Notes on Boundaries

A. C. Quillen + Aidan Bachmann

July 28, 2024

Contents

1 Fluid/Boundary interactions

The fluid exerts a force on the boundary that arises from the stress tensor. If we write conservation of momentum as

$$\partial_t(\rho \mathbf{u}) = -\nabla \cdot \boldsymbol{\sigma} \tag{1}$$

where our shorthand $\partial_t = \frac{\partial}{\partial t}$, the mass density is ρ and the fluid velocity vector is $\mathbf{u}$. The density and velocity are functions of position and time $\mathbf{x}, t$. In a Cartesian coordinate

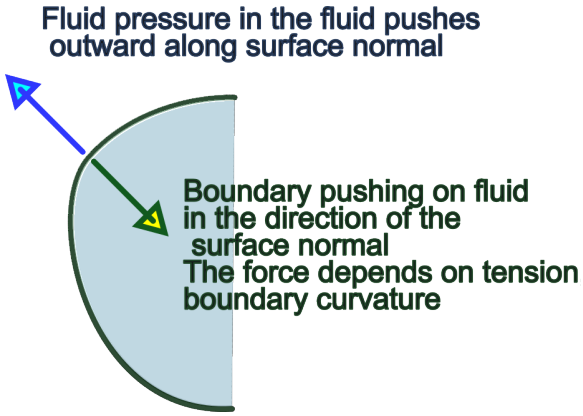

Figure 1: Our expectation for a fluid boundary surface interaction.

system, the stress tensor has components

$$\sigma_{ij} = p\delta_{ij} + \rho u_i u_j + \text{viscous terms} \tag{2}$$

where p is the pressure. The viscous terms depend on the gradient of the velocity vector $\partial_i u_j + \partial_j u_j$ (made symmetrical).

In terms of components and neglecting viscosity, equation 1 is equal to

$$\partial_t(\rho u_i) = -\sum_j \left[\partial_j p + \partial_j(\rho u_i u_j) + ...\right]. \tag{3}$$

Here shorthand $\partial_j = \frac{\partial}{\partial x_j}$.

The equation for conservation of mass

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{4}$$

Conservation of mass along with equation 1 or 3 for conservation of momentum gives. Euler's equation, and if viscous forces are taken into account we arrive at the Navier-Stokes equation

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla P}{\rho} + \nu \Delta \mathbf{u}. \tag{5}$$

Here ν is the kinematic viscosity and Δ, the Laplacian is equal to ∇^2.

We can gain intuition on boundary interactions by integrating Euler's equation (the Navier-Stokes equation without viscosity) in a domain Ω

$$\int_\Omega \partial_t(\rho \mathbf{u})\, dV = -\int_\Omega \nabla \cdot \boldsymbol{\sigma}\, dV. \tag{6}$$

We use Gauss' law

$$\int_\Omega \partial_t(\rho \mathbf{u})\ dV = -\int_{\partial\Omega} \boldsymbol{\sigma} \cdot d\mathbf{A}. \tag{7}$$

To make it clear what we mean by the right hand side, we can write the above equation in terms of components

$$\int_\Omega \partial_t(\rho u_i)\ dV = -\int_{\partial\Omega} \sum_j \sigma_{ij} dA_j. \tag{8}$$

Note that the inner product of a tensor and a vector is a vector. See here for some properties of tensors and how they operate on vectors. In this case, σ_{ij} is the ith component of the force on the jth direction.

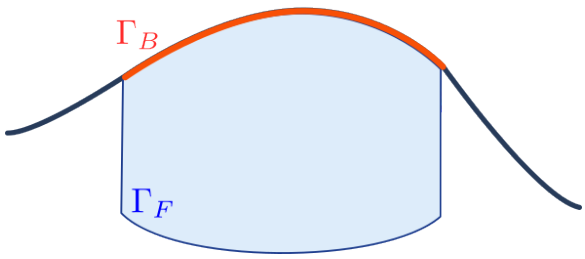

Figure 2: A fluid element that is up against a boundary.

