Lecture notes: Active matter

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1 What is active matter?

Active matter consists of some kind of distributed stuff, like particles, cells, birds, bacteria or fish, 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 matter. 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 or conventional global conserved quantities.

As energy is locally consumed, active matter systems differ from systems where energy is injected into the system from a particular location, for example, a heat source, an electric field or a flapping boundary.

Active systems can display self-organized behavior that is not present in equilibrium settings. Examples include flocking, synchronization, metachronal waves (like those in systems of cilia), jammed or circulating states, vortices, and spontaneous flow or turbulence in active neumatic gels. Active matter includes organization and growth of cells in tissue or for structures within cells.

2 Self-propelled particles

Self-propelled particles are a type of *dry* active matter. The ambient medium through which the particles move is often 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 forces that cause it 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 an integer that labels a specific boid which we can think of as a moving point particle. The forces are labelled by i to make it clear that the forces are different for each boid. Each boid has a mass and boid i has mass m_i. In the above equation the acceleration vector is $\ddot{\mathbf{r}} = \frac{d^2\mathbf{r}}{dt^2}$. The velocity vector is $\mathbf{v} = \frac{d\mathbf{r}}{dt} = \dot{\mathbf{r}}$. The velocity vector of particle i is the vector $\mathbf{v}_i$. The positions, velocities and accelerations of each boid are functions of time. Equation 1 is a set of coupled ordinary differential equation which are also the equations of motion.

The *propel* force strives to keep the boid moving at the same speed

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

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 and total energy is not conserved! An equal an opposite force is neglected. Some kind of interaction with the background substrate must take place otherwise momentum would not be globally conserved. However, this interaction is not specified in the model.

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 could exhibit some cohesion and as they could actively 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. That means the force between two particles would depend upon

[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

the distance between them and would be equal and opposite on each particle in the pair. This type of interaction is conventional in physics. Other types of interactions could also be adopted in a model!

Each boid has a velocity $\mathbf{v}_i(t)$. To numerically integrate a boid model, boid positions and velocities are typically updated on a time-step Δt using a low order integration scheme (often first order Eulerian or slightly more complicated second order scheme). For boid i, we write its position as $\mathbf{r}_i$. 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

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

which is a first order (in time) approximation to the velocity.

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 boid 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. Boids could attract if they are distant and repel if they get too close together so that they avoid collision. In models of flocking birds, the angular dependence of a bird's vision can be taken into account as well as other quantities (status of each bird, time to react, etc ...).

The Vicsek model is similar to the Boid model except the particle velocity is maintained a particular speed, only particle position and heading are adjusted each time-step and the velocity can be randomly perturbed. 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 or jammed 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 a coherent structure called a vortex. A flock can move together in one direction, breaking rotational symmetry. Notably these types of organized states would spontaneously arise even if the initial condition had all boids stationary or moving in random directions.

N-body models are often chaotic. A system of boids that evolves 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. The dynamical system can be chaotic. By adding noise to a boid model of ordinary differential equations one could control the level of *ergodic* behavior. If the self-propelled particle system contains a noise term, it can be called *Brownian* or *stochastic*.

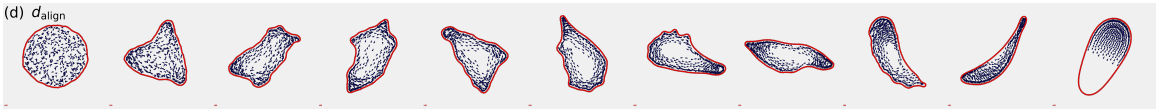

Figure 1: A series of simulations showing gas like behavior on the left and crystalline behavior on the right with more fluid-like circulating behavior in the middle. Here confinement of the flock by a flexible loop gives behavior similar to attraction. The series of particle based simulations from has 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`

What phenomena are exhibited by self-propelled particles? Phase transitions (gas like, jammed, flowing and circulating). Clumping. Density waves. Vortices. Concentrations can form at boundaries or be repelled by boundaries.

In the boid model, particle acceleration is equal to a sum of forces. **When are equations used that depend on acceleration (the second time derivative of position)**

[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`

and when are equations used that only depend on velocity (the first time derivative of position)? Consider a damped harmonic oscillator

$$m\ddot{x} + m\gamma\dot{x} + kx^2 = 0. \tag{9}$$

Here γ describes a velocity dependent damping term. If the damping term exceeds the acceleration then the system is strongly damped and the equation of motion can be approximated with

$$\dot{x} \sim -\frac{kx^2}{m\gamma}. \tag{10}$$

3 Other forms of particle based and dry active matter

Consider a particle swarm. Each particle can contain degrees of freedom other than position and velocity that affect their interaction and their motion. Self-propelled particles (boids) are considered *polar* because in addition to a position and velocity each particle is also described with a specific direction or angle. This direction determines interactions between it and neighboring particles. The direction could be the same as its current velocity or heading or it could refer to a particle body orientation and this direction could differ from its current velocity. The particle could be elongated and its shape could affect its interactions with neighboring particles. If particles interact in a way that is sensitive to their body orientation they can be called *neumatic*.

3.1 Interacting Oscillators

A particle could contain an internal oscillator, which case it would also be described by a phase of oscillation. Neighboring particles could influence each other's oscillations. For example, some species of fire-flies synchronize their flashing. Synchronization of neurons firing or muscle cells contracting occurs in heart muscle and in the brain.

Consider a collection of phases or angles θ_i where index i lets us refer to one of them. Here the angle $\theta_i \in [0, 2\pi)$ and is periodic. Equivalently each phase can be described as being on the unit circle or as being on the real line but modulo 2π.

