1. Governing Equations for Active Nematics

Refer to paper [1] and paper [2]

1.1. Smoluchowski Equation and mean-field model

Consider a suspension of active Brownian swimmers with mean number density n confined in a domain Ω with fixed boundary $\partial\Omega$ and characteristic size H. The swimmers self-propel with constant velocity V_s along their unit director $\mathbf{p}$, with constant translational and rotational diffusivities d_t and d_r. They exert a net symmetric force dipole on the suspending fluid with stresslet strength σ_0. The suspending fluid is assumed to be Newtonian and incompressible with density ρ and dynamic viscosity μ.

Distribution function $\Psi(\mathbf{x},\mathbf{p},t)$ is used to describe a swimmer at position $\mathbf{x}$ with orientation $\mathbf{p}$ at time t.

The evolution of the distribution function $\Psi(\mathbf{x},\mathbf{p},t)$ is governed by the Smoluchowski equation:

$$\partial_t\Psi + \nabla_x\cdot(\dot{\mathbf{x}}\Psi) + \nabla_p\cdot(\dot{\mathbf{p}}\Psi) = 0 \tag{1.1}$$

where $\dot{\mathbf{x}}$ and $\dot{\mathbf{p}}$ represent the translational and orientational flux velocities, ∇_x and ∇_p are the spatial and orientational gradient operators.

$\nabla_x\cdot(\dot{\mathbf{x}}\Psi)$**:** the Translational flux divergence
$\nabla_p\cdot(\dot{p}\psi)$**:** the Orientational flux divergence.

The translational flux velocity $\dot{\mathbf{x}}$ is given by:

$$\dot{\mathbf{x}} = V_s\mathbf{p} + \mathbf{u} - d_t\nabla_x \ln\Psi \tag{1.2}$$

accounts for self propulsion of the swimmers V_s, $\mathbf{u}$ is the background fluid velocity acts as advection, and d_t is the translational diffusivity. why is here a ”ln” term?

The orientational flux velocity $\dot{\mathbf{p}}$ is given by:

$$\dot{\mathbf{p}} = (\mathbf{I}-\mathbf{pp})\cdot(\zeta\mathbf{E}-\mathbf{W})\cdot\mathbf{p} - d_r\nabla_p \ln\Psi \tag{1.3}$$

where ζ is Bretherton's constant which characterizes the shape of particle (0 for spheres and 1 for slender particles). $\mathbf{E} = \frac{1}{2}(\nabla\mathbf{u}+\nabla\mathbf{u}^T)$ and $\mathbf{W} = \frac{1}{2}(\nabla\mathbf{u}-\nabla\mathbf{u}^T)$ are the rate-of-strain and vorticity tensors, here acts as rotational diffusion. d_r is the rotational diffusivity.

The boundary condition for $\Psi(\mathbf{x},\mathbf{p},t)$ is given by:

$$n\cdot\dot{\mathbf{x}} = 0 \quad \text{on} \quad \partial\Omega\times C \tag{1.4}$$

which ensures no flux across the boundaries.

1.2. Dimensionless Groups

Using H as the length scale, d_r^{-1} as time scale, non-dimensionalization of the governing equations yields the following dimensionless groups:

$$\mathrm{Pe}_s = \frac{V_s}{d_rH}, \quad \alpha = \frac{\sigma_0 n}{\mu d_r}, \quad \Lambda = \frac{d_rd_t}{V_s^2}, \quad \mathrm{Re} = \frac{\rho H^2 d_r}{\mu} \tag{1.5}$$

Peclet number Pe_s denotes the ratio of the persistence length of swimmer trajectories to the characteristic size of the domain.

α is a comparation of effect of active stresses exerted by the swimmers on the fluid, to the dissipation effects of viscosity and rotational diffusion. $\alpha > 0$ is so-called pullers such as certain micro-algae, that exert a thrust with their anterior flagella, in such case the fluid field flows towards the particle. $\alpha < 0$ is so-called pushers such as bacteria, they exert a thrust with their flagellar tail, in such case the fluid field flows away from the direction of particle movement.

Swimming-specific Λ compares the strength of propulsion to Brownian diffusion, $\Lambda \to 0$ describes purely ballistic swimmers, while $\Lambda \to \infty$ corresponds to purely diffusive swimmers.

Renolds number Re the inertia force to viscous force, typically small in active suspensions.

1.3. Moments and Closure Approximation

Moment is used here to describe the statistical properties of the distribution function, also to reduce the computational complexity, since the original Smoluchowski equation is high-dimensional in space, orientation and time.

