Lecture notes: Active matter

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Contents

1 What is active matter?

Active matter consists of some kind of distributed stuff, like particles, that consume energy. The locally expended energy is converted into something like motion or forces or shape changes and not all the locally consumed energy is recovered by the distributed stuff. The systems are described as being *out of equilibrium*. Non-equilibrium active systems usually lack a simple free energy integral or an equation of state.

As energy is locally consumed, active matter systems are different from systems where energy is injected into the system from a particular location. For example, a heat source or a flapping boundary.

Active systems can display self organized behavior that is not present in equilibrium settings. Examples include flocking, synchronization, organization of metachronal waves (think cilia) and spontaneous flow in active neumatic gels. Active matter includes organization and growth of cells in tissue or even constituents of cells.

2 Self-propelled particles

Self-propelled particles are a type of *dry* active matter. The ambient medium through which the particles move is neglected.

Two related models are the Boid model (Reynolds 87)[1] `https://dl.acm.org/doi/pdf/10.1145/37401.37406` and the Vicsek model (Vicsek+95)[2] `https://arxiv.org/abs/cond-mat/0611743`. In both models each particle strives to move at a fixed speed, v_0.

We take $\mathbf{r}_i(t)$ to be the i-th particle's position at time t.

The original paper by Reynolds is more descriptive rather than specific, referring to updates of the velocity vector in terms of 'steering'. But we could also describe variations in a velocity vector as an acceleration that is derived from forces. In the Boid model each particle (or boid) feels a bunch of forces that cause the boid to accelerate

$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_{i,propel} + \mathbf{F}_{i,steer} + \mathbf{F}_{i,attract} + \mathbf{F}_{i,repel}. \tag{1}$$

The index i is used to make it clear that the forces are different for each boid. Each boid has a mass m_i. In the above equation $\ddot{\mathbf{r}} = \frac{d^2\mathbf{r}}{dt^2}$. The velocity $\mathbf{v} = \frac{d\mathbf{r}}{dt} = \dot{\mathbf{r}}$.

The propel force keeps the boid moving at the same speed

$$\mathbf{F}_{i,propel} \propto -(\mathbf{v}_i - v_0\hat{\mathbf{v}}_i) \tag{2}$$

[1] Reynolds, Craig (1987). Flocks, herds and schools: A distributed behavioral model. Proceedings of the 14th annual conference on Computer graphics and interactive techniques. Association for Computing Machinery. pp. 25-34.

[2] Vicsek, Tamás; Czirók, András; Ben-Jacob, Eshel; Cohen, Inon; Shochet, Ofer (1995-08-07). Novel Type of Phase Transition in a System of Self-Driven Particles. Physical Review Letters. 75 (6): 1226-1229. arXiv:cond-mat/0611743

where $\mathbf{v}_i$ is the i-th boid's velocity and $\hat{\mathbf{v}}_i = \mathbf{v}_i/|\mathbf{v}_i|$ is a unit vector with the same direction as the velocity. The boid speeds up if it is moving slower than v_0 and it slows down if its speed is faster than v_0. As the propel force depends upon velocity, it is not a conservative force.

The steer force depends on the average of the headings (directions of motion) of nearby boids. The boid adjusts its heading direction to be closer to that of its neighbors. Reynolds referred to the steer force as *velocity matching*.

Boids repel each other if they get too close to each other but they also exhibit some cohesion and will steer towards groups of other boids. Reynolds referred to these forces as *collision avoidance* and *flock centering*. The repel and attract force could be implemented with conservative forces that are derived from a position dependent potential energy function.

Each boid has a velocity $\mathbf{v}_i(t)$. To integrate a boid model, boid positions and velocities are updated on a time-step Δt using a low order integration scheme (often first order Eulerian). At each time step, each boid position is updated using its current velocity vector

$$\mathbf{r}_i^{n+1} = \mathbf{r}_i^n + \Delta t \mathbf{v}_i^n. \tag{3}$$

Here the upper index n refers to a discrete value of time, in intervals of the time-step. the above equation is consistent with

$$\mathbf{v}_i^n \sim \frac{d\mathbf{r}_i^n}{dt} \sim \frac{\mathbf{r}_i^{n+1} - \mathbf{r}_i^n}{\Delta t}. \tag{4}$$

The forces are computed from the positions and velocities of nearby boids. The velocity is updated by applying an acceleration

$$\mathbf{v}_i^{n+1} = \mathbf{v}_i^n + \frac{\Delta t}{m_i}\left(\mathbf{F}_{i,attract} + \mathbf{F}_{i,repel} + \mathbf{F}_{i,steer} + \mathbf{F}_{i,propel}\right) \tag{5}$$

The forces are computed from the particle velocities and positions at timestep n and I have neglected the super script for time on the right hand side of the equation in the description of the forces. The steer force can be something like

$$\mathbf{F}_{i,steer} \propto \langle \hat{\mathbf{v}} \rangle_{nn,i} - \hat{\mathbf{v}}_i \tag{6}$$

where $\langle \hat{\mathbf{v}} \rangle_{nn,i}$ is the average heading of nearest neighbors to boid i. The steer force steers the boid to match the headings of its neighbors. The attraction and repel forces can be similar to that of a conventional N-body or molecular dynamics model

$$\mathbf{F}_{i,attract/repel} \propto \sum_{j \neq i} -\frac{dU(r_{ij})}{dr_{ij}} \hat{\mathbf{r}}_{ij} \tag{7}$$

where $\mathbf{r}_{ij}$ is the vector between particle i and particle j, and $U(r_{ij})$ is a pairwise potential that is a function of distance between a pair of particles. The sign of U determines whether two boids attract or repel each other.