The i-th oscillator could advance in phase with a characteristic frequency ω_i

$$\dot{\theta}_i = \omega_i. \tag{11}$$

A famous model of interacting oscillators which can synchronize is the **Kuramoto model**[4] where

$$\dot{\theta}_i = \omega_i + \sum_j K_{ij} \sin(\theta_j - \theta_i). \tag{12}$$

[4]Kuramoto, Yoshiki (1975). H. Araki (ed.). Lecture Notes in Physics, International Symposium on Mathematical Problems in Theoretical Physics. Vol. 39. Springer-Verlag, New York. p. 420.

The interaction term is important when the two phases are not similar. So if $\theta_i \sim \theta_j$ then the ith oscillator does not speed up. But if $\theta_j > \theta_i$ (and both are small), then for positive K_{ij} $\dot{\theta}_j > 0$. This tends to push θ_i to be closer to θ_j leading to synchronization. The coefficients K_{ij} are a set of interaction coefficients. Whether or not the ensemble synchronizes Depends upon initial conditions, the distributions of intrinsic frequencies and interaction strengths. A noise term can be added to equation 12.

We found that a chain of noisy and similar oscillators with lopsided interactions was more likely to enter a wave like state, called a *metachronal wave*, where each oscillator lagged in phase compared to its neighbor [5]

3.2 Swarmallators

Particles that both both move and oscillate are called *swarmalators* [6] `https://arxiv.org/abs/1701.05670`. An organism that undulates to move (a snake or nematode) can be described with a phase of oscillation. In general, many types of locomotion can described with a series of motions that are repeated periodically (walking, galloping, swimming, flying). Groups of organisms can synchronize their gait. Cilia on the surface of a Paramecium can synchronize to form waves that allow them to propel themselves.

Consider a collection of self-propelled oscillators. Each particle i has position $\mathbf{x}_i$ and velocity $\mathbf{v}_i = \dot{\mathbf{x}}_i$ and a phase $\theta_i \in [0, 2\pi)$ which is an angle. In the absence of any interactions, a particle's phase would advance at a constant rate, given by phase velocity ω_i. Neighboring particles attract and repel each other, but these interactions could depend upon the particles relative phases. Neighboring particles also influence each others's phase velocity. In that sense the oscillators interact. The positions and phases can be described with the Viscek model, along with an extra degree of freedom. To equation 1 for the self-propelled particle model, we add an additional force

$$\mathbf{F}_{phase} = \sum_j \mathbf{f}(\mathbf{x}_i - \mathbf{x}_j, \theta_i, \theta_j). \tag{13}$$

We also need to update phases of each particle,

$$\dot{\theta}_i = \omega_i + \sum_j g(\mathbf{x}_i - \mathbf{x}_j, \theta_i, \theta_j). \tag{14}$$

Here functions $\mathbf{f}, g$ describe the interactions and the sums are over neighboring particles j that are within a particular distance of particle i. A popular model for would be one that has strength dependent on $|\mathbf{x}_i - \mathbf{x}_j|$ which is the distance, between particles i and j is in the direction aligned with the vector between the two particles $\hat{\mathbf{x}}_{ij} = \frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|}$ and is also a sinusoidal function of the phase difference $\theta_i - \theta_j$.

With the addition of noise, swarmalator models can be Brownian.

[5] Quillen, A. 2023, Physical Review E, Volume 107, Issue 3, article id.034401. `https://ui.adsabs.harvard.edu/abs/2023PhRvE.107c4401Q/abstract`.

[6] O'Keeffe, Hong and Strogatz, *Oscillators that Sync and Swarm*, Nature Communications, 8, 1504 (2017)

4 Lagrangian and Eulerian views

Fluid simulations are often characterized by whether they are particle based or continuum based. Often particle based simulations are called *Lagrangian*.

An example of a particle based fluid simulation technique is called *smooth particle hydrodynamics* (SPH). The fluid is modeled with a collection of particles. Pressure is computed by locally averaging over the properties (number, mass and velocity) of the particle distribution and then a force from its gradient applied when updating the positions and velocities of each particle. SPH simulations are commonly used in cosmological simulations.

An alternative to a particle based approach is to model a large collection particles by locally estimating its locally **averaged** properties. For example mass density can be computed from an average in a particular region by computing the total mass of particles in that region and dividing by the area or volume of that region. Velocity can be computed as the average velocity of particles in a particular region. Pressure could be computed using an equation of state and the locally averaged mass density.

For a particle based methods, we keep track of a list of particles. For example particles can be indexed by an integer i. Particle properties such as position $\mathbf{r}_i(t)$ are functions of time and updated during the simulation. The equations we integrate are a list of coupled ordinary differential equations that contain first order and optionally second order time derivatives.

In contrast we could consider the evolution of continuum properties such as density $\rho(\mathbf{x}, t)$ and velocity $\mathbf{v}(\mathbf{x}, t)$ which are functions of both position and time. The equations that we would integrate are partial differential equations (PDEs).

Between particle and continuum approaches are those that model evolution of a distribution function. For example we can consider a distribution $f(\mathbf{x}, \mathbf{v}, t$ that gives the numbers of particles in a region in space and in a region in velocity space. Distribution functions can be useful to model transport properties, such as thermal conduction, or examine whether the particle distribution contains or develops a high velocity tail.

5 The simplest continuum models (PDEs)

5.1 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

$$\partial_t \psi = -a \partial_x \psi. \tag{15}$$

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 $\partial_x \psi = f'$.

Often **advection** terms in a PDE are called **convective** terms.

