Notes on Boundaries

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Contents

1 Brief Introduction to Fluids

Before discussing boundaries, we will give a brief introduction to fluid dynamics. This discussion is based on Part 5 of Modern Classical Physics by Thorne and Blanford, as well as the introduction to Principles of Astrophysical Fluid Dynamics by Clarke and Carswell.

1.1 The Fluid Approximation

The fluid approximation is a useful tool for predicting the dynamics of continuum systems. For the approximation, instead of dealing with the dynamics of individual particles, we work with "fluid parcels" over which we average to compute local quantities such as density, pressure, and temperature. For this approximation to hold, we require two scale conditions:

1. The length scale of the fluid parcel l_{parcel} is smaller than the scale over which our local properties vary. In other words, for a quantity q, $l_{parcel} \ll \frac{q}{|\nabla q|}$.
2. l_{parcel} is large enough to ignore statistical fluctuations between individual particles. In other words, parcel of volume l_{parcel}^3 has to contain many particles.

So, for a fluid we define the fluid parcel large enough to have robust averaging for our fluid quantities, but small enough such that these properties are constant over the scale of the parcel. For a fluid to be "collisional" (particles obey a Maxwellian), we additionally require that the average distance traveled between collisions, known as the mean free path λ, be smaller than the length scale of the fluid L. In other words, $\lambda \ll L$.

In fluid problems, we usually deal with fluid density ρ, pressure p, temperature T, bulk velocity u, and energy E. We evolve these variables using a collection of coupled partial differential equations describing conservation of mass, momentum and energy. Additionally, we take an equation of state which relates T, p, and ρ.

1.2 Conservation of Mass

We will use bold quantities to denote vectors. For density ρ contained within a volume Ω bounded by the surface $\partial\Omega$, the total mass M is given by $M = \int_\Omega \rho d\tau$. Then, the rate of change of mass in the volume is

$$\frac{\partial M}{\partial t} = \frac{\partial}{\partial t}\int_\Omega \rho d\tau = \int_\Omega \frac{\partial \rho}{\partial t} d\tau.$$

Additionally, the rate of change of mass within Ω is equal to the amount of mass leaving (or entering) through the surface $\partial\Omega$. This mass flux (per unit area) is given by $\rho\mathbf{u}$, so the total amount of mass leaving through the surface is $\int_{\partial\Omega} \rho\mathbf{u} \cdot d\mathbf{S}$. Through divergence theorem, this yields the equality

$$\int_\Omega \frac{\partial \rho}{\partial t} d\tau = -\int_{\partial\Omega} \rho\mathbf{u} \cdot d\mathbf{S} = -\int_\Omega \nabla \cdot (\rho\mathbf{u}) d\tau.$$

From this integral equation, we get our mass continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{1}$$

This equation can be recast using the Lagrangian derivative by expanding the second term in the above equation using the product rule. For a quantity Q, the Lagrangian (total) derivative is given by

$$\frac{dQ}{dt} = \frac{\partial Q}{\partial t} + (\mathbf{u} \cdot \nabla) Q.$$

With this definition, we can write

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} = \frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{u} = 0. \tag{2}$$

With the equation in this form, we can see that when $\nabla \cdot \mathbf{u} = 0$, the Lagrangian derivative is also zero. This is called incompressible, or divergence free, flow. Conservation of momentum and energy will be briefly addressed below, and more thoroughly discussed later.

1.3 Conservation of Momentum

Momentum conservation takes a similar form. The time rate of change of momentum density in some volume is equal to momentum flux through the bounding surface. Momentum flux can be written as the divergence of the stress tensor $\boldsymbol{\sigma}$:

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \boldsymbol{\sigma} = 0. \tag{3}$$

The components of the stress tensor can include viscous terms as well as pressure terms (both ram pressure and thermal pressure). The right hand side of the above equation can also include external forcing terms (for example, gravitational force), which will become relevant in our discussion of boundaries.

