NPTEL
NATIONAL PROGRAMME ON
TECHNOLOGY ENHANCED LEARNING

IIT BOMBAY

CDEEP
IIT BOMBAY

Phase field modeling; the materials science, mathematics and computational aspects

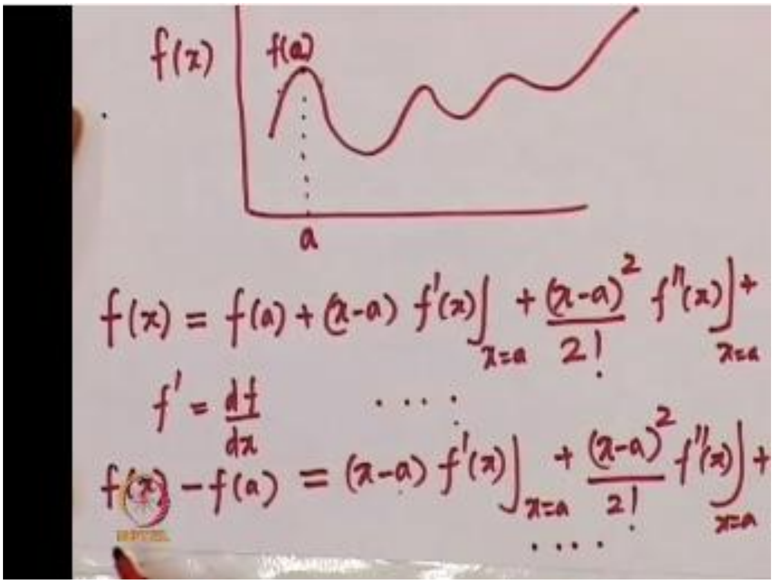
Prof. M P Gururajan
Department of Metallurgical Engineering
And materials Science, IIT Bombay

Module No.13
Lecture No.53
Variational calculus

Welcome we have been looking at some mathematical concepts; we looked at what is a group? What is symmetry? What is point group symmetry? How to define symmetry for a physical property? And how the point group symmetry of a crystal is related to the symmetry of the physical properties of that crystal?

So that is one mathematical idea that we would need to understand face real models, the other important mathematical idea is related to functional and their minimization, so in this lecture we will try to understand what is a functional? And how does one understand minimization of functional to start? With we will start with the Taylor series expansion, and for a function which looks something like this okay. So let us consider some, f(x) and it looks something like this

(Refer Slide Time: 01:12)



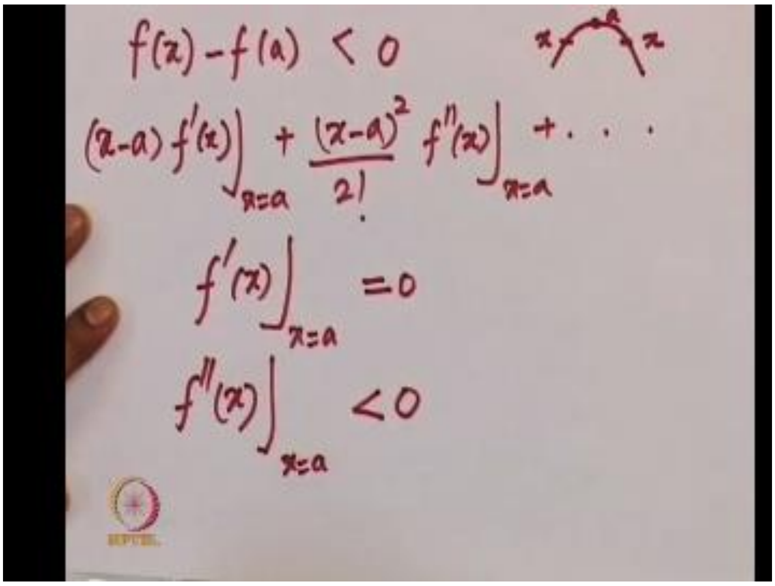
Okay so f(x) look something, so if you have a function like this and if we wanted to know where the maxima and minima of this function are, then the conditions for such maxima and minima there are necessary conditions, there are sufficiency conditions and they can be obtained $^{/}$ looking at the Taylor series expansion.

Let us say that I am looking at a point a, which is an extrimum point okay, so let me say that this is an extremum point, so this is f (a) this is, and so I do a Taylor series expansion about, so a, I consider a point X so, and so that is nothing but f (a) + f ` that is X - a (f `) X evaluated at X =a + X - a $^{2\ /}$2! f ` ` (x) evaluated at X =a + ..., and where f ` (x) is nothing but d $^{/}$dx.