Why is equation 15 advective? Consider a quantity $\psi(y)$ but let position $y(t)$ as if ψ is being carried along by a particle that happens to have position $y(t)$. The instantaneous velocity of the particle is $\frac{dy}{dt}$. We compute

$$\frac{d\psi}{dt} = \frac{d\psi}{dy}\frac{dy}{dt}. \tag{16}$$

This is in the same form as equation 15 but we associate $\frac{dy}{dt}$ with the speed of the particles that are carrying ψ.

In more than one dimension ($\mathbf{x} \in \mathbb{R}^{\mathbf{d}}$ for dimension d with $\psi(\mathbf{x}, t)$)

$$\partial_t \psi = -\mathbf{a} \cdot \nabla \psi. \tag{17}$$

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 $f(x \pm at)$.

An advective term in a PDE looks like

$$(\mathbf{v} \cdot \boldsymbol{\nabla})(\mathrm{Q}) \tag{18}$$

where $\mathbf{v}$ is the velocity of the medium and Q is the quantity that is pushed around.

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

$$\partial_t u + u\partial_x u = 0 \tag{19}$$

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

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = 0. \tag{20}$$

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

5.2 Diffusion

Suppose u is a temperature that depends on x, t. The gradient of temperature is $\frac{du}{dx}$. We assume that heat flux goes in the direction opposite to the gradient $F \propto -\frac{du}{dx}$. If there is a constant heat flux then the temperature does not change. But if there is a gradient in the

heat flux at some location then heat will either be dumped into that location or removed from it. The temperature will locally increase or decrease. This gives $\frac{\partial u}{\partial t} \propto \frac{dF}{dx} \propto \frac{d^2u}{dx^2}$.

The diffusion (or heat) equation in 1 dimension is

$$\partial_t u = D\partial_{xx} u \tag{21}$$

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

$$u(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}. \tag{22}$$

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

$$\partial_t u = D\Delta u \tag{23}$$

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

$$\Delta = \partial_{xx} + \partial_{yy} + \partial_{zz}. \tag{24}$$

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.

5.3 Conservation laws

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

$$\partial_t \rho = -\nabla \cdot \mathbf{F} \tag{25}$$

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

$$\frac{dM}{dt} = \dot{M} = \int_S \mathbf{F} \cdot d\mathbf{A} \tag{26}$$

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

$$\int_V \partial_t \rho \; dV = -\int_S \mathbf{F} \cdot d\mathbf{A} \tag{27}$$

We apply Gaus' law

$$\int_S \mathbf{F} \cdot d\mathbf{A} = \int_V \nabla \cdot \mathbf{F} \; dV \tag{28}$$

The previous two equations together give equation 25.

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

$$\partial_t \rho = -\nabla \cdot (\rho \mathbf{v}). \tag{29}$$

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

Why is $\nabla \cdot \mathbf{v}$ equivalent to incompressibility? We expand the mass continuity equation 29

$$\partial_t \rho = -\rho \nabla \cdot \mathbf{v} - (\mathbf{v} \cdot \nabla)\rho \tag{30}$$

If $\nabla \cdot \mathbf{v} = 0$ then equation 30 is an advective equation. The density is just carried around by the velocity field, which means that the density of any particular fluid parcel remains constant while that parcel moves around.

An incompressible fluid is usually assumed to have nearly constant density.

6 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

$$\frac{Df}{Dt} = \partial_t f + \nabla f \cdot \mathbf{v} - \nabla_v f \cdot \nabla U = \frac{df}{dt}_{collisions}. \tag{31}$$

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

Toner and Tu[7] 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

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{32}$$

$$\begin{aligned} \partial_t \mathbf{v} + \lambda_1 (\mathbf{v} \cdot \nabla)\mathbf{v} + \lambda_2 (\nabla \cdot \mathbf{v})\mathbf{v} + \lambda_3 \nabla v^2 = (\alpha - \beta v^2)\mathbf{v} - \nabla P/\rho + \text{noise} \\ + D_0 \nabla^2 \mathbf{v} + D_1 \nabla(\nabla \cdot \mathbf{v}) + D_2 (\mathbf{v} \cdot \nabla)^2 \mathbf{v}. \end{aligned} \tag{33}$$

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 $v_0 = \sqrt{\alpha/\beta}$.

[7] 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.

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. By stiff, we mean it has a large gradient near a particular density value.

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

If $\lambda_2 < 0$, particles speed up where the flow is divergent.

If $\lambda_3 > 0$, particles are pushed 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.

There are no fourth order derivatives in the Toner and Tu model, which facilitates numerical models.

6.2 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.

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.

6.3 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;

$$\mathbf{p} = \langle \hat{\mathbf{v}}_j \rangle. \tag{34}$$

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 33. This term can also be written in terms of a potential gradient $\nabla_v U(v)$ where $\nabla_v = \left(\frac{\partial}{\partial v_x}, \frac{\partial}{\partial v_y}\right)$ in 2d

$$U(v) = -\frac{\alpha}{2}v^2 + \frac{\beta}{4}v^4 \tag{35}$$

$$-\nabla_v U(v) = \alpha\mathbf{v} - \beta v^2 \mathbf{v}. \tag{36}$$

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

$$\partial_t \mathbf{v} \sim -\nabla_v U(v). \tag{37}$$

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 33.

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

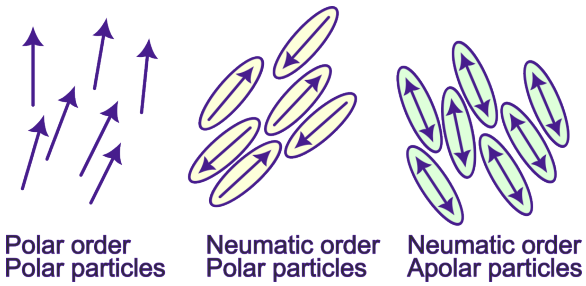

Figure 2: Polar particles move in a particular direction. Polar particles with polar order align their direction of motion with their neighbors, as shown on the left. Repulsive and attractive interactions between particles only depend on particle position, not particle orientation. The Vicsek/Toner-Tu/Boid 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.