1.4 Energy Conservation

The energy equation is more complicated, but it boils down to the same formula: time rate of change of energy is equal to energy flux. For an ideal fluid, the energy has three terms: kinetic, internal energy of the system ϵ, and energy associated with an external potential ϕ, such as gravity. The energy U is thus

$$U = \rho(\frac{1}{2}\mathbf{u} \cdot \mathbf{u} + \epsilon + \phi). \tag{4}$$

Here, the first term is kinetic energy. The energy flux takes a similar form, given by

$$F = \rho \mathbf{u}(\frac{1}{2}\mathbf{u} \cdot \mathbf{u} + h + \phi) \tag{5}$$

where

$$h = \epsilon + \frac{P}{\rho} \tag{6}$$

is the enthalpy per unit mass. Enthalpy can be thought of as a measure of total system energy, usually written as $H = E+PV$ where E is the internal energy, P is the pressure, and V is the volume. So, it is internal energy plus energy from work done by thermal pressure. This can be found by applying the Legendre transform to the first law of thermodynamics. This equation is difficult to deal with an can sometimes be circumvented using an equation of state.

1.5 Equation of State

An equation of state (EOS) is an equation which relates state variables such as T, p, and ρ. In certain scenarios, this can be taken as the closure to the fluid equations instead of the energy equation. The simplest, and most famous equation of state, is the ideal gas law:

$$p = Nk_BT \tag{7}$$

where N is the number density and k_B is the Boltzmann constant. This equation of state is valid for a sufficiently dilute gas. Another common equation of state taken is a polytropic equation of state:

$$p = K\rho^{1+\frac{1}{n}} \tag{8}$$

where K is a proportionality constant and n is the polytropic index. This equation of state is relevant in many astrophysical systems and can be used to described stars in hydrostatic equilibrium.

2 Fluid/Boundary interactions

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

$$\partial_t(\rho\mathbf{u}) = -\nabla \cdot \boldsymbol{\sigma} \tag{9}$$

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 system, the stress tensor has components

$$\sigma_{ij} = p\delta_{ij} + \rho u_i u_j + \text{viscous terms} \tag{10}$$

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).

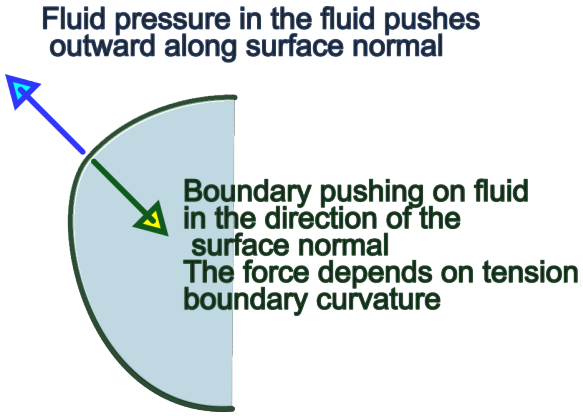

Figure 1: Our expectation for a fluid boundary surface interaction.

In terms of components and neglecting viscosity, equation 9 is equal to

$$\partial_t(\rho u_i) = -\sum_j \left[\partial_j p \delta_{ij} + \partial_j(\rho u_i u_j) + ...\right]. \tag{11}$$

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

The equation for conservation of mass

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

Conservation of mass along with equation 9 or 11 for conservation of momentum gives Euler's equation, and if viscous forces are taken into account we arrive at the Navier-Stokes equation

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla P}{\rho} + \nu \Delta \mathbf{u}. \tag{13}$$

Here ν is the kinematic viscosity and Δ, the Laplacian, is equal to ∇^2. Getting to the equation equation above from equation 11 just requires expanding terms in mass and momentum conservation using the product rule and careful bookkeeping of indices.

