GEOL 2300

Introduction

In this class, we learn how to apply proficiently concepts of maths & physics to your research.

Some of you are directly interested to study & solve equations such

$$\frac{\partial p}{\partial t} = \Lambda \frac{\partial T}{\partial t} + \frac{1}{S}\frac{\partial}{\partial x}\left(\frac{k(p)}{\mu}\frac{\partial p}{\partial x}\right)$$

$$\rho\frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j}\left[\frac{1}{2} C_{ijkl}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right)\right]$$

$$\frac{\partial C}{\partial t} = \nabla\cdot(D\nabla C) - R(C - C_0)$$

$$\begin{cases} \rho\left[\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u}\right] = -\nabla p + \rho\vec{g} + \mu\nabla^2\vec{u} \\ \nabla\cdot\vec{u} = 0 \end{cases}$$

and many more ...

- What do they have in common?

$\Rightarrow$ differential equations.

Physics is about predicting / extrapolating the state of a system and <u>especially</u> its variation with space & time!

Variations $\rightarrow$ introduce differential operators.

The first two modules of this class

(1) Tensor calculus

(2) Continuum mechanics

are designed to provide the tools to derive, use & solve differential equations that we commonly face in the Earth, Environmental & Planetary Science.

The language of physics is calculus ....

Feynman asked once a journalist doing research on the Manhattan Project whether he knew calculus ....
Feynman said "It's the language God talks"...
Calculus provides a language where differential equations are sentences to study & understand the world around us.

Einstein: "The eternal mystery of the world is its comprehensibility".

Wigner: "The miracle of the appropriateness of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve."

(see more in "Infinite Powers" S. Strogatz)

Our roddmap:

(1) Fundamental theorem of calculus

- what is it?
- What does it mean?
- Why should I care?

=> answer: in a nutshell it formalizes how one approaches solving physics problems:

↳ derivation of differential equation (ex. statement of conservation laws)

↳ solution by integration.

(2) Continuous functions are vectors! Using some simple linear algebra to solve differential equations

- What is a vector? A vectorial space?
- How do you choose a vectorial basis for continuous functions?
  - (•) Taylor series
  - (•) Fourier series
  - (•) Trigonometric series.
  - (•) Legendre polynomial / spherical harmonics
  - (•) Bessel functions.

(3) Differential operators & Integrals are linear operators

(4) From 1 to N Dimensions - multivariate calculus

(•) Partial derivatives
(•) Vector calculus, div, grad, curl
(•) tensors and some aspect of symmetry

(5) Continuum mechanics

(•) Eulerian vs Lagrangian ref frame
(•) Gauss theorem, Reynolds transport theorem
(•) Generic Conservation laws (continuity, Cauchy ...)

(•) Closure equations
(i) Linear transport theory
(ii) intuition & symmetry

(•) Buckingham - Π theorem & dimensional analysis

The Fundamental theorem of Calculus

<u>Idea:</u> Integrals & derivatives are related to each other, they are opposites.

<u>why do we care?</u>

(a) derivatives are easy to compute, not the case for integrals → can use inference with guesses from our understanding of derivatives to solve integrals analytically

e.g. $\int [3x^2 + 2x + 5]\, dx = ?$

$$\int 3x^2 dx + \int 2x dx + \int 5 dx$$

$\frac{d}{dx}(x^3) = 3x^2 \qquad \frac{d}{dx}(x^2) = 2x \qquad \frac{d}{dx}(5x) = 5$

$$\Rightarrow \int \frac{d(x^3)}{dx} dx + \int \frac{d}{dx}(x^2) dx + \int \frac{d(5x)}{dx} dx$$

$$= x^3 + x^2 + 5x$$ using fundamental th. of calculus.

(b) $\mu \frac{d^2 v}{dx^2} = \frac{dp}{dx}$

$\frac{dv}{dy} = 0$

} Stokes flow (unidirectional) with incompressible fluid

⇒ Differential Equations

solving $p(x)$ & $v(x)$ requires integration!

more generally physical laws are expressed generally as differential equations
↳ Solution(s) require integration.

