BE 159: Signal Transduction and Mechanics in Morphogenesis

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9 Continuum mechanics: active complex fluids

Last time we derived 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), the we can define the flux tensor we need to specify. For conservation of momentum, this flux tensor is the stress tensor.

$$\rho \frac{\mathrm{d}v_i}{\mathrm{d}t} = -\partial_j \sigma_{ij} \tag{9.1}$$

9.1 Physical interpretation of the stress tensor

The stress tensor describes forces resulting from relative motion of a material. It has units of force per area, or momentum flux. To see this, note that momentum has dimension of ML/T. A flux introduces dimension of $1/L^2T$. Putting it together, the stress has units of M/LT^2, or force per area.

To understand how it describes forces due to relative motion consider for example the case where part of the material moves left and another part moves right, we have a stretching motion. The material pulls in resistance to this motion. The component of the stress tensor describing resistance to this mode of relative motion is σ_{xx}.

9.2 Constitutive relations for an elastic solid

We first consider a homogeneous elastic solid. The stress tensor is given in terms in the **strain** tensor, which we will first characterize.

9.2.1 Elastic strain tensor

We define by x_i the position of a piece of the solid in space. We then deform the solid such that that same piece is now at position x'_i. We define the **displacement**, $u_i = x'_i - x_i$. If an object changes shape, then the displacement varies across the solid. If u_i is constant across the solid, the solid is not being deformed; rather, it is being translated in the direction of u_i. However, if u_i varies in space, we do have a deformation. So, the quantity $\partial_i u_j$ reflects local deformations in the solid.

To investigate the magnitude of deformations, we consider the differential squared distance between neighboring points in the solid.

$$\mathrm{d}\ell^2 = \mathrm{d}x_i\,\mathrm{d}x_i. \tag{9.2}$$

If we have a deformation, this distance changes by

$$
d\ell'^2 = dx'_i \, dx'_i. \tag{9.3}
$$

For small deformations,

$$
dx'_i - dx = u_i - u'_i \approx (\partial_j u_i) dx_j, \tag{9.4}
$$

by the chain rule. Then, we have

$$
\begin{aligned}
d\ell'^2 &= \left(dx_i + (\partial_j u_i) dx_j\right) \left(dx_i + (\partial_k u_i) dx_k\right) \\
&= dx_i \, dx_i + (\partial_j u_i) dx_j \, dx_i + (\partial_k u_i) dx_k \, dx_i + (\partial_j u_i)(\partial_k u_i) dx_j \, dx_k \\
&= d\ell^2 + \left[\partial_i u_j + \partial_j u_i + (\partial_i u_k)(\partial_j u_k)\right] dx_i \, dx_j,
\end{aligned} \tag{9.5}
$$

where in the last line we have renamed indices to collect terms multiplying $dx_i \, dx_j$. We can write this down as

$$
d\ell'^2 - d\ell^2 = 2\, \varepsilon_{ij} \, dx_i \, dx_j, \tag{9.6}
$$

where we have defined the **strain tensor** as

$$
\varepsilon_{ij} = \frac{1}{2} \left(\partial_i u_j + \partial_j u_i + (\partial_i u_k)(\partial_j u_k)\right). \tag{9.7}
$$

The last term in the strain tensor is small for small displacements, so we have, to linear order in $\partial_i u_i$,

$$
\varepsilon_{ij} \approx \frac{1}{2} (\partial_i u_j + \partial_j u_i). \tag{9.8}
$$

9.2.2 Elastic stress tensor

We have established that the strain describes deformations of the solid. We can derive a relationship between the stress tensor, which describes the forces necessary to achieve the deformations, using thermodynamic arguments. Instead, we will just start with Hooke's law, which is valid for small deformations. As Hooke said, "*ut tensio sic vis*," or the force is proportional to extension. Because the stress tensor is a rank 2 tensor, as is the strain tensor, to write a linear relationship between the two, most generally, we need a rank 4 tensor.

$$
\sigma_{ij} = C_{ijkl} \, \varepsilon_{kl}. \tag{9.9}
$$

There are $3^4 = 81$ entries in the tensor C_{ijkl}. This looks really intimidating, but by symmetry arguments, we can show that the entries are not all independent. For example, because the strain tensor ε_{ij} is symmetric, $\varepsilon_{ij} = \varepsilon_{ji}$. The stress tensor must also show this symmetry, so therefore so must C_{ijkl}. This implies that $C_{ijkl} = C_{jikl} = C_{ijlk}$. We will not go through all of the symmetry arguments here, but in the end, we find that there are only two independent parameters. Generally, it can be shown that a linear relationship between two rank 2 symmetric tensors that remains invariant under change of coordinates has the form

$$\sigma_{ij} = \lambda\, \varepsilon_{kk}\delta_{ij} + 2\mu\, \varepsilon_{ij}, \tag{9.10}$$

where the constants λ and μ are called the **Lamé coefficients**. This gives us our constitutive relation for an elastic solid.