6.4 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 involves: (1) find an order parameter; (2) expand the free energy in the vicinity of the transition with respect to the (assumed small) order parameter; and (3) find the minima of the free energy at each temperature, pressure, and other variables, 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[8], PDEs describing a system of active polar

[8]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`

particles depends on density ρ and polarization vector $\mathbf{p}$

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{p}) = 0 \tag{38}$$

$$\partial_t \mathbf{p} + \lambda_1 (\mathbf{p} \cdot \nabla)\mathbf{p} = -\frac{\delta F_p}{\delta \mathbf{p}} + \text{noise} \tag{39}$$

are written in terms of the free energy functional

$$F_p[\mathbf{p}] = \int dV \Big(-\frac{\alpha}{2} p^2 + \frac{\beta}{4} p^4 + \frac{K}{2} \sum_{jk} (\partial_j p_k)(\partial_j p_k) - v_1 \nabla \cdot \mathbf{p} \frac{\rho - \rho_0}{\rho_0} + \frac{\lambda}{2} p^2 \nabla \cdot \mathbf{p} \Big). \tag{40}$$

In Equation 39 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 40 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.

An approach to describing a system with a free energy is to expand a function in a Taylor series of powers of the fields of interest (density, order parameter, phase if you have oscillating active matter, field in active field theories) and also in terms of different gradients. If there is a symmetry (such as neumatic symmetry) then you would only consider terms that obey the symmetry. The Toner-Tu approach is to consider a lot of terms in the free energy. Alternatively one could search for the simplest model that you can explore that seems to have nice phenomenology or is motivated by a real system.

6.5 A quick note on functional derivatives

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

$$L[q] = \int_a^b \mathcal{L}(x, q(x), q'(x)) dx \tag{41}$$

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 $q \to q + \delta q$.

$$\begin{aligned} \delta L[q] &= \int_a^b \mathcal{L}\left(x, q + \delta q, \frac{d}{dx}(q + \delta q)\right) dx - L[q] \\ &= \int_a^b \frac{\partial \mathcal{L}}{\partial q} \delta q \; dx + \int_a^b \frac{\partial \mathcal{L}}{\partial q'} \frac{d}{dx} \delta q \; dx. \end{aligned} \tag{42}$$

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

$$\delta L[q] = \int_a^b \left(\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dx}\frac{\partial \mathcal{L}}{\partial q'} \right) \delta q \; dx. \tag{43}$$

We associate

$$\frac{\delta L[q]}{\delta q(x)} = \frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dx}\frac{\partial \mathcal{L}}{\partial q'} \tag{44}$$

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 40. Equation 40 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

$$\mathcal{L}(\mathbf{p}, \nabla \mathbf{p}) = -\frac{\alpha}{2}p^2 + \frac{\beta}{4}p^4 + \frac{K}{2}\sum_{jk}(\partial_j p_k)(\partial_j p_k) - v_1 \nabla \cdot \mathbf{p}\frac{\rho - \rho_0}{\rho_0} + \frac{\lambda}{2}p^2 \nabla \cdot \mathbf{p} \tag{45}$$

we compute

$$\frac{\partial \mathcal{L}}{\partial p_k} = -\alpha p_k + \beta p^2 p_k + \lambda p_k \nabla \cdot \mathbf{p} \tag{46}$$

$$\frac{\partial \mathcal{L}}{\partial(\partial_j p_k)} = K\partial_j p_k - v_1 \frac{(\rho - \rho_0)}{\rho_0}\delta_{jk} + \frac{\lambda}{2}p^2 \delta_{jk} \tag{47}$$

$$\frac{d}{dx_j}\frac{\partial \mathcal{L}}{\partial(\partial_j p_k)} = K\partial_{jj} p_k - (\partial_j \rho)\frac{v_1}{\rho_0}\delta_{jk} + \frac{\lambda}{2}\partial_j p^2 \delta_{jk} \tag{48}$$

$$\frac{\delta F_d}{\delta \mathbf{p}} = (-\alpha + \beta p^2)\mathbf{p} - K\nabla^2 \mathbf{p} + v_1 \frac{\nabla \rho}{\rho_0} - \frac{\lambda}{2}\nabla p^2 + \lambda \mathbf{p} \nabla \cdot \mathbf{p} \tag{49}$$

Inserting this into equation 39 we find

$$\partial_t \mathbf{p} + \lambda_1(\mathbf{p} \cdot \nabla)\mathbf{p} = (\alpha - \beta p^2)\mathbf{p} + K\nabla^2 \mathbf{p} + v_1 \frac{\nabla \rho}{\rho_0} + \frac{\lambda}{2}\nabla p^2 - \lambda \mathbf{p} \nabla \cdot \mathbf{p} \tag{50}$$

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. If our focus is confined systems, then we are striving to pay attention to the boundary terms and we don't necessarily want to discard them!

6.6 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

$$\mathcal{L}_B = \partial_x f. \tag{51}$$

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

$$L[q]_B = \int_a^b dx\ \mathcal{L}_\mathcal{B} = f(b) - f(a). \tag{52}$$

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

$$\mathcal{L}_B = \nabla \cdot \mathbf{f} \tag{53}$$

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

$$L[q]_B = \int_\Omega \nabla \cdot \mathbf{f}\ dv = \int_{\partial\Omega} \mathbf{f} \cdot d\mathbf{A}. \tag{54}$$

In two dimensions

$$L[q]_B = \int_\Omega \nabla \cdot \mathbf{f}\ dA = \int_{\partial\Omega} \mathbf{f} \cdot d\mathbf{s}. \tag{55}$$

In summary, terms that are important on boundaries tend to involve a divergence.