So by looking at this we can find out what is the necessary condition, for example for an extremum to do that let us rewrite this part a little bit differently, so f(x) - F(a) right have taken f(a) onto this side is nothing but X – a, times F ` of X with X =a + X - a $^{2\ /}$ 2 ! f ` ` (x) at X = a + ..., and so forth if you look at this f(x) – f (a), if suppose I am at a Maxima point then we see that if I choose x to the left of a or to the right of a, in both cases f (a) is going to be larger than fx(a) a so fx - fa has to be, so these are the X points.

So fx - fa has to be a negative quantity right so, so we know from the geometry for example, from the curve for example, how it looks? so if you are at a maximum point so any nearby point you go and evaluate the value of the function, if you take the difference of the function at a nearby point the - the maximum point, that has to be negative, that it has to be less than zero right. So we have this condition.

(Refer Slide Time: 04:45)



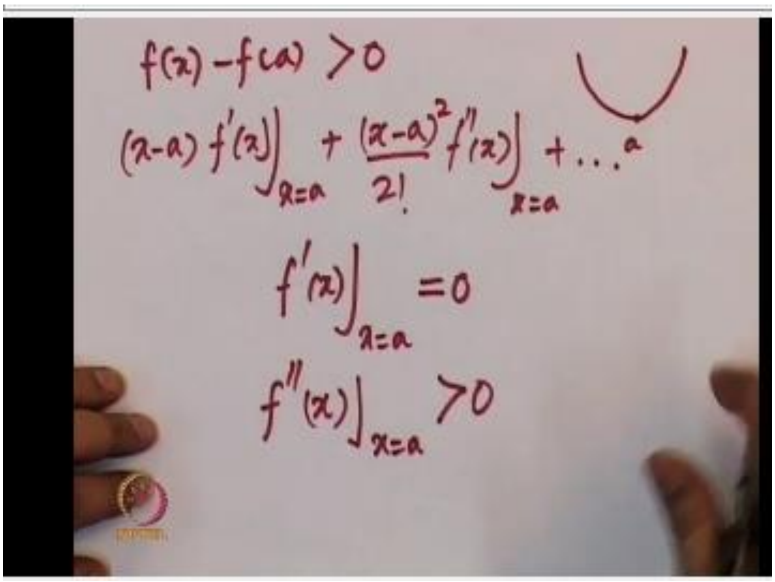
So f(x) -f (a) <0, that should be negative but this quantity is nothing but this, x – a f ` (x) evaluated at x = a + X - a $^{2\,/}$ 2! F ` ` (x) at x =a + ..., now if this quantity has to be negative and this has to be negative irrespective of whether the X that I choose, so I am at a maxima point this is my a sometimes I might choose an x here, sometimes I might choose an x here, when I choose to the left, and when I choose to the right, then the x- a is going to have opposite signs.

If I have chosen x here then this x - a is going, to be negative but if I have chosen x here this x - a is going to be positive, so this quantity will become positive or negative, depending on where I choose x, but this quantity has to be necessarily less than 0, which means the only way that condition is satisfied is if F ` (x) at x = a =0.

Now because this has to be negative, and because x - a ^{2} irrespective of whether you choose x to the left of a or right of a, that is going to be a positive quantity, 2! Is nothing but 2 so that that is a positive quantity so this entire coefficient here is positive quantity, which automatically implies that F `` of x evaluated at x =a, < 0 if that is more than 0 then this would not be satisfied.

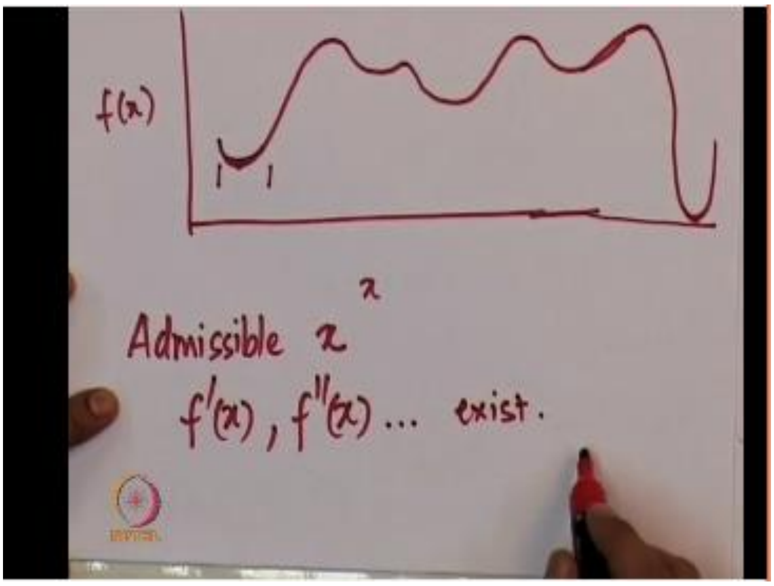
So if you can pick an X which is quite close to a, in such a way that all the higher order terms can be neglected, then the Taylor series expansion tells that it is essential that f ` (x) is 0 and f `` (x) <0, for this function to be having maxima at a b, the same argument using a similar argument if suppose I say that a is not a maxima point but a minimum point a point that looks like that.

