GEO 441 Notes

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Introduction

This document contains notes taken for the class GEO 441: Computational Geophysics at Princeton University, taken in the Spring 2025 semester. These notes are primarily based on lectures by Professor Jeroen Tromp. This class covers finite-difference, finite-element, and spectral methods for numerical solutions to the wave and heat equations. Since these notes were primarily taken live, they may contains typos or errors.

Chapter 1

Continuum Mechanics and the Equations of Motion

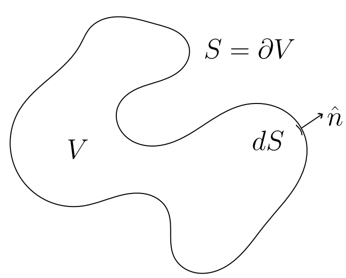
In this class, we will primarily focus on the wave and heat equations, which are important in the study of geophysics, and more broadly, continuum mechanics. As such, we will begin with an introduction to basic continuum mechanics to better understand the role of the differential equations we study.

Continuum mechanics are primarily governed by four conservation laws:

1. Conservation of mass,
2. Conservation of linear momentum,
3. Conservation of angular momentum,
4. Conservation of energy.

The wave and heat equations arise as a result of (2) and (4), respectively, but in actual applications it is often the case that coupled systems of conservation laws must be solved.

1.1 Conservation of Mass



We consider a "comoving volume" V. By "comoving volume", one can imagine a bag of some fluid mass deposited in a river, which can be deformed as it moves, but nevertheless maintains a constant mass throughout. We also denote the surface of V by $S = \partial V$, and for small surface elements $\mathrm{d}S$ we denote the unit outward normal vector by $\hat{n}$.[1]

We also adopt the Einstein summation convention, in which repeated indices that are not otherwise used are implied to be summed over:

$$\vec{u} = u^i e_i$$

If we consider a change of basis to some new basis $\{e_1', e_2'\}$, this can then be written as

$$\vec{u} = u^{i'} e_i'$$

where $u^{i'}$ denotes the ith component of $\vec{u}$ in the new basis.

While $\vec{u}$ is invariant under change of basis, the components are of course not. The way that they transform under change of basis is given by the change of basis matrix λ, and this relationship is expressed under Einstein summation notation by

$$\begin{aligned} u^i &= \lambda^i_{i'} u^{i'} \\ e_i &= \lambda^i_{i'} e_i' \end{aligned}$$

The reverse transformation may be denoted by Λ. The fact that they are inverses may be expressed by the equation

$$\lambda^i_{i'} \Lambda^{i'}_j = \delta^i_j$$

where δ^i_j is the Kronecker delta (in coordinates, the RHS is the identity matrix). This then allows us to express the reverse relationships for change of basis:

$$\begin{aligned} u^{i'} &= \Lambda^{i'}_i u^i \\ e_i' &= \Lambda^{i'}_i e_i \end{aligned}$$

Now, to formalize the notion of the mass of V, we first consider the mass density, considered as a function $\rho(\vec{x}, t)$ of both space and time (with respect to some coordinate system). For an infinitesimal volume element $\mathrm{d}V$, the mass of the volume is given by $\rho\,\mathrm{d}V$. Notice that the dimensions of mass density is

$$[\rho] = \frac{\mathrm{kg}}{\mathrm{m}^3}$$

so that the dimensions of mass are

$$[\rho]\,[\mathrm{d}V] = \mathrm{kg}$$

More generally, the mass of V is given by integrating against mass density,

$$M = \int_V \rho\,\mathrm{d}V$$

[1] In this course we adopt the convention that a vector is denoted by $\vec{v}$, a unit vector by $\hat{v}$, and the ith component of a vector by v_i or v^i. (The distinction is the distinction between covariant and contravariant indices, but is not necessary for this course). Moreover, we denote the standard basis vectors in the x and y directions by $e_x = \hat{x}$ and $e_y = \hat{y}$, respectively.

In Cartesian coordinates this is

$$M = \int_V \rho(x, y, z, t)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

Notice that the integrand is time dependent. Moreover, we allow V to deform over time as well, so that this equation might be more appropriately written as

$$M(t) = \int_{V(t)} \rho(x, y, z, t)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

Then the conservation of mass law is expressed as the ODE

$$0 = \frac{\mathrm{d}M}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int_{V(t)} \rho\,\mathrm{d}V$$

If V is constant (that is, if we allow for no deformation), then Feynman's trick give us

$$\frac{\mathrm{d}M}{\mathrm{d}t} = \int_V \frac{\partial \rho}{\partial t}\,\mathrm{d}V$$

However, because V is time-dependent, this fails to hold. Instead, we first appeal to the single-dimensional case by considering Leibniz's rule, which handles integration with time-dependent limits and integrand of the form

$$I(t) = \int_{a(t)}^{b(t)} f(x, t)\,\mathrm{d}x$$

In this case, by considering I as the area under the curve, it is clear that (at least for continuous a, b) the value $\frac{\mathrm{d}I}{\mathrm{d}t}$ must take into account both the values $\frac{\partial f}{\partial t}|_{[a,b]}$, but also the area which is added or removed by the change in a, b.

