

The finite element method for the Navier-Stokes equations

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Chapter 1

Mechanics

Corpus omne perseverare in statu suo quiescendi vel movendi uniformiter in directum, nisi quatenus a viribus impressis cogitur statum suum mutare.

Mutationem motus proportionalem esse vi motrici impressae, & fieri secundum lineam rectam qua vis illa imprimitur.

Actioni contrariam semper & aequalem esse reactionem: sive corporum duorum actiones in se mutuo semper esse aequales & in partes contrarias dirigi.

Newton [1]

1.1 Newton's laws of motion

Newton's three laws, namely those of inertia, force, and equilibrium, have found universal success in application to mechanical systems such as the pendulum, the motion of a rigid body, the evolution of a bending beam, and, as we shall see, the motion of a fluid. *Mechanics* could be thought of as the study of physical motion, but the word “physical” might be misleading. Newton's principles are mathematical in nature, applicable to the study of motion in a general sense as some unambiguously measurable state which evolves in time.

1.1.1 Symmetry, momenta, and inertia

Mechanics as a theory of physical motion will require a definition of physical motion. A first attempt might be to posit that “physical states” are representable as points in a finite-dimensional manifold, which we call the configuration space C , which is the case for typical notions of state such as the two angles in a double pendulum, or the position and orientation of a rigid body. We might define a motion as a continuous time-parameterised curve

$$\gamma : [t_1, t_2] \rightarrow C.$$

We start in the middle:

$$\text{Total force} = \text{change of momentum.} \tag{1.1}$$

In this form, Newton's second law of motion states that a (non-explanatory) measurement of change of momentum will be called “force”.

1.2 The Euler-Lagrange equations: From $F = ma$ to $\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} = 0$

1.2.1 A Lagrangian of a mechanical system

Force is an intensive measurement of the change in momentum. In the language of calculus,

$$\int_{s_1}^{s_2} F dt = \mathcal{P}(s_2) - \mathcal{P}(s_1) \quad (1.2)$$

for all time subintervals $[s_1, s_2] \subset [t_1, t_2]$. If we restrict F to be conservative and a function only of position q , then we may let $F = -\frac{\partial V}{\partial q}$ for some potential function V . Suppose also that $\mathcal{P} = \frac{\partial T}{\partial \dot{q}}$ for some potential function (called the “kinetic energy”) independent of position q . We then define a Lagrangian of the mechanical system to be

$$\mathcal{L}(q, \dot{q}, t) = T(\dot{q}, t) - V(q, t) = \text{kinetic} - \text{potential}.$$

By definition, we have the force equation (1.2) as

$$-\int_{s_1}^{s_2} \frac{\partial \mathcal{L}}{\partial q} dt = \frac{\partial \mathcal{L}}{\partial \dot{q}}(s_2) - \frac{\partial \mathcal{L}}{\partial \dot{q}}(s_1).$$

The step toward the calculus of variations (—)

$$\int_{s_1}^{s_2} \frac{\partial \mathcal{L}}{\partial q} h dt + \int_{s_1}^{s_2} \frac{\partial \mathcal{L}}{\partial \dot{q}} \frac{dh}{dt} dt = 0 \quad \equiv \quad \left\langle \frac{\partial \mathcal{L}}{\partial q}, h \right\rangle + \left\langle \frac{\partial \mathcal{L}}{\partial \dot{q}}, \frac{dh}{dt} \right\rangle = 0. \quad (1.3)$$

Adjointness of differential operator $\frac{d}{dt}$ to $-\frac{d}{dt}$, and integration by parts. (—) By linearity, we then get the reformulation of (1.3) as

$$\left\langle \frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}}, h \right\rangle = 0$$

for all perturbation functions h .

1.2.2 The first variation of a functional

In the calculus of variations, $\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}}$ is an instance of the *Gâteaux derivative*, also called the “first variation” of the functional

$$S[q] := \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}, t) dt.$$

The first variation measures response of the value of S , called the *action*, to perturbations of the (differentiable) input function q , and is denoted

$$\frac{\delta S}{\delta q(t)} := \frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}}. \quad (1.4)$$

The first variation is linear in the perturbation function, and so another term for the Gâteaux derivative could be “functional gradient”. Setting this to zero gives the Euler-Lagrange equations, and the practice of determining trajectories of motions as stationary curves of the action is called the “principle of stationary action”.

1.2.3 From the Lagrangian to the equations of motion

In the framework of Lagrangian mechanics, $\mathcal{P} := \frac{\partial \mathcal{L}}{\partial \dot{q}}$ is the momentum. If there are d degrees of freedom in the mechanical system, and we suppose that q_1, \dots, q_d are (local) variables of state, then we say that $\mathcal{P}_i := \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$ are *conjugate* to the q_i .

(—) By inducing the equations of motion by a Lagrangian, we get systems with a “physical interpretation” with “physically meaningful” force measurements.

1.2.4 Why —?

These variational ideas appear because, no matter if our configuration space is finite-dimensional, time forms a continuum, and therefore if we globally consider the calculus of the motion as a whole, it must be a “variational” calculus. (—)

(—) Physical process, conservation laws, conservative forces (hint at thermodynamics limiting the range of stress tensors?)

When we consider mechanical models of continuum processes, we will see that these same ideas appear in the spatial dimensions too. A variational understanding of a continuum mechanics model leads very easily to a class of methods called Galerkin methods for solving the corresponding (PDE) equations of motion.

Chapter 2

Continuum mechanics

2.1 Transport

Before considering continuum processes in the framework of Newtonian and Lagrangian mechanics, we will look at a fundamental notion of a “motion” of a point in a function space. Many continuum models in physics, such as the heat equation, Maxwell’s equations, and the equations of fluid motion, are formed by *conservation equations*. These laws posit that the evolution of the state (represented by a function) is due to the transport of the quantity that the function measures, which is either pushed around (by some flux either predetermined or dependent on the current state) or created and destroyed at sources and sinks.

(figure of some manifold embedded in space, and some vector field pushing quantity around)

We consider here the transport of quantities (scalar, vector, and tensor) on a general finite-dimensional manifold M , colloquially called “the continuum”. All transporting vector fields (or flux functions) are considered to be tangent to this manifold M .

2.1.1 Continuity equations and conservation laws

The integral form of a continuity equation

Consider some spatial quantity ϕ on M and a flux function j which by which this quantity flows around M . For clarity, we will begin by specializing ϕ to be a scalar, although later we will find it useful to transport vector quantities such as momentum. By definition we want this flux function to just push quantity around, and not create or destroy it: the creation and destruction of quantity is determined by some arbitrary source function s (of the same kind as ϕ). These variables are related by the conservation condition

$$\frac{d}{dt} \int_{\Omega_0} \phi \, dx = \int_{\Omega_0} s \, dx + \int_{\partial\Omega_0} \phi j \cdot (-\hat{n}) \, dx \quad (2.1)$$

for arbitrary control volumes Ω_0 in the continuum. The term $-\hat{n}$ denotes the inward-pointing normal to the boundary of the control volume. This simply says that the change in the total quantity in the fixed control volume is accounted for exactly by that quantity pushed through the boundary by the flux function j , and the internal sources and sinks of quantity s .

The differential form of a continuity equation

A common technique in continuum modelling is the use of Stokes' theorem to simplify integral expressions. Equation (2.1) becomes

$$\frac{\partial \phi}{\partial t} = s - \nabla \cdot (\phi j) \quad (2.2)$$

assuming that ϕj is sufficiently differentiable such that the limiting integral exists. It should be noted that Stokes' theorem and its specialisations are really *definitions* of pointwise quantities such as the divergence and curl as limits of these integral expressions for arbitrarily small regions. Continuity relations are most naturally expressed in form (2.1), while the form (2.2) may be more useful for techniques such as finite differences. For example, it is a theorem of Gauss that in Euclidean space ($M = \mathbb{R}^3$) we have

$$\nabla \cdot j = \frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} + \frac{\partial j_z}{\partial z}, \quad (2.3)$$

and we get (2.2) in the form

$$\frac{\partial \phi}{\partial t} = s - \nabla \phi \cdot j - \phi \left(\frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} + \frac{\partial j_z}{\partial z} \right), \quad (2.4)$$

by the product rule. As one equation in a system of PDEs, (2.4) is readily discretised by finite differences. For example, using forward difference in time and central differences in space, our discrete scheme is

$$\begin{aligned} \frac{\phi(t + \Delta t) - \phi(t)}{\Delta t} = s - & \frac{\phi(\hat{x} + e_1 \Delta x/2) - \phi(\hat{x} - e_1 \Delta x/2)}{\Delta x} j_x \\ & - \frac{\phi(\hat{x} + e_2 \Delta y/2) - \phi(\hat{x} - e_2 \Delta y/2)}{\Delta y} j_y \\ & - \frac{\phi(\hat{x} + e_3 \Delta z/2) - \phi(\hat{x} - e_3 \Delta z/2)}{\Delta z} j_z \\ & - \frac{j_x(\hat{x} + e_1 \Delta x/2) - j_x(\hat{x} - e_1 \Delta x/2)}{\Delta x} \phi \\ & - \frac{j_y(\hat{x} + e_2 \Delta y/2) - j_y(\hat{x} - e_2 \Delta y/2)}{\Delta y} \phi \\ & - \frac{j_z(\hat{x} + e_3 \Delta z/2) - j_z(\hat{x} - e_3 \Delta z/2)}{\Delta z} \phi \end{aligned} \quad (2.5)$$

for e_1, e_2, e_3 the standard basis vectors in \mathbb{R}^3 . Later, when we discuss numerical methods for solving continuum models, we will not take this route. The methods of interest, *Galerkin* methods, work naturally with the integral form (2.1). It will be seen later that some constructions in the presentation of Galerkin methods, such as the “weak form” of a PDE, simply undo the differentialisation of the original integral form of physical PDEs.