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

$$\int_\Omega \partial_t(\rho \mathbf{u})\ dV = -\int_\Omega \nabla \cdot \boldsymbol{\sigma}\ dV. \tag{14}$$

We use Gauss' law

$$\int_\Omega \partial_t(\rho \mathbf{u})\ dV = -\int_{\partial\Omega} \boldsymbol{\sigma} \cdot d\mathbf{A}. \tag{15}$$

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

$$\int_\Omega \partial_t(\rho u_i)\ dV = -\int_{\partial\Omega} \sum_j \sigma_{ij} dA_j. \tag{16}$$

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.

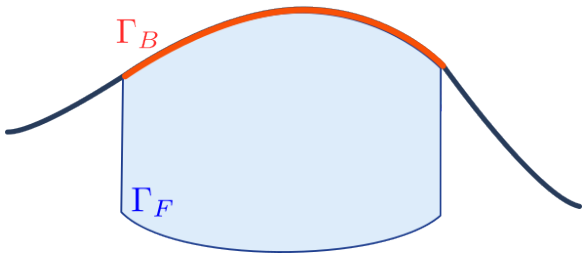

Figure 2: A fluid element that is up against a boundary.

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

$$\int_\Omega \partial_t(\rho \mathbf{u})\ dV + \int_{\Gamma_F+\Gamma_B} \boldsymbol{\sigma} \cdot d\mathbf{A} = \mathbf{F}_b. \tag{17}$$

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

$$\int_{\Gamma_B} \boldsymbol{\sigma} \cdot d\mathbf{A} \tag{18}$$

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)

$$\int_{\Gamma_B} p\ d\mathbf{A} + \rho\mathbf{u}(\mathbf{u} \cdot d\mathbf{A}). \tag{19}$$

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 19 vanishes and the force from the boundary onto the fluid must be

$$\mathbf{F}_b = -p \; d\mathbf{A}. \tag{20}$$

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.

2.1 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

$$\varepsilon = \frac{1}{2} \left(\nabla u + \nabla u^T \right) \tag{21}$$

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

$$\boldsymbol{\varepsilon} = \frac{1}{2} \left(\partial_i u_j + \partial_j u_i \right). \tag{22}$$

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

$$\boldsymbol{\sigma}_\nu = 2\mu\boldsymbol{\varepsilon} \tag{23}$$

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

$$\boldsymbol{\sigma}_\nu \cdot d\mathbf{A} = 2\mu dA(\partial_n \mathbf{u} + \nabla u_n) = -\mathbf{F}_{b,\nu}. \tag{24}$$

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.

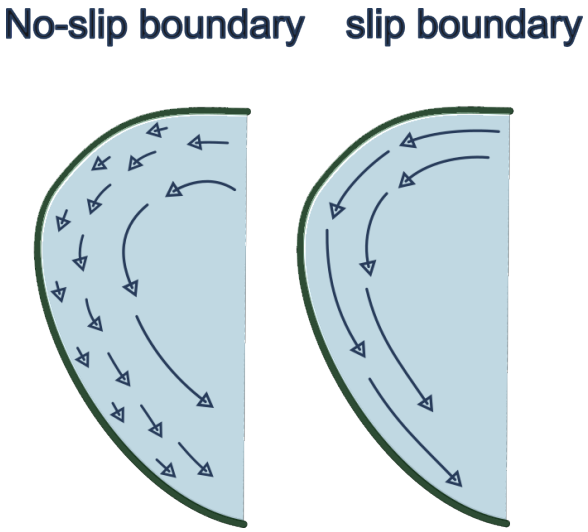

Figure 3: Illustration of a no-slip boundary on the left and one that allows motion right up against the boundary (on the right).

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

$$Re = \frac{\rho u L}{\mu} \tag{25}$$

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.

2.2 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

$$\mathbf{V}(\mathbf{s}, t) = \mathbf{u}(\mathbf{x}(\mathbf{s}, t)). \tag{26}$$

2.3 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

$$\mathbf{F} = \zeta_\perp \mathbf{v}_\perp + \zeta_\parallel \mathbf{v}_\parallel \tag{27}$$

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

2.4 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

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{v}. \tag{28}$$

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

$$\nabla p = \mu \Delta \mathbf{v} \tag{29}$$

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

$$\Delta \boldsymbol{\omega} = 0 \tag{30}$$

where $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is the **vorticity**. Equation 30 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

$$\Delta^2 \psi = 0 \tag{31}$$

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.