Theorem 1.1: Leibniz's Rule

Let $f(x, t)$ be jointly continuous with $\frac{\partial}{\partial t} f(x, t)$ also jointly continuous in some region given by $a(t) \le x \le b(t)$, $t_0 \le t \le t_1$. If a, b are both continuously differentiable, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{a(t)}^{b(t)} f(x, t)\,\mathrm{d}x\right) = \int_{a(t)}^{b(t)} \frac{\partial f}{\partial t}(x, t)\,\mathrm{d}x + f(b(t), t)\frac{\mathrm{d}b}{\mathrm{d}t}(t) - f(a(t), t)\frac{\mathrm{d}a}{\mathrm{d}t}(t)$$

This can be derived using the limit formulation of the derivative by writing

$$\frac{\mathrm{d}I}{\mathrm{d}t} = \lim_{\Delta t \to 0} \frac{1}{\Delta t}\left[\int_{a(t+\Delta t)}^{b(t+\Delta t)} f(x, t + \Delta t)\,\mathrm{d}x - \int_{a(t)}^{b(t)} f(x, t)\,\mathrm{d}x\right]$$

As a first order approximation for the change in area if the integration limits are constant, Feynman's rule holds and we have

$$\int_{a(t)}^{b(t)} \frac{1}{\Delta t} \lim_{\Delta t \to 0} [f(x, t + \Delta t) - f(x)]\,\mathrm{d}x + O((\Delta t)^2) = \int_{a(t)}^{b(t)} \frac{\partial f}{\partial t}(x, t)\,\mathrm{d}x$$

At the upper limit, f is also near constant, so the change in area is approximated to first order by

$$f(b(t),t)\lim_{\Delta t\to 0}\frac{1}{\Delta t}\left[b(t+\Delta t)-b(t)\right]=f(b(t),t)\frac{\mathrm{d}b}{\mathrm{d}t}(t)$$

The lower limit is similar with a negative sign. Combining the three approximations, we get

$$\frac{\mathrm{d}I}{\mathrm{d}t}=\int_{a(t)}^{b(t)}\frac{\partial f}{\partial t}(x,t)\,\mathrm{d}x+f(b(t),t)\frac{\mathrm{d}b}{\mathrm{d}t}(t)-f(a(t),t)\frac{\mathrm{d}a}{\mathrm{d}t}(t)$$

Now, we return to the case of our comoving volume. Taking inspiration from Leibniz's rule, the main term that we have to adjust in the 2-dimensional case is the change in boundary area. This is approximated by considering the volume over which a surface element moves within an infinitesimal time interval.

For a given surface element $\mathrm{d}S(t)$, we consider both the associated normal $\hat{n}(t)$ and the velocity vector $\vec{v}$. Then the component of the velocity of $\mathrm{d}S(t)$ in the normal direction is given by

$$\vec{v}\cdot\hat{n}(t)=v^i(t)n^i(t)$$

Note that, as usual we also define the length of u by

$$\|\vec{u}\|^2=(u^i)^2$$

Now, the flux of mass through $\mathrm{d}S(t)$ in the period $[t,t+\Delta t]$ is then

$$\rho|_{\mathrm{d}S(t)}\vec{v}\cdot\hat{n}$$

Then we can now include the correct error term to calculate $\frac{\mathrm{d}M}{\mathrm{d}t}$:

$$\frac{\mathrm{d}M}{\mathrm{d}t}=\frac{\mathrm{d}}{\mathrm{d}t}\int_{V(t)}\rho\,\mathrm{d}V=\int_{V(t)}\frac{\partial\rho}{\partial t}\,\mathrm{d}V+\int_{S(t)}\rho\vec{v}\cdot\hat{n}\,\mathrm{d}S$$

(where S is equipped with the outward-facing orientation). Lastly, we can replace the second term with an integral over $V(t)$ using the divergence theorem:

$$\int_S\vec{u}\cdot\hat{n}\,\mathrm{d}S=\int_V\nabla\cdot\vec{u}\,\mathrm{d}V$$

We combine the integrals:

$$\frac{\mathrm{d}M}{\mathrm{d}t}=\int_{V(t)}\left[\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\vec{v})\right]\mathrm{d}V$$

Note that the divergence is taken against $\rho\vec{v}$, since this is the quantity which is dotted against $\hat{n}$.