The Vicsek model is similar to the Boid model except the particle velocity is maintained a particular speed and only particle position and heading are adjusted each time-step. Each time-step the heading (direction of motion) of each boid is set to the average value of its neighbors with the addition of noise;

$$\hat{\mathbf{v}}_i^{n+1} = \langle \hat{\mathbf{v}} \rangle_{nn,i} + \text{noise}. \tag{8}$$

The noise can be drawn from a probability distribution that has a mean of zero and a desired variance.

In the original Vicsek model, particles do not attract or repel. A characteristic number density of particles is used to describe the system. Confinement can cause behavior similar to that of attraction (e.g., [3]). Noise tends to cause gas-like rather than fluid-like or solid-like behavior. Because the boids can't rest (birds fall out of the air if they stop flying) self-organized states involve motion. A school of fish can swim in a circle forming something like a vortex. A flock can move together in one direction, breaking rotational symmetry.

N-body models are often chaotic. A boid model without the addition of noise can act as if it is noisy. After a series of pair-wise encounters, memory of the initial conditions is lost. By adding noise to a boid model one could control the level of 'ergodic'-like behavior. If the self-propelled particle system contains a noise term, it can be called 'Brownian'.

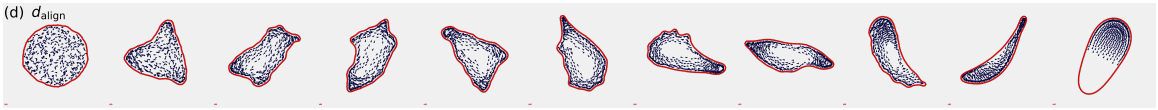

Figure 1: A series of simulations showing gas like behavior on the left and crystalline behavior on the right with more fluid-like circulating behavior in the middle. Here confinement of the flock by a flexible loop gives behavior similar to attraction. The series of particle based simulations from has similar parameters except the extent of the alignment force is increased on the right compared to simulations on the left. From Quillen+20 `https://arxiv.org/abs/2002.00536`

[3] Quillen, Smucker, Peshkov, 2020, Boids in a loop: Self-propelled particles within a flexible boundary, Phys Rev E 101, 052618, `https://arxiv.org/abs/2002.00536`

3 The simplest continuum models (PDEs)

3.1 Advection

We start with a field $\psi(x,t) \in \mathbb{R}$ with $x,t \in \mathbb{R}$ (in 1 dimension) and we assume that dynamics can be described with a single time derivative

$$\partial_t \psi = -a\partial_x \psi. \tag{9}$$

Here we use short hand $\partial_t = \frac{\partial}{\partial t}$. This partial differential equation is advective. Waves travel in one direction at a speed a. For example $\psi(x,t) = f(x-at)$ is a solution because $\partial_t \psi = -af'$ and $\partial_x \psi = f'$. In more than one dimension ($\mathbf{x} \in \mathbb{R}^{\mathbf{d}}$ for dimension d with $\psi(\mathbf{x},t)$)

$$\partial_t \psi = -\mathbf{a} \cdot \nabla \psi. \tag{10}$$

has solution $\psi(\mathbf{x},t) = f(\mathbf{x}-\mathbf{a}t)$. This follows as $\partial_t \psi = -(a_x \partial_x f + a_y \partial_y f + a_z \partial_z f)$ and this is equal to $-\mathbf{a} \cdot \nabla \psi$.

To model a wave equation where waves can travel in both directions, you can use two fields instead of one; $\partial_t u = a\partial_x v$, $\partial_t v = -a\partial_x u$ giving $\partial_{tt} u = -a^2 \partial_{xx} u$ which is the wave equation. Solutions include $f(x \pm at)$.

If the field itself is advecting the flow then in 1d we would get Burger's equation

$$\partial_t u + u\partial_x u = 0 \tag{11}$$

The field is u and it is acting like a velocity that advects itself. However, this is a non-linear equation.

In three dimensions, if the field is to act like a velocity it must be three dimensional. That means a velocity vector $\mathbf{u}$ should have the same dimensions as the domain points $\mathbf{x}$. Burger's equation becomes

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = 0. \tag{12}$$

The Euler equation and Navier-Stokes equations for hydrodynamics have these advective terms in them.

3.2 Diffusion

The diffusion (or heat) equation in 1 dimension is

$$\partial_t u = D\partial_{xx} u \tag{13}$$

for $u(x,t)$ and diffusion coefficient D which has units of x^2/t. A solution is

$$u(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}. \tag{14}$$

Notice that the solution spreads out but its integral over space is conserved $\int_{-\infty}^{\infty} u(x,t)dx = 1$.