3 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;

$$\rho c_P \partial_t u + \nabla \cdot \mathbf{F}_T = 0. \tag{32}$$

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

$$\partial_t u = \kappa \Delta u \tag{33}$$

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

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

$$\begin{aligned} \partial_t u &= \kappa \Delta u \qquad \text{on } \Omega \\ u &= 0 \qquad \text{on } \partial\Omega \\ u(\mathbf{x}, t=0) &= \text{initial condition} \end{aligned} \tag{34}$$

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

$$\nabla u \cdot \hat{\mathbf{n}} = 0 \tag{35}$$

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

$$\frac{\partial u}{\partial n} = 0. \tag{36}$$

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.

4 Boundaries relevant for active matter

4.1 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

$$\mathbf{F}_{boundary} = -\nabla U_b(\mathbf{x}) \tag{37}$$

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.

4.2 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

$$\mathbf{U} = f(\mathbf{x})(\hat{\mathbf{n}} \cdot \hat{\mathbf{p}}) \tag{38}$$

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.

5 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

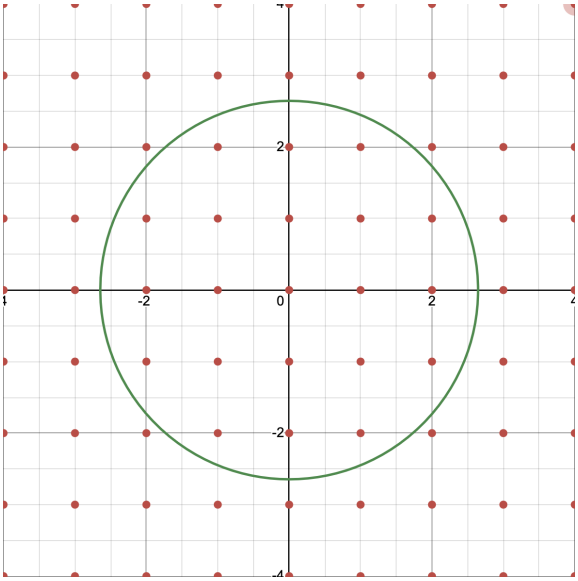

Figure 4: Spherical boundary on rectangular grid. No boundary points lie along grid nodes.

along the boundary is non-trivial and requires interpolation. In IBMs, this is commonly

done through point tagging. Points are 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 within the fluid. The first external points, then, are the collection of points denoting the first fluid cell adjacent to the boundary. Using an appropriate interpolation scheme, state parameters at boundary nodes can be estimated. Additionally, virtual forcing terms can be added to enforce boundary conditions, such as a no-slip condition. This methods are a computationally efficient way to solve flow problems on irregular geometries. Additionally, since re-meshing a domain is computationally expensive, this method is extremely useful for problems with moving boundaries. An example of this is given by Deng et al. in their 2006 paper.

6 Loops and Balloons

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

6.1 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 $u = \frac{dw}{dt} = \dot{w}$.

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 $\mathcal{L}$ per unit length and integrate it to create a Lagrangian $L[w]$;

$$L[w] = \int \mathcal{L}(w, \dot{w}, \partial_s w, \partial_s^2 w) ds \; dt$$

$$\mathcal{L} = \frac{\lambda}{2}(\dot{w})^2 - \frac{T}{2}(\partial_s w)^2 - \frac{B}{2}(\partial_s^2 w)^2 - q(s,t)w. \tag{39}$$

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 $\frac{\lambda}{2}(\dot{w})^2$. The function $q(s,t)$ is an applied force per unit length, applied in the direction perpendicular to the loop tangent so that it can cause a displacement w. Force times distance is work so q is multiplied by displacement w to give an energy density. The B term is an energy density term that depends on the *curvature* of the displacement. Conventionally the Lagrangian is $T - V$ which is kinetic energy subtracted by potential energy. That is why all terms are negative except the kinetic energy term.