Because the integral must be zero for all possible V, the integrand is identically zero. Thus we express the conservation of mass law for a comoving volume (also known as the **continuity equation**) by

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\vec{v})=0$$

We can expand this using summation notation as

$$\partial_t \rho + v^i \nabla_i \rho + \rho \nabla_i v^i = 0$$

The first two terms $\partial_t \rho + v^i \nabla_i \rho$ is known as the **material derivative**

$$D_t \rho = \partial_t \rho + \vec{v} \cdot \nabla \rho$$

where the first term is the local change in density, and the second is the advection term (which is the directional derivative of the density in the direction of velocity). In other words, the rate of change of local mass along a path is given by the pointwise rate of change together with the change given by the motion of the path against the gradient. We then rephrase the continuity equaiton as

$$D_t \rho + \rho \nabla \cdot \vec{v} = 0$$

or equivalently

$$\frac{1}{\rho} D_t \rho = -\nabla \cdot \vec{v}$$

This essentially says that the relative change in density along a path is the negative of the velocity divergence. This makes sense because when divergence is positive, mass is moving away and density decreases, while density increases with velocity divergence is negative. In particular, if the mass is incompressible, $\nabla \cdot \vec{v} = 0$, so that density is constant along any path. In this case, we don't need to worry about conservation of mass.

1.2 Conservation of Linear Momentum

Linear momentum is given by the product of mass with velocity. In continuum mechanics this is given by $\rho \vec{v} \, \mathrm{d}V$. Thus the total momentum of a volume is simply

$$p = \int_{V(t)} \rho \vec{v} \, \mathrm{d}V$$

The statement of conservation of linear momentum is essentially that the only way to change linear momentum is to apply (external) forces to our volume. This is basically Newton's second law, written as $\vec{F} = \dot{p}$. One can consider a body force $\vec{f}$ which pulls on small volume elements $\mathrm{d}V$. We can also consider forces $\vec{t}$ which act only on the surface of the volume. Thus we write

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V(t)} \rho \vec{v} \, \mathrm{d}V = \int_{V(t)} f \, \mathrm{d}V + \int_{S(t)} \vec{t} \, \mathrm{d}S$$

We can differentiate the left hand side the same way as we did in the conservation mass equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V(t)} \rho \vec{v} \, \mathrm{d}V = \int_{V(t)} \partial_t (\rho \vec{v}) \, \mathrm{d}V + \int_{S(t)} (\rho \vec{v}) \hat{n} \cdot \vec{v} \, \mathrm{d}S$$

To conceptualize the surface-acting forces, we consider the **stress tensor**, which is a rank 2 tensor (or matrix) T such that $T \cdot \vec{n}$ gives the traction force on $\mathrm{d}S$, if the unit outward normal of $\mathrm{d}S$ is $\hat{n}$. In indices, this is

$$t_i = T_{ij} \hat{n}_j \, \mathrm{d}S$$

(Note that in general $T_{ij}\hat{n}_j \neq \hat{n}_j T_{ji}$, but this is true if T is a symmetric tensor). Then the right hand side of our equation is writen as

$$\int_{V(t)} \vec{f}\,\mathrm{d}V + \int_{S(t)} T\cdot\hat{n}\,\mathrm{d}S$$

Once again we use the divergence theorem to convert these to volume integrals, so that our equation is given by

$$\int_{V(t)} \left[\partial_t(\rho\vec{v}) + \nabla\cdot(\rho\vec{v}\otimes\vec{v})\right]\mathrm{d}V = \int_{V(t)} \left[\vec{f} + \nabla\cdot T\right]\mathrm{d}V$$

Note that both integrals are vector quantities. In components, the integrand on the left can be given by

$$\partial_t\rho v^i + \nabla_j\cdot\left(\rho v^i v^j\right)$$

(By convention, the divergence theorem is written in indices as $\int_S u^i\hat{n}_i\,\mathrm{d}S = \int_V \nabla_i u^i\,\mathrm{d}V$).