2.1.2 The Reynolds transport theorem

The integral form of Reynolds transport

With our integral formulation of a continuity relation (2.1), the control volume Ω_0 is fixed. We may change our perspective by considering, in addition to the flux function j (which transports quantity ϕ), another vector field \hat{u} which will transport our control volume Ω_0 . The rate of change of some time-dependent quantity γ in this *moving* control volume is expressed as

$$\frac{d}{dt} \int_{\Omega_0(t)} \gamma \, dx, \quad (2.6)$$

where $\Omega_0(t)$ implicitly denotes that Ω_0 is being transported under the flow of \hat{u} . Clearly, this rate of change of quantity γ is due to the motion of the control volume,

(a picture of positive and negative contributions at the boundary)

as well as internal changes of γ inside the (fixed) control volume. The formal expression of these contributions to the rate of change (2.6) is

$$\left. \frac{d}{dt} \left[\int_{\Omega_0(t)} \gamma dx \right] \right|_{t=0} = \int_{\Omega_0(0)} \frac{\partial \gamma}{\partial t} dx + \int_{\partial \Omega_0(0)} \gamma \hat{u} \cdot \hat{n} dx. \quad (2.7)$$

This result is called the *Reynolds transport theorem*, a generalisation of Feynman’s popularised “differentiation under the integral sign” [10], otherwise named the Leibniz integral rule. See, for example, [8] for a formal derivation of (2.7).

The differential form of Reynolds transport

In the limit, with the routine application of Stokes’ theorem, we can differentialise (2.7) to get

$$\left. \frac{d}{dt} \left[\int_{\Omega_0(t)} \gamma dx \right] \right|_{t=0} \longrightarrow \frac{\partial \gamma}{\partial t} + \nabla \cdot (\gamma \hat{u}), \quad (2.8)$$

as Ω_0 becomes small. The right-hand-side of (2.8) measures the change in volume of a quantity when a small control volume around the point of evaluation is moved, expanded or contracted by the flow field \hat{u} .

Reynolds transport applied to a continuity equation

Letting our quantity γ in (2.7) be the quantity ϕ transported by flux function j , described in continuity equation (2.1), we get a specialised form of the Reynolds transport theorem for continuity equations. Term $\frac{\partial \gamma}{\partial t}$ in (2.7) becomes $\frac{\partial \phi}{\partial t}$ in the differential form of the continuity equation (2.2), giving

$$\begin{aligned} \left. \frac{d}{dt} \left[\int_{\Omega_0(t)} \phi dx \right] \right|_{t=0} &= \int_{\Omega_0(0)} -\nabla \cdot (\phi j) + s dx + \int_{\partial \Omega_0(0)} \phi \hat{u} \cdot \hat{n} dx \\ &= \int_{\Omega_0(0)} s dx + \int_{\partial \Omega_0(0)} \phi (\hat{u} - j) \cdot \hat{n} dx \end{aligned} \quad (2.9)$$

by Stokes’ theorem. This has a clear interpretation. The $\hat{u} - j$ term is due to us wanting to measure the contributions to the total ϕ due to the moving boundary of Ω_0 , where the motion that matters is *relative* to the flux of the quantity j . Specifically, if we move the control volume by the same flux function j (letting $\hat{u} = j$), we get

$$\left. \frac{d}{dt} \left[\int_{\Omega_0(t)} \phi dx \right] \right|_{t=0} = \int_{\Omega_0(0)} s dx. \quad (2.10)$$

In fact, (2.10) is just another form for the conservation law (2.1), where the “frame of reference” for measurement of ϕ follows the transport of ϕ . This simply means that as we follow some volume of quantity original situated in Ω_0 , a conservation law posits that the only change detected is due to the source function s . In differential form (2.10) becomes

$$\frac{\partial \gamma}{\partial t} + \nabla \cdot (\gamma \hat{u}) = s, \quad (2.11)$$

a succinct equivalent to (2.2). The idea of following the flow while making measurements is called the *Lagrangian* perspective, in contrast to the *Eulerian*, fixed, perspective.

2.1.3 Incompressible and compressible transport

Analogous to constraints on the motion of a finite mechanical system, we can constrain possible movement of our continuous quantity to *incompressible transport*. Much like how, in the framework of Lagrangian mechanics, constraints on motion are implicitly enforced by strong “virtual forces”, constraining transport to be non-compressing will lead to the notion of *pressure*, when we later consider the dynamics of the continuum.

Incompressibility

Incompressibility of control volumes gives a constraint on the form of a flux function j . We call this constrained flux function j non-compressing. By incompressibility we mean that a control volume being transported by j will have constant volume. While j may transport other quantities, we express incompressibility by requiring the flux function to transport a constant “volume quantity” with a corresponding null source function,

$$\phi_{\text{vol}} = 1, \quad s_{\text{vol}} = 0.$$

The corresponding conservation law, in differential form (2.2), is

$$\frac{\partial \phi_{\text{vol}}}{\partial t} = -\nabla \cdot (\phi_{\text{vol}} j) + s_{\text{vol}} \quad \Rightarrow \quad \nabla \cdot j = 0. \quad (2.12)$$

This is our non-compressing constraint on j , and has a clear interpretation, as there is a non-zero divergence of j if and only if there is an inward or outward flux which would contract or expand a transported control volume.

The material derivative

We define here a differential operator which will be useful later. Assuming an non-compressing flux function j which transports quantity ϕ , the “convective derivative” in (2.11) following a control volume becomes

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi j) = \frac{\partial \phi}{\partial t} + j \cdot \nabla \phi + \cancel{\phi \nabla \cdot j}. \quad (2.13)$$

We define the *material derivative* to be

$$\frac{D}{Dt} := \frac{\partial}{\partial t} + j \cdot \nabla. \quad (2.14)$$

It is a convention to leave the vector field j implicit, as material derivatives are usually taken with respect to some unambiguous velocity field. The material derivative may be taken with respect to a compressing flux j , in which case it measures change from the perspective of an ideal point mass with no extent under the flow of j . As j has no extent, it can not expand under the flow of j .

(figure of a point mass flowing along a scalar field, and a mass with extent being compressed)

2.1.4 Transport of vector and tensor quantities

All previous discussion on the transport of scalar quantities applies trivially to vector and tensor quantities. This will soonest be of use in the discussion of conservation of linear momentum, a vector quantity. However, some notational discussion is needed in order to establish differentialised forms of continuity equations and the Reynolds transport theorem.

Reynolds transport of vector and tensor quantities

For a general tensor quantity Γ , the integral form of Reynolds transport (2.7) is trivially

$$\frac{d}{dt} \left[\int_{\Omega_0(t)} \Gamma \, dx \right] \Big|_{t=0} = \int_{\Omega_0(0)} \frac{\partial \Gamma}{\partial t} \, dx + \int_{\partial \Omega_0(0)} \Gamma (\hat{u} \cdot \hat{n}) \, dx. \quad (2.15)$$

The step to the differential form (2.8), however, needs some thought as rearranging

$$“\Gamma (\hat{u} \cdot \hat{n}) = (\Gamma \hat{u}) \cdot \hat{n}”$$

in order to apply the divergence theorem makes no sense. However, the divergence $\nabla \cdot$ was *defined* to evaluate the limit of this boundary integral for arbitrarily small Ω_0 . We therefore have a natural generalisation of the divergence for arbitrary tensors Ψ , as the limit of the boundary integral of the *contraction* of Ψ with the outward normal \hat{n} (which is a contravariant vector). The divergence of a rank n tensor is then a rank $n - 1$ tensor,

$$\int_{\Omega_0} \nabla \cdot \Psi \, dx := \int_{\partial \Omega_0} \Psi : \hat{n} \, dx. \quad (2.16)$$

We can then rewrite $\Gamma (\hat{u} \cdot \hat{n})$ in (2.15) as

$$\Gamma (\hat{u} \cdot \hat{n}) = (\Gamma \otimes \hat{u}) : \hat{n},$$

where the tensor product \otimes “defers contraction” of \hat{u} with \hat{n} , by storing it as a component of product tensor $\Gamma \otimes \hat{u}$. This leads to a differentialisation of (2.15),

$$\frac{d_{\hat{u}} \Gamma}{d_{\hat{u}} t} = \frac{\partial \Gamma}{\partial t} + \nabla \cdot (\Gamma \otimes \hat{u}). \quad (2.17)$$

Conservation equations for vector and tensor quantities

With the previous ideas from tensor algebra, it will be easy to describe continuity relations for transport of tensors. The integral form of the scalar continuity equation (2.1), generalised to transported tensor Φ , trivially becomes

$$\frac{d}{dt} \int_{\Omega_0} \Phi \, dx = \int_{\partial \Omega_0} \Phi (j \cdot (-\hat{n})) \, dx + \int_{\Omega_0} s \, dx. \quad (2.18)$$

By the same tensor algebra as above we have

$$\Phi (j \cdot (-\hat{n})) = -(\Phi \otimes j) : \hat{n},$$

giving (2.18) differentialised as

$$\frac{\partial \Phi}{\partial t} = -\nabla \cdot (\Phi \otimes j) + s. \quad (2.19)$$

2.2 The kinematics of the continuum

Transport equations are just one notion of “physical motion” in a continuum model. These transport equations, with prescribed flux and source functions, determine a continuous process on a fixed domain M . These conserved quantities are time-varying maps from M to some measurement space of scalars or tensors. Each map is a component of the total configuration space C , which clearly must be infinite-dimensional. We now consider another component of C which will let us model a physical domain with alterable shape. In our discussion we will consider a fixed time interval $[t_1, t_2]$ in which our physical motions will take place.