We consider a fluid volume element that has an area of its boundary that is an interface with another fluid or up against a membrane or a solid surface, as shown in Figure 2. We divide the boundary of the element into two pieces, that inside the fluid and that on the interface $\partial\Omega = \Gamma_F + \Gamma_B$. Because the fluid parcel is up against the boundary there could also be a force exerted by the boundary onto the fluid which we call $\mathbf{F}_b$. Conservation of momentum gives

$$\int_\Omega \partial_t(\rho \mathbf{u})\ dV + \int_{\Gamma_F+\Gamma_B} \boldsymbol{\sigma} \cdot d\mathbf{A} = \mathbf{F}_b. \tag{9}$$

The equation is a vector equation. The force exerted by the fluid onto the boundary element Γ_B is

$$\int_{\Gamma_B} \boldsymbol{\sigma} \cdot d\mathbf{A} \tag{10}$$

and this is equivalent to $\mathbf{F}_b$ due to Newton's third law (equal and opposite forces).

Ignoring viscosity, the stress tensor contains a pressure term and a ram pressure term, which gives a force (from the fluid onto the boundary)

$$\int_{\Gamma_B} p \; d\mathbf{A} + \rho \mathbf{u}(\mathbf{u} \cdot d\mathbf{A}). \tag{11}$$

The term on the left is a force that depends on the pressure and the area of the surface element and it is in the direction of the normal to the boundary, as intuitively expected from Figure 1. If the boundary is fixed then because the fluid cannot cross the boundary and $\mathbf{u} \cdot d\mathbf{A} = 0$. This implies that the right hand side of equation 11 vanishes and the force from the boundary onto the fluid must be

$$\mathbf{F}_b = -p \; d\mathbf{A}. \tag{12}$$

It is helpful to recall that the units of pressure are energy density $\frac{J}{m^3}$, or equivalently $\frac{N}{m^2}$, which is force per area. So pressure integrated over a surface corresponds to a force associated with thermal motion while the (aptly named) ram pressure term is force associated with bulk flow.

1.1 What if there is viscosity?

The stress due to viscosity is described with a gradient of the velocity field. The strain rate tensor is free of solid body rotation as solid body rotation would not give any stress. To get rid of rotation we use

$$\varepsilon = \frac{1}{2} \left(\nabla u + \nabla u^T \right) \tag{13}$$

where ^{T} refers to the transpose of the matrix. In terms of components

$$\boldsymbol{\varepsilon} = \frac{1}{2} \left(\partial_i u_j + \partial_j u_i \right). \tag{14}$$

The strain rate tensor can be decomposed into a traceless and a traced part. The part of ε that contains the trace is $(\nabla \cdot \mathbf{u}) \frac{\delta_{ij}}{3}$ (in 3 dimensions) and we can ignore it if the fluid is incompressible. If the fluid is compressible it is conventional to describe the stress tensor with two types of viscosity, one associated with volume changes and the other associated with shear. For an incompressible fluid, the viscous part of stress tensor is

$$\boldsymbol{\sigma}_\nu = 2\mu\boldsymbol{\varepsilon} \tag{15}$$

where μ is the dynamic shear viscosity. It is often convenient to write $\mu = \nu\rho$ where ν is the kinematic shear viscosity.

Let's define a normal direction $d\mathbf{A} \propto \hat{\mathbf{n}}$. We compute a force per unit area on the boundary due to the viscous part of the stress tensor

$$\boldsymbol{\sigma}_\nu \cdot d\mathbf{A} = 2\mu dA(\partial_n \mathbf{u} + \nabla u_n) = -\mathbf{F}_{b,\nu}. \tag{16}$$

The components parallel to the boundary don't necessarily vanish which implies that we have a traction or drag force. Ignoring the velocity component toward the boundary, the term $\propto \partial_n \mathbf{u}$ is due to velocity shear.

