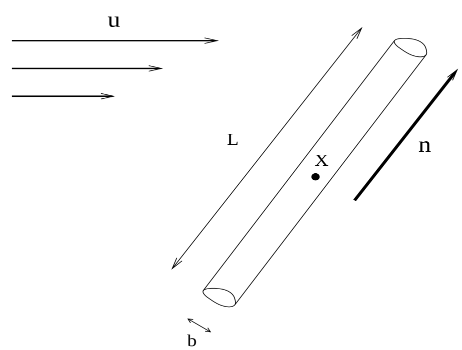
Experimental work by Metzger-Butler-Guazzelli, JFM 07 video

Analytical work on modeling, linearized stability, Koch-Shaqfeh JFM 89, Butler-Shaqfeh JFM 02

Particle simulations Tornberg-Gustafson 06

Modeling and simulation of active suspensions Saintillan - Shelley 07

Suspension of rods in solvent under gravity



$$dx = udt + \underbrace{\left(\frac{1}{\zeta_{||}} n \otimes n + \frac{1}{\zeta_{\perp}} (I - n \otimes n)\right)}_{\frac{1}{\zeta}(n)} G\, dt + \sqrt{2D(n)}\, dW$$

$$dn = P_{n^{\perp}} (\nabla_x u n)\, dt + \sqrt{2D_r}\, dB$$

$$\zeta_{\perp} = 2\zeta_{||}, \qquad D(n) = k_B T \tfrac{1}{\zeta}(n),$$

$f = f(t, x, n)$ distribution function of position and orientation of rods

Moment closure system

Suspension of rods in solvent under gravity

Kinetic equation for the microstructure coupled to Navier-Stokes

$$\partial_t f + \nabla_x \cdot (uf) + \nabla_n \cdot (P_{n^\perp} \nabla_x u n f) - \nabla_x \cdot ((I + n \otimes n)\, \vec{e}_2 f)$$
$$= \Delta_n f + \gamma \nabla_x \cdot (I + n \otimes n)\, \nabla_x f$$
$$\sigma = \int_{S^{d-1}} (dn \otimes n - I)\, f\, dn$$
$$Re\,(\partial_t u + (u \cdot \nabla_x)\, u) = \Delta_x u - \nabla_x p + \delta\gamma \nabla_x \cdot \sigma - \delta \int_{S^{d-1}} f\, dn \vec{e}_2$$
$$\nabla_x \cdot u = 0$$

Dimensionless parameters Re, γ and δ

$\gamma = \frac{\text{elastic forces}}{\text{boyancy}} = \frac{1}{Pe}$ $\qquad$ $\delta = \frac{\text{boyancy}}{\text{viscous force of solvent}} \sim N = \text{number of rods}$

Questions:

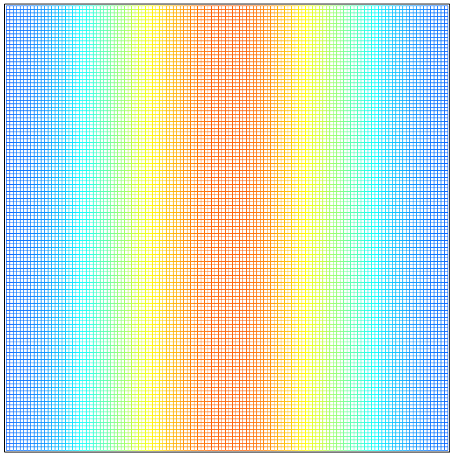
- Stability of quiescent flow $u \equiv 0$, $f = \frac{1}{4\pi}$
- Emergence of structures in long times

Linearized Stability Analysis

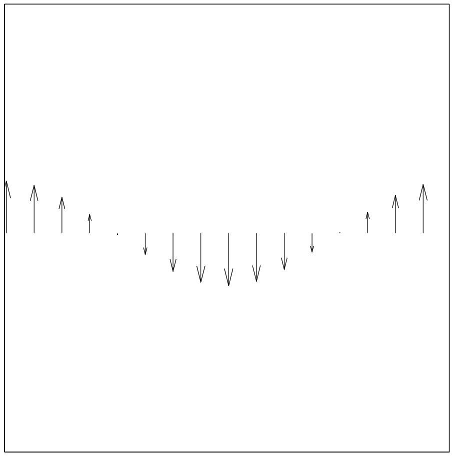
$$\partial_t f + \nabla_n \cdot (P_{n^\perp} \nabla_x u n) \frac{1}{2\pi} - D(n) e_2 \cdot \nabla_x f = \Delta_n f + \gamma \nabla_x \cdot D(n) \nabla_x f$$