2.2.1 Position maps

We may consider the manifold M as the parametric domain of some points living in an ambient manifold N . We will call this the “position map”

$$y : M \times [t_1, t_2] \rightarrow N.$$

In general, y needs not be continuous, differentiable, or invertible. These restrictions are only introduced in accord to the physical meaning of the position map. For example, models of small beam deflections may require continuity, and invertibility to prevent self-intersections.

(figure of abstract square domain mapping to a bent beam, and a figure of a map from a reference configuration to itself.)

As an example, suppose we are modelling the heat distribution of a 2D beam supporting a point load which is also a heat source. We could model the beam geometry as a smooth invertible map $y : [0, 1]^2 \rightarrow \mathbb{R}^2$, letting $M = [0, 1]^2$ and $N = \mathbb{R}^2$. The heat distribution on the beam could be represented by a function $h : M \rightarrow \mathbb{R}$, and a heat flux function j could be pulled back to M from N .

(picture of this)

Although this model is so far hopelessly incomplete, we can see that position maps and transport equations are fundamental tools used for modelling the *geometry* of a problem.

2.2.2 Velocity

As in the mechanics of a particle, each component of our state $q \in C$ will have a corresponding velocity which “generates” a physical motion of that component. In the case of the position map $y : M \times [t_1, t_2] \rightarrow N$, the velocity will be given by a vector in the tangent space of N at $y(x)$ for each parameter $x \in M$. This vector field is denoted \dot{y} . This is the *Lagrangian* description of motion. We will find it useful to instead use the *Eulerian* description, where we measure the velocity of the position map in the position domain N . Formally we denote this Eulerian velocity by the letter u , ubiquitous in fluid mechanics, and let

$$u(y, t) := \dot{y}(y^{-1}(y, t), t) \quad \text{for all valid } y \in N.$$

(draw this)

For some transported scalar quantity $\phi : M \times [t_1, t_2] \rightarrow \mathbb{R}$, the tangent space at each point of \mathbb{R} is \mathbb{R} , and therefore our velocity is represented by a scalar function $\frac{\partial \phi}{\partial t}$ giving local change in time of $\phi(x)$ for each $x \in M$.

(draw this)

We may denote our total velocities as a state variable \dot{q} . When we have state q , the corresponding velocity \dot{q} will be in the tangent space of C at q , denoted $T_q C$. We can then define the space of velocities as the *tangent bundle* of the configuration space,

$$TC = \bigcup_{q \in C} T_q C.$$

2.2.3 The deformation and velocity gradients

We may think of the mechanics of a particle as a special case of our continuum model, where M is a single point. In this case we have only one $x \in M$, so we cannot vary x . However, for a continuum parameter domain M we can take derivatives with respect to our parameter as well as time. We can extract important geometric/kinematic information from the spatial derivatives of our position map y .

The deformation gradient

The gradient of the position map y with respect to parameter $x \in M$ is called the *deformation gradient*

$$\nabla y. \quad (2.20)$$

The deformation gradient is equivalent to the *Jacobian matrix*, used to compute the *pushforward* of tangent vectors under the displacement map.

(draw this)

The determinant of the Jacobian matrix is usually denoted $J = \det(\nabla y)$, and is called the Jacobian.

The velocity gradient

Letting u be our Eulerian velocity as defined above, we may express the position map through an ODE,

$$\frac{d}{dt}y(x, t) = u(y(x, t), t), \quad y(x, 0) = y_0(x). \quad (2.21)$$

It is common, especially in flow problems, to let M be a subset of N which is the “initial geometry”. In this case we could let the initial position map be the identity map

$$y_0(x) = x \in M \subset N.$$

For example, given an initial disc in \mathbb{R}^2 , we may prescribe a constant Eulerian velocity field u and see how the original disc is “mixed”.

(draw this)

We can see that, in this case, it is meaningful to take spatial gradients in (2.21) to derive an ODE for the deformation gradient ∇y :

$$\nabla \frac{d}{dt}y(x, t) = \nabla u(y(x, t), t), \quad \nabla y(x, 0) = I, \quad (2.22)$$

where I is the identity tensor. This is easily visualised.

(draw this)

We can see that the term ∇u is a “differential generator” of the deformation gradient. We call ∇u , the spatial gradient of the Eulerian velocity, the *velocity gradient*.

2.3 The dynamics of the continuum

2.3.1 Conservation of mass

We will take for granted that there is some initial mass density function $\rho_0 : M \rightarrow \mathbb{R}^+$ which we would like to conserve.

The Lagrangian form of mass conservation

As the position map y evolves, for example under the action of Eulerian velocity field u in the ODE (2.21), we would like a mass density function $\rho : N \rightarrow \mathbb{R}^+$ to be greater if the position map “compresses” the material, and smaller if it “stretches” the material. Our aim is that the total mass measured in a control volume of N is the same as in its initial configuration. We can express this by the integral equation

$$\int_{\Omega_0} \rho_0(x) dx = \int_{y(\Omega_0, t)} \rho(y, t) dy, \quad (2.23)$$

where $y(\Omega_0, t)$ denotes the domain pushed forward by the position map. By the usual change of variables formula we have

$$\int_{\Omega_0} \rho_0(x) dx = \int_{\Omega_0} \det(\nabla y) \rho(y(x, t), t) dx, \quad (2.24)$$

where $J = \det(\nabla y)$ is the Jacobian, measuring the local change in the volume element due to the change of variables.

(draw this)

As (2.24) must hold identically for all Ω_0 , we have the localised conservation law

$$\rho_0 = \det(\nabla y) \rho. \quad (2.25)$$

The Eulerian form of mass conservation

Conservation law (2.25) is simple. However, it is given in terms of absolute deformation gradient ∇y . Instead of asking how mass is distributed in comparison to its initial configuration, we can ask how mass is transported by u . This gives an instance of the continuity equation (2.1), where we have no source:

$$\frac{d}{dt} \int_{\Omega_0} \rho dx + \int_{\partial\Omega_0} \rho u \cdot \hat{n} dx = 0. \quad (2.26)$$

With application of Stokes' theorem we have

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0. \quad (2.27)$$

Following [8], there is a more geometrical statement of this equation, which will be useful when we discuss “material points” By a divergence product rule (2.27) is equivalent to

$$\frac{\partial \rho}{\partial t} + u \cdot \nabla \rho + \rho \nabla \cdot u = 0 \quad \Rightarrow \quad \frac{D\rho}{Dt} = -\rho \nabla \cdot u, \quad (2.28)$$

where $\frac{D}{Dt}$ is the material derivative as defined in (2.14).

2.3.2 Conservation of linear momentum

If we conserve the linear momentum ρu , a “quantity of motion”, under the flow of u , then we get a continuity equation

$$\frac{d}{dt} \left[\int_{\Omega_0(t)} \rho u \, dx \right] \Big|_{t=0} = \int_{\Omega_0(0)} \rho g \, dx + \int_{\partial\Omega_0(0)} \hat{t} \, dx, \quad (2.29)$$

a specific realisation of the Lagrangian continuity equation (2.10). The Lagrangian perspective is convenient as it allows us to factor out certain forces on a moving piece of material. The term g is a regular body force per unit mass, where ρg corresponds to the source term s in (2.10). The boundary term involving \hat{t} , however, has no analogue in the scalar continuity equation (2.10). This vector term \hat{t} is called the *traction* in continuum mechanics, and measures a local force exerted across the boundary of the control volume due to the immediately adjacent material.

The Euler-Cauchy stress principle

Clearly, in accord with Newton, we would like that two Ω_0 and Ω'_0 which share a boundary element should have equal and opposite tractions across that boundary element. Since the normal \hat{n} represents a boundary element, and is negative for the opposite element, if \hat{t} is linear in \hat{n} we have this required property. We can then let (2.29) become

$$\frac{d}{dt} \left[\int_{\Omega_0(t)} \rho u \, dx \right] \Big|_{t=0} = \int_{\Omega_0(0)} \rho g \, dx + \int_{\partial\Omega_0(0)} \sigma : \hat{n} \, dx \quad (2.30)$$

where σ is termed the *Cauchy stress tensor*.