In $\mathbb{R}^d$, the diffusion equation is

$$\partial_t u = D\Delta u \tag{15}$$

where the Laplacian operator $\Delta = \nabla \cdot \nabla$ is the divergence of the gradient. In 3D Cartesian coordinates

$$\Delta = \partial_{xx} + \partial_{yy} + \partial_{zz}. \tag{16}$$

If the diffusion coefficient $D < 0$ the model is unstable! For a negative D, we rescale space or/and time to get rid of the diffusion coefficient, giving $\partial_t u = -\partial_{xx} u$. Suppose we start with an initial condition near zero, and with a very small perturbation $u(x,t) = \epsilon e^{\sigma t + ikx}$ which is exponential in time and wave-like in space. We plug this into the differential equation, finding $\sigma = k^2$. The parameter $\sigma > 0$ for all $k \neq 0$. This implies that the amplitude of the perturbation would exponentially grow with growth rate σ. Sometimes active materials can give diffusive terms that cause instability, and to stabilize the system you would need to take into account additional derivatives or/and non-linear terms.

3.3 Conservation laws

A conservation law for a quantity, say density $\rho(\mathbf{x}, t)$ looks like

$$\partial_t \rho = -\nabla \cdot \mathbf{F} \tag{17}$$

where $\mathbf{F}(\mathbf{x}, t)$ is the mass flux. If I choose a small area element, A, and a normal to this small area element $\hat{\mathbf{n}}$, I can construct a vector $d\mathbf{A} = A\hat{\mathbf{n}}$. The amount of mass passing through this area element per unit time is $\dot{M} = \mathbf{F} \cdot d\mathbf{A}$.

Consider a blob with volume V which has a surface S. The amount of mass that is leaving that volume is

$$\frac{dM}{dt} = \dot{M} = \int_S \mathbf{F} \cdot d\mathbf{A} \tag{18}$$

where we integrate over the surface of volume V. To conserve mass

$$\int_V \partial_t \rho \; dV = -\int_S \mathbf{F} \cdot d\mathbf{A} \tag{19}$$

We apply Gaus' law

$$\int_S \mathbf{F} \cdot d\mathbf{A} = \int_V \nabla \cdot \mathbf{F} \; dV \tag{20}$$

The previous two equations together give equation 17.

Question: Can the diffusion equation be written as a conservation law?

Answer: Yes. This follows because the Laplacian operator is the divergence of a gradient operator. The heat equation can be described as energy transport. Heat flux depends on the gradient of temperature and the diffusion coefficient is proportional to the thermal conductivity and inversely proportional to the density and specific heat.

Mass flux in a fluid is $\mathbf{F} = \rho\mathbf{v}$ giving mass conservation

$$\partial_t \rho = -\nabla \cdot (\rho \mathbf{v}). \tag{21}$$

If density ρ remains constant then $\nabla \cdot \mathbf{v} = 0$ and the system is said to be **incompressible**.

4 Continuum models for active matter

Suppose instead of describing a self-propelled particle system with particle positions and headings, we describe the system with fields, the number density of particles $\rho(\mathbf{x}, t)$ (the number of particles per unit area or volume) and a velocity field $\mathbf{v}(\mathbf{x}, t)$.

If the system behaves as if it were incompressible we can ignore ρ, though in some regimes some models predict large fluctuations in density and so are definitely not incompressible.

How do we relate a particle system to a system described with fields? A field can be constructed from a sum of delta functions, where each delta function is contributed by a single particle. Alternatively, we can compute the average of a quantity such as velocity of a population of self-propelled particles in a small volume element. This is like smoothing over the sum of delta functions within a volume element. The density is the number of particles per volume element.

What size volume element (or smoothing length) is used? The length scale should be larger than the typical distance between particles. The length should be large enough that the fluctuations due to different numbers of particles within each volume element are not significant.

Kinetic theory involves describing a particle system with a distribution function $f(\mathbf{x}, \mathbf{v}, t)$ that is a function of position and velocity (and possibly other quantities such as ionization state). The pressure in a fluid arises from the distribution of velocities in a particular volume element. In the limit of large particle number, the equations for hydrodynamics can be derived from the Boltzmann equation (often used in plasma physics) which can look something like this

$$\frac{Df}{Dt} = \partial_t f + \nabla f \cdot \mathbf{v} - \nabla_v f \cdot \nabla U = \left.\frac{df}{dt}\right|_{collisions}. \tag{22}$$

4.1 Toner and Tu's continuum model for self-propelled particles

Toner and Tu[4] proposed a continuum model for self-propelled particles. The model describes density $\rho(\mathbf{x}, t)$ and velocity $\mathbf{v}(\mathbf{x}, t)$ which are as a function of position and time, and gives PDEs that contain a large number of terms

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{23}$$

$$\partial_t \mathbf{v} + \lambda_1 (\mathbf{v} \cdot \nabla)\mathbf{v} + \lambda_2 (\nabla \cdot \mathbf{v})\mathbf{v} + \lambda_3 \nabla v^2 = (\alpha - \beta v^2)\mathbf{v} - \nabla P + \text{noise} + D_0 \nabla^2 \mathbf{v} + D_1 \nabla(\nabla \cdot \mathbf{v}) + D_2 (\mathbf{v} \cdot \nabla)^2 \mathbf{v}. \tag{24}$$

Toner and Tu motivated the collection of terms using symmetry arguments.

The noise, averaged over a particular volume element, could be a Wiener process `https://en.wikipedia.org/wiki/Wiener_process`. With the addition of noise, the coupled PDEs are *stochastic* equations.