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

$$ds = \sqrt{dx^2 + dz^2} = dx\sqrt{1 + \frac{dz^2}{dx^2}} \sim dx\left(1 + \frac{1}{2}\left(\frac{dw}{dx}\right)^2\right) \tag{40}$$

The term in the energy density $T(\partial_s w)^2$ that is the square of the derivative arises if energy density depends on length.

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

We take functional derivatives to find a function that minimizes the integrated function called the Lagrangian L. The resulting function is also the equations of motion. Energy $(T+V)$ can be conserved, not minimized, which why the potential energy is subtracted for the Lagrangian 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

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w} &= -q \\
\frac{\partial \mathcal{L}}{\partial \dot{w}} &= \lambda \dot{w} \\
\frac{\partial \mathcal{L}}{\partial \partial_s w} &= -T\partial_s w \\
\frac{\partial \mathcal{L}}{\partial \partial_s^2 w} &= -B\partial_s^2 w.
\end{aligned} \tag{41}$$

We expand the integral of the Lagrangian

$$\begin{aligned}
\delta L &= \int \mathcal{L}(w+\delta, \dot{(}w+\delta), \partial_s(w+\delta), \partial_s^2(w+\delta))dsdt - \mathcal{L}ds\ dt \\
&= \int [\lambda \dot{w}\dot{\delta} - T\partial_s w \partial_s(\delta) - B\partial_s^2 w \partial_s^2 \delta - q]ds\ dt \\
&= \int [-\lambda \ddot{w} + T\partial_s^2 w - B\partial_s^4 w - q]\delta ds\ dt
\end{aligned} \tag{42}$$

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

$$-\lambda\ddot{w} + T\partial_s^2 w - B\partial_s^4 w = q(s,t). \tag{43}$$

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.

6.2 Weak form of a PDE for a 1dimensional loop or segment

6.2.1 The wave equation

We first start with the wave equation so $B = 0$. We construct a velocity so we evolve two fields

$$\begin{aligned} \dot{w} &= u \\ \lambda\dot{u} &= T\partial_s^2 w - q(s,t). \end{aligned} \tag{44}$$

The weak form for the second PDE is

$$\int_\Omega \lambda\dot{u}v ds = \int_\Omega T(\partial_s^2 w)v ds - \int_\Omega qv ds \tag{45}$$

Integrating the first term on the right by parts

$$\int_\Omega \lambda\dot{u}v ds = T(\partial_s w)v\Big|_{\partial\Omega} - \int_\Omega T(\partial_s w)(\partial_s v)ds - \int_\Omega qv ds \tag{46}$$

for $v \in H^1$ with H^1 the Sobolev space containing functions v such that $|v|^2$ and $|\partial_s|^2$ have finite integrals over Ω.

For a loop, we don't have a boundary, so we could ignore the boundary term.

If we were working on a segment and using Dirichlet boundary conditions: We set the value of the field on then ends of the segment and only consider w in a space of functions that have our specified values on the boundary. We require the test functions v to vanish where w is specified, which in this case is on the ends of the segment.

If we were working on a segment and using Neumann boundary conditions: If $\partial_s w = 0$ on the ends of the segment, then the boundary condition can be neglected. In this case we don't restrict the class of test functions v and we don't add anything to the equation to solve.

If $\partial_s w \neq 0$ then we need to add a term to the equation we are solve taking into account the values on the boundary.

The space is restricted to a discrete set of values (vertices!). We restrict test and trial solutions to discrete values at these locations. The weak form of equation 46 is then turned into an operator (or matrix) equation (convert the gradient into an operator on the array of positions) which we would solve, updating w for each time step.

