BE 159: Signal Transduction and Mechanics in Morphogenesis

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12 Continuum mechanics III: active complex fluids

We have conservation laws for mass and linear momentum. In both cases, we showed that the conservation law is of the same form. The time rate of change of a quantity is given by the divergence of a flux, plus some generation term for nonconserved quantities. When written in the comoving frame (that is, using the material derivative), we can define the flux tensor we need to specify. For conservation of linear momentum, this flux tensor is the stress tensor. The specification of the stress tensor is called a constitutive relation, and we have reasoned our way to them thus far (really, without proof). Now, we will move on to active fluids, which are a central topic in the papers we will read and discuss on the polarization of the *C. elegans* zygote.

12.1 Isotropic active viscous fluid

Our immediate goal is to model the acto-myosin cortex of the developing *C. elegans* embryo. The cortex is an example of an **active fluid**, in that it can exert stresses upon itself. This is achieved through the activity of motor proteins that cross-link actin filaments. Working together, the motors serve to compress the actin meshwork. We therefore add an active stress to the stress tensor. We will define the magnitude of this active stress to be σ_a. In general, this can be a function of myosin motor concentration or the concentration of any other factor that regulates actin or motor activity. We stipulate however that it is not a function of fluid velocity. So, the active stress in an isotropic fluid is a scalar quantity depending only on other scalar quantities. It therefore appears in the stress tensor must like the pressure, as $\sigma_a \delta_{ij}$. In this section, we will show that such a fluid cannot have any interesting dynamics beyond a passive fluid to motivate the need for the broken symmetry of a nematic active fluid.

Augmenting the stress tensor with the active stress, we have

$$\sigma_{ij} = -p\,\delta_{ij} + 2\eta\, v_{ij} + \sigma_a\,\delta_{ij}. \tag{12.1}$$

As a reminder, $v_{ij} = (\partial_i v_j + \partial_j v_i)/2$ is the symmetric part of the velocity gradient tensor. Apparently, from the definition of the stress tensor, the active stress is indistinguishable from the hydrostatic pressure, since they always appear together as a sum. Let us investigate this further by writing the equation of motion with the new stress tensor (again, assuming the dynamics are intertialess).

$$\eta\,\partial_j\partial_j v_i - \partial_i(p - \sigma_a) = 0. \tag{12.2}$$

As a step in exposing the active stress independence of the dynamics, we take the curl of both sides of the equation.

$$\varepsilon_{kli}\partial_k\left(\eta\,\partial_j\partial_j v_i - \partial_i(p - \sigma_a)\right) = \eta\,\partial_j\partial_j\,\omega_i = 0, \tag{12.3}$$

where we have defined the curl of the velocity field as the **vorticity**, ω_i (not to be confused the the antisymmetric part of the velocity gradient tensor, ω_{ij}). This tells us that the dynamics of the vorticity are given by

$$\partial_j \partial_j \omega_i = 0, \tag{12.4}$$

meaning that the motion is entirely determined by the boundary conditions.

Now, we will take the divergence of both sides of the equation of motion.

$$\partial_i \left(\eta \partial_j \partial_j v_i - \partial_i (p - \sigma_a) \right) = \eta \partial_j \partial_j [\partial_i v_i] - \partial_i \partial_i (p - \sigma_a) = 0. \tag{12.5}$$

The bracketed term is zero for an incompressible fluid by the continuity equation. Thus, the difference between the pressure and active stress are set by

$$\partial_i \partial_i (p - \sigma_a) = 0. \tag{12.6}$$

This equation must hold regardless of what the velocity field is to enforce incompressibility. Therefore, the quantity $p - \sigma_a$ is set entirely by incomressibility and the active stress can have no effect on the fluid dynamics that is distinguishable from the hydrostatic pressure. So, we cannot really model the cortex as an active incompressible isotropic fluid because this is indistinguishable from a non-active fluid.