or in one-space dimension

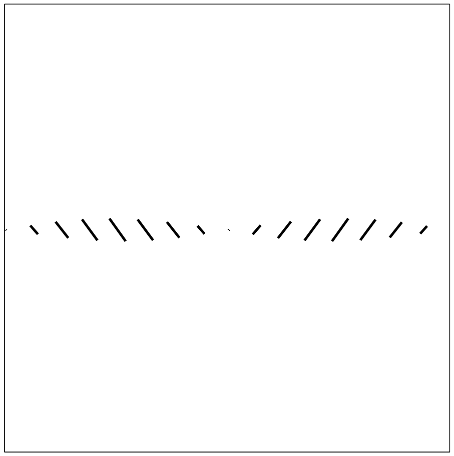
$$\partial_t f + \partial_\theta \left(v_x \cos^2 \theta f_0 \right) - \partial_x (\sin\theta \cos\theta f) = \partial_{\theta\theta} f + O(\gamma)$$



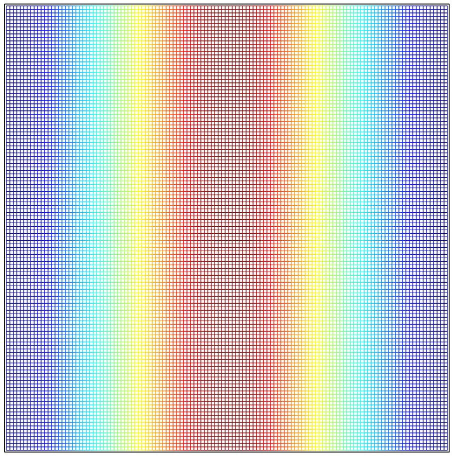
(g) initial density modulation



(h) velocity field



(i) microscopic orientation



(j) increased density modulation at later time

Moment closure linearized system

Laplace Beltrami operator $\triangle_n$ has eigenfunctions spherical harmonics
It is natural to derive moment equations and to truncate them at some level.
In 2-d the simplest meaningful system emerges when one truncates at the level of 2nd order moments

$$\rho = \int f d\theta \quad \sigma = \int f \cos 2\theta d\theta \quad s = \int f \sin 2\theta d\theta$$

$$\begin{aligned}
\partial_t \rho &= s_x - c_y + \gamma\left(\frac{3}{2}(\rho_{xx} + \rho_{yy}) + c_{xx} - c_{yy} + 2s_{xy}\right) \\
\partial_t c &= -\frac{1}{8}\rho_y + \frac{1}{4}(u_x - v_y) - 4c + \gamma\left(\frac{1}{8}(\rho_{xx} - \rho_{yy}) + \frac{3}{2}(c_{xx} + c_{yy})\right) \\
\partial_t s &= \frac{1}{8}\rho_x + \frac{1}{4}(u_y + v_x) - 4s + \gamma\left(\frac{1}{4}\rho_{xy} + \frac{3}{2}(s_{xx} + s_{yy})\right).
\end{aligned}$$

Linearized Instability of the solution $f_0 = \frac{1}{4\pi}$, $u_0 = 0$

- Solution is unstable (for the linear second moment system)
- numerical calculation of the spectral abscissae indicates

  $Re = 0$ max eigenvalue at $\xi = 0$. Most unstable wave length of the size of the calculation box.

  $Re > 0$ max eigenvalue at $\xi_1 > 0$.

For $0 < Re << 1$ the change of the eigenvalue (at $\xi_2 = 0$, ξ_1 variable) is described by an asymptotic expansion of the form

$$\lambda = \lambda_0 + (Re)\lambda_1 + \dots$$

where

$$\lambda_0 = \frac{1}{4}\left(-8 + \sqrt{64 + 4\delta - 2\xi_1^2}\right)$$

$$\lambda_1 = -\frac{\delta}{\frac{2\xi_1^2}{(2\delta - \xi_1^2)}\left(8 + \sqrt{64 + 4\delta - 2\xi_1^2}\right)^2 + 4\xi_1^2}.$$

Aggregate response at long times

Hyperbolic Limit

$$x = \frac{1}{\delta}\hat{x},\ t = \frac{1}{\delta}\hat{t},\ u = \hat{u},\ p = \hat{p}.$$

$$\delta\partial_t f + \delta u \cdot \nabla_x f - \delta D(n)\vec{e}_2 \cdot \nabla_x f + \delta\nabla_x \cdot (P_{n^\perp}\nabla_x u n f)$$
$$= \Delta_n f + \delta^2\gamma\nabla_x \cdot D(n)\nabla_x f$$
$$-\delta^2\Delta_x u + \delta\nabla_x p - \delta^2\gamma\nabla_x \cdot \sigma = -\delta\left(\int_{S^2} f dn\right)\vec{e}_2$$

where $D(n) = I + n \otimes n$.