Functions of a single variable

$F(x)$ is an anti-derivative of $f(x)$ if

$$\frac{d}{dx} F(x) = f(x)$$

(there is an infinite number of them for any well-behaved $f(x)$)

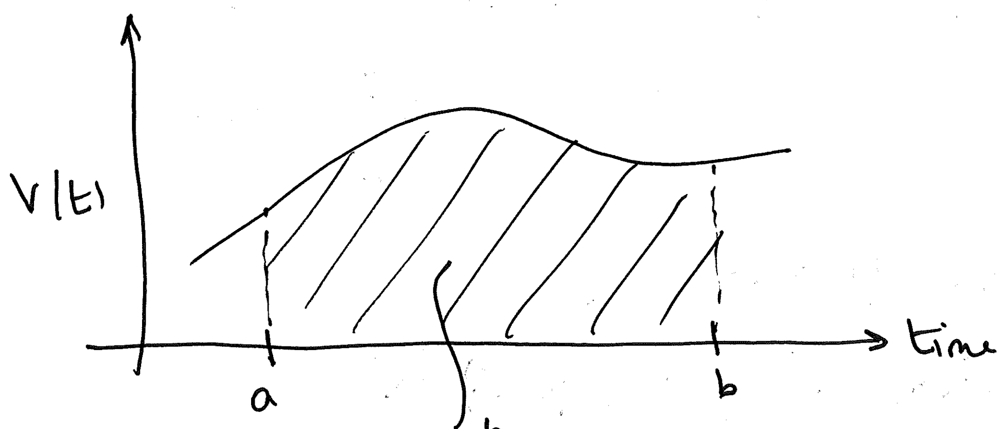
One statement of the Fundamental theorem of Calculus reads

$$\int_a^b f(x)\,dx = F(b) - F(a)$$

Let's build some intuition into it, assume you're running around on the campus from position $x=a$ to $x=b$
(we can assume a pseudo 1D trajectory for this idealized case)
There are hills & flat portions such that your instantaneous velocity $v(x)$ can vary a lot. You want to compute your average velocity $\langle v \rangle$

We can use 2 approaches / pts of view

how fast did I go? Well, I can use a GPS-running watch to measure my "instantaneous" velocity $v(t)$ at differnt times



$$\langle v \rangle = \frac{1}{b-a} \int_a^b v(t)\, dt \qquad (*)$$

Alternatively if I know the distance I ran & the time it took $(b-a)$ then

$$\langle v \rangle = \frac{x(t=b) - x(t=a)}{b-a} \qquad (**)$$

Equating $(*)$ & $(**)$

$$\frac{1}{b-a} \int_a^b v(t)\, dt = \frac{x(t=b) - x(t=a)}{b-a}$$

$$\Rightarrow \int_a^b v(t)\, dt = x(t=b) - x(t=a)$$

with $x(t) \Rightarrow$ related to $v(t)$ by

$\frac{dx}{dt} = v(t)$ (x is anti-derivative of v)

In a nutshell that is the fundamental theorem of calculus

$$F(b) - F(a) = \int_a^b f(x)\,dx \quad \text{when} \quad \frac{dF}{dx} = f(x)$$

let's go further

$$F(x) - F(a) = \int_a^x f(x')\,dx'$$

d/dx (

$$\frac{dF(x)}{dx} = f(x) \quad \text{as we know } \&$$

$$\frac{dF(x)}{dx} = \frac{d}{dx}\left[\int_a^x f(x')\,dx'\right]$$

$$\Rightarrow \frac{d}{dx}\left[\int_a^x f(x')\,dx'\right] = f(x)$$ which is another way to frame the theorem.

What does it mean?

(1) Derivatives & integrals are opposites

(2) Because they are opposite & derivatives are much easier to compute we can compute integrals by guessing the correct anti-derivative ...

(3) Every function $f(x)$ that can be written in terms of a primitive function $F(x)$ such that $\frac{dF}{dx} = f(x)$

is such that its integral (definite) is equal to the value of the difference of F at the 2 bounds. (b & a).

In more than 1-D if $f(\vec{x})$ is a function (here a scalar function for the sake of simplicity) of multiple variables

e.g. $\vec{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ position ; $\vec{x} = \underbrace{\begin{pmatrix} P \\ T \end{pmatrix}}_{\text{pressure \& temperature}}$ thermodynamics

Intuitively, the fundamental theorem would suggest that

$$(1) \qquad F(\vec{X}_b) - F(\vec{X}_a) = \int_{\mathcal{C}} f(\vec{x})\, \underbrace{d\ell}$$

$\mathcal{C}$ ↑ path integral

$d\ell$: integrate over a trajectory in $\vec{x}$ space

Well that would be great because it would mean

(a) that the integral is independent of the path $\mathcal{C}$ as long as it starts from $\vec{X_a}$ and ends at $\vec{X_b}$

(b) if $\vec{X_b} = \vec{X_a}$ → (1) implies that for a closed path

$$\oint_{\mathcal{C}} f(\vec{x})\, d\ell = 0$$

For a 1-D function $f(x)$, we saw that the condition is that

$$\frac{dF}{dx} = f(x) \qquad F = \text{anti-derivative of } f$$

What condition(s) need(s) to be fulfilled in more dimensions with $f(\vec{x})$ & $F(\vec{x})$?

