AE 760AA: Micromechanics and multiscale modeling

Lecture 8 - Variational Calculus

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schedule

- Feb 18 Variational Calculus
- Feb 20 Variational Calculus
- Feb 25 Bounds and Boundary Conditions (HW 3 Due)
- Feb 27 -

outline

- lagrange multipliers
- calculus of variations

lagrange multipliers

differential and variational statements

- A differential statement includes a set of governing differential equations established inside a domain and a set of boundary conditions to be satisfied along the boundaries
- A variational statement is to find stationary conditions for an integral with unknown functions in the integrand
- Variational statements are advantageous in the following aspects
 - Clear physical meaning, invariant to coordinate system
 - Can provide more realistic descriptions than differential statements (concentrated loads)
 - More easily suited to solving problems numerically or approximately
 - Can be more systematic and consistent than building a set of differential equations

stationary problems

- If the function $F(u_1)$ is defined on a domain, then at $\frac{dF}{du_1} = 1$ it is considered to be stationary
- This stationary point could be a minimum, maximum, or saddle point
- We use the second derivative to determine which of these it is: >0 for a minimum, <0 for a maximum and =0 for a saddle point
- For a function of *n* variables, $F(u_n)$ the stationary points are

$$\frac{\partial F}{\partial u_i} = 0$$

for all values of i

and to determine the type of stationary point we use

$$\sum_{i,j=1,n} rac{\partial^2 F}{\partial u_i \partial u_j}$$

lagrange multipliers

• Let us now consider a function of several variables, but the variables are subject to a constraint

$$f(u_1, u_2, ...) = 0$$

- Algebraically, we could use each provided constraint equation to reduce the number of variables
- For large problems, it can be cumbersome or impossible to eliminate some variables
- The Lagrange Multiplier method is an alternative, systematic approach

lagrange multiplier

For a constrained problem at a stationary point we will have

$$dF = rac{\partial F}{\partial u_1} du_1 + \ldots + rac{\partial F}{\partial u_n} du_n = 0$$

• The relationship between du_i can be found by differentiating the constraint

$$df=rac{\partial f}{\partial u_1}du_1+\ldots+rac{\partial f}{\partial u_n}du_n\,=0$$

• We can combine these two equations using a Lagrange Multiplier

$$\left[rac{\partial F}{\partial u_1}du_1\!+\!\ldots\!+\!rac{\partial F}{\partial u_n}du_n\,+\lambda\left[rac{\partial f}{\partial u_1}du_1\!+\!\ldots\!+\!rac{\partial f}{\partial u_n}du_n
ight]$$

• We can re-group terms as

$$\sum_{i=1}^n \left[rac{\partial F}{\partial u_i} + \lambda rac{\partial f}{\partial u_i}
ight] du_i = 0$$

lagrange multiplier

- The Lagrange Multiplier, λ is an arbitrary function of u_i
- We can choose the Lagrange Multiplier such that

$$\frac{\partial F}{\partial u_n} + \lambda \frac{\partial f}{\partial u_n} = 0$$

• Which now leaves

$$rac{\partial F}{\partial u_i} + \lambda rac{\partial f}{\partial u_i} = 0 \qquad i = 1, 2, \ldots, n-1$$

• We now define a new function $F^* = F + \lambda f$

lagrange multiplier

- This converts a constrained problem in n variables to an unconstrained problem in n + 1 variables
- Notice that while the stationary values of F^* will be the same as the stationary values to F, they will not necessarily correspond
- For example, a minimum in F^* might be a maximum in F
- This provides a systematic method for solving problems with any number of variables and constraints, and is also well-posed for numeric solutions

example

- Design a box with given surface area such that the volume is maximized
- The box has no cover along one of the surfaces (open-face box)
- This gives the surface area as A = xy + 2yz + 2xz = C
- worked example

calculus of variations

functional

• A functional of some unknown function y(x) is defined as

$$I = I[y(x)]$$

- A functional depends on all values of y(x) over some interval
- We will often use the form