Differentializing the Cauchy momentum equation

By application of the Reynolds transport theorem (2.15) to (2.30) we get

$$\int_{\Omega_0(0)} \frac{\partial(\rho u)}{\partial t} \, dx + \int_{\partial\Omega_0(0)} \rho u (u \cdot \hat{n}) \, dx = \int_{\Omega_0(0)} \rho g \, dx + \int_{\partial\Omega_0(0)} \sigma : \hat{n} \, dx. \quad (2.31)$$

Differentializing (2.31), by our previously derived tensor identities, gives

$$\frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u \otimes u) = \rho g + \nabla \cdot \sigma. \quad (2.32)$$

This is called the *conservative form* of the Cauchy momentum equation. We can derive another, possibly more convenient form of (2.32) using the fact that ρ is conserved and has no source. Here, this will be derived purely algebraically, although the final form of the equation has a useful interpretation. Expanding the partial derivative

$$\frac{\partial(\rho u)}{\partial t} = \rho \frac{\partial u}{\partial t} + u \frac{\partial \rho}{\partial t}$$

is simple. The tensor divergence $\nabla \cdot (\rho u \otimes u)$ is defined such that

$$\int_{\Omega_0} \nabla \cdot (\rho u \otimes u) \, dx = \int_{\partial\Omega_0} (\rho u \otimes u) : \hat{n} \, dx = \int_{\partial\Omega_0} \rho u (u \cdot \hat{n}) \, dx$$

for arbitrary control volumes Ω_0 . As Ω_0 becomes small, we can separately assume u and ρu are constant to derive

$$\int_{\partial\Omega_0} \rho u (u \cdot \hat{n}) \, dx = u \int_{\partial\Omega_0} (\rho u) \cdot \hat{n} \, dx + \rho u \cdot \int_{\partial\Omega_0} u \hat{n} \, dx \quad + \quad \dots$$

where a trailing term becomes negligible for a small control volume. This gives a “tensor product rule” for the divergence,

$$\nabla \cdot (\rho u \otimes u) = u \nabla \cdot (\rho u) + \rho u \cdot \nabla u. \quad (2.33)$$

Equation (2.32) then becomes

$$\rho \frac{\partial u}{\partial t} + u \frac{\partial \rho}{\partial t} + u \nabla \cdot (\rho u) + \rho u \cdot \nabla u = \rho g + \nabla \cdot \sigma.$$

Noting that $\frac{\partial \rho}{\partial t}$ is already given by continuity equation (2.27)

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho u),$$

as mass is transported by u and has no source, we get

$$\rho \frac{\partial u}{\partial t} - \underbrace{u \nabla \cdot (\rho u)} + \underbrace{u \nabla \cdot (\rho u)} + \rho u \cdot \nabla u = \rho g + \nabla \cdot \sigma.$$

Finally, the material derivative as defined in section (ref) is helpful in simplifying the above to

$$\rho \frac{Du}{Dt} = \rho g + \nabla \cdot \sigma. \quad (2.34)$$

This form of (2.32) is called the *convective form* of the Cauchy momentum equation, and is more obviously a form of $F = ma$. Recall that the material derivative is defined as

$$\frac{D}{Dt} := \frac{\partial}{\partial t} + u \cdot \nabla,$$

which measures the rate of change of a pointwise quantity from the perspective of a particle moving with the flow field u . The equation (2.34) then says that, if the continuum consists of idealised points each with a certain linear momentum (in the particle sense), deflection of their inertial path is due only to the application of a body force ρg at this point, and a total traction force exerted by the surrounding material.

The system of conservation laws

The conservation equations derived are conservation of mass (2.27) and conservation of linear momentum (2.34). Here the equations are given in their typical differential form for flow problems, with the Eulerian perspective of mass conservation, and the convective form of linear momentum conservation.

$$\begin{aligned} \frac{D\rho}{Dt} + \rho \nabla \cdot u &= 0 \quad (\text{Conservation of mass}), \\ \rho \frac{Du}{Dt} &= \rho g + \nabla \cdot \sigma \quad (\text{Conservation of linear momentum}). \end{aligned} \quad (2.35)$$

The unknowns include mass density ρ and velocity u , described by $1 + d$ scalar functions where d is the dimension of the domain. We can see there are $1 + d$ equations by expanding u in terms of components in some basis.

$$\begin{aligned} \rho \frac{Du_i}{Dt} &= \rho g_i + (\nabla \cdot \sigma)_i \quad (\text{Conservation of linear momentum components}), \\ i &= 1, \dots, d. \end{aligned}$$

When g and σ are known, this system is well-formed, but not very interesting. This effectively models a continuum of non-interacting material points, with a linear-momentum-introducing source function $\rho g + \nabla \cdot \sigma$. However, we usually let g be known (as this is a per-mass external body force, for example gravity), and the Cauchy stress tensor σ be unknown. This gives d^2 more unknowns, so the system is heavily underdetermined. In effect, the system (2.35) is really underdetermined because we don't have a specific material in mind.

2.3.3 Constitutive relations

We here investigate possible forms of the Cauchy stress tensor. A specification of σ is called a *constitutive relation*, as σ depends on the “material constitution”. A constitutive relation specifies how the kinematics of the continuum relate to its dynamics, as in, how the material configuration induces forces on the material. With σ specified, the Cauchy momentum equation (2.34) becomes well-posed (however, in general, σ may depend on new variables such as temperature, requiring further equations).

The notion of a material point

The system (2.35) is given in terms of the material derivative $\frac{D}{Dt} := \frac{\partial}{\partial t} + u \cdot \nabla$.

Deviatoric and volumetric stresses

Suppose that the tractions are determined only by the velocity gradient,

$$\sigma = \sigma(\nabla u).$$

We have the symmetric-antisymmetric splitting of the velocity gradient

$$\nabla u = \frac{1}{2} (\nabla u + \nabla u^T) + \frac{1}{2} (\nabla u - \nabla u^T).$$

The symmetric term $\frac{1}{2} (\nabla u + \nabla u^T)$ can be thought of as differential generator of stretching (as the exponential of a symmetric matrix is symmetric-positive-definite), and the antisymmetric term $\frac{1}{2} (\nabla u - \nabla u^T)$ can be thought of as a differential generator of rotations (as the exponential of an antisymmetric matrix is orthogonal).

Pressure in incompressible materials

The concept of pressure will be very important in our discussion of the Navier-Stokes equations, so we introduce it here. A detailed derivation of the pressure is given in terms of Stokes flow in section 4.4.

If we require the velocity field u of the position map x to be non-compressing (as described in section (ref)), then we add to our model equations the constraint

$$\nabla \cdot u = 0. \tag{2.36}$$

We proceed by analogy to a simple mechanical system. The state of a pendulum of mass m might be described by two spatial variables X and Y with a constraint

$$X^2 + Y^2 = 1.$$

Given a differentiable pendulum motion, the linear momenta mv_X and mv_Y clearly cannot be constant, as then the pendulum would “fly out” of its arc. From the perspective of the X, Y coordinate system there exists “virtual forces” which are exactly those that are needed to maintain constraints. These forces have no necessary physical interpretation, as the pendulum model does not explicitly reference the tension of the pendulum rod, but are rather those strong forces that must “come from somewhere” such that the constraints are satisfied.

(figure)

From a constraint on position (X, Y) we can derive a constraint on velocity (v_X, v_Y) by noting that the velocity must stay inside the tangent plane in the configuration space. In this case, we require

$$Xv_X + Yv_Y = 0. \quad (2.37)$$

(— add Lagrange multipliers to the system, then pressure here is a sort of Lagrange multiplier). The continuum velocity constraint (2.36) is completely analogous to (2.37). Motions of x are restricted to those which do not compress mass. Clearly, our (per-point) linear momentum ρu cannot be constant except in simple parallel flows, implying the existence of some virtual (per-point) force. We call this force the *pressure* p , and we are now solving for ρ , u , and p in a coupled system of equations (2.34) and (2.36), repeated here:

$$\rho \frac{Du}{Dt} = \rho g + \nabla \cdot \sigma, \quad \nabla \cdot u = 0.$$

As there is no explicit mention of p , it must be part of the constitutive relation for σ . We let σ be

$$\sigma = -pI + \tau \quad \Rightarrow \quad \nabla \cdot \sigma = -\nabla p + \nabla \cdot \tau,$$

where I is the identity tensor and τ is called the *deviatoric* component of the Cauchy stress tensor. τ is chosen such that the pressure p entirely encapsulates the isotropic forces which push material volumes apart.

Completing our equations

We have so far been working quite generally with the forms of continuum mechanics models and their constraints. Although we have made some assumptions (for example, we require σ to be a purely local function, an idealisation due to Cauchy [ref]), we must so far leave our systems underdetermined. In the next chapter, we will investigate an important constitutive relation for the deviatoric stress τ , forming what is called a *Navier-Stokes fluid*, giving a complete system of equations called the *Navier-Stokes equations*.