6.7 More complicated polar systems

Polar materials can have extra terms in the free energy

$$F_p[\mathbf{p}] = \int dV \Bigg(\frac{K_1}{2}(\nabla \cdot \mathbf{p})^2 + \frac{K_2}{2}(\mathbf{p} \cdot (\nabla \times \mathbf{p}))^2 + \frac{K_3}{2}(\mathbf{p} \times (\nabla \times \mathbf{p}))^2 + \frac{K_4}{2}\nabla \cdot [(\mathbf{p} \cdot \nabla)\mathbf{p} - \mathbf{p}(\nabla \cdot \mathbf{p})] + v\nabla \cdot \mathbf{p} + \frac{h_\parallel}{2}(p^2 - 1) \Bigg). \tag{56}$$

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 $h_{\|}$ 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 $h_{\|}p^2/2$. 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`

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 40. In this case the sum of the three terms simplifies to

$$\frac{K}{2}[(\nabla \cdot \mathbf{p})^2 + (\nabla \times \mathbf{p})^2]. \tag{57}$$

So far the free energy terms only have a single gradient operator of the order parameter (with the exception of 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.

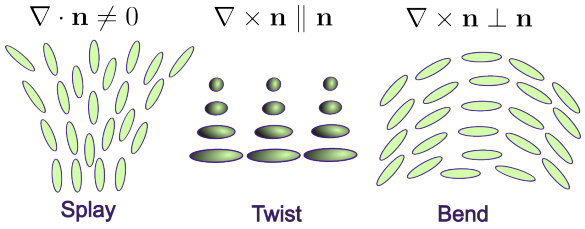

Figure 3: Relevant for the Frank constants for neumatic materials.

7 Active neumatics

An active neumatic system can resemble a liquid crystal but can exhibit behavior such as spontaneously generated directed flow or/and turbulence that is not seen in an equilibrium

system.

7.1 Bipolar particles

A neumatic particle exhibits a 180° symmetry. If you take origin the center of the particle and flip the particle $\mathbf{x} \to -\mathbf{x}$, the equations of motion should not change. This type of particle is also called **bipolar**. A neumatic particle can be described with an orientation angle or a unit vector that specifics the orientation of the particle's long axis, $\hat{\mathbf{n}}$, known as the director. Equations of motion should obey a symmetry $\mathbf{n} \to -\mathbf{n}$.

Active bipolar particles are assumed to move along the particle's orientation direction, (velocity $\mathbf{v} \propto \mathbf{n}$) but they are equally likely to move in the $+\mathbf{n}$ direction as in the $-\mathbf{n}$ direction. In a particle based model, the particle is equally likely to move in either direction along its long axis. One way to simulate an particle based active neumatic, is to randomly chose a direction of motion for each particle on a particular timescale. Equivalently the direction of motion (along the particle's long axis) is 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[9] did this in their paper on dry active neumatics on a sphere).

7.2 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

$$\begin{aligned} \mathbf{Q} &= s(\mathbf{nn} - \frac{1}{d}\mathbf{I}) \\ Q_{ij} &= s(n_i n_j - \frac{1}{d}\delta_{ij}) \end{aligned} \tag{58}$$

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

[9] 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`

take z aligned with the director $\hat{\mathbf{n}}$ and take θ to be a co-latitude. The scalar order parameter

$$s = \langle \frac{1}{2}(3\cos^2\theta - 1)\rangle, \tag{59}$$

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 $\hat{\mathbf{n}}$.

7.3 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

$$\begin{aligned} F_p[Q] = \text{constant} &+ \frac{A}{2}\sum_{ij} Q_{ij}Q_{ij} + \frac{B}{3}\sum_{ijk} Q_{ij}Q_{jk}Q_{ki} + \frac{C}{4}\sum_{ijkl} Q_{ij}Q_{jk}Q_{kl}Q_{li} + ... \\ &+ K_Q \sum_{ijk} \partial_i Q_{ij}\partial_k Q_{kj} + K'_Q \sum_{ijk} \partial_i Q_{jk}\partial_i Q_{jk} + K''_Q \sum_{ijk} \partial_i Q_{jk}\partial_k Q_{ji} + ... \\ &+ B_Q \sum_{ij} (\partial_i Q_{ij} Q_{ji} + \partial_i Q_{jj} Q_{ji} + \partial_i Q_{ii} Q_{jj} ....)? \end{aligned} \tag{60}$$

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.

$$\begin{aligned} \frac{\partial F_p[Q]}{\partial(\partial_a Q_{bc})} &= K_Q \delta_{ia}\delta_{bi}\delta_{cj}\delta_k Q_{kj} + ... \\ &= 2K_Q \delta_{ab} \sum_k \partial_k Q_{kc} + 2K'_Q \partial_a Q_{bc} + 2K''_Q \partial_c Q_{ba} \end{aligned} \tag{61}$$

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

The K coefficients of equation 56 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 absent. This probably means that it is possible to equivalently write the gradient terms in terms of the Q order parameter.

7.4 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.

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

$$\partial_t \mathbf{Q} = -\Gamma \frac{\delta \mathcal{F}_p(\mathbf{Q}, \rho)}{\delta \mathbf{Q}} + \text{noise} \tag{62}$$

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`

7.5 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, $\mathbf{Q}$ and the other for the evolution of the order parameter.

$$\begin{aligned} \frac{D\mathbf{v}}{dt} &= \nabla \sigma(\mathbf{Q}) \\ \frac{D\mathbf{Q}}{dt} &= -\frac{\delta F}{\delta \mathbf{Q}} \end{aligned} \tag{63}$$

Here $\frac{D}{dt}$ represents a Lagrangian derivative which allows you to advect quantities. The stress tensor could be sensitive to the order parameter allowing the neumatic to push the fluid around. The free energy could allow the neumatic particles to interact.