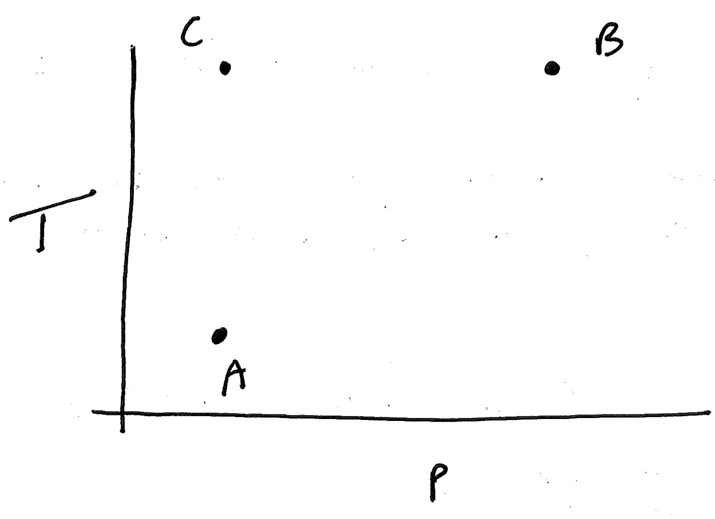
We will use 2 examples drawn from physics:

(A) thermodynamics - Gibbs free energy

(B) Gravity (conservative) versus friction (non-conservative)

(A) <u>Path invariance in thermodynamics</u>

Assume a closed system is initially in state A given by (T_A, p_A) (temperature/pressure) and is changing to a state B defined by (T_B, p_B), then the change in Gibbs free energy experienced by the system is independent of the (T, p) path followed to go from $A \longrightarrow B$



Let's define a change in Gibbs free energy

$$dG\,\cancel{f}(T,p) = \alpha(T,p)\,dT + \beta(T,p)\,dp$$

where α, β are functions that will assume "special" properties to ensure path independence.

Let's define a transitional state $C \to (T_C,\ p_C = p_A)$

along the path from $A \to C$

$$dG = \alpha(T,p)\,dT \quad , \text{ because } dp = 0$$

$$\Delta_{A\to C} G = \int_{T_A}^{T_C} \underbrace{\alpha(T,p)\,dT}_{\equiv\, dG \text{ at fixed pressure}}$$

similarly $\displaystyle \Delta_{C\to B} G = \int_{p_C}^{p_B} (dG)_{\text{fixed } T} = \int_{p_C}^{p_B} \beta(T,p)\,dp$

Path independence

$$\Delta_{A\to B} G = \int_A^B dG \overset{\text{path independence}}{=} \int_{T_A}^{T_C} \alpha(T,p)\,dT + \int_{p_C}^{p_B} \beta(T,p)\,dp$$

it works only if $\alpha(T,p) = \left(\frac{\partial G}{\partial T}\right)_{\text{fixed } p}$ & $\beta = \left(\frac{\partial G}{\partial p}\right)_{\text{fixed } T}$

$\Rightarrow$ path independence when integrating a multivariate function like Gibbs free energy changes dG is satisfied if and only if

$$dG(x,y,z) = \frac{\partial G}{\partial x}dx + \frac{\partial G}{\partial y}dy + \frac{\partial G}{\partial z}dz = \nabla G \cdot \vec{dx}$$

$$\nabla G \equiv \begin{pmatrix} \partial G/\partial x \\ \partial G/\partial y \\ \partial G/\partial z \end{pmatrix}$$

in that case dG is said to be a total derivative and

$$G(\vec{x}_B) - G(\vec{x}_A) = \int_A^B \nabla G \cdot \vec{dx}$$

Same fundamental theorem of calculus and

for functions such as dG (total derivative)

$$\oint \nabla G \cdot \vec{dx} = 0$$

over a closed path
$\Rightarrow$ reversibility!

so $$G(\vec{x}_B) - G(\vec{x}_A) = \int_A^B \vec{f} \cdot \vec{dx}$$

works if $\vec{f}$ is the gradient of G

$$\vec{f} = \begin{pmatrix} \partial G/\partial x \\ \partial G/\partial y \\ \partial G/\partial z \end{pmatrix}$$

Interesting properties of total derivatives:

$$dG = \overset{\alpha}{\frac{\partial G}{\partial T}}\, dT + \overset{\beta}{\frac{\partial G}{\partial p}}\, dp$$ for example

$$\frac{\partial \alpha}{\partial p} = \frac{\partial \beta}{\partial T}$$ (simple check)

Because $$\frac{\partial \alpha}{\partial p} = \frac{\partial}{\partial p}\left(\frac{\partial G}{\partial T}\right) = \frac{\partial}{\partial T}\left(\frac{\partial G}{\partial p}\right)$$ exchange of limits

$$\frac{\partial \beta}{\partial T} = \frac{\partial}{\partial T}\left(\frac{\partial G}{\partial p}\right)$$