The $\lambda_1 > 0$ term is the velocity $\mathbf{v}$ advecting itself. If $\lambda_1 < 1$ then the advection is not very strong. This is when there is a drag or friction force with an external medium?

The parameter $D_0 > 0$ is like a shear viscosity.

The parameter D_1 is like a bulk viscosity that dissipates energy if compression or expansion takes place.

The $\alpha, \beta > 0$ term gives a self-propel force which strives to maintain a constant speed $v_0 = \sqrt{\alpha/\beta}$.

The pressure can be related to density via an equation of state. If an incompressible system is desired, a very stiff equation of state can be chosen.

If the system behaves as if it were incompressible, we can neglect the $\lambda_2, \lambda_3, D_1$ terms.

If $\lambda_1 > 1$, particles speed up where the flow is divergent.

The $\lambda_3 > 0$ term, pushes particles to regions where the velocity is lower.

I don't have a nice intuitive feel for the D_2 term! It seems advective of the advection.

The terms that are **non-linear** are those with $\lambda_1, \lambda_2, \lambda_3, \beta$ and D_2. This is relevant when implementing a numerical model.

4.2 Wet vs Dry

Active materials consume energy. By definition energy is not conserved. If they conserve momentum (which implies interactions by equal and opposite forces) then they are usually called 'dry'. If many but not all of the forces in a particle based model are applied in an equal and opposite manner then the active material can still be described as dry. Steer forces for boids don't necessarily conserve momentum, but self-propelled particle systems are usually described as dry. Note a particle based model could still experience a strong drag force (and would not conserve momentum) and it still would be described as dry.

[4] Toner, John; Tu, Yuhai (1995). Long-Range Order in a Two-Dimensional Dynamical XY Model: How Birds Fly Together. Physical Review Letters. 75 (23): 4326–4329.

Particle based simulations are usually dry.

Wet models are usually modeled with PDEs because the particles are embedded in a fluid which is described with a velocity field.

In the continuum model, if you see the density as a field that evolves, then the system is dry.

In continuum wet systems, the particle density is usually neglected. Instead the order parameter is advected by a fluid which is described with only a velocity. I think the models described as active gels by Marcetti+12 are just wet continuum models.

4.3 Polarization as an order parameter

The Toner and Tu model describes two fields density ρ and velocity, $\mathbf{v}$, which are functions of position and time $\mathbf{x}, t$. How do we relate a system of moving point particles to these fields? As mentioned above the density is the number of particles per unit volume and the velocity can be the average particle velocity in a volume element. Neither of these quantities describe how ordered the system is. For example, the average velocity could be much lower than the individual velocities of each particle within a volume element.

An order parameter describes how ordered the system is locally. If all the particles are moving in the same direction, then the order parameter is high. If the particles are moving randomly, then the order parameter should be low.

Order parameters are often used in the context of phase transitions. The transition between ordered and disordered states or between states with different types of order can be temperature dependent. For example, consider a collection of spins that can take one of two values, up or down. This is also called the Ising model. At high temperature the spins are essentially random and the average spin (also called the magnetization in this context) is zero. Below a particular temperature interactions cause all the spins to align. In this case the order parameter is a binary digit that is a function of position.

In liquid crystals, elongated molecules are not arranged in a crystalline lattice so are not ordered in position, but they can be ordered in terms of their orientation. In this case an order parameter would describe statistics of alignment.

One way to create an order parameter for a self-propelled particle system is to define a polarization vector from the velocities. However, instead of simply taking the average velocity we take an average of the particle heading directions. We take $\hat{\mathbf{v}}_i$ to be a unit vector of particle i such that its velocity $\mathbf{v}_i = |\mathbf{v}|_i \hat{\mathbf{v}}_i$. A *polarization* vector can be defined as the average value of $\hat{\mathbf{v}}$ computed within a volume element;

$$\mathbf{p} = \langle \hat{\mathbf{v}}_j \rangle. \tag{25}$$

If all particles are moving at the same velocity but in different directions, then the sum of their velocity headings (the unit vector $\hat{\mathbf{v}}$) would be low. The polarization would be low. If all the particles are moving in the same direction, then the polarization is equal to 1 and

has the same direction as their velocity An order parameter is a measure of the degree of order.

Look again at the term $(\alpha - \beta v^2)\mathbf{v}$ in the equation 24. This term can also be written in terms of a potential a gradient $\nabla U(v)$ where

$$U(v) = -\frac{\alpha}{2}v^2 + \frac{\beta}{4}v^4 \tag{26}$$

$$-\nabla U(v) = \alpha\mathbf{v} - \beta v^2\mathbf{v}. \tag{27}$$

If we only consider the time dependent term and the potential term then,

$$\partial_t \mathbf{v} \sim -\nabla U(v). \tag{28}$$

Assuming that $\alpha, \beta > 0$, a steady state is reached at the potential minimum which is where $|\mathbf{v}| = \sqrt{\alpha/\beta}$. The potential minimum has a direction. If we interpret the velocity field as the average of particle velocities in a particular region the non-zero static state implies that there is order in the system. Most particles in a particular region are moving together. For example, microorganisms could exhibit head-tail asymmetries and associated interactions that favor alignment. The self-propel force and the alignment forces in the boid model are mimicked by the $(\alpha - \beta v^2)\mathbf{v}$ term in equation 24.

The boid/Vicsek/Toner-Tu model is said to describe **polar** particles as each particle has a particular direction for its motion.