As is commonly done, is is convenient to write the Lamé coefficients in a different form. We define

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \tag{9.11}$$

$$\mu = \frac{E}{2(1+\nu)}, \tag{9.12}$$

where E is called the Young's modulus and ν is the Poisson ratio. The resulting expression for the stress tensor is

$$\sigma_{ij} = \frac{E}{1+\nu}\left(\varepsilon_{ij} + \frac{\nu}{1-2\nu}\,\varepsilon_{kk}\delta_{ij}\right), \tag{9.13}$$

The second law of thermodynamics dictates that $E \geq 0$ and $-1 \leq \nu \leq 1/2$ (which we will not derive here). Thus, the stress associated with an elastic deformation is of order $E\varepsilon$.

9.2.3 Equation of motion for an elastic solid

Now that we have our constitutive relation, we can write the equation of motion from the statement of conservation of linear momentum. The local velocity, v_i, is related to the displacement as $v_i = \partial_t u_i$. Thus, we can write

$$\rho\,\frac{\mathrm{d}v_i}{\mathrm{d}t} = \rho\left(\partial_t^2 u_i + (\partial_t u_j)\partial_j\partial_t u_i\right) = -\partial_j\sigma_{ij}, \tag{9.14}$$

where the t's denote time derivatives and are not summed over. Evidently, this is a wave equation in the displacement. The dynamics then describe elastic waves through the solid. We know these waves as sound. The dynamics are usually very fast compared to biological time scales of interest, so we usually neglect the left hand side of the equation of motion. Typically with elastic solids, we will study only statics, as governed by the constitutive relation itself.

9.3 Constitutive relation for an isotropic viscous fluid

If we look at the expression for the elastic stress, we see that it scales like the displacement, $\sigma \sim E\varepsilon$. For a fluid, we would not expect this to be the case. If we displace a fluid and then let it rest, we do not have to exert any more force to maintain the displacement. Instead, we expect that the stress we need to exert on a fluid to move it will be related to the *rate* at which we make deformations, $\partial_t \partial_i u_i$. In other words, if we want to move a fluid more rapidly, it will require more force than to move it slowly. The actual magnitude of the displacement will not matter; only the rate at which we make displacements. We then define the velocity gradient tensor $\partial_i v_j$, on which the stress tensor will surely depend. This tensor can be written as

$$\partial_i v_j = \frac{1}{2}(\partial_i v_j + \partial_j v_i) + \frac{1}{2}(\partial_i v_j - \partial_j v_i) = \frac{1}{2}(v_{ij} + \omega_{ij}). \tag{9.15}$$

The first term is v_{ij}, a symmetric tensor ($v_{ij} = v_{ji}$), and the second term is usually written as ω_{ij} and is an antisymmetric tensor ($\omega_{ij} = -\omega_{ji}$). Due to the symmetry of an isotropic fluid and conservation of angular momentum (which we will not formally consider here), the stress tensor must be symmetric, whic means that ω_{ij} does not contribute to it.

We might also expect the stress to include the hydrostatic pressure, p. After all, pumps move fluids around by exerting pressure on them. So, we additionally have a $-p\,\delta_{ij}$ term in the stress tensor. For an isotropic viscous fluid, then, we have

$$\sigma_{ij} = -p\,\delta_{ij} + C_{ijkl} v_{kl}. \tag{9.16}$$

Again, we use the fact that a linear relationship between two rank 2 symmetric tensors that remains invariant under change of coordinates can be written with Lamé coefficients.

$$\sigma_{ij} = -p\,\delta_{ij} + \lambda\, v_{kk}\,\delta_{ij} + 2\mu\, v_{ij}. \tag{9.17}$$

We will define η and η_v such that $\mu = \eta$ and $\lambda = (\eta_v - 2\eta)/3$. Then, we have

$$\sigma_{ij} = -p\,\delta_{ij} + 2\eta\left(v_{ij} - \frac{v_{kk}}{3}\,\delta_{ij}\right) + \frac{\eta_v}{3}\, v_{kk}\,\delta_{ij}. \tag{9.18}$$

The quantity η is called the **viscosity**, or shear viscosity, and η_v is called the bulk viscosity. It is clear that η_v determines the contribution of isotropic compression to the stress. For am incompressible fluid, the continuity equation (8.23) gives that $v_{kk} = \partial_k v_k = 0$, so the stress tensor is

$$\sigma_{ij} = -p\,\delta_{ij} + 2\eta\, v_{ij} = -p\,\delta_{ij} + \eta\,(\partial_i v_j + \partial_j v_i). \tag{9.19}$$

9.4 Equation of motion for an incompressible isotropic viscous fluid

Now that we have the constitutive relation, we can write down the equation of motion for an incompressible isotropic viscous fluid. This is the statement of conservation of linear momentum.