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

8 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

$$\frac{D\mathbf{u}}{dt} = \partial_t + (\mathbf{v}\cdot\nabla)\mathbf{u} = -\frac{\nabla p}{\rho} + \nabla\boldsymbol{\sigma} \tag{64}$$

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

$$\nabla p = \nabla\cdot\sigma + \text{noise} \tag{65}$$

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

$$(\partial_t + \mathbf{v}\cdot\nabla)\mathbf{Q} = S(\nabla\mathbf{v}) - \frac{\delta F_p}{\delta\mathbf{Q}} \tag{66}$$

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

8.1 Advecting a tensor via fluid rotation

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

$$\frac{D\mathbf{Q}}{Dt} = \partial_t\mathbf{Q} + (\mathbf{v}\cdot\nabla)\mathbf{Q} + \boldsymbol{\Omega}\cdot\mathbf{Q} - \mathbf{Q}\cdot\boldsymbol{\Omega} \tag{67}$$

where

$$\boldsymbol{\Omega} \equiv \frac{1}{2}(\nabla\mathbf{v} - \nabla\mathbf{v}^T). \tag{68}$$

The derivative in equation 67 is sometimes called the co-moving co-rotational derivative of the Q-tensor. Let's be specific about the indexing.

$$\Omega_{ij} = \frac{1}{2}(\partial_i v_j - \partial_j v_i) \tag{69}$$

$$\boldsymbol{\Omega}\cdot\mathbf{Q} = \sum_{ij}\Omega_{ij}Q_{ij}. \tag{70}$$

8.2 Oscillating polar materials

We follow the spirit of the paper by Brato Chakrabarti and collaborators `https://ui.adsabs.harvard.edu/abs/2023PhRvL.13018202C/abstract` `https://arxiv.org/pdf/2206.04035` [10] exploring active oscillating neumatic materials.

We can describe a population of swarmalators with a polarization $\mathbf{p}$, which sets the direction of motion and a density ρ. We could modify the Toner and Tu model to include a

We describe the density distribution for our oscillating particles with a function of position, time, and phase; $\rho(\mathbf{x}, t, \phi)$. Conservation of particle number would be

$$\partial_t \rho + (\mathbf{v} \cdot \nabla)\partial_x \rho + \dot{\phi}\partial_\phi \rho = D\Delta\rho \tag{71}$$

where on the right hand side I added a diffusion coefficient. On the left we essentially differentiate ρ w.r.t. to all its dependent variables.

We need an equation for the oscillator phase velocity

$$\dot{\phi} = \Omega_0 + \xi(\phi)Q :: (\nabla v + (\nabla v)^T) - g\nabla_\phi \rho \tag{72}$$

Here the particle alignment influences the phase velocity and so does the particle density.

Finally for the fluid itself in the Stoke's limit

$$\mu\Delta\mathbf{v} = \nabla p/\rho + \nabla\sigma(Q) \tag{73}$$

where σ is stress generated on the fluid by the active particles.

There are (I think) other possible choices for what you choose to evolve for continuum models of active oscillating systems.

8.3 A possible model

How about the following. We let the particle orientation oscillate? The particle orientation is the velocity. A vector perpendicular to velocity would be $\nabla \times \hat{\mathbf{v}}$.

$$\partial_t v = f(\dot{\theta})(\nabla \times \hat{v}) \tag{74}$$

9 Active scalar model

We consider a density ρ for a material that has an order parameter describing its orientation $\mathbf{Q}$ or $\mathbf{p}$, depending upon whether you want it to be polar or neumatic and a phase that oscillates.

The active scalar model advects an active scalar quantity ρ.

9.1 A compendium of models

10 Conserved quantities and Lyapunov functions

Consider an integrated function over the domain Ω

$$T = \int_{\Omega} d\mathbf{x} f(\mathbf{x}, t, \mathbf{v}, \mathbf{Q}.....),$$

where the function f depends on the fields present in the active or pattern formation system. Suppose in addition that you can show that

$$\frac{dT}{dt} < 0.$$

Then a fixed point of the system is a minimum of T. Such a function T is known as a Lyapunov function. Once the system reaches a minimum value for T then it must stay at that value. This can mean that the attractors, or long lived asymptotic states of the system would not exhibit temporal behavior. The system would converge to a fixed state. For some pattern formation models, there exists a Lyapunov function (e.g., versions of the Swift-Hohenburg model).

10.1 A Lyapunov function for the Swift-Hohenberg pattern formation model

For example, the Swift-Hohenberg pattern formation model

$$\partial_t u = ru - (1 + \nabla)^2 u + u^3 \tag{75}$$

has a potential function

$$V = \int dxdy \left(-\frac{1}{2} ru^2 + \frac{1}{4} u^2 + \frac{1}{2} [(\nabla^2 + 1)u]^2 \right) \tag{76}$$

that satisfies

$$\frac{dV}{dt} = -\int dxdy (\partial_t u)^2 \tag{77}$$

which is always less than or equal to zero. (See Cross's book page 180).