$$I[y] = \int_a^b F(x,y(x),\dot{y}(x)) dx$$

bernoulli

- The original problem that motivated study of variational calculus
- Bernoulli 1696
- Design a chute between two points, A and B
- such that a particle sliding without friction under its own weight
- travels from A to B in the shortest time

variational statement

• To solve Bernoulli's problem we denote the arc length as *s*, speed as

$$v=rac{ds}{dt}$$

• And we can find the total time as

$$t=\int_A^B rac{ds}{v}$$

variational statement

• The arc length *s* can be found from

$$ds=\sqrt{dx^2+dy^2}$$

- Since y=y(x) we can write $dy = \dot{y} dx$
- We can now re-write ds as

$$ds=\sqrt{1+\dot{y}^2}dx$$

variational statement

• From the conservation of energy we can also say that

$$rac{1}{2}mv^2=mgy$$

• Such that

$$v=\sqrt{2gy}$$

• We now need to find some function y(x) which minimizes the integral

$$t=\int_0^arac{\sqrt{1+\dot{y}^2}}{\sqrt{2gy}}dx$$

- Now we develop a method for finding y(x)
- Consider the functional

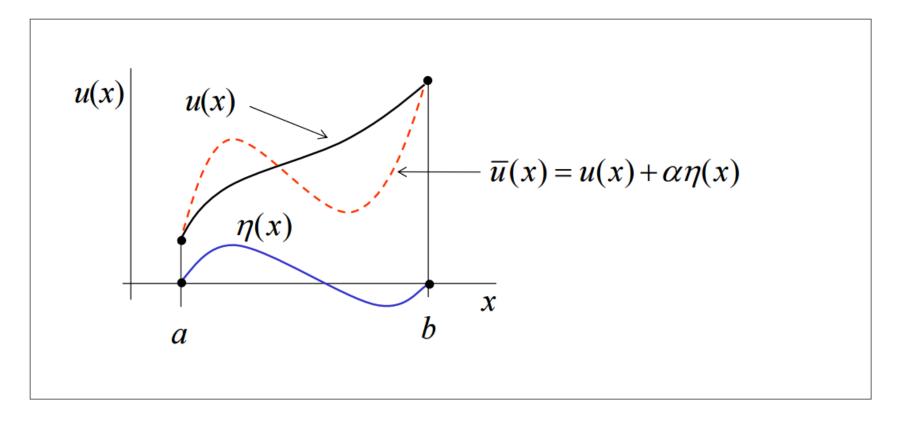
$$I[y] = \int_{x_0}^{x_1} F(x,y,\dot{y}) dx$$

• Where y(x) is subject to boundary conditions

$$y(x_0) = y_0$$
$$y(x_1) = y_1$$

$$y(x_1)=y_1$$

- We assume that there is some solution, y(x) for which I is stationary
- We also assume that y(x) is continuous and differentiable in the problem domain
- Let us now choose some trial function $\bar{y}(x) = y(x) + \alpha \eta(x)$
- Where $\eta(x)$ is some arbitrary continuous function which vanishes at the boundaries



• We can take the derivative of \bar{y} to find

$$\dot{ar{y}} = \dot{y}(x) + lpha \dot{\eta}(x)$$

• This now gives

$$I[lpha]=\int_{x_0}^{x_1}F(x,ar{y},\dot{ar{y}})dx=\int_{x_0}^{x_1}F(x,y(x)+lpha\eta(x),\dot{y}(x)+lpha\dot{\eta}(x))dx$$

• Once y(x) and $\eta(x)$ are chosen, I is a function of α

• We find the stationary function by letting $\frac{dI}{d\alpha} = 0$

$$rac{dI}{dlpha} = \int_{x_0}^{x_1} rac{\partial F}{\partial lpha} dx = \int_{x_0}^{x_1} \left(rac{\partial F}{\partial ar{y}} rac{\partial ar{y}}{\partial lpha} + rac{\partial F}{\partial \dot{ar{y}}} rac{\partial \dot{ar{y}}}{\partial lpha}
ight) dx$$