The zeroth-order moment which represents the concentration field, is defined as:

$$c(\mathbf{x},t) = \int_C \Psi(\mathbf{x},\mathbf{p},t)d\mathbf{p} \tag{1.6}$$

The first-order moment, representing the polarization vector, is defined as:

$$\mathbf{m}(\mathbf{x},t) = \int_C \mathbf{p}\Psi(\mathbf{x},\mathbf{p},t)d\mathbf{p} \tag{1.7}$$

The second-order moment, representing the nematic alignment tensor, is defined as:

$$\mathbf{D}(\mathbf{x},t) = \int_C \left(\mathbf{pp} - \frac{\mathbf{I}}{2}\right)\Psi(\mathbf{x},\mathbf{p},t)d\mathbf{p} \tag{1.8}$$

Evolution of Moments

Taking the zeroth-order moment of the Smoluchowski equation yields the evolution equation for concentration:

$$\partial_t c = -\nabla \cdot F_c \tag{1.9}$$

where F_c is the flux of concentration.

Taking the first-order moment of the Smoluchowski equation and considering the contribution from the orientational flux, we obtain the evolution equation for polarization:

$$\partial_t \mathbf{m} = -\nabla \cdot F_m + H_m - \mathbf{m} \tag{1.10}$$

The term $-\mathbf{m}$ represents the natural relaxation of polarization due to rotational diffusion.

Similarly, taking the second-order moment yields the evolution equation for the nematic tensor:

$$\partial_t \mathbf{D} = -\nabla \cdot F_D + H_D - 4D \tag{1.11}$$

The three translational fluxes is given by

$$F_c = \mathbf{u}c + \mathrm{Pe}_s\mathbf{m} - \lambda \mathrm{Pe}_s^2 \nabla c \tag{1.12}$$

$$F_m = \mathbf{um} + \mathrm{Pe}_s \left(\mathbf{D} + \frac{c\mathbf{I}}{2} \right) - \lambda \mathrm{Pe}_s^2 \nabla \mathbf{m} \tag{1.13}$$

$$F_D = \mathbf{uD} + \mathrm{Pe}_s \left(\mathbf{T} - \frac{\mathbf{mI}}{2} \right) - \lambda \mathrm{Pe}_s^2 \nabla \mathbf{D} \tag{1.14}$$

The source terms H_m and H_D come from Jeffery's equation, describe particle alignment by the flow

$$H_m = \frac{1}{2}\zeta \mathbf{E} \cdot \mathbf{m} - \mathbf{W} \cdot \mathbf{m} \tag{1.15}$$

$$H_D = \frac{1}{2}\zeta c\mathbf{E} + \frac{2}{3}\zeta \mathbf{E} \cdot \mathbf{D} - \frac{1}{3}\zeta (\mathbf{D} : \mathbf{E})\mathbf{I} + \mathbf{D} \cdot \mathbf{W} - \mathbf{W} \cdot \mathbf{D} \tag{1.16}$$

Closure Approximation

To reduce the dimensionality, we use a closure approximation for the distribution function $\Psi(\mathbf{x}, \mathbf{p}, t)$:

$$\Psi(\mathbf{x}, \mathbf{p}, t) \approx \frac{1}{2\pi} \left(c(\mathbf{x}, t) + 2\mathbf{p} \cdot \mathbf{m}(\mathbf{x}, t) + 4\mathbf{pp} : \mathbf{D}(\mathbf{x}, t) \right) \tag{1.17}$$

where $c(\mathbf{x}, t)$ is the concentration, $\mathbf{m}(\mathbf{x}, t)$ is the polarization, and $\mathbf{D}(\mathbf{x}, t)$ is the nematic tensor.

In the translational flux for $\mathbf{D}$ contains a third-order moment $\mathbf{T}$, base on the closure approximation, it can be related to the polarization as

$$T_{ijk} = \frac{1}{4} \left(m_i \delta_{jk} + m_j \delta_{ik} + m_k \delta_{ij} \right) \tag{1.18}$$

The fourth-order moment based on this closure approximation is

$$\begin{aligned} S_{ijkl} = {} & \frac{c}{8}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ & + \frac{1}{4}(\delta_{ij}\delta_{kl}D_{jl} + \delta_{ik}\delta_{jl}D_{jk} + \delta_{il}\delta_{jk}D_{il} + \delta_{jl}\delta_{ik}D_{kl} + \delta_{il}\delta_{jk}D_{jl} + \delta_{kl}\delta_{ij}D_{ij}) \end{aligned} \tag{1.19}$$

1.4. Fluid motion

Assume that the suspending flow satisfy the Stokes equation

$$-\Delta \mathbf{u} = -\nabla p + \alpha \nabla \cdot \mathbf{D} \tag{1.20}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{1.21}$$

note an acive stress tensor $\alpha\mathbf{D}$ is included to capture the effect of the force dipoles exerter by the swimmers on the fluid.