Viscosity often is only important in a shallow sheet called a boundary layer. If we take into account viscosity in a boundary layer we expect the velocity to go to zero at a fixed boundary as shown in the no-slip boundary case of Figure 3. If you ignore the boundary layer or assume the viscosity is really low you could adopt a boundary with slip as shown in the right hand side of this figure.

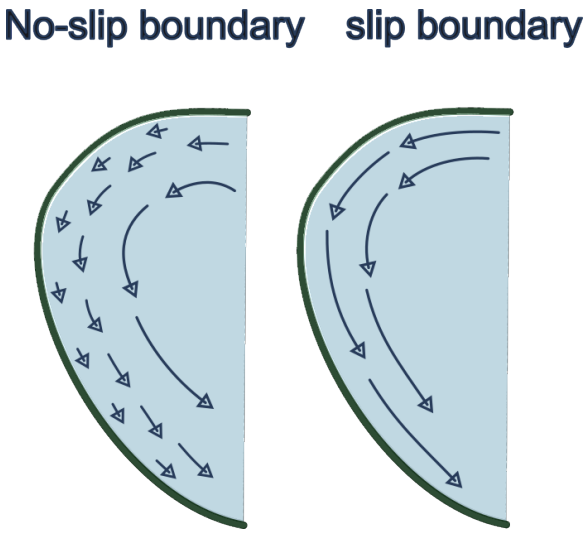

Figure 3: Illustration of a no-slip boundary on the left and one that allows motion right up against the boundary (on the right).

Boundary layers pose a significant challenge to numerical simulations, especially in the inviscid, or high Reynolds number, limit. In this limit, boundary layers are thin, so if a no-slip condition is imposed, then large velocity gradients may develop on small length scales. This requires increasingly fine meshes, which are computationally expensive. One example of such a system is macroscopic flows of air. The Reynolds number is given by

$$Re = \frac{\rho u L}{\mu} \tag{17}$$

where ρ is density, u is velocity, L is a characteristic length scale, and μ is viscosity. For human-scale air flows, for instance in an HVAC system, u, L, and ρ are on the order of 10^0

or 10^1 (in MKS units), while $\mu \sim 10^{-5}$, so the Reynolds number is large and flows tend to be turbulent. Another result of this fact, via Kelvin's circulation theorem, indicates that vorticity flux Γ is conserved instead of being diffused into in the medium by the viscosity. This is why smoke rings are so long lived! — and a motivation for studing boundary/flow interactions. In hydrodynamics, because vorticity is conserved everywhere but at a boundary, boundaries tend to start or stop or drive interesting flow patterns.

1.2 What if the boundary is moving?

We require that the fluid is moving with the boundary. We parameterize positions on the boundary with a coordinate $\mathbf{s}$. The position in real space $\mathbf{x}(\mathbf{s}, t)$ would describe a moving boundary. The velocity of the boundary $\mathbf{V}(\mathbf{s})$ should be equal to that of the fluid right next to it. If there is no slip then

$$\mathbf{V}(\mathbf{s}, t) = \mathbf{u}(\mathbf{x}(\mathbf{s}, t)). \tag{18}$$

1.3 Slender body and resistive force theory

Note: *slender body theory* and *resistive force theory* are attempts to directly relate the motion of a small moving surface element or slender object to the force on it. These are derived with drag coefficients or point solutions to Stokes flow to take into account viscosity. The idea is to ignore the global flow pattern and approximate the flow near the boundary with a few coefficients.

In resistive force theory a friction force (per unit length?) depends on velocity components perpendicular and parallel to a slender body or filament

$$\mathbf{F} = \zeta_\perp \mathbf{v}_\perp + \zeta_\parallel \mathbf{v}_\parallel \tag{19}$$

where $\zeta_\perp, \zeta_\parallel$ are friction or drag coefficients.