Similarly, the divergence of T is given by contracting the gradient against the last index of T, so that the integrand on the right is given in indices by

$$f^i + \nabla_j\cdot T^{ij}$$

Equating the integrands again, the conservation of linear momentum law is thus given by

$$\partial_t(\rho\vec{v}) + \nabla\cdot(\rho\vec{v}\otimes\vec{v}) = \nabla\cdot T + \vec{f}$$

Some equivalent formulations are

$$\begin{aligned}\partial_t(\rho\vec{v}) &= \nabla\cdot(T - \rho\vec{v}\otimes\vec{v}) + \vec{f}\\ \partial_t(\rho\vec{v}) + \nabla\cdot(\rho\vec{v}\otimes\vec{v} - T) &= \vec{f}\end{aligned}$$

The last formulation is the Eulerian form, which expresses the conservation law as the pointwise time derivative of a quantity plus its flux being equated to the source term.

Expressing this with the chain rule gives

$$(\partial_t\rho)\vec{v} + \rho\partial_t\vec{v} + \nabla\cdot(\rho\vec{v})\vec{v} + \rho\vec{v}\nabla\cdot\vec{v} = \nabla\cdot T + \vec{f}$$

The first and third term are zero by conservation of mass. Thus this is equivalent to

$$\rho\left(\partial_t\vec{v} + \vec{v}\nabla\cdot\vec{v}\right) = \nabla\cdot T + \vec{f}$$

The parenthetical term is again the material derivative, this time of velocity, so this is

$$\rho D_t\vec{v} = \nabla\cdot T + \vec{f}$$

As formulated, the coupling of the conservation of mass and momentum laws gives four scalar equations. Even if body forces are given, this leaves as unknowns the mass density, velocity, and stress tensor. Thus we need constitutive relationships, which express some of these (particularly the stress tensor) in terms of the others in order to solve these. This makes sense given that the actual results will depend on material properties, which are specified in the stress tensor but nowhere else.

To do this, we consider stress and strain. Fix some origin point and let $\vec{x}$ denote the starting point of some particle. Let $\vec{r}(\vec{x}, t)$ denote the position of particle $\vec{x}$ at time t. By definition $\vec{r}(\vec{x}, 0) = \vec{x}$. Define $\vec{s}(\vec{x}, t) = \vec{r}(\vec{x}, t) - \vec{x}$ to be the displacement vector. Suppose we consider two initially neighboring particles $\vec{x}, \vec{x} + \mathrm{d}\vec{x}$. As time progresses, their displacement becomes $\mathrm{d}\vec{r} = \vec{r}(\vec{x} + \mathrm{d}\vec{x}, t) - \vec{r}(\vec{x}, t)$. We take the first order Taylor expansion:

$$\mathrm{d}\vec{r} \approx \vec{r}(\vec{x}, t) + \mathrm{d}\vec{x} \cdot \nabla \vec{r}(\vec{x}, t) - \vec{r}(\vec{x}, t) = \mathrm{d}x^i \nabla_i \vec{r} = \mathrm{d}\vec{x} \cdot \nabla \vec{r}$$

We can express this as a tensor by

$$\nabla_j r^i \, \mathrm{d}x^j = F^i_j \, \mathrm{d}x^j$$

where $F^i_j = \nabla_j r^i$, or equivalently $F = (\nabla \vec{r})^T$. The tensor F is known as the **deformation gradient**. Recalling that $\vec{r} = \vec{x} + \vec{s}$, we have

$$F = [\nabla(\vec{x} + \vec{s})]^T = [\nabla \vec{x} + \nabla s]^T$$

Since $\nabla \vec{x}$ is taken against $\vec{x}$ itself, its matrix formulation is just the identity:

$$I = \nabla \vec{x} = \hat{x} \otimes \hat{x} + \hat{y} \otimes \hat{y} + \hat{z} \otimes \hat{z} = (\delta_{ij})$$

In summary, we can write

$$F = I + (\nabla \vec{s})^T$$

which is the identity plus the transpose of the displacement gradient. Physically, the displacement gradient represents the separation or convergence of material, or equivalently the deviation from uniform motion. Noting that

$$\mathrm{d}\vec{r} = F \cdot \mathrm{d}\vec{x}$$

we have

$$\mathrm{d}\vec{r} = \left[I + (\nabla \vec{s})^T \right] \mathrm{d}\vec{x} = \mathrm{d}\vec{x} + (\nabla \vec{s})^T \cdot \mathrm{d}\vec{x}$$

In general the tensor may not be symmetric; however we can always decompose a matrix into its symmetric and antisymmetric parts as

$$A = \frac{1}{2}\left(A + A^T\right) + \frac{1}{2}\left(A - A^T\right)$$

In particular, we can write F as

$$F = I + \varepsilon + \omega$$

where ε, ω are the symmetric and antisymmetric parts of $(\nabla \vec{s})^T$, respectively. ε is called the **strain** and ω the **vorticity**.

Definitions