• This simplifies to

$$\int_{x_0}^{x_1} \left(rac{\partial F}{\partial ar{y}} \eta + rac{\partial F}{\partial \dot{ar{y}}} \dot{\eta}
ight) dx \, .$$

• Now we know that I will be stationary when $\alpha=0$, in which case $\bar{y}=y$, therefore we can write

$$\int_{x_0}^{x_1} \left(rac{\partial F}{\partial y}\eta + rac{\partial F}{\partial \dot{y}}\dot{\eta}
ight) dx = 0.$$

• And now we perform integration by parts on the second term

integration by parts

Recall that

$$\int u dv = uv - \int v du$$

• We choose

$$u=rac{\partial F}{\partial \dot{y}} \ du=rac{d}{dx}igg(rac{\partial F}{\partial y}igg) \ v=\eta(x) \ dv=\dot{\eta}dx$$

integration by parts

• This gives (for the second term)

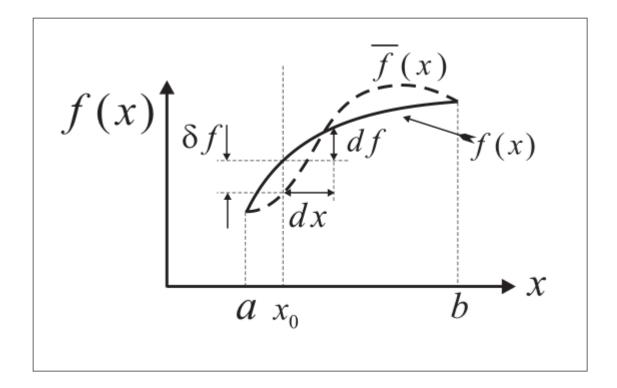
$$\int_{x_0}^{x_1} rac{\partial F}{\partial \dot{y}} \dot{\eta} dx = rac{\partial F}{\partial \dot{y}} \eta|_{x_0}^{x_1} - \int_{x_0}^{x_1} rac{d}{dx} igg(rac{\partial F}{\partial y}igg) \eta(x) \, dx$$

• Combining with the original equation and simplifying gives

$$\int_{x_0}^{x_1} \left[rac{\partial F}{\partial y} - rac{d}{dx} igg(rac{\partial F}{\partial y} igg)
ight] \eta dx + rac{\partial F}{\partial \dot{y}} \eta |_{x_0}^{x_1} = 0.$$

- We already know that $\eta|_{x_0}^{x_1}=0$, so we only need concern ourselves with the terms inside the integral
- Since this must be true for any arbitrary function, η , we can say that $\frac{\partial F}{\partial y} \frac{d}{dx} \left(\frac{\partial F}{\partial y} \right) = 0$
- This is known as the Euler-Lagrange equation
- A solution to the Euler-Lagrange equation is called an extremal, and an extremal which satisfies the boundary conditions is called a stationary function

- In variational calculus, we define the first variation as $\delta y = \bar{y} y$
- Note: while the variation follows many of the same rules as differentiation, it does not correspond to any slope, since η is completely arbitrary



• Variational laws are analogous to differentiation

$$egin{align} \delta(F_1F_2) &= F_1\delta F_2 + \delta F_1F_2 \ \delta\left(rac{F_1}{F_2}
ight) &= rac{F_2\delta F_1 - F_1\delta F_2}{F_2^2} \ \end{aligned}$$

• The variation and derivative are commutative

$$rac{d}{dx}(\delta u) = \delta\left(rac{du}{dx}
ight)$$

• Similarly, the variation is commutative with the integral

$$\delta \int F dx = \int \delta F dx$$

• We can also take the variation of a functional

$$\Delta F = F(x,y+lpha\eta,\dot{y}+lpha\dot{\eta}) - F(x,y,\dot{y})$$

Expanding this function via a Taylor series gives

$$\Delta F = \left[F(x,y,\dot{y}) + \left(\delta y rac{\partial F}{\partial y} + \delta \dot{y} rac{\partial F}{\partial \dot{y}} + \dots
ight)
ight] - F(x,y,\dot{y})$$