Ansatz

$$f = \delta f_0 + \delta^2 f_1 + \ldots$$
$$u = u_0 + \delta u_1 + \ldots$$

leading order $O(\delta)$: $\triangle_n f_0 = 0$

$$f_0(t,x,n) = \frac{1}{4\pi}\int_{S^2} f_0 dn = \frac{1}{4\pi}\rho_0(t,x)$$

$\rho = \int_{S^2} f_0 dn$ and $u = u_0$ satisfy the Boussinesq system

$$\partial_t \rho + \nabla_x \cdot (u\rho) - \frac{1}{4\pi}\Big(\int D(n)dn\Big)\vec{e}_2 \cdot \nabla_x \rho = 0$$

$$-\Delta_x u + \nabla_x p = -\rho\vec{e}_2$$

$$\nabla_{\vec{x}} \cdot u = 0$$

Diffusive Scale

Consider a rectilinear vertical flow

$$u = (0, v(t,x,z), 0) \qquad f = f(t,x,z)$$

The hydrodynamic limit is trivial. Consider the diffusive scale

$$x = \frac{1}{\delta}\hat{x},\ t = \frac{1}{\delta^2}\hat{t},\ u = \hat{u},\ p = \hat{p}$$

$$O(\delta) \qquad \Delta_n f_0 = 0 \quad \Longrightarrow \quad f_0 = \frac{1}{4\pi}\rho_0$$

$$O(\delta^2) \qquad -\left(D(n) - \frac{1}{4\pi}\int_{S^2} D(n)dn\right)\vec{e}_2 \cdot \nabla_x f_0 + \nabla_{\vec{n}} \cdot (P_{n^\perp}\nabla_x u_0 n f_0) = \Delta_n f_1$$

$$O(\delta^3) \qquad \partial_t \rho_0 = \nabla_x \cdot \int_{S^2}\left(D(n) - \frac{1}{4\pi}\int_{S^2} D(n)dn\right)\vec{e}_2 f_1\, dn + \gamma\nabla_x \cdot (\frac{1}{4\pi}\int_{S^2} D(n)dn)\nabla_x \rho_0$$

The leading order terms in the Hilbert expansion $\rho_0 = \int f_0 dn$ and v_0 satisfy the Keller-Segel system

$$
\begin{aligned}
\partial_t \rho_0 &= \alpha \nabla_{(x,z)} \cdot \big(\rho_0 \nabla_{(x,z)} v_0 \big) + \beta \triangle_{(x,z)} \rho_0 \\
\Delta_{(x,z)} v_0 &= \rho_0
\end{aligned}
$$

BGK models for KS system Chalub-Markowich-Perthame-Schmeiser

Effective response

$$\frac{\partial f}{\partial t} = -\nabla_n \big(P_{n^\perp} \kappa n f\big) + \triangle_n f$$

$$\sigma = \int (3n \otimes n - I) f dn =< 3n \otimes n - I > , \qquad \sigma^T = \sigma$$

Compute the equation for the polymeric stress

$$\frac{\partial \sigma}{\partial t} = -6\sigma + \frac{1}{2}(\kappa + \kappa^T) + \kappa\sigma + \sigma\kappa^T - 6 < n \otimes n(n \cdot \kappa n) >$$

Oldroyd model

$$\underbrace{\partial_t \sigma + (u \cdot \nabla)\sigma - \nabla u \sigma - \sigma \nabla u^T}_{upper\ convected\ Maxwell} = -\lambda\sigma + \mu(\nabla u + \nabla u^T)$$

Consider a shear flow in 2-d $f = f(t,x)$, $v = v(t,x)$, neglect translational Brownian motion

$$\partial_t f + \partial_\theta \left((v_x + v_x \cos 2\theta) f \right) - \partial_x (\sin 2\theta f) = \partial_{\theta\theta} f$$
$$v_{xx} = \delta \rho$$

Compute moments and truncate to moments of second order

$$\rho = \int f d\theta \quad c = \int \cos 2\theta f d\theta \quad s = \int \sin 2\theta f d\theta$$

Moment system

$$\begin{aligned} \partial_t \rho &= \partial_x s \\ \partial_t c + v_x s &= -4c \\ \partial_t s - v_x c - v_x \rho - \rho_x &= -4s \end{aligned}$$

Quasi-dynamic approximation

$$v_x s = -4c$$
$$-v_x c - v_x \rho - \rho_x = -4s$$

The "equilibrium" response is described by

$$s = \frac{v_x}{1+v_x^2}\rho + \frac{1}{1+v_x^2}\rho_x$$

and thus

$$\partial_t \rho = \partial_x \left(\frac{v_x}{1+v_x^2}\rho + \frac{1}{1+v_x^2}\rho_x \right)$$
$$v_{xx} = \delta\rho$$