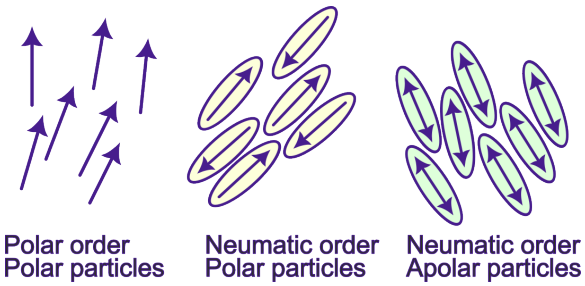

Figure 2: Polar particles move in a particular direction. Polar particles with polar order align their direction of motion with their neighbors, as shown on the left. Repulsive and attractive interactions between particles only depend on particle position, not particle orientation. The Vicsek/Toner-Tu/Boid model of self-propelled particles is in this class. A particle could also have an ellipse or rod shape. Nearby particles could orient their shapes so that their long axes are parallel to each other. In this case, the particles are said to have neumatic order, as shown in in the middle and right panels. Repulsive and attractive interactions depend upon particle orientation. The middle panel shows self-propelled rods and the right panel shows an apolar active rod. The apolar particle can move in both directions along its long axis.

4.4 Free energy

According to the second law of thermodynamics, conventional systems are likely to minimize a function called the free energy. Thermodynamic equilibrium is equivalent to minimization of free energy. The phenomenological Landau theory of phase transitions has three steps: (1) finding a proper order parameter; (2) expanding the free energy in the vicinity of the transition with respect to the (small) order parameter; and (3) finding the minima of the free energy at each temperature, pressure, and so on, as functions of the order parameter.

Even though they are out of equilibrium, sometimes active matter systems are described, in part, using a free energy functional that might be used to describe a related non-active statistical system. Many of the terms in the PDEs describing the dynamics of the active system are computed using a functional derivative of a free energy functional that depends on an order parameter.

Following the review by Marchetti+12[5], PDEs describing a system of active polar particles depends on density ρ and polarization vector $\mathbf{p}$

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{p}) = 0 \tag{29}$$

$$\partial_t \mathbf{p} + \lambda_1 (\mathbf{p} \cdot \nabla)\mathbf{p} = -\frac{\delta F_p}{\delta \mathbf{p}} + \text{noise} \tag{30}$$

are written in terms of the free energy functional

$$F_p[\mathbf{p}] = \int dV \Big(-\frac{\alpha}{2} p^2 + \frac{\beta}{4} p^4 + \frac{K}{2} \sum_{jk} (\partial_j p_k)(\partial_j p_k) - v_1 \nabla \cdot \mathbf{p} \frac{\rho - \rho_0}{\rho_0} + \frac{\lambda}{2} p^2 \nabla \cdot \mathbf{p} \Big). \tag{31}$$

In Equation 30 The derivative $\frac{\delta F_p}{\delta \mathbf{p}}$ is a functional derivative (see `https://en.wikipedia.org/wiki/Functional_derivative`).

With coefficients for the terms that depend upon temperature and setting $\frac{\delta F_p}{\delta \mathbf{p}} = 0$, we could describe a conventional material that would display phase transitions.

As we will show below, this model generates a PDE that looks similar to the Toner-Tu model, but describing evolution of the polarization vector $\mathbf{p}$ instead of the average particle velocity. In this continuum model $\mathbf{p}$ simultaneously plays the role of the orientational order parameter of the system and the particle velocity field.

[5] M.C. Marchetti, J.F. Joanny, S. Ramaswamy, T.B. Liverpool, J. Prost, Madan Rao, and R. Aditi Simha, Hydrodynamics of soft active matter, , Reviews of Modern Physics, vol. 85, Issue 3, pp. 1143-1189, `https://arxiv.org/abs/1207.2929`

4.5 A quick note on functional derivatives

Consider the function $q(x)$ and the integral

$$L[q] = \int_a^b \mathcal{L}(x, q(x), q'(x))dx \tag{32}$$

where $\mathcal{L}$ is a function of x and the function $q(x)$ and its derivative $q' = \frac{dq}{dx}$ at x. We vary the function q by taking $q \to q + \delta q$.

$$\begin{aligned}\delta L[q] &= \int_a^b \mathcal{L}\left(x, q + \delta q, \frac{d}{dx}(q + \delta q)\right) dx - L[q] \\ &= \int_a^b \frac{\partial \mathcal{L}}{\partial q}\delta q \; dx + \int_a^b \frac{\partial \mathcal{L}}{\partial q'}\frac{d}{dx}\delta q \; dx. \end{aligned} \tag{33}$$

We integrate the right hand term by parts and assume that everything vanishes on the boundary

$$\delta L[q] = \int_a^b \left(\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dx}\frac{\partial \mathcal{L}}{\partial q'}\right)\delta q \; dx. \tag{34}$$

We associate

$$\frac{\delta L[q]}{\delta q(x)} = \frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dx}\frac{\partial \mathcal{L}}{\partial q'} \tag{35}$$

where the derivatives on the right hand side are evaluated at x. If $\frac{\delta L[q]}{\delta q(x)} = 0$ then the free energy is minimized.