=> Maxwell's relations in thermodynamics

$$dG = -S\, dT + V\, dp$$ (fixed mass)

$$(\alpha = -S \; ; \; \beta = V)$$

thermal expansion coefficient

$$\Rightarrow \quad -\left(\frac{\partial S}{\partial p}\right)_T = \left(\frac{\partial V}{\partial T}\right)_p = +\gamma_T V$$

little game: what is the temperature profile ~~of~~ in a convecting fluid where adiabatic fluid ascent is assumed?

adiabatic means no heat exchange with surrounding

depending on conjugate variable we want to use

$$\delta Q = T\, dS = c_p\, dT = 0$$

$$\left(\frac{\partial T}{\partial S}\right)_p = \frac{T}{c_p}$$

$$\left(\frac{\partial T}{\partial p}\right)_S = -\left(\frac{\partial T}{\partial S}\right)_p \left(\frac{\partial S}{\partial p}\right)_T = \frac{\gamma_T T V}{C_p}$$

dG is expressed as an energy/mass

so V is a volume/unit mass

$$V = \frac{1}{\rho}$$

$$\left(\frac{\partial T}{\partial p}\right)_S = \frac{\gamma_T T}{\rho C_p}$$ is the adiabatic T profile in a fluid

$$\left(\frac{\partial T}{\partial z}\right)_S = \left(\frac{\partial T}{\partial p}\right)\left(\frac{\partial p}{\partial z}\right)$$

if pressure profile is <u>near</u> hydrostatic ...
(can it be hydrostatic?)

$$\Rightarrow \frac{\partial p}{\partial z} \sim \rho g$$

$$\Rightarrow \left(\frac{\partial T}{\partial z}\right)_S = \frac{\gamma_T T g}{C_p}$$

B <u>Gravity a conservative force</u>

Conservative forces are often said to "derive" from a potential (e.g. $\psi(\vec{x})$)

so if $\vec{f} = -\nabla\psi$ is a force associated with potential ψ (← gradient)

$$\left(\nabla\psi = \begin{pmatrix} \partial\psi/\partial x \\ \partial\psi/\partial y \\ \partial\psi/\partial z \end{pmatrix} \right)$$

such a force is said to be conservative if

$$\text{work around closed path} = \oint \vec{f} \cdot \vec{dl} = 0$$

$$\text{check} \quad -\oint \nabla\psi \cdot \vec{dl} = \psi(x_0) - \psi(x_0) = 0$$

↑ Fundamental th. of calculus.

e.g. Gravity force $\vec{f_g} = -m\nabla V_g$

where $V_g(\vec{x})$ is the gravitational potential

$V_g(\vec{x})$ & or using radial (spherical)

coordinates centered on the object "creating" the potential

$$V_g(r) = -\frac{GM}{r} \rightarrow \vec{f_g} = -\frac{GMm}{r^2}\hat{r}$$

$$\oint \vec{f_g} \cdot \vec{dl} = -m\oint \nabla V_g \cdot \vec{dl} = -m\,[\underbrace{V_g(\vec{x}_{end}) - V_g(\vec{x}_0)}_{=0 \text{ on closed loop}}]$$

Now, let's consider friction (linear)

$$\vec{f} = -\mu \frac{d\vec{x}}{dt} \qquad (-\mu \vec{v})$$

Let's assume that we follow a circular trajectory and compute the net work performed by this force

$$W = \oint \vec{f} \cdot \vec{dl} \quad , \quad \vec{dl} = \frac{d\vec{x}}{dt} dt$$

$$\left.\begin{array}{l} x = \cos(2\pi t) \\ y = \sin(2\pi t) \end{array}\right\} \quad \frac{d\vec{x}}{dt} = \begin{pmatrix} -2\pi \sin(2\pi t) \\ 2\pi \cos(2\pi t) \end{pmatrix}$$

$$\oint \vec{dl} \longrightarrow \int_0^1 \frac{d\vec{x}}{dt} dt$$

$$W = -\int_0^1 \mu \frac{d\vec{x}}{dt} \cdot \frac{d\vec{x}}{dt} dt = -\mu 4\pi^2 \int_0^1 \underbrace{[\sin^2(2\pi t) + \cos^2(2\pi t)]}_{=1} dt$$

$$= -4\pi^2 \mu \neq 0 \quad \Rightarrow \text{ not a conservative force}$$

$\vec{f}$ cannot be written as the gradient of a potential

$$\vec{f} \neq \nabla \psi \Rightarrow \text{so}$$

Fundamental theorem of calculus <u>doesn't</u> apply.