1.5. Summary for governing equations

Using incompressibility, rewrite the coupled non-linear equations as

$$\partial_t c + \mathbf{u}\cdot\nabla c = \Lambda Pe_s^2 \Delta c - Pe_s \nabla\cdot\mathbf{m}, \tag{1.22}$$

$$\partial_t \mathbf{m} + \mathbf{u}\cdot\nabla\mathbf{m} = \Lambda Pe_s^2 \Delta\mathbf{m} - \mathbf{m} - Pe_s\nabla\cdot\left(\mathbf{D} + c\frac{\mathbf{I}}{2}\right) + \mathbf{H}_m, \tag{1.23}$$

$$\partial_t \mathbf{D} + \mathbf{u}\cdot\nabla\mathbf{D} = \Lambda Pe_s^2 \Delta\mathbf{D} - 4\mathbf{D} - Pe_s\nabla\cdot\left(\mathbf{T} - \mathbf{m}\frac{\mathbf{I}}{2}\right) + \mathbf{H}_D, \tag{1.24}$$

$$-\Delta\mathbf{u} = -\nabla p + \alpha\nabla\cdot\mathbf{D}. \tag{1.25}$$

1.6. Numerical Method

Pseudo-spectral discretization with 2/3 anti-aliasing rule is used to discretize eq ?-? on spatial domain. A second-order implicit-explicit backward differentiation time-stepping scheme (SBDF2) is performed on time domain, where the linear terms are handled implicitly and the nonlinear terms explicitly,

$$\frac{3A^{n+2} - 4A^{n+1} + A^n}{2\Delta t} = L(A^{n+1}) + N(A^n) \tag{1.26}$$

An iterative method is implemented to tackle the non-linearity in hydrodynamic terms $\mathbf{H}_m$ and $\mathbf{H}_D$. Specifically, when computing the solution for step t_{n+1}, initialize the values using the solution from previous step, then correct it iteratively using the new value solved implicitly. Using subscript indicating the iteration number and supscript for time step:

$$\left(\frac{3}{2\Delta t}\mathbf{I} - \Lambda Pe_s^2\Delta\right) c_{k+1}^{n+1} = -\mathbf{u}_k^{n+1}\cdot\nabla c^n - \frac{-2}{\Delta t}c^n - \frac{-1}{2\Delta t}c^{n-1} - Pe_s\nabla\cdot\mathbf{m}_k^{n+1}, \tag{1.27}$$

$$\begin{aligned}\left((1+\frac{3}{2\Delta t})\mathbf{I} - \Lambda Pe_s^2\Delta\right)\mathbf{m}_{k+1}^{n+1} = &-\mathbf{u}_k^{n+1}\cdot\nabla\mathbf{m}^n - \frac{-2}{\Delta t}\mathbf{m}^n - \frac{-1}{2\Delta t}\mathbf{m}^{n-1} \\ &- Pe_s\nabla\cdot\left(\mathbf{D}_k^{n+1} + c_{k+1}^{n+1}\frac{\mathbf{I}}{2}\right) + \mathbf{H}_{m,k}^{n+1},\end{aligned} \tag{1.28}$$

$$\begin{aligned}\left((4+\frac{3}{2\Delta t})\mathbf{I} - \Lambda Pe_s^2\Delta\right)\mathbf{D}_{k+1}^{n+1} = &-\mathbf{u}_k^{n+1}\cdot\nabla\mathbf{D}^n - \frac{-2}{\Delta t}\mathbf{D}^n - \frac{-1}{2\Delta t}\mathbf{D}^{n-1} \\ &- Pe_s\nabla\cdot\left(\mathbf{T}_{k+1}^{n+1} - \mathbf{m}_{k+1}^{n+1}\frac{\mathbf{I}}{2}\right) + \mathbf{H}_{D,k}^{n+1},\end{aligned} \tag{1.29}$$

$$-\Delta\mathbf{u}_{k+1}^{n+1} = -\nabla p + \alpha\nabla\cdot\mathbf{D}_{k+1}^{n+1}. \tag{1.30}$$

Eq 2.2 - 2.5 is updated iteratively. The iteration process terminates when the difference between two concentration values is less than an error tolerance.

Appendix

Orientation and topological defects

$\mathbf{D}$ (or $\mathbf{Q} = \frac{\mathbf{D}}{c}$) is a coarse-grained order parameter describing the orientation field. It's relation with orientation field $\mathbf{n}$

$$\mathbf{Q} = \frac{d}{d-1} q(\mathbf{nn} - \mathbf{I}/d) \tag{1.31}$$

where q is the magnitude of order, d is the dimension of space and $\mathbf{I}$ is the identity matrix.

Topological defects is induced by the neighbouring nematic unit have different direction which leads to singularities in the orientation field. For a two dimensional nematic fields, the two types of topological defects are defined by it's winding number: comet-like(+1/2) of trefoil-like(-1/2). It is defined by the change in orientation of molecules around a singular point along a 360 rotation: +1/2 or -1/2 defects when the molecule turn through +180 or -180.