12.2 Active nematic viscous fluid

The cortex consists of crosslinked filaments of actin. It therefore stands to reason that it is *not* isotropic because it consists of these stick like structures. We can define a local vector, called a **director** that describes the average orientation of the filaments in a small volume element. We will call this vector n_i and specify that it is a unit vector ($n_i n_i = 1$). We could define the local order in terms of n_i itself, but instead we will consider the case where the *sign* of the direction of the director is immaterial. Physically, this means that the "sticks" in the fluid do not have arrowheads; pointing in the positive x direction is the same as pointing in the negative x direction. In this case, we need to construct a **nematic order parameter** that respects this nondirectionality. As shown by de Gennes in the study of liquid crystals, this order parameter is a rank 2 tensor that can be constructed from the director as

$$Q_{ij} = S \left(n_i n_j - \frac{1}{3} \delta_{ij} \right). \tag{12.7}$$

Here, S is the magnitude of the local order. The nematic order parameter is symmetric and traceless.

Now that we have this order parameter that describes the fluid, we no longer have the isotropy we enjoyed when writing down the stress tensor for a simple fluid. We need to add an extra term to the stress tensor that takes into account nematic order.

$$\sigma_{ij} = -p \delta_{ij} + 2\eta v_{ij} + \sigma_{ij}^{\text{nematic}}. \tag{12.8}$$

We will assume that we are above a critical temperature such that the filaments tend to be disordered. In other words, in a relaxed, equilibrium state, the order parameter tends toward zero. We might then write the nematic stress as a Taylor series about the $Q_{ij} = 0$ state, noting that the first order term should vanish because the nematic stress is minimal with $Q_{ij} = 0$.

$$\sigma_{ij}^{\text{nematic}} = A_{ijkl}Q_{kl} + B_{ijklmn}\partial_k\partial_l Q_{mn}. \tag{12.9}$$

From symmetry arguments and other approximations we will not go into here, the higher order tensors in the expansion can be reduced to scalars. As is traditionally done, we can define constants β_1, χ, and L and write the passive nematic stress as

$$\sigma_{ij}^{\text{nematic}} = \beta_1(\chi - L\partial_k\partial_k)Q_{ij}. \tag{12.10}$$

Here, χ is referred to as an inverse susceptibility and L is related to the Frank elastic constants from the theory of liquid crystals. The coefficient β_1 is an Onsager coefficient. We will not go into the details of these terms here (and this hand-wavy Taylor series expansion is not a careful derivation at all), but we write it this way because this is how it appears in the literature. So, the stress tensor for a passive nematic viscous fluid is

$$\sigma_{ij} = -p\,\delta_{ij} + 2\eta\, v_{ij} + \beta_1(\chi - L\partial_k\partial_k)Q_{ij}. \tag{12.11}$$

Next, we will write the active stress in terms of the order parameter. We can write it to linear order as a Taylor expansion.

$$\sigma_{\text{active}} = \sigma_a^0\,\delta_{ij} + \sigma_a Q_{ij}. \tag{12.12}$$

The first term describes the isotropic contraction due to active stresses. This is the same term as in the isotropic case and is indistinguishable from the pressure. We will therefore absorb it into the pressure and define $\Pi = p - \sigma_a^0$. The last term is directional stress exerted along the nematic order. So, our stress tensor for an active nematic fluid is

$$\sigma_{ij} = -\Pi\,\delta_{ij} + 2\eta\, v_{ij} + \beta_1(\chi - L\partial_k\partial_k)Q_{ij} + \sigma_a Q_{ij}. \tag{12.13}$$

The equation of motion is then, considering again the interialess limit for an incompressible fluid,

$$\partial_j\sigma_{ij} = 0 = -\partial_i\Pi + \eta\,\partial_j\partial_j v_i + \beta_1(\chi - L\partial_k\partial_k)\partial_j Q_{ij} + \partial_j(\sigma_a Q_{ij}). \tag{12.14}$$

12.3 Two-and-one-dimemsional active nematic fluid

In the homework, you will derive the equation of motion for an active nematic fluid that is confined to two dimensions. You will then make some assumptions about the symmetry of the flow to reduce the result to a one-dimensional equation. This is the equation used in the Mayer, et al. and the Gross, et al. papers to describe the cortex dynamics. Specifically, you will derive that

$$-\eta\,\partial_x^2 v_x + \gamma v_x = \partial_x \sigma_a, \tag{12.15}$$

where γ is a friction coefficient. This equation means that gradients in active stress drive cortical flow against viscous dissipation and frictional losses.

Note that Q_{ij} does not appear in this equation. Nonetheless, to derive the equation of motion for the cortex, we do need to explicitly take into account nematic order.