1.4 What is Stokes flow?

Stokes flow is a high viscosity (or low Reynolds number) limit of the Navier-Stokes equation for an incompressible fluid. The Stokes limit is good for studying swimming microbes. The Naviers Stokes equation

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{v}. \tag{20}$$

In the Stokes limit, inertial terms (those on the left) are ignored giving

$$\nabla p = \mu \Delta \mathbf{v} \tag{21}$$

where $\mu = \rho\nu$ and $\Delta = \nabla^2$. The pressure is whatever it needs to be so that $\nabla \cdot \mathbf{u} = 0$ which is obeyed by an incompressible fluid. If we operate with a curl, we find

$$\Delta\boldsymbol{\omega} = 0 \tag{22}$$

where $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is the **vorticity**. Equation 22 is called Laplace's equation and solutions in 2D are often called **harmonic**. If you specify some information for the field on the boundary $\partial\Omega$ of a volume Ω, the solution inside Ω is essentially determined.

In two dimensions the condition $\nabla \cdot \mathbf{u} = 0$ is nicely satisfied by adopting a stream function ψ that gives $\mathbf{u} = (\partial_y\psi, -\partial_x\psi)$. With a stream function, Stokes flow becomes

$$\Delta^2\psi = 0 \tag{23}$$

where Δ is the Laplacian. This equation is called a biharmonic equation. Solutions to the biharmonic equation also satisfy Laplace's equation.

Point discontinuities that are solutions to Laplace's equation everywhere except at a point (Stokeslet, forcelets) are sometimes used to construct solutions.

If you have a thin fluid layer and integrate over the vertical direction, you get what is called Hele-Shaw flow.

2 Boundaries for the Heat equation

We start with a quantity $u(x,t)$ that is real and a function of position $\mathbf{x}$ and time t. The quantity u could be temperature. The heat flux we assume is proportional to the gradient $\mathbf{F} = -K_T\nabla u$, with the minus sign so that heat flows from hot to cold. The constant K_T is the thermal conductivity. We conserve energy with a conservation law;

$$\rho c_P \partial_t u + \nabla \cdot \mathbf{F}_T = 0. \tag{24}$$

Here ρ is density, c_P is specific heat and ∂_t is short hand for $\frac{\partial}{\partial t}$. This gives the Heat equation

$$\partial_t u = \kappa\Delta u \tag{25}$$

with diffusion coefficient $\kappa = K_T/(\rho c_P)$.

A time dependent problem to solve might be something like this:

$$\begin{aligned} \partial_t u &= \kappa\Delta u \qquad \text{on } \Omega \\ u &= 0 \qquad \text{on } \partial\Omega \\ u(\mathbf{x}, t=0) &= \text{initial condition} \end{aligned} \tag{26}$$

Here Ω is the domain and $\partial\Omega$ is the boundary of the domain.

The PDE is second order so at least one quantity must be set on the boundary to specify a solution for the static problem with $\partial_t u = 0$.

In the above example, the temperature is set on the boundary and the boundary condition is called a Dirichlet boundary condition. The boundary is connected to a heat bath. Think of your domain floating in a lake that is at a fixed temperature because it is so big.

Instead of connecting a region of the boundary to a heat bath, we could blanket it with an insulator. In this case, there would be no heat flux through that portion of the boundary, giving

$$\nabla u \cdot \hat{\mathbf{n}} = 0 \tag{27}$$

where $\hat{\mathbf{n}}$ is a unit vector normal to the boundary. This type of boundary condition is known as a Neumann boundary condition. This type of boundary condition is sometimes written like this

$$\frac{\partial u}{\partial n} = 0. \tag{28}$$

More complicated boundary conditions involve setting the heat flux to a quantity that is sensitive to the temperature itself. For example a surface that is radiating to space has a heat flux that depends on temperature. You could use a black body formula to compute the rate that energy is lost.