[10] Chakrabarti, Shelley, Fürthauer (2023), Collective Motion and Pattern Formation in Phase-Synchronizing Active Fluids, Physical Review Letters, Volume 130, Issue 12, article id.128202

10.2 The winding number for systems of coupled oscillators

Suppose

$$\frac{dT}{dt} = 0.$$

Then T is a conserved quantity. Even if an energy like functional is not conserved, other quantities could be conserved. For example, in 1d coupled oscillating systems with periodic boundaries, the winding number which is the integral of $d\phi/dx$ is conserved. The winding number can be considered a topological quantity making it an interesting parameter to think about.

For example consider a 1d periodic space $x \in [0, 2\pi)$ with a phase function $\phi(x, t)$ that satisfies

$$\partial_t \phi = F(\phi, \partial_x \phi, \partial_{xx} \phi, ..) \tag{78}$$

for some continuous function F. This describes Kuramoto-like oscillators, all in a linear chain, in the continuum limit.

We define a winding number

$$w = \frac{1}{2\pi} \int_0^{2\pi} \frac{d\phi}{dx} dx \tag{79}$$

The winding number must be an integer if ϕ is continuous.

$$\begin{aligned} \frac{dw}{dt} &= \frac{d}{dt} \frac{1}{2\pi} \int_0^{2\pi} \frac{d\phi}{dx} dx \\ &= \frac{1}{2\pi} \int_0^{2\pi} \partial_x \dot{\phi} dx \\ &= \frac{1}{2\pi} \int_0^{2\pi} \partial_x F dx \\ &= \frac{1}{2\pi} \Big|_0^{2\pi} F \\ &= 0. \end{aligned} \tag{80}$$

The winding number is a conserved quantity and so is set by initial conditions.

11 Problems

- Examples of making your own mesh with points and a Delaunay triangulation and importing into skfem: `https://github.com/kinnala/scikit-fem/discussions/705` Make your own 2D mesh and solve a pattern formation model on it. Explore how boundary shape affects the patterns.

- See if we can solve the heat equation with FEM and an interesting static boundary. (in skfem?) If this works, try reaction diffusion equations on a triangular mesh with interesting static boundary shapes and different boundary conditions (Neumann and Dirichlet).
- Classify all behavior caused by different shapes/boundaries for a pattern formation or active matter system. Predict behavior and test predictions via numerical studies.
- Examine/explore the dynamics of defects near boundaries.
- Explore static boundary related behavior in the biharmonic Swift-Hohenberg equation.
- Explore oscillating active mater PDEs.
- Explore ways to let boundaries move.
- Try to make a 1d loop, in 2d space that exhibits waves in FEM. Try connecting it to a 2d continuous system and letting the two systems interact.
- Try moving a boundary that is coupled to a PDE on a mesh.
- Try FEM models for some active matter systems on a mesh.
- Add or adjust noise an explore related behavior.
- Try FEM models for some active matter systems with interesting boundaries.
- Try creating a 2d mesh with holes in it. Can posts be used to control an active medium? There is a body of experimental work with posts causing clumps/solid transitions in self-propelled particle systems.
- Explore evolution of defects on boundary for 3D meshes. Topological surface properties? Skyrmions?
- Find and numerically implement a system that exhibits temporal behavior. Explore time dependent models and patterns near boundaries.
- Effect of boundaries on effective parameters.
- Pattern formation/active matter models on curved surfaces with boundaries.
- Design an abstract model for a controllable muscle (think of reagent parameters as free parameters? Couple motion to orientation?).
- Design an abstract model for a controllable active matter powered pump.

- Explore defects in active oscillating mater (probably not much done).
- Explore pattern formation with local point sources adding reagents or setting field or gradient values.
- Generalize models to work on curved surfaces.

Post workshop comments:

We succeeded in integrating PDEs of pattern formation models using finite element methods on meshes of 2d triangles that cover different shapes (hexagon, circle, triangle).

We succeeded in simulating reaction diffusion equations such as the Brusselator and Gray Scott pattern formation models (with two coupled fields) and the complex Ginzburg-Landau model (with one complex field).

We think that meshes that contain corner triangles that have two facets on the boundary could cause difficulties with non-invertible matrices. There is a work-around.

The boundary in the Brusselator models seems to strongly influence the forming patterns across a few wavelengths of grown patterns. With a zero Neumann boundary condition and square or triangular domain, we saw periodic patterns, resembling crystals, that were not formed on a similar sized circular domain. With Dirichlet or non-zero Neumann boundary conditions patterns tended to be aligned with the boundary.

In contrast, the Gray Scott model, which is quite similar to the Brusselator model, is insensitive to the nearby boundary. No crystalization and the boundary influenced the pattern across a distance less than a pattern wavelength.

12 Some numerical notes

12.1 On mesh generation

We can use `pygmsh` `https://pypi.org/project/pygmsh/` for mesh generation as it seems to work and popular using for `fenics` and `skfem` applications. `Ngsolve` `https://docu.ngsolve.org/latest/index.html` has similar mesh generating routines that are available as part of its `netgen` package.

12.2 Check the Peclet number

Advective problems may be sensitive to the Peclet number which is the ratio of the rate of advective flux to diffusive transport flux. If ν is a kinematic viscosity, V a transport velocity and L a length scale, the Peclet number is

$$Pe \equiv \frac{VL}{\nu}. \tag{81}$$

In a numerical method, a relevant Peclet number would have L equal to the grid spacing.

Depending upon the numerical method, with $Pe > 1$ you could have numerical instability. In this case, check the Peclet number and try increasing the viscosity to lower the Peclet number.