Chapter 3

Some functional analysis

3.1 Weak solutions to PDEs

3.2 Sobolev spaces

Chapter 4

The Navier-Stokes equations

4.1 The kinematics of flow

4.1.1 Vorticity

4.1.2 The Helmholtz decomposition

The stream function

The velocity potential

4.2 Deriving the Navier-Stokes equations

The incompressible Navier-Stokes equations model the motion of a common kind of viscous fluid called a *Newtonian fluid*. They are:

- The Cauchy momentum equation (2.34) for mass density ρ and velocity u ,
- an incompressibility constraint $\nabla \cdot u = 0$ and unknown pressure p ,
- and a concrete constitutive relation for the deviatoric stress τ .

In anticipation, their common form is

$$\rho \frac{Du}{Dt} = -\nabla p + \nabla \cdot \tau + \rho g, \quad \nabla \cdot u = 0, \quad (4.1)$$

where τ is defined by Stokes' constitutive relation

$$\tau = \mu (\nabla u + \nabla u^T), \quad (4.2)$$

where μ is called the *viscosity*, and ∇u is the velocity gradient measuring the local deformation of a small control volume under the flow of u . Alongside a domain and appropriate initial and boundary conditions, the Navier-Stokes equations (4.1) form a concrete flow problem which can be solved numerically, or in special situations analytically.

4.3 Scaling and dimension

4.3.1 The Reynolds number

4.4 Stokes flow and the meaning of pressure

If we assume that the advective term $u \cdot \nabla u$ in the incompressible Navier-Stokes equations is “small”, we can ignore it and derive the linear *unsteady Stokes equations*:

$$\rho \frac{\partial u}{\partial t} = \mu \Delta u + \rho g - \nabla p, \quad \nabla \cdot u = 0. \quad (4.3)$$

We are assuming validity for low Reynolds number $Re \ll 1$, where convective behaviour is negligible compared to the viscous forces, which for a Navier-Stokes fluid “diffuse” the linear momentum. Setting the left-hand-side of (4.3) to zero results in the *steady Stokes equations*

$$\mu \Delta u + \rho g - \nabla p = 0, \quad \nabla \cdot u = 0. \quad (4.4)$$

Time-dependent equation (4.3) can be thought of as a “gradient descent” to find the steady Stokes flow (4.4). The steady Stokes equation is a constrained vector Poisson equation, where we have introduced pressure p explicitly. It is well-known, by Dirichlet’s principle, that we can think of a weak solution to the unconstrained vector Poisson equation as a minimiser of the Dirichlet energy,

$$\underset{u}{\text{minimize}} \quad E(u) = \frac{\mu}{2} \langle \nabla u, \nabla u \rangle - \langle u, \rho g \rangle. \quad (4.5)$$

We can validate this by computing the Euler-Lagrange equations:

$$\frac{\delta E}{\delta u} = \frac{\partial \mathcal{L}}{\partial u} - \frac{d}{dx} \frac{\partial \mathcal{L}}{\partial u_x} = -\rho g - \mu \Delta u = 0.$$

We now introduce the incompressibility constraint $\nabla \cdot u = 0$, giving the constrained minimization

$$\begin{aligned} \underset{u}{\text{minimize}} \quad & E(u) = \frac{\mu}{2} \langle \nabla u, \nabla u \rangle - \langle u, \rho g \rangle \\ \text{subject to} \quad & \nabla \cdot u = 0. \end{aligned} \quad (4.6)$$

It is not immediately obvious how to form the constrained Euler-Lagrange equations here, as $\nabla \cdot$ is a differential operator. We cannot just write

$$\frac{\delta E}{\delta u} = \lambda \nabla \cdot$$

for scalar function λ , as we can with a pointwise linear constraint such as $u \cdot v = 0$ for some vector field v . However, this is just a problem of notation. The evaluation of energy change with perturbations is defined as

$$\left\langle \frac{\delta E}{\delta u}, \delta u \right\rangle = \int_{\Omega} \frac{\delta E}{\delta u} \cdot \delta u \, dx.$$

We want this measure of energy change to be purely a divergence measure, up to a scalar multiplier λ :

$$\int_{\Omega} \frac{\delta E}{\delta u} \cdot \delta u \, dx = \int_{\Omega} \lambda \nabla \cdot \delta u \, dx. \quad (4.7)$$

This means that virtual displacements with $\nabla \cdot \delta u = 0$ will not cause an energy change, which is the condition that we want for a stationary point. We can now apply integration by parts to (4.7), assuming that δu vanishes on the boundary of the domain, to get

$$\int_{\Omega} \frac{\delta E}{\delta u} \cdot \delta u \, dx = - \int_{\Omega} \nabla \lambda \cdot \delta u \, dx. \quad (4.8)$$

We can now reasonably apply the localisation step to get the constrained Euler-Lagrange equations

$$\frac{\delta E}{\delta u} = -\nabla \lambda \quad \equiv \quad \mu \Delta u + \rho g - \nabla \lambda = 0. \quad (4.9)$$

Along with the constraint $\nabla \cdot u = 0$, this is just the steady Stokes equations (4.4), where $\lambda = p$! We can see that the pressure p is actually a Lagrange multiplier, which measures a virtual force that responds to virtual displacements which would break the constraint of incompressibility. In fact, we may think of this as a derivation of the pressure.

Alternative direct derivation in terms of a modified energy

Previously, we emphasized the meaning of the Lagrange multiplier. One utility of Lagrange's methods is their automated calculational power. It is standard to express that a solution to the optimization problem (4.6), with a differentiable equality constraint, is a stationary point of the modified energy

$$L(u, \lambda) := \frac{\mu}{2} \langle \nabla u, \nabla u \rangle - \langle u, \rho g \rangle - \langle \lambda, \nabla \cdot u \rangle. \quad (4.10)$$

We can take an evaluated first variation with respect to u to get

$$\left\langle \frac{\delta L}{\delta u}, \delta u \right\rangle = \langle -\rho g - \mu \Delta u, \delta u \rangle - \langle \lambda, \nabla \cdot \delta u \rangle,$$

which by integration by parts becomes

$$\left\langle \frac{\delta L}{\delta u}, \delta u \right\rangle = \langle -\rho g - \mu \Delta u + \nabla \lambda, \delta u \rangle. \quad (4.11)$$

We then get

$$\begin{aligned} \frac{\delta L}{\delta u} &= -\rho g - \mu \Delta u + \nabla \lambda = 0, \\ \frac{\delta L}{\delta \lambda} &= -\nabla \cdot u = 0, \end{aligned} \quad (4.12)$$

which are the steady Stokes equations (4.4) with pressure $p = \lambda$.

4.4.1 Application to hydrostatics

For example, we may imagine the steady Stokes equations modelling a calm sea with a flat seabed. We can let the body force be gravity described by a potential ϕ :

$$\rho g = -\nabla \phi.$$

If we make a perturbed displacement of the velocity field at the bottom of the ocean, supposing that some volume of water is beginning to expand, we are working against gravity as well as our virtual force, pressure.

(draw this)

Chapter 5

The finite element method

5.1 Introduction

Consider a single conservation law as described in section 2.1.1. This law was given in two forms, “integral” (2.1):

$$\frac{d}{dt} \int_{\Omega_0} \phi \, dx = \int_{\Omega_0} s \, dx + \int_{\partial\Omega_0} \phi j \cdot (-\hat{n}) \, dx,$$

and “differential” (2.2):

$$\frac{\partial \phi}{\partial t} = s - \nabla \cdot (\phi j).$$

Thinking about (2.1) will lead to Galerkin methods, which include finite volumes, finite elements, and spectral methods. Thinking about (2.2) will lead, primarily, to the finite difference method, historically the first and still very important in applications. We will discuss the latter first.

5.1.1 Discretization of the differential form

The finite difference method will take equation (2.2) and, for example, expand the divergence by Gauss’ theorem (2.3):

$$\nabla \cdot j = \frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} + \frac{\partial j_z}{\partial z}.$$

The approximate solution may be represented by a number of samples on the domain, for example, a grid. The term j_x above could then be approximated by a secant, for example a central difference.

(draw this)

However, we have not necessarily given a real interpretation of what the solution samples at grid points say about the solution everywhere. They could be a coefficients of, for example, hat basis functions.

(draw this)

Yet a finite difference discretization of (2.2) may not take this into account at all. One might feel that limits have been taken too soon, and that the integral form (2.1) gives clearer routes to discretizations which have geometric meaning.

5.1.2 Discretization of the integral form

The integral conservation law (2.1) is a geometric statement about fluxes of quantity ϕ by j , quantified over arbitrary control volumes Ω_0 . We have an infinite number of control volumes, and therefore equations which must hold, and an infinite-dimensional space of solutions to choose from. A key idea, then, is to choose a finite number of equations and a finite-dimensional subspace of possible solutions. A supposed solution will be represented by the coefficients of some choice of basis functions for the subspace. Each equation will be checked exactly against this supposed solution.

(figure)

Finite element methods, and more generally Galerkin methods, live comfortably in the language of weak solutions, integral forms of partial differential equations, and the calculus of variations. Some methods of this kind will be derived in the subsequent sections, investigating discretizations of the integral forms of some physical PDEs. In order:

- The linear Poisson equation: Finite volumes, finite elements, linear systems.
- The linear Stokes equations: FEM with constraints, time-dependence.
- A non-linear Poisson equation: Non-linear FEM.
- A non-linear heat equation: Non-linear, time-dependent FEM.
- The Burgers equation: Introduces shocks and the numerical effect of viscosity.