6.2.2 The bending wave equation including tension

We construct a velocity so we evolve two fields

$$\begin{aligned} \dot{w} &= u \\ \lambda \dot{u} &= T\partial_s^2 w - B(\partial_s^4 w) - q(s,t). \end{aligned} \tag{47}$$

The weak form for the second PDE is

$$\int_\Omega \lambda \dot{u} v ds = \int_\Omega \left[T(\partial_s^2 w) - B(\partial_s^4 w) - q \right] v ds. \tag{48}$$

We integrate by parts the term proportional to B

$$\begin{aligned} \int_\Omega (\partial_s^4 w) v ds &= (\partial_s^3 w) v \Big|_{\partial\Omega} - \int_\Omega (\partial_s^3 w)(\partial_s v) ds \\ &= \left[(\partial_s^3 w) v - (\partial_s^2 w)(\partial_s v) \right] \Big|_{\partial\Omega} + \int_\Omega (\partial_s^2 w)(\partial_s^2 v) ds. \end{aligned} \tag{49}$$

We insert this into equation 48

$$\begin{aligned} \int_\Omega \lambda \dot{u} v ds = \int_\Omega &\left[T(\partial_s^2 w) v - qv - B(\partial_s^2 w)(\partial_s^2 v) \right] ds \\ &- \left[(\partial_s^3 w) v - (\partial_s^2 w)(\partial_s v) \right] \Big|_{\partial\Omega}. \end{aligned} \tag{50}$$

For PDEs with 4th order derivatives, one can use elements that are quadratic and contain both field and gradient values. The test function v is in Sobolov space H^2. We can compute gradients of the trial (for w) and test functions (v). The terms with first and second order derivatives are inner products and again we can think of the problem as solving a linear (i.e., matrix) equation.

The analogy of the Dirichlet boundary condition is restricting the trial solution space to have specific values of w and $\partial_s w$ on the ends of the segment. If w is set on the boundary then the beam or membrane is *fixed*. If the gradient is set on the boundary, then the boundary is *clamped*.

The analogy for the Neumann boundary condition involves evaluating the two boundary terms (which depend upon the Laplacian and third order derivatives) when solving the system. The Laplacian term gives what is called the bending moment. The derivative of the *bending moment* gives the *shear stress* on the boundary.

6.3 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. A Lagrangian energy density would be surface area times surface tension that is in units of energy per unit area. The surface could resist bending and that would give an energy that depends on the curvature. We again assume that there is an equilibrium position and define a scalar quantity $w(x, y, z, t)$ that describes the displacement (perpendicular to the rest position) of each position on the balloon. A position on the surface $\mathbf{s}$ in two dimensions. For the gradient we would take the components in the tangent space at a point. We generalize the Lagrangian density for the loop but not integrating over the surface area of the balloon

$$\begin{aligned} L[w] &= \int dA\ dt\ \mathcal{L}(w, \dot{w}, \nabla w, \Delta w) \\ \mathcal{L} &= \frac{\lambda}{2}\dot{w}^2 - \frac{\gamma}{2}(\nabla w)^2 - \frac{D}{2}(\Delta w)^2 - qw. \end{aligned} \tag{51}$$

Here λ is mass per unit area, γ is either surface tension or just tension in the case of a drum membrane and D is the flexural stiffness for a plate (as in homogenous, thin and equal thickness, Kirchhoff-Love plates). The function $q(\mathbf{s}, t)$ is the applied force per unit area.

We take some functional derivatives

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial w} &= -q \\ \frac{\partial \mathcal{L}}{\partial \dot{w}} &= \lambda \dot{w} \\ \frac{\partial \mathcal{L}}{\partial \partial_i w} &= -\gamma \partial_i w \\ \frac{\partial \mathcal{L}}{\partial \partial^2_{ij} w} &= -D\Delta w \delta_{ij}. \end{aligned} \tag{52}$$

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

$$-\lambda \ddot{w} + \gamma \Delta w - D\Delta^2 w - q(\mathbf{s}, t) = 0. \tag{53}$$

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 used.