Dry active matter Shaebani+19

Contiuum model	Governing equations		Parameters
Toner-Tu Model [62,63] (dry polar flocks)	$\partial_t n + \nabla\cdot(v_0\, n\, \boldsymbol{p} + \boldsymbol{J}_{\text{passive}}) = 0$	A1	v_0: propulsion speed λ: coefficient of convective derivative $\boldsymbol{J}_{\text{passive}}$: particle flux χ: random noise vector $\mathcal{F}[n,\boldsymbol{p}]$: free energy functional
	$\partial_t \boldsymbol{p} + \lambda(\boldsymbol{p}\cdot\nabla)\boldsymbol{p} + \cdots = -\Gamma_r \dfrac{\delta\mathcal{F}[n,\boldsymbol{p}]}{\delta\boldsymbol{p}} + \chi$	A2	
Models of dry active nematics [67,68]	$\mathbf{Q}(\mathbf{r},t) = S\left(\boldsymbol{p}\otimes\boldsymbol{p} - \frac{1}{d}\mathbf{I}\right)$	A3	S: magnitude of the order parameter $\mathcal{F}[n,\mathbf{Q}]$: free energy functional Λ: white noise tensor ζ: coefficient of active current
	$\partial_t \mathbf{Q} = -\Gamma_r \dfrac{\delta\mathcal{F}[n,\mathbf{Q}]}{\delta\mathbf{Q}} + \Lambda$	A4	
	$\partial_t n + \nabla\cdot(\zeta\nabla\cdot\mathbf{Q} + \boldsymbol{J}_{\text{passive}}) = 0$	A5	
Scalar active model B+ [72-75]	$\phi = (2n - n_H - n_L)/(n_H - n_L)$	A6	n_H, n_L: densities of high and low density coexisting phases λ, ξ terms break time-reversal symmetry.
	$\partial_t\phi + \nabla\cdot\left(-\lambda\nabla\left((\nabla\phi)^2\right) + \xi(\nabla^2\phi)\nabla\phi + \boldsymbol{J}_{\text{passive}} + \chi\right) = 0$	A7	

Active particles in fluid

Contiuum model	Governing equations		Parameters
	incompressible Navier-Stokes equations: $\begin{cases}\rho\,(\partial_t + \boldsymbol{v}\cdot\nabla)\boldsymbol{v} = -\nabla P + \nabla\cdot\boldsymbol{\sigma} + \mathbf{f} \\ \nabla\cdot\boldsymbol{v} = 0\end{cases}$	B1	$\mathbf{f}$: force density $\boldsymbol{\sigma} = \boldsymbol{\sigma}^a + \boldsymbol{\sigma}^d + \boldsymbol{\sigma}^r$: stress tensor $\boldsymbol{\sigma}^a$: ative stress $\boldsymbol{\sigma}^d = 2\eta\mathbf{E}$: dissipative stress $\mathbf{E} = \frac{1}{2}(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T)$: rate of strain tensor $\boldsymbol{\sigma}^r$: reversible stress due to free energy functional
	Stokes equation: $\nabla P - \nabla\cdot\boldsymbol{\sigma} - \mathbf{f} = 0$	B2	
Polar active gel models [1-3, 178-183]	$D_t\,\boldsymbol{p} + \lambda_1\,(\boldsymbol{p}\cdot\nabla)\,\boldsymbol{p} + \cdots = \lambda\,\mathbf{E}\cdot\boldsymbol{p} - \Gamma_r \dfrac{\delta\mathcal{F}}{\delta\boldsymbol{p}}$	B3	D_t: convected corotational time derivative λ_1: strength of advection by polarization λ: flow alignment coefficients $\mathcal{F}[\boldsymbol{p}]$: free energy functional containing Frank elastic terms and terms controlling the order-disorder transition
	$\partial_t n + \nabla\cdot[(\boldsymbol{p} + \boldsymbol{v})n] = 0$	B4	
Active nematic gel models [1-3, 90, 184-187]	$(\partial_t + \boldsymbol{v}\cdot\nabla)\mathbf{Q} = \mathbf{S}(\mathbf{E},\boldsymbol{\Omega}) + \Gamma\mathbf{H}$	B5	$\mathbf{H}$: variational derivative of the free energy $\boldsymbol{\Omega}$: vorticity tensor $\mathbf{S}$ describes the competition between rotation and flow alignment.
Generalized Navier-Stokes models [183, 188-193]	$\mathbf{f} = \dfrac{\delta F[\boldsymbol{v}]}{\delta\boldsymbol{v}}$	B6	$F[\boldsymbol{v}]$: biquadratic Landau-like free energy ζ:activity parameter $\boldsymbol{\sigma}^d$ is a generalized dissipative stress.
	$\boldsymbol{\sigma}^a = -\zeta\left[\boldsymbol{v}\otimes\boldsymbol{v} - \dfrac{v^2}{d}\mathbf{I}\right]$	B7	
	$\boldsymbol{\sigma}^d = 2\left[\Gamma_0 - \Gamma_2\nabla^2 + \Gamma_4\left(\nabla^2\right)^2\right]\mathbf{E}$	B8	
Scalar active model H [194,195]	$\partial_t\phi + \boldsymbol{v}\cdot\nabla\phi = \Gamma_t\,\nabla^2\mu$	B9	ϕ: scalar order parameter μ: chemical potential $\lambda(\nabla\phi)^2$: active contribution to μ $\tilde{\kappa} = \kappa + \zeta \neq \kappa$
	$\mu = a\phi + b\phi^3 - \kappa\nabla^2\phi + \lambda\,(\nabla\phi)^2$	B10	
	$\boldsymbol{\sigma} = -\tilde{\kappa}\left[(\nabla\phi)\otimes(\nabla\phi) - \frac{(\nabla\phi)^2}{d}\mathbf{I}\right]$	B11	

Figure 4: From Shaebani et al. 2020, Computational models for active matter, Nature Reviews Physics, 2, pages 181-199 (2020), `https://arxiv.org/abs/1910.02528`