Armed with this quick introduction, we attempt to compute the functional derivative of the free energy function of equation 4.4. Equation 4.4 is an equation that would be obeyed if the kinetic energy subtracted by the free energy (the Lagrangian) is a minimum. The difference is used so that total energy is a conserved quantity.

First we compute some derivatives. With

$$\mathcal{L}(\mathbf{p}, \nabla\mathbf{p}) = -\frac{\alpha}{2}p^2 + \frac{\beta}{4}p^4 + \frac{K}{2}\sum_{jk}(\partial_j p_k)(\partial_j p_k) - v_1\nabla\cdot\mathbf{p}\frac{\rho - \rho_0}{\rho_0} + \frac{\lambda}{2}p^2\nabla\cdot\mathbf{p} \tag{36}$$

we compute

$$\frac{\partial \mathcal{L}}{\partial p_k} = -\alpha p_k + \beta p^2 p_k + \lambda p_k \nabla\cdot\mathbf{p} \tag{37}$$

$$\frac{\partial \mathcal{L}}{\partial(\partial_j p_k)} = K\partial_j p_k - v_1\frac{(\rho - \rho_0)}{\rho_0}\delta_{jk} + \frac{\lambda}{2}p^2\delta_{jk} \tag{38}$$

$$\frac{d}{dx_j}\frac{\partial \mathcal{L}}{\partial(\partial_j p_k)} = K\partial_{jj}p_k - (\partial_j\rho)\frac{v_1}{\rho_0}\delta_{jk} + \frac{\lambda}{2}\partial_j p^2\delta_{jk} \tag{39}$$

$$\frac{\delta F_d}{\delta \mathbf{p}} = (-\alpha + \beta p^2)\mathbf{p} - K\nabla^2\mathbf{p} + v_1\frac{\nabla\rho}{\rho_0} - \frac{\lambda}{2}\nabla p^2 + \lambda\mathbf{p}\nabla\cdot\mathbf{p} \tag{40}$$

Inserting this into equation 30 we find

$$\partial_t\mathbf{p} + \lambda_1(\mathbf{p}\cdot\nabla)\mathbf{p} = (\alpha - \beta p^2)\mathbf{p} + K\nabla^2\mathbf{p} + v_1\frac{\nabla\rho}{\rho_0} + \frac{\lambda}{2}\nabla p^2 - \lambda\mathbf{p}\nabla\cdot\mathbf{p} \tag{41}$$

Except for some constants that can be absorbed into units, this is essentially consistent with equation 5 by Marchetti+12 and contains terms similar to those in the Toner+Tu model.

Is there any advantage to writing the equations of motion in terms of a free energy functional? Sometimes it helps to think about the equations of motion in terms of energy and minimizing energy. For example, the quadratic function $-\alpha p^2 + \beta p^4$ looks like the potential energy function we discussed in the previous section.

In using the free energy to compute functional derivatives, we dropped boundary terms, as is conventionally done with the assumption that most things go to zero at infinity. $\langle !\#^*\#! \rangle$. If our focus is confined systems, then we are striving to pay attention to the boundary terms and we don't want to discard them!

4.6 Terms in the free energy that are important on the boundary

Suppose that the free energy of a 1d system contains a term that can be written as a derivative of some function

$$\mathcal{L}_B = \partial_x f. \tag{42}$$

The contribution of this term to free energy is the integral of this term over the domain, and in 1dimension

$$L[q]_B = \int_a^b dx\ \mathcal{L}_\mathcal{B} = f(b) - f(a). \tag{43}$$

This is only sensitive to the function f on the boundary. In 2 or 3 dimensions if

$$\mathcal{L}_B = \nabla\cdot\mathbf{f} \tag{44}$$

then we can use Stokes theorem to write the contribution in terms of an integral over the boundary. In three dimensions

$$L[q]_B = \int_\Omega \nabla\cdot\mathbf{f}\ dv = \int_{\partial\Omega}\mathbf{f}\cdot d\mathbf{A}. \tag{45}$$

In two dimensions

$$L[q]_B = \int_\Omega \nabla\cdot\mathbf{f}\ dA = \int_{\partial\Omega}\mathbf{f}\cdot d\mathbf{s}. \tag{46}$$

4.7 More complicated polar systems

Polar materials can have extra terms in the free energy

$$F_p[\mathbf{p}] = \int dV \left(\frac{K_1}{2}(\nabla \cdot \mathbf{p})^2 + \frac{K_2}{2}(\mathbf{p} \cdot (\nabla \times \mathbf{p}))^2 + \frac{K_3}{2}(\mathbf{p} \times (\nabla \times \mathbf{p}))^2 + \frac{K_4}{2}\nabla \cdot [(\mathbf{p} \cdot \nabla)\mathbf{p} - \mathbf{p}(\nabla \cdot \mathbf{p})] + v\nabla \cdot \mathbf{p} + \frac{h_\parallel}{2}(p^2 - 1) \right) \tag{47}$$

The K_1 term is the free energy of splay deformation (think of a fan).

The K_2 term is the free energy of twist deformation (only in 3d).

The K_3 term is the free energy of bend deformation.

The K_4 term is a divergence, known as 'saddle-splay' (?) and is associated with the surface.

The $h_\parallel$ term is a Lagrange multiplier and there to ensure that the polarization vector remains at or near length 1. I have made the term look like a Lagrange multiplier, though in equation 32 by Marcetti+12, the term was $h_\parallel p^2/2$. When you take the functional derivative, the constant term drops out so maybe it does not matter which way you write it.