This is in order to build up concepts to solve the non-linear time-dependent Navier-Stokes equations.

5.2 Solving the Poisson equation

Poisson's equation is a steady-state version of the heat equation. Through this investigation we will derive many of the tools and ideas underlying general Galerkin methods. In particular we will derive a *finite volume method* and a *finite element method* from first principles. In anticipation, some results are shown below:

(visualisations)

We will defer the important step of analysis of our methods' convergence and stability to a later section.

5.2.1 Deriving the Poisson equation through diffusion processes

A diffusion process “levels out” some quantity, such as temperature or some chemical concentration. We can intuitively think of a diffusion as a progressive “blurring” such as in a camera defocus, and in fact many common image processing techniques use diffusion PDEs from physics [16]. We will stick with the notion of temperature h as the diffused quantity. *Fick's law of diffusion* is a constitutive relation giving the bulk flux of temperature h as proportional to the negative gradient:

$$hj = -\mu \nabla h,$$

where μ is called the diffusion coefficient. This is one way of saying that the temperature tends to level out. If we form a continuity equation (2.1) for temperature, with source s , we get

$$\frac{d}{dt} \int_{\Omega_0} h \, dx = \int_{\Omega_0} s \, dx + \int_{\partial\Omega_0} \mu \nabla h \cdot \hat{n} \, dx, \quad (5.1)$$

which by application of Stokes' theorem becomes

$$\frac{dh}{dt} = s + \nabla \cdot (\mu \nabla h). \quad (5.2)$$

If we further assume that the diffusion coefficient μ is constant, we get

$$\frac{dh}{dt} = s + \mu \nabla \cdot \nabla h = s + \mu \Delta h, \quad (5.3)$$

which is the standard heat equation. The steady-state heat equation is then

$$-\Delta h = f, \quad (5.4)$$

where we let $f = s/\mu$ in the above. Equation (5.4) is called the Poisson equation, which models steady-state diffusion processes and can be used to calculate gravitational or electrostatic potential fields. In integral form, “undoing” the application of Stokes' theorem above, the Poisson equation is

$$\int_{\partial\Omega_0} -\nabla h \cdot \hat{n} \, dx = \int_{\Omega_0} f \, dx. \quad (5.5)$$

Form (5.5) clearly shows that we are calculating a steady state, as we are solving for h such that the amount of heat that leaves Ω_0 is the amount created by the source function. This form will be the most convenient for our numerical methods.

5.2.2 Discretizing the Poisson equation

Equation (5.5) is quantified over arbitrary control volumes Ω_0 . A simple idea is to break the domain Ω up into small cells $\Omega_1, \dots, \Omega_n$, and check that the flux integral holds over each of these. We will then have n equations on h . As this system will be underdetermined (h has infinite degrees of freedom), we must restrict h to what we will call a “test space”,

$$\Phi = \text{span} \{ \phi_1, \dots, \phi_n \}.$$

The basis functions ϕ_i should generate a “good” space of approximations, such that our linear system is non-singular. We then have a discrete system of equations

$$\int_{\partial\Omega_j} -\nabla \left(\sum_{i=1}^n h_i \phi_i \right) \cdot \hat{n} \, dx = \int_{\Omega_j} f \, dx, \quad j = 1, \dots, n,$$

which by linearity can be written as

$$\sum_{i=1}^n h_i \int_{\partial\Omega_j} -\nabla \phi_i \cdot \hat{n} \, dx = \int_{\Omega_j} f \, dx, \quad j = 1, \dots, n. \quad (5.6)$$

We see here that there must be some restrictions on the ϕ_i . Formally, our basis functions must be in the Sobolev space $H^1(\Omega)$. This simply means that they must have a gradient defined “almost everywhere”. It does not matter if the gradient is not defined at isolated lower-dimensional subsets, as these make no contribution to the integral. Since the source

f , our domain decomposition Ω_j , and the basis functions ϕ_i are known, we can pre-compute the majority of (5.6) to give a matrix system

$$A\hat{h} = \begin{bmatrix} \int_{\partial\Omega_1} -\nabla\phi_1 \cdot \hat{n} \, dx & \cdots & \int_{\partial\Omega_1} -\nabla\phi_n \cdot \hat{n} \, dx \\ \vdots & & \vdots \\ \int_{\partial\Omega_n} -\nabla\phi_1 \cdot \hat{n} \, dx & \cdots & \int_{\partial\Omega_n} -\nabla\phi_n \cdot \hat{n} \, dx \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_{n-1} \\ h_n \end{bmatrix} = \begin{bmatrix} \int_{\Omega_1} f \, dx \\ \int_{\Omega_2} f \, dx \\ \vdots \\ \int_{\Omega_{n-1}} f \, dx \\ \int_{\Omega_n} f \, dx \end{bmatrix} = \hat{f}. \quad (5.7)$$

If our domain decomposition $\Omega_1, \dots, \Omega_n$ and test space $\Phi = \text{span}\{\phi_1, \dots, \phi_n\}$ are chosen well, this linear system will be non-singular and hopefully well-conditioned. In all cases we have a conservative system of balanced fluxes, but it is another question whether our approximation $\Phi\hat{h}$ is good.

Choosing a domain decomposition and test space

Possibly the simplest scheme is to triangulate Ω as $\Omega = \bigsqcup T_i$ such that we have n nodal points. Each nodal point p_i will be associated with a piecewise “hat” basis function ϕ_i which is 1 at p_i and 0 at its neighbours.

(draw this)

As we typically have more triangles than vertices, we cannot use the T_i as our domain decomposition. However, we may associate to each p_i a domain Ω_i called the *Voronoi cell*.

(draw this)

This scheme has found some success, especially in the domain of geometry processing [14]. By Stokes’ theorem, the matrix A in (5.7) can be thought of as a negative discrete Laplacian. If we compute these integrals, we will find a very simple closed form for the entries of A .

In geometry processing this matrix is called the “cotangent Laplacian” [14], and it is typically applied to surface meshes in \mathbb{R}^3 , which can be thought of as triangulations of a smooth surface.

Results and visualisation

(results and visualisation)

We have worked through an instance of a *finite volume method* [4]. Finite volume methods are characterised by an exact domain partition and computation of flux integrals. Finite volume methods are typically *conservative*, due to the “flux network” nature of the discretisation.

5.2.3 The notion of a trial function

The matrix equation (5.7) consists of linear equations

$$\int_{\partial\Omega_1} -\nabla \left(\sum_{i=1}^n h_i \phi_i \right) \cdot \hat{n} \, dx = \int_{\Omega_1} f \, dx,$$

and so on. We cannot compute flux integrals over all arbitrary control volumes, but we can take a number of “trial” flux integrals over the finite number of cells Ω_i . We can take linear combinations of these equations to get more equations which must hold on a solution. For example,

$$\int_{\partial\Omega_1} -\nabla \left(\sum_{i=1}^n h_i \phi_i \right) \cdot \hat{n} \, dx + \int_{\partial\Omega_2} -\nabla \left(\sum_{i=1}^n h_i \phi_i \right) \cdot \hat{n} \, dx = \int_{\Omega_1} f \, dx + \int_{\Omega_2} f \, dx \quad (5.8)$$

must hold. At first sight, (5.8) cannot directly be interpreted as a statement about a “flux integral”, but rather about a sum of flux integrals. However, a key idea is to regard (5.8) as a flux integral over a *formal sum* of domains,

$$\Omega_1 + \Omega_2.$$

We now have the equation

$$\int_{\partial\Omega_1 + \partial\Omega_2} -\nabla \left(\sum_{i=1}^n h_i \phi_i \right) \cdot \hat{n} \, dx = \int_{\Omega_1 + \Omega_2} f \, dx. \quad (5.9)$$

Formally $\Omega_1 + \Omega_2$ is called a *chain*. For example, we may visualise $\Omega_1 + 2\Omega_2 + 0.5\Omega_4$ as:

(draw this)

We define the boundary operator ∂ to be linear in formal sums e.g.,

$$\partial(\Omega_1 + \Omega_2) = \partial\Omega_1 + \partial\Omega_2.$$

If Ω_1 and Ω_2 share a boundary, we would like $\Omega_1 + \Omega_2$ to represent their union, such that a flux integral over $\partial(\Omega_1 + \Omega_2)$ evaluates to zero on the shared boundary. This can be done by thinking of the boundary as *oriented*, as in, consisting of oriented “surface elements” over which flux integrals can be taken. For example, the \hat{n} in a flux integral denotes the outward-pointing normal, which represents an “outward-flux-measuring surface element”. The opposite $-\hat{n}$ then represents the “inward-flux-measuring surface element”, which is outward from the perspective of an adjacent cell.