(Refer Slide Time: 07:18)



And this is my a then also you can look at the f(x) - F(a), right so if I'm at a minima either way I go, f(x) - F(a) > 0 if that is so, then I have x - a f ` (x) at x =a + X - a $^{2\,/}$ 2 ! f ` ` (x) evaluated at x =a +..., now again if I choose x to the left of a or to the right of at his is going to change a sign, but we want this quantity to be positive so this means that f ` of x evaluated at x =a, should necessarily b =0, that is 0 and because this coefficient is always positive the sign of f(x) - F(a) is determined by f’’ of x provided you choose x small enough that higher order terms can be neglected, in which case f’’ of x > 0 for this to be a minimum. So these are conditions that you, can derive from a simple Taylor series expansion, there is one more notion that is the local extrema.

(Refer Slide Time: 08:43)



So we considered a function for example, f(x) as a function of x so you have something like that for example, right. So when we are looking at these x's about the minima point, so there is an admissible value of x okay, there is an admissible x okay, so for example if I am trying to see if this is a minimal or Maxima, I cannot do it because I mean it can so happen that this function goes and then go somewhere below and then comes right.

So I cannot compare the f(x) at this a value with an x which is very far away, I mean that I should look in the vicinity, this is also important because I am Taylor expanding and I am going to throwaway higher order terms, so I should be as close to x as possible in the admissible values assuming that I already have an extrema art F(a), because that is what helped us decide whether f(x) - F(a) should be greater than 0 or less than 0, because I assume that it is an extreme are depending on then whether it is a minima or maxima.

We in any case irrespective of whether it is minima maxima, we find that this quantity the first derivative has to be 0, and the second derivative sign actually decides whether it is a minima or Maxima, so these are local extrema and if you can find all the extrema, for a given function and whichever is the lowest is known as the global extrema, in this case this is a global minima maybe this is the global Maxima rest of them are all maximize and minimize.

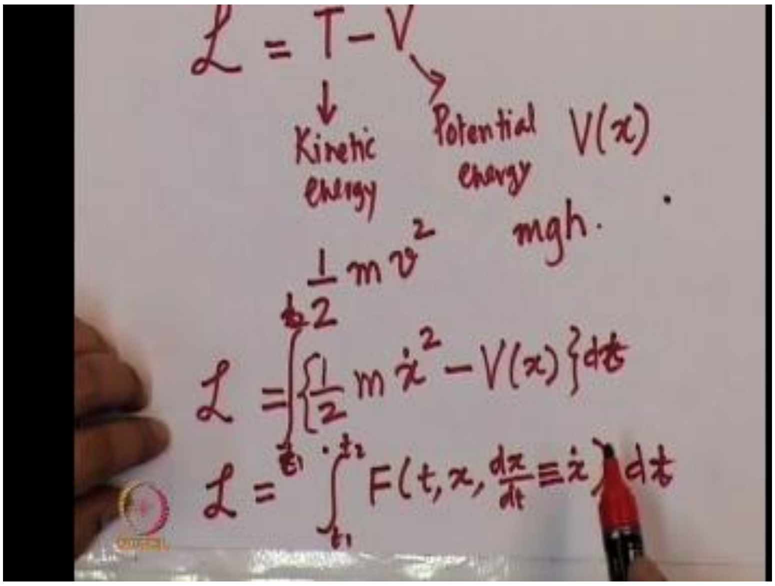
So this is as far as a function, is concerned so we have what is a function? there is a independent variable x and for every value of that x you have f(x) and we have also assumed that that though we define the Taylor series expansion which consisted of F ` (x) and F ` ` of (x) which means that these derivatives exist right, so f ` (x) f` ` (x) etcetera exist if those derivatives do not exist you cannot write that Taylor series expansion.