The K coefficients are called Frank constants `https://en.wikipedia.org/wiki/Distortion_free_energy_density`

The K coefficients describe all possible low order derivative terms that obey the $\mathbf{n} \to -\mathbf{n}$ neumatic symmetry. Terms with a single gradient don't obey this symmetry and so are lacking. This probably means that it is possible to equivalently write the gradient terms in terms of the Q order parameter.

Sometimes people set the K_1, K_2, K_3 Frank constants to be identical and lump them together in one term, as in the free energy of equation 4.4. In this case the sum of the three terms simplifies to

$$\frac{K}{2}[(\nabla \cdot \mathbf{p})^2 + (\nabla \times \mathbf{p})^2]. \tag{48}$$

So far the free energy terms only have a single gradient operator of the order parameter (with the exception o the K_4 term which is a divergence). When taking the functional derivative, this gives PDEs with a Laplacian or second order spatial derivatives in them. The coupled fields can have diffusive terms and non-linear potential terms so we could imagine similarities to reaction diffusion equations. We would have to expand the free energy to higher order derivatives to pick up fourth order derivatives, such as appear in the Swift-Hohenberg pattern formation model. If the diffusive terms cause instability, (a negative viscosity), then terms with higher order derivatives are needed to stabilize the model.

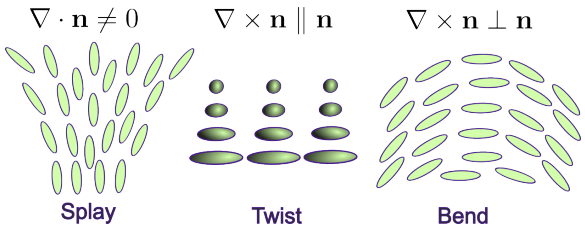

Figure 3: Relevant for the Frank constants for neumatic materials.

5 Active neumatics

An active neumatic system can resemble a liquid crystal but can exhibit behavior such as spontaneous flow that is not seen in an equilibrium system.

5.1 The neumatic order parameter

A neumatic system is not polar, so instead of choosing an order parameter that is a vector, the order parameter is a symmetric tensor (with two indices), similar to a quadrupole moment or a moment of inertia tensor.

The neumatic order parameter $\mathbf{Q}$ depends on the local orientation vector which is described with a unit vector $\hat{\mathbf{n}}(\mathbf{x}, t)$ that is a function of position and time. The order parameter is a two index, traceless and symmetric tensor

$$\mathbf{Q} = s(\mathbf{nn} - \frac{1}{d}\mathbf{I})$$
$$Q_{ij} = s(n_i n_j - \frac{1}{d}\delta_{ij}) \tag{49}$$

where $d = 2$ in two dimensions and $d = 3$ in three dimensions (so that $\mathrm{tr}\mathbf{Q} = \sum_j Q_{jj} = 0$). In the above equation $\mathbf{I}$ is the identity matrix. The definition for $\mathbf{Q}$ has the

$$\mathbf{n} \to -\mathbf{n}$$

nematic symmetry built-in.

The parameter s, called the *scalar order parameter*, describes the degree of alignment and depends on an average of the orientations of particles in a local volume element. We take z aligned with the director $\hat{\mathbf{n}}$ and take θ to be a co-latitude. The scalar order parameter

$$s = \langle \frac{1}{2}(3\cos^2\theta - 1) \rangle, \tag{50}$$

where the average is over the particle angles and it is integrated over solid angle. The function is designed so that an isotropic distribution $f(\theta, \phi) = \frac{1}{4\pi}$ gives $s = 0$. The scalar order parameter $s \in [-1/2, 1]$ in 3D with the value of -1/2 for $\theta = \pi/2$ and when particles are perpendicular to $\hat{\mathbf{n}}$.

5.2 Free energy

For a generic uniaxial neumatic material (uniaxial means the order parameter only depends on $\hat{\mathbf{n}}$ and not on an additional direction) the free energy typically contains terms like

$$\begin{aligned} F_p[Q] = \text{constant} + \frac{A}{2}\sum_{ij} Q_{ij}Q_{ij} + \frac{B}{3}\sum_{ijk} Q_{ij}Q_{jk}Q_{ki} + \frac{C}{4}\sum_{ijkl} Q_{ij}Q_{jk}Q_{kl}Q_{li} + ... \\ + K_Q \sum_{ijk} \partial_i Q_{ij}\partial_k Q_{kj} + K'_Q \sum_{ijk} \partial_i Q_{jk}\partial_i Q_{jk} + K''_Q \sum_{ijk} \partial_i Q_{jk}\partial_k Q_{ji} + ... \\ + B_Q \sum_{ij} (\partial_i Q_{ij} Q_{ji} + \partial_i Q_{jj} Q_{ji} + \partial_i Q_{ii} Q_{jj} ....)? \end{aligned} \tag{51}$$

where coefficients depend upon temperature or/and density.

The term with coefficient A is sometimes written $\mathbf{Q} : \mathbf{Q} = \text{tr } \mathbf{Q}^2$.

The term with coefficient B could be written as tr $\mathbf{Q}^3$.

The terms with coefficients K might be written confusingly as $(\nabla \mathbf{Q})^2$.