(draw this)

We may now define

$$\Psi = \text{span} \{ \Omega_1, \dots, \Omega_n \}$$

to be the *trial space*, where the span is taken with respect to formal sums. As with any linear space, we may choose from many possible bases. For example,

$$\Psi = \text{span} \{ \Omega_1, \Omega_2, \Omega_3 \} = \text{span} \{ \Omega_1 + \Omega_2, 2\Omega_2, \Omega_3 \}.$$

A key idea, leading to Galerkin methods, is to allow freedom in the choice of our trial space Ψ . Notably, we do not need Ψ to be a space of formal sums of domains. The Poisson equation is discretised over flux integrals around cell boundaries in the linear system (5.6), which we repeat here:

$$\sum_{i=1}^n h_i \int_{\partial\Omega_j} -\nabla \phi_i \cdot \hat{n} \, dx = \int_{\Omega_j} f \, dx, \quad j = 1, \dots, n.$$

Applying Stokes' theorem, we get

$$\sum_{i=1}^n h_i \int_{\Omega_j} -\Delta \phi_i dx = \int_{\Omega_j} f dx, \quad j = 1, \dots, n.$$

We can think of these integrals as over the *entire domain* Ω , giving the form

$$\sum_{i=1}^n h_i \int_{\Omega} -\Delta \phi_i \cdot \chi(\Omega_j) dx = \int_{\Omega} f \cdot \chi(\Omega_j) dx, \quad j = 1, \dots, n.$$

where $\chi(\Omega_j)$ is the indicator function of Ω_j ,

$$\chi(\Omega_j)(x) := \begin{cases} 0 & \text{if } x \in \Omega_j \\ 1 & \text{if } x \notin \Omega_j. \end{cases}$$

Note that we can now think of our trial space Ψ as a span of functions, instead of a span of domains:

$$\Psi = \text{span} \{ \chi(\Omega_1), \dots, \chi(\Omega_n) \}.$$

Now we can instead let

$$\Psi = \text{span} \{ \psi_1, \dots, \psi_n \}$$

where the ψ_j need not be the indicator functions of a domain decomposition. We now have the system of equations

$$\sum_{i=1}^n h_i \int_{\Omega} -\Delta \phi_i \psi_j dx = \int_{\Omega} f \psi_j dx, \quad j = 1, \dots, n.$$

By integration by parts we have

$$\sum_{i=1}^n h_i \int_{\Omega} -\nabla \phi_i \cdot \nabla \psi_j dx = \int_{\Omega} f \psi_j dx, \quad j = 1, \dots, n, \quad (5.10)$$

and we see that we still only require the ϕ_i to be in $H^1(\Omega)$. We can see that equation (5.10) is very similar to the exact fluxes in (5.6). There is a real geometric sense in which (5.10) is a “blurred convolution” of flux integrals.

Integrating over trial functions versus integrating over domains

The reasoning here is in the spirit of Green's functions. While this is more readily formalised with the notion of a distribution, or generalised function, we will work with the Dirac delta function, defined by

$$\int_{\Omega_0} \delta_y dx = \begin{cases} 1 & \text{if } y \in \Omega_0 \\ 0 & \text{otherwise.} \end{cases}$$

For example, possibly under some regularity assumptions, we may represent a trial function ψ_j on Ω as

$$f = \int_{\Omega} \delta_x f(x) dx,$$

which we may call “Riemann-integral-like”. We may instead represent ψ_j in a “Lebesgue-integral-like” way by defining

$$L_y(\psi_j) := \{ z \in \Omega \mid \psi_j(z) = y \}$$

to be a level set of ψ_j , the points of Ω for which $\psi_j = y$. We can then express ψ_j as

$$\psi_j = \int_{-\infty}^{\infty} \left[\int_{L_y(\psi_j)} y \delta_x dx \right] dy.$$

This gives ψ_j as the totality of its level sets. For example, if we let Ψ be spanned by the hat functions on some triangulation, each hat function ψ_j can be thought of as a totality of level sets culminating in the point-set of $\psi_j(p_j) = 1$.

(draw this)

The discretised Poisson equation (5.10) involves an integral over $\nabla \phi_i \cdot \nabla \psi_j$, and we can compute this as

$$\begin{aligned} \int_{\Omega} \nabla \phi_i \cdot \nabla \psi_j dx &= \int_{-\infty}^{\infty} \int_{\Omega} \nabla \phi_i \cdot \nabla \left[\int_{L_y(\psi_j)} y \delta_z dz \right] dx dy \\ &= \int_{-\infty}^{\infty} y \int_{L_y(\psi_j)} \nabla \phi_i \cdot \hat{n} dx dy. \end{aligned} \tag{5.11}$$

We have this final equality by noting that the gradient of ψ_j at x , where $\psi_j(x) = y$, is orthogonal to the level set $L_y(\psi_j)$, and has length y :

(draw this)

We can think of the “flux trial” (5.10) as involving “blurred fluxes” as in (5.11). For example, if we let $\Phi = \Psi$ be the set of hat functions on some triangulation of Ω , then form and solve the matrix system, we get a generally non-conservative system of fluxes. We have lost conservativeness by the “blurring” of the flux integrals, but we may have gained advantages in terms of stability and convergence: in this case, the linear system will be symmetric-positive-definite, and stably solvable by, for example, conjugate gradients.

Visualisation and results

(visualisation and results)

We have worked through an instance of a *finite element method*. Finite element methods are characterised by a test space Φ and trial space Ψ with basis functions of *compact support*, where Φ and Ψ typically consist of continuous functions in some Sobolev space, constructed over a domain tessellation. We will formally define a “finite element method”, following Ciarlet [15], after one more example, the steady Stokes equations.

5.3 Solving the Stokes equations

The Stokes equations (4.3), which are solved for a stable incompressible Navier-Stokes flow, assume the Reynolds number is $Re \ll 1$ and thus convective processes are negligible in comparison to viscous processes. We will begin with the steady-state form (4.4). Due to this simplification, the Steady stokes equations (4.4), repeated here:

$$\mu \Delta u + \rho g - \nabla p = 0, \quad \nabla \cdot u = 0,$$

form a constrained linear equation. As we saw in section 4.4, the pressure term p is a Lagrange multiplier introduced with the constraint $\nabla \cdot u = 0$. We will begin by discretizing the *unconstrained* steady Stokes equations, which are a vector Poisson equation:

$$-\mu \Delta u = \rho g. \quad (5.12)$$

5.3.1 Discretizing the vector Poisson equation

In principle we should keep the Stokes equation in integral form (using the conservative-form Cauchy momentum equation (2.31)), and continue as we did in section 5.2.3. However, we will take a formal step to skip the reasoning of section 5.2.3, typical of finite element method derivations. As we start with the *differential* equation (5.12), we can introduce a trial space Ψ and then “weaken” the equation by integrating against $v \in \Psi$, and removing the Laplacian by integration by parts:

$$\int_{\Omega} -\mu \Delta u \cdot v \, dx = \int_{\Omega} \rho g \cdot v \, dx \quad \equiv \quad \int_{\Omega} -\mu \nabla u : \nabla v \, dx = \int_{\Omega} \rho g \cdot v \, dx. \quad (5.13)$$

Noting that the left-hand-side of (5.13) is a bilinear form in u and v , and the right-hand-side is a linear functional in ψ , it is standard practice (ref) to write this kind of equation as

$$a(u, v) = f(v). \quad (5.14)$$

Our subsequent derivations are much the same as in 5.2.2, simplified by our new notation. We can now approximate u in the test space Φ as $\hat{u} = \sum_{i=1}^n u_i \phi_i$. By linearity we only need to compute trials over the basis trial functions ψ_j . We then have the linear system of equations

$$\sum_{i=1}^n u_i a(\phi_i, \psi_j) = f(\psi_j), \quad j = 1, \dots, n, \quad (5.15)$$

which can be written in matrix form as

$$A\hat{u} = \begin{bmatrix} a(\phi_1, \psi_1) & \cdots & a(\phi_1, \psi_n) \\ \vdots & & \vdots \\ a(\phi_n, \psi_1) & \cdots & a(\phi_n, \psi_n) \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} f(\psi_1) \\ f(\psi_2) \\ \vdots \\ f(\psi_{n-1}) \\ f(\psi_n) \end{bmatrix} = \hat{f}. \quad (5.16)$$

We can solve (5.16) to get a velocity field $\sum_{i=1}^n u_i \phi_i$, although in general this will not satisfy $\nabla \cdot u = 0$. As some preliminary analysis, if $\Phi = \Psi$ and have the same basis functions, we have a symmetric-positive-definite system. This form of linear system is known to be stably solvable, for example by the conjugate gradient method.