3 Boundaries relevant for active matter

3.1 Bordertaxis

Bordertaxis is attraction to a surface. How would we describe that in a system of self-propelled particles? To an equation for the particle acceleration in particle based models we can add a position dependent force that is important near the boundary

$$\mathbf{F}_{boundary} = -\nabla U_b(\mathbf{x}) \tag{29}$$

where the potential energy function $U_b()$ is a function of distance from the boundary. For a continuum (PDE) model for active matter we can add a position dependent force term to an equation for the time dependent evolution of the velocity field or polarization vector or neumatic order parameter. The sign of the potential function would determine whether or not the boundary is attracting or repelling. Equivalently, for continuum descriptions of active matter, the potential energy function could be added to the free energy functional.

Bordertaxis occurs for microswimmers due to hydrodynamic forces (you can sometimes model motion a boundary, with an image particle that is on the other side of the boundary surface). A surface that has a coating could either repel or attract swimmers.

3.2 Orientation dependent attraction or repulsion to the boundary

The level of attraction or repulsion can depend upon the orientation of the active matter with respect to the boundary normal $\hat{\mathbf{n}}$. Suppose the medium orientation can be described with a vector $\mathbf{p}$ which we can call the polarization.

A possible boundary condition might be

$$\mathbf{p} \cdot \hat{\mathbf{n}} = 0$$

where $\mathbf{n}$ is the surface normal. This would mean the orientation vector $\mathbf{p}$ is perpendicular to the surface.

Another possible boundary condition could be

$$\mathbf{p} \times \hat{\mathbf{n}} = 0$$

giving polarization parallel to the boundary.

If attraction or repulsion to the boundary is dependent upon the distance to the boundary forces can dependent on a potential that is sensitive to the distance to the boundary and the orientation of the active material. For example, an angular dependent attraction or repulsion force can be described with a potential

$$\mathbf{U} = f(\mathbf{x})(\hat{\mathbf{n}} \cdot \hat{\mathbf{p}}) \tag{30}$$

that is both a function of position and orientation vector. Here $f(\mathbf{x})$ is a function of position which could just be a function of the distance to the boundary.

4 Immersed Boundary Methods

Immersed Boundary Methods (IBMs) are a broad category of methods employed when solving problems where nodes of the mesh do not necessarily fall along the domain boundary (i.e., a mesh that is not body-fitted). For example, evaluating a flow around a cylinder using a Cartesian mesh (for example, Figure 4). In such a system, evaluating flow parameters along the boundary is non-trivial and usually requires interpolation. In IBMs, points are usually classified into three categories at the boundary: first internal, interface, and first external. The first internal points are the points closest to the boundary outside the fluid. The interface points are the collection of nodes that lie along, or closest to the boundary. The first external points, then, are the collection of points denoting the first fluid cell adjacent to the boundary.

5 Loops and Ballooons

If we are working with a two-dimensional continuum system, then the boundary is a 1-dimensional object. If we are working with a three-dimensional continuum system, then

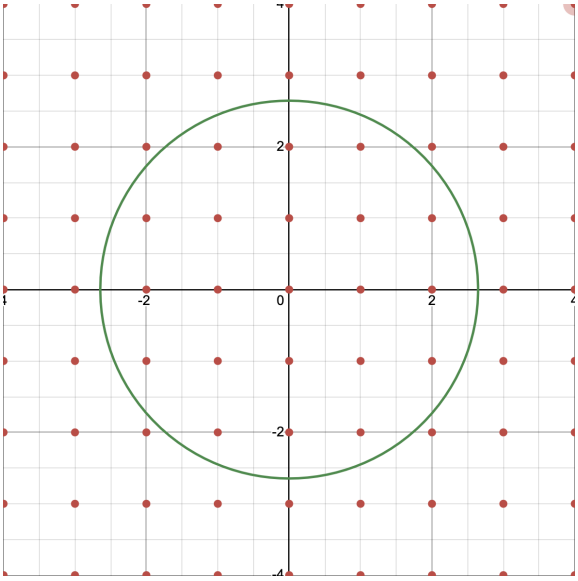

Figure 4: Spherical boundary on rectangular grid. No boundary points lie along grid nodes.

the boundary is a 2-dimensional object. The boundary could have mass, stretch, be under tension, and resist bending.