A model lacking the gradient terms can be used to model the nematic to isotropic phase transition.

$$\begin{aligned} \frac{\partial F_p[Q]}{\partial(\partial_a Q_{bc})} &= K_Q \delta_{ia}\delta_{bi}\delta_{cj}\delta_k Q_{kj} + ... \\ &= 2K_Q \delta_{ab} \sum_k \partial_k Q_{kc} + 2K'_Q \partial_a Q_{bc} + 2K''_Q \partial_c Q_{ba} \end{aligned} \tag{52}$$

These terms might be related to the terms previously discussed in terms of polarization.

5.3 Dry active nematics

Models are often classified as a dry active neumatic or as an active neumatic gel, depending upon the role of the background fluid.

In a particle based model, the particle is equally likely to move in either direction along its long axis. Often the direction of motion (along the particle's long axis) is simply occasionally reversed. For example, a coin can be flipped every once in a while to randomly choose the direction of motion (for example, Henke+17[6] did this in their paper on dry active neumatics on a sphere).

A continuum model can be constructed for the free energy containing terms with both polarization and neumatic order tensor (Q).

[6] Dynamical patterns in active nematics on a sphere, Silke Henkes, M. Cristina Marchetti and Rastko Sknepnek, 2017, Phys. Rev. E 97, 042605, `https://arxiv.org/abs/1705.05166`

$$\partial_t \mathbf{Q} = -\Gamma \frac{\delta \mathcal{F}_p(\mathbf{Q}, \rho)}{\delta \mathbf{Q}} + \text{noise} \tag{53}$$

If coupled to the density the model can exhibit particle fluctuations and propagation of defects. This equation along with one describing evolution of the density is described as a dry model.

I found this useful to discuss both models and numerics `https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.129.258001#supplemental`

5.4 Active neumatic gels

These are in the category of wet models.

The thing called an active neumatic gel is I think just two equations, one for the velocity and consistent with a fluid and the second advecting the order parameter, $\mathbf{Q}$.

Active gels can exhibit spontaneous flow and generate turbulence (and there is a real system based on actin filaments that actually does this).

6 Active fluid systems

The setting is suspensions of active rodlike or elongated objects (e.g. swimming organisms, cytoskeleton, or tissues) embedded in a momentum-conserving solvent that generate stresses on the fluid.

In a wet system, we use the equations for hydrodynamics (conservation of mass and momentum) which depend on density ρ and velocity $\mathbf{v}$. Many models adopt a incompressible fluid so there only an equation for the velocity, with the constraint that $\nabla \cdot \mathbf{v} = 0$.

To conservation of momentum for the fluid we add a term in the stress tensor that depends on the active particles. The active particles push the fluid.

We add a third equation for the evolution of an order parameter describing the orientation of the active particles. The order parameter is advected by the fluid. Its equation of motion takes into account interactions between active particles.

Firstly the fluid equations, in general

$$\frac{D\mathbf{u}}{dt} = \partial_t + (\mathbf{v} \cdot \nabla)\mathbf{u} = -\frac{\nabla p}{\rho} + \nabla \boldsymbol{\sigma} \tag{54}$$

Here the stress tensor depends upon velocity $\mathbf{u}$ and the order paremeter of the active material $\mathbf{Q}$,

$$\sigma(\mathbf{u}, \mathbf{Q}).$$

An example is called an *active neumatic gel* at low Reynold's number. Starting with Stokes flow

$$\nabla p = \nabla \cdot \sigma + \text{noise} \tag{55}$$

we add an equation for evolution of an order parameter $\mathbf{Q}$

$$(\partial_t + \mathbf{v} \cdot \nabla)\mathbf{Q} = S(\nabla \mathbf{v}) - \frac{\delta F_p}{\delta \mathbf{Q}} \tag{56}$$

where S is a function that depends on the gradient of the velocity, possibly including the vorticity.

6.1 Advecting a tensor

Ordinarily in a fluid, one does not keep track of the vorticity when advecting a quantity. However, if that quantity has orientation, the vorticity (fluid circulation) causes the advected quantity to rotate. If $\mathbf{Q}$ is the neumatic order parameter (a tensor) then when advected by the fluid

$$\frac{D\mathbf{Q}}{Dt} = \partial_t \mathbf{Q} + (\mathbf{v} \cdot \nabla)\mathbf{Q} + \mathbf{\Omega} \cdot \mathbf{Q} - \mathbf{Q} \cdot \mathbf{\Omega} \tag{57}$$

where

$$\mathbf{\Omega} = \frac{1}{2}(\nabla \mathbf{v} - \nabla \mathbf{v}^T) \tag{58}$$

The derivative in equation 57 is sometimes called the co-moving co-rotational derivative of the Q-tensor. Let's be specific about the indexing.

$$\Omega_{ij} = \frac{1}{2}(\partial_i v_j - \partial_j v_i) \tag{59}$$

$$\Omega \cdot \mathbf{Q} = \sum_{ij} \Omega_{ij} Q_{ij}. \tag{60}$$

7 Active oscillating materials

Many systems consist of individual oscillating elements. For example cilia, heart muscle, fire flies. Collective behavior leads to synchronization or wave-like phenomena.

Swarmallators are self propelled particles that also oscillate. O'Keefe.

Brato's paper!

8 Active scalar model

The active scalar model advects an active scalar quantity ϕ.