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = -\partial_j \sigma_{ij} = \partial_i p - \eta\, \partial_j \partial_j v_i, \tag{9.20}$$

We can nondimensionalize this equation, choosing $x = \ell \tilde{x}$, $v_i = U\tilde{v}_i$, and $p = \tilde{p}\,\eta\, U/\ell$. The resulting equation is

$$\begin{aligned}\frac{\rho\,\ell^2}{\eta\tau}\,\partial_t \tilde{v}_i + \frac{\rho U \ell}{\eta}\,\tilde{v}_j \partial_j \tilde{v}_j &= \partial_i \tilde{p} - \partial_j \partial_j \tilde{v}_i \\ = \mathrm{Re}\,(\mathrm{Sr}\,\partial_t + \partial_j \tilde{v}_j)\,\tilde{v}_i &= \partial_i \tilde{p} - \partial_j \partial_j \tilde{v}_i,\end{aligned} \tag{9.21}$$

where the derivatives are now over dimensionless variables and we have defined the **Reynolds number** $\mathrm{Re} = \rho U \ell/\eta$ and the **Strouhal numbers**, $\mathrm{Sr} = (\ell/U)/\tau$. The Reynolds number is the ratio of the inertial energy, $\rho U^2 \ell^3$, to the energy loss due to viscous dissipation, $\eta U \ell^2$. The Strouhal number is the ratio of the advective time scale, ℓ/U to any other pertinent time scale of interest, τ. If $\mathrm{Re} \ll 1$ and $\mathrm{Re}\,\mathrm{Sr} \ll 1$, then the left hand side of the equation of motion is negligible compared to each term in the right hand side. In cell and developmental biology, this is generally the case. We can estimate it. The density of our material is close to that of water, or 10^3 kg/m^3. The smallest viscosity is that of water, which is about 10^{-3} kg-m/s. The longest length scale we generally consider in early embryos is about 1 mm = 10^{-3} m. The faster speeds could conceivably be that of the fastest motor proteins, about 100 µm/s = 10^{-4} µm/s. Putting this together gives a Reynolds number of $\mathrm{Re} = 0.1$. We have intentionally overestimated this, since most fluid-like embryonic movements more more slowly, over shorter distances, and with much higher viscosity. So, we are generally justified in neglecting the left hand side of the equation of motion, and we have

$$\partial_j \sigma_{ij} = 0. \tag{9.22}$$

We will talk in more depth about dynamics of isotropic incompressible viscous fluids at low Reynolds number when we study the He, at al. paper toward the end of the course. Now, we will move on to active fluids.

9.5 Isotropic active viscous fluid

Out 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 of motor activity. So, our updated stress tensor is

$$\sigma_{ij} = -p\delta_{ij} + 2\eta v_{ij} + \sigma_a \delta_{ij}. \tag{9.23}$$

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).

$$\eta \partial_j \partial_j v_i - \partial_i (p - \sigma_a) = 0. \tag{9.24}$$

We take the curl of both sides of the equation.

$$\varepsilon_{kli} \partial_k \left(\eta \partial_j \partial_j v_i - \partial_i (p - \sigma_a) \right) = \eta \partial_j \partial_j \omega_i = 0, \tag{9.25}$$

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

$$\partial_j \partial_j \omega_i = 0, \tag{9.26}$$

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.

$$\partial_i \left(\eta \partial_j \partial_j v_i - \partial_i (p - \sigma_a) \right) = \eta \partial_j \partial_j [\partial_i v_i] - \partial_i \partial_i (p - \sigma_a) = 0. \tag{9.27}$$

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

$$\partial_i \partial_i (p - \sigma_a) = 0. \tag{9.28}$$

This equation must hold regardless 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.

9.6 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. 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

$$Q_{ij} = S\left(n_i n_j - \frac{1}{3}\,\delta_{ij}\right). \tag{9.29}$$

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. Deriving the stress tensor is a bit more difficult, but under certain assumptions, we can write it as

$$\sigma_{ij} = -p\,\delta_{ij} + 2\eta\, v_{ij} + \beta_1(\chi - L\partial_k\partial_k)Q_{ij}. \tag{9.30}$$

The last term describes the tendency for the order parameter to return to zero, meaning that the filaments have a tendency to be randomly oriented.

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

$$\sigma_{\text{active}} = \sigma_a^0\,\delta_{ij} + \sigma_a Q_{ij}. \tag{9.31}$$

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

$$\sigma_{ij} = -\Pi\,\delta_{ij} + 2\eta\, v_{ij} + \beta_1(\chi - L\partial_k\partial_k)Q_{ij} + \sigma_a Q_{ij}. \tag{9.32}$$

The equation of motion is then, considering again the interialess limit,

$$\partial_j\sigma_{ij} = 0 = -\partial_i\Pi + \eta\,\partial_j\partial_j v_i + \beta_1(\chi - L\partial_k\partial_k)\partial_j Q_{ij} + \partial_j(\sigma_a Q_{ij}). \tag{9.33}$$

9.7 Two-and-one-dimemsional active nematic fluid

In homework 4, 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. paper to describe the cortex dynamics. Specifically, you will derive that

$$-\eta\,\partial_x^2 v_x + \gamma\, v_x = \partial_x \sigma_a, \tag{9.34}$$

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