5.1 Loops

The two-dimensional space the loop resides in is $\mathbb{R}^2$ with a point $\mathbf{x} = (x, y)$. If we are interested in dynamics, our space also contains time t, also in $\mathbb{R}$.

Suppose there is an equilibrium loop configuration $\mathbf{X}_0(s)$ where s gives distance along the loop.

A point on the loop can be displaced from the equilibrium position by a distance w. We let w be a scalar in this discussion, but more generally it could be a vector. Since we use a scalar we can approximate the system with w a displacement radially away from the loop center.

The loop has a linear mass density λ.

The velocity of a particle on the loop $v = \frac{dw}{dt} = \dot{w}$.

The mass of an element of length ds on the loop is $dm = \lambda ds$.

One way to derive equations of motion is to define a Lagrangian density per unit length

and integrate it

$$L[w] = \int \mathcal{L}(w, \dot{w}, \partial_s w, \partial_s^2 w) ds \; dt$$
$$\mathcal{L} = \frac{\lambda}{2}(\dot{w})^2 - \frac{T}{2}(\partial_s w)^2 - \frac{B}{2}(\partial_s^2 w). \tag{31}$$

here T is the tension, and B is what is called the flexural rigidity (related to the Young's modulus and the second moment of area to take into account beam area in the context of Euler-Bernoulli beam theory). The kinetic energy per unit length is $\frac{\lambda}{2}(\dot{w})^2$.

Consider a curve $z = w(x)$ where w is small. What is the length of the curve? Each distance dx has length

$$ds = \sqrt{dx^2 + dz^2} = dx\sqrt{1 + \frac{dz^2}{dx^2}} \sim dx \left(1 + \frac{1}{2}\left(\frac{dw}{dx}\right)^2\right) \tag{32}$$

Terms in the energy that are squares of a gradient arise if energy is related to the length of the loop.

Note that the B term is an energy term that depends on the *curvature* of the displacement.

We integrate over both space and time because $\mathcal{L}$ is a function of both. If we were interested in a static system we would be minimizing potential energy and would not integrate over time.

The idea is that we take functional derivatives to find functions that minimize an integrated function called the Lagrangian. The resulting functions are the equations of motion. Energy can be conserved, not minimized, which why the potential energy is subtracted rather than added. If the Lagrangian is independent of time then Noether's theorem implies that energy would be a conserved quantity.

An alternative approach would be to compute forces on each element of the loop, rather than use *functional derivatives* and *calculus of variations*.

We take some functional derivatives

$$\frac{\partial \mathcal{L}}{\partial w} = 0$$
$$\frac{\partial \mathcal{L}}{\partial \dot{w}} = \lambda \dot{w}$$
$$\frac{\partial \mathcal{L}}{\partial \partial_s w} = -T\partial_s w$$
$$\frac{\partial \mathcal{L}}{\partial \partial_s^2 w} = -B\partial_s^2 w. \tag{33}$$

We expand the integral of the Lagrangian

$$\begin{aligned}\delta L &= \int \mathcal{L}(w+\delta, \dot{(}w+\delta), \partial_s(w+\delta), \partial_s^2(w+\delta))dsdt - \mathcal{L}ds\ dt \\ &= \int [\lambda \dot{w}\dot{\delta} - T\partial_s w \partial_s(\delta) - B\partial_s^2 w \partial_s^2 \delta]ds\ dt \\ &= \int [-\lambda \ddot{w} + T\partial_s^2 w - B\partial_s^4 w]\delta ds\ dt \end{aligned} \tag{34}$$

where we have integrated by parts and dropped all boundary terms. The equation of motion is

$$-\lambda \ddot{w} + T\partial_s^2 w - B\partial_s^4 w = 0. \tag{35}$$

If we set $B = 0$ we recover the wave equation. If we set $T = 0$ we recover the dynamical equation for an elastic beam that bends as in Euler-Bernoulli beam theory.