• And thus we call the variation of *F*

$$\delta F = rac{\partial F}{\partial y} \delta y + rac{\partial F}{\partial \dot{y}} \delta \dot{y} + \epsilon_1$$

• Where ϵ_1 are terms of higher order than $\sqrt{(\delta y)^2 + (\delta \dot{y})^2}$ and are neglected in the first variation

• We can use variational notation to find the Euler-Lagrange equation

$$I[y] = \int_{x_0}^{x_1} F(x,y,\dot{y}) dx$$

• and taking the variation

$$\delta I = \int_{x_0}^{x_1} \left[rac{\partial F}{\partial y} \delta y + rac{\partial F}{\partial \dot{y}} \delta \dot{y}
ight] dx = 0$$

Using integration by parts on the second term, as before, we find

$$\delta I = \int_{x_0}^{x_1} \left[rac{\partial F}{\partial y} - rac{d}{dx} igg(rac{\partial F}{\partial \dot{y}} igg)
ight] \delta y dx = 0$$

- Since $\delta y(x_0) = \delta y(x_1) = 0$
- Since this must be true for any arbitrary variation, we have

$$rac{\partial F}{\partial y} - rac{d}{dx} igg(rac{\partial F}{\partial \dot{y}}igg)$$

• If the functional, F, does not depend on x explicitly (i.e. the only x dependence comes from y(x)) then we can say

$$rac{d}{dx}igg(F-\dot{y}rac{\partial F}{\partial \dot{y}}igg)=0$$

• or, similarly

$$F-\dot{y}rac{\partial F}{\partial \dot{y}}=C$$

brachistochrone problem

• If we return now to Bernoulli's problem, we had found

$$t=\int_0^arac{\sqrt{1+\dot{y}^2}}{\sqrt{2gy}}dx$$

• Since this does not depend on *x* explicitly, we can use the simpler form of the Euler-Lagrange equation.

$$F=rac{\sqrt{1+\dot{y}^2}}{\sqrt{2gy}}$$

with

$$F-\dot{y}rac{\partial F}{\partial \dot{y}}=C$$

brachistochrone problem

Computing the partial derivative we find

$$rac{\partial F}{\partial \dot{y}} = rac{\dot{y}}{\sqrt{2gy}\sqrt{1+\dot{y}^2}}$$

• Which gives in the Euler-Lagrange equation

$$rac{\sqrt{1+\dot{y}^2}}{\sqrt{2gy}}-rac{\dot{y}^2}{\sqrt{2gy}\sqrt{1+\dot{y}^2}}=C$$

brachistrochrone problem

• Simplifying gives

$$rac{1}{\sqrt{2gy}\sqrt{1+\dot{y}^2}}=C$$

• We can square both sides and lump constants together

$$y(1+\dot{y}^2)=rac{1}{2gc^2}=c_1$$

• And solving for \dot{y} , taking only the positive solution

$$\dot{y}=rac{\sqrt{c_1-y}}{\sqrt{y}}$$

brachistochrone problem

• The Brachistochrone problem can be solved using parametric equations

$$x = k^2(\theta - \sin \theta)$$

$$y = k^2 (1 - \cos \theta)$$

example

- We can also use variational calculus to prove that the shortest distance between to points is a straight line
- The distance along a curve is given by

$$L=\int_a^b ds$$

- ullet Where $ds=\sqrt{dx^2+dy^2}=\sqrt{1+\dot{y}^2}\,dx$
- So we can find the minimum of the functional

$$I[y] = \int_a^b \sqrt{1+\dot{y}^2} dx$$

group problems

• Find the Euler-Lagrange equation for

$$I[y] = \int y \sqrt{1 + \dot{y}^2} dx$$

• Find the Euler-Lagrange equation for

$$I[y]=\int [\dot{y}^2+y^2+2xy]dx$$

next class

- Boundary conditions
- Multi-variate variational calculus
- Approximate solutions
- Variational Asymptotic Method