5.3.2 Discretizing the steady Stokes equations

As described in section 4.4, the pressure p is a Lagrange multiplier that appears when solving the optimization problem (4.6):

$$\begin{aligned} & \underset{u}{\text{minimize}} && E(u) = \frac{\mu}{2} \langle \nabla u, \nabla u \rangle - \langle u, \rho g \rangle \\ & \text{subject to} && \nabla \cdot u = 0. \end{aligned}$$

As a first idea, we can introduce p as a variable to solve for. Pressure then needs to be discretized, so we introduce another test space Φ_{pressure} . To get a weak form of the steady Stokes equations (4.4), which are two equations including the constraint $\nabla \cdot u = 0$, we

introduce another trial space $\Psi_{\text{constraint}}$, whose functions will be integrated against $\nabla \cdot u$. The weak form is then

$$\begin{aligned} \int_{\Omega} (\mu \Delta u + \rho g - \nabla p) \cdot v \, dx &= 0, \\ \int_{\Omega} (\nabla \cdot u) q \, dx &= 0, \quad \text{where } v \in \Psi, q \in \Psi_{\text{constraint}}, \end{aligned}$$

which by integration by parts can be written as

$$\begin{aligned} \int_{\Omega} -\mu \nabla u : \nabla v - (\nabla \cdot v) p \, dx &= \int_{\Omega} \rho g \cdot v \, dx, \\ \int_{\Omega} (\nabla \cdot u) q \, dx &= 0, \quad \text{where } v \in \Psi, q \in \Psi_{\text{constraint}}. \end{aligned} \tag{5.17}$$

As in section 5.3.1, we introduce notation for the bilinear and linear forms in (5.17):

$$\begin{aligned} a(u, v) &:= \int_{\Omega} -\mu \nabla u : \nabla v \, dx, \quad \text{for } u \in \Phi, v \in \Psi, \\ \hat{b}(p, v) &:= \int_{\Omega} -(\nabla \cdot v) p \, dx, \quad \text{for } p \in \Phi_{\text{pressure}}, v \in \Psi, \\ b(u, q) &:= \int_{\Omega} -(\nabla \cdot u) q \, dx, \quad \text{for } u \in \Phi, q \in \Psi_{\text{constraint}}, \\ f(v) &:= \int_{\Omega} \rho g \cdot v \, dx \quad \text{for } v \in \Psi. \end{aligned} \tag{5.18}$$

Although they have the same form, b and \hat{b} are distinguished as they take inputs in different function spaces. We now have a simplified notation for the weak form (5.17),

$$\begin{aligned} a(u, v) + \hat{b}(p, v) &= f(v), \\ b(u, q) &= 0, \quad \text{where } v \in \Psi, q \in \Psi_{\text{constraint}}. \end{aligned} \tag{5.19}$$

Working with discrete function spaces, we get a $2n \times 2n$ linear system in the unknowns u_1, \dots, u_n and p_1, \dots, p_n ,

$$\begin{aligned} \sum_{i=1}^n u_i a(\phi_i, \psi_j) + \sum_{i=1}^n p_i \hat{b}(\phi_i^C, \psi_j) &= f(\psi_j), \\ \sum_{i=1}^n u_i b(\phi_i, \psi_j^C) &= 0, \quad j = 1, \dots, n. \end{aligned} \tag{5.20}$$

To emphasize the linear system structure of (5.19), the block matrix form is:

$$\begin{aligned} M \hat{x} &= \begin{bmatrix} A & \hat{B} \\ B & 0 \end{bmatrix} \hat{x} \\ &= \left[\begin{array}{ccc|ccc} a(\phi_1, \psi_1) & \cdots & a(\phi_1, \psi_n) & \hat{b}(\phi_1^C, \psi_1) & \cdots & \hat{b}(\phi_1^C, \psi_n) \\ \vdots & & \vdots & \vdots & & \vdots \\ a(\phi_n, \psi_1) & \cdots & a(\phi_n, \psi_n) & \hat{b}(\phi_n^C, \psi_1) & \cdots & \hat{b}(\phi_n^C, \psi_n) \\ \hline b(\phi_1, \psi_1^C) & \cdots & b(\phi_1, \psi_n^C) & 0 & \cdots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ & & \vdots & \vdots & & \vdots \\ b(\phi_n, \psi_1^C) & \cdots & b(\phi_n, \psi_n^C) & 0 & \cdots & 0 \end{array} \right] \begin{bmatrix} u_1 \\ \vdots \\ u_n \\ p_1 \\ \vdots \\ p_n \end{bmatrix} = \begin{bmatrix} f(\psi_1) \\ \vdots \\ f(\psi_n) \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \hat{b}. \end{aligned} \tag{5.21}$$

Is this method reasonable?

For the vector Poisson equation, letting $\Phi = \Psi$, we ended up with a symmetric-positive-definite system (5.16), which is known to be stably solvable. We can ask how reasonable it is to solve (5.21), and what trial and test spaces we should use. In fact, in the problem (5.19), and more generally in a “saddle point problem”, arising in Lagrange-multiplier methods for constrained PDEs, we should not choose just any test and trial spaces. The Ladyzhenskaya–Babuška–Brezzi condition, discussed later, enforces restrictions on choices that result in a stable method. We will until then continue with computations.

Results and visualisation

(results and visualisation)

5.3.3 Discretizing the unsteady Stokes equations

The steady Stokes above are the stable state of the time-dependent Stokes flow, after the transient flow behaviour settles down. The unsteady Stokes equations (4.3) are

$$\rho \frac{\partial u}{\partial t} = \mu \Delta u + \rho g - \nabla p, \quad \nabla \cdot u = 0.$$

These form an initial-boundary-value problem, and this will be our first attempt at discretizing a PDE in time. We could think of solving with the test and trial spaces over the domain $\Omega \times [0, T]$, but this is typically not done due to the memory costs, and different qualitative meaning of the time variable. Instead, we will use an implicit-Euler finite difference in time:

$$\frac{\rho}{\Delta t} (u^{(n)} - u^{(n-1)}) = \mu \Delta u^{(n)} + \rho g - \nabla p^{(n)}, \quad \nabla \cdot u^{(n)} = 0, \quad (5.22)$$

where Δt is a fixed time step, and $u^{(n)}$ and $p^{(n)}$ is the solution at time $t_n = n\Delta t$. We can weaken each step (5.22) by integrating against trial functions $v \in \Psi$ and $q \in \Psi_{\text{constraint}}$, performing integration by parts as in section 5.3.2, and rearranging the knowns and unknowns. We can also let u be $u^{(n)}$, p be $p^{(n)}$, and u_{prev} be $u^{(n-1)}$ in the above to simplify subsequent notation. The weak form of (5.22) is then:

$$\begin{aligned} \int_{\Omega} \frac{\rho}{\Delta t} u \cdot v - \mu \nabla u : \nabla v - (\nabla \cdot v) p \, dx &= \int_{\Omega} \frac{\rho}{\Delta t} u_{\text{prev}} \cdot v + \rho g \cdot v \, dx, \\ \int_{\Omega} (\nabla \cdot u) q \, dx &= 0, \end{aligned} \quad (5.23)$$

We can define the linear forms as

$$\begin{aligned} a(u, v) &:= \int_{\Omega} \frac{\rho}{\Delta t} u \cdot v - \mu \nabla u : \nabla v \, dx, \quad \text{for } u \in \Phi, v \in \Psi, \\ \hat{b}(p, v) &:= \int_{\Omega} -(\nabla \cdot v) p \, dx, \quad \text{for } p \in \Phi_{\text{pressure}}, v \in \Psi, \\ b(u, q) &:= \int_{\Omega} -(\nabla \cdot u) q \, dx, \quad \text{for } u \in \Phi, q \in \Psi_{\text{constraint}}, \\ f(v) &:= \int_{\Omega} \frac{\rho}{\Delta t} u_{\text{prev}} \cdot v + g \cdot v \, dx \quad \text{for } v \in \Psi \end{aligned} \quad (5.24)$$

to reexpress (5.23) in the notation

$$\begin{aligned} a(u, v) + \hat{b}(p, v) &= f(v), \\ b(u, q) &= 0, \quad \text{where } v \in \Psi, q \in \Psi_{\text{constraint}}. \end{aligned} \quad (5.25)$$

This is the same structure as in the steady Stokes system (5.19), and so the matrix block structure is the same as in (5.21). Therefore, every step we need to solve a linear system that is very similar to the steady Stokes problem. In fact this step can be thought of as successively introducing the momentum source ρg (ignoring convection), while solving for the new pressure force needed to keep the fluid non-compressed.

Discretizing the initial condition

We may have some analytically determined, or otherwise, initial velocity field u with $\nabla \cdot u = 0$. We would like to form $u^{(0)}$ in order to start the iteration. The velocity u should be projected in some way into the test space Ψ . Enforcing $u^{(0)}$ to give the same “blurred average” value when evaluated against a trial function,

$$\int_{\Omega} u^{(0)} \cdot v \, dx = \int_{\Omega} u \cdot v \, dx, \quad \forall v \in \Psi, \quad (5.26)$$

gives a linear system

$$\sum_{i=1}^n u_i^{(0)} \int_{\Omega} \phi_i \cdot \psi_j \, dx = \int_{\Omega} u \cdot \psi_j \, dx, \quad j = 1, \dots, n. \quad (5.27)$$

Solving this linear system for the $u_i^{(0)}$ gives $u^{(0)} = \sum_{i=1}^n u_i^{(0)} \phi_i$ as a projection of u onto Φ . This projection is orthogonal if $\Phi = \Psi$, and therefore could be considered the “best” such projection under the Euclidean norm. This is the standard Gramian matrix construction for projection in approximation theory [20].

5.4 Solving non-linear equations

5.4.1 A non-linear Poisson equation

5.4.2 A non-linear heat equation

5.4.3 The Burgers equation

Chapter 6

Solving the Navier-Stokes equations

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