To allow longitudinal waves to propagate, we would need to allow displacements in directions parallel to the loop's rest state as well as perpendicular to it.

If we exert a transverse force (perpendicular to loop) per unit area $q(s,t)$ on the loop at a particular location, then equation 35 becomes

$$-\lambda \ddot{w} + T\partial_s^2 w - B\partial_s^4 w = q. \tag{36}$$

5.2 Balloons

Surface tension gives an energy that depends upon the surface area. Similarly if you have a membrane under tension, like a drum head, then you would have an energy that depends upon the surface area. The surface could resist bending and that would give an energy that depends on the curvature. A Lagrangian energy density would be surface are times surface tension that is in units of energy per unit area. We again assume that there is an equilibrium position and define a scalar quantity $w(x,y,z,t)$ that describe the displacement (perpendicular to the rest position) of each position. We generalize the Lagrangian density for the loop

$$L[w] = \int \mathcal{L}\left(\frac{\lambda}{2}\dot{w}^2 - \frac{\gamma}{2}(\nabla w)^2 - \frac{D}{2}(\Delta w)^2\right) dV\ dt \tag{37}$$

where λ is mass per unit area, γ is either surface tension and D is the flexural stiffness for a plate (as in homogenous, thin and equal thickness, Kirchhoff-Love plates).

We take some functional derivatives

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial w} &= 0 \\ \frac{\partial \mathcal{L}}{\partial \dot{w}} &= \lambda \dot{w} \\ \frac{\partial \mathcal{L}}{\partial \partial_i w} &= -\gamma \partial_i w \\ \frac{\partial \mathcal{L}}{\partial \partial^2_{ij} w} &= -D\Delta w \delta_{ij}. \end{aligned} \tag{38}$$

The last expression is found using $(\Delta w)^2 = (\sum_j \partial_{jj} w)(\sum_k \partial_{kk} w)$. When inserted into an expression for δL, integrating by parts and discarding boundary terms

$$-\lambda \ddot{w} + \gamma \Delta w - D\Delta^2 w = 0. \tag{39}$$

To compute the Laplacian at a particular point on the membrane, we could locally define a coordinate system. The membrane is not necessarily flat, so a generalization of the Laplacian operator, called the Laplace Beltrami operator can be compute.d Equivalently we can

Again if we exert a force per unit area $q(\mathbf{x}, t)$ at a point $\mathbf{x}$ on the membrane then equation 39 becomes

$$-\lambda \ddot{w} + \gamma \Delta w - D\Delta^2 w = q. \tag{40}$$

6 Questions and things to do

- 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 boundaries for some different reaction diffusion equations. Predict behavior and test predictions via numerical studies.
- Examine dynamics of defects near boundaries.
- Explore static boundary behavior in the biharmonic Swift-Hohenberg equation.
- Explore oscillating active mater PDEs.
- Try to make a 1d loop, in 2d space that exhibits waves in FEM.
- Try moving a boundary that is coupled to a PDE on a mesh.

- Why is phase not used as a variable in the common active matter PDEs?
- Try FEM models for some active matter systems on a mesh.
- Try FEM models for some active matter systems with interesting boundaries.
- Try knocking holes in a mesh by removing some triangles. Can posts in a rink be used to control the medium? There is a body of work with posts to cause clumps in self-propelled particle systems.
- Evolution of defects on boundary for 3D meshes. Topological surface properties? Skyrmions?
- Focus on/explore time dependent models and patterns near boundaries in those?
- Effect of boundaries on effective parameters.
- Pattern formation on curved surfaces with boundaries.
- Make a controllable muscle model (think of reagent parameters as free parameters? Couple motion to orientation?).
- defects in active oscillating mater (probably not much done).