So Taylor series expansion actually helps us understand where the minima or Maxima for a function is, and it is a single-valued function, it just took a scalar x and for that exit gave you what is a function value, and by looking at Taylor series expansion of this function about an extreme appoint, it would be a minimum point or Maxima point and by looking at points quite close to that.

So that higher order terms can be neglected and then one can make comments and this can be generalized, for example it is possible that for some function f ` is 0 f ` ` is 0, and then you look at f ``` and then what happens? So there is also this notion of saddle point, so these things are possible.

Now what we are interested in, is what is known as a functional what is a functional is actually a function of a function, so what is this idea of a functional and once we define what is a functional, then we would like to understand how to find out its extreme a point, so that is what we want to do with this lecture, the easiest way to understand functional for example is to look at the quantity called action, which is defined in classical mechanics.

(Refer Slide Time: 12:16)



So action is defined as some T – V, where so this classical mechanics T is the kinetic energy and B is the potential energy, now you can see that what is kinetic energy? suppose if you consider a particle the kinetic energy of the particle will be 1/2 mv^2, and potential energy is typically a function of position right, for example if you are considering in the gravitational potential then depending on the height of this particle with respect to some reference.

If it is h then you will have the potential energy as mgh, for example in general potential energy can be thought of so the potential energy is nothing but a function of position, and what is velocity? so it is ½ mx^2, so the so-called action is nothing but ½ mx^2- V (x),okay now if you integrate this quantity, over x this action can also be written as, suppose you are integrating it some from position x1 to x2.

So this can also be written, as a functional of T which is a time x this is a position, and dx/dt, which is what is noted as x dot, and integrated or dx, this we now call as a functional it is a functional because what we are saying is that the T is the independent variable, for every time there is a position, and even though there is a derivative which is the derivative of position with respect to time which is the velocity, we consider that as an independent variable.

Why do we consider that as an independent variable? we consider that as an independent variable because, for example I might be at this position at some time t, and t and x are fixed but my velocity at this point, could be anything that is a completely independent quantity, for example I might be stationary point in which case x dot is 0. I might be having a velocity to the left which is say 10meter per second, then we use 10 meter per second to the left, and I might have10 meter per second to the right, I might have two meter per second at an angle which makes a 30 degrees, with the x-axis.

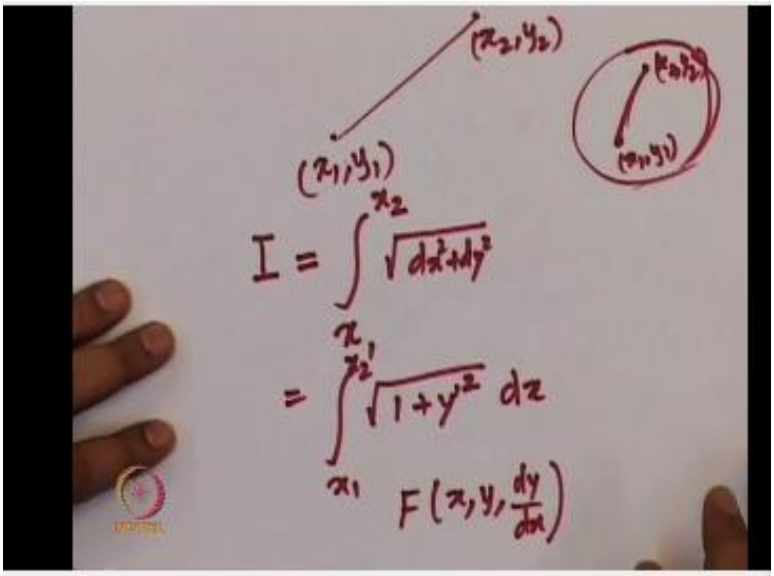
So everything is possible, so we just because I have fixed my position and fixed my time, does not mean that I have also fixed my velocity, becomes another independent variable. Because of which if you look at this quantity, now it is a function of a function right, the position itself is a function of time, and the velocity is a function of the position, so at different positions it might have different values and so they all have to be, so the independent variable is t but x and x dot both have to be considered as dependent variables.

But they are not fixed by fixing x I am not fixing x dot even though for every t I can give you an x, but at that x point what is the velocity is still independent variable, so this is known as a functional, so functional is a function of a function, and typically it has this form typically a functional is an integral from some point to some other point, in this case it is it is whatever from position I have made a mistake.

So if this t is going to be the this thing, so we have to integrate with respect to t, and this is dt right so this is t 1 to t 2, and then d t, so typically a functional has this form integral some from points to some point, so that is a variable which is getting integrated and then some f and then that is that independent variable, and then the variable that depends on that variable, and another variable which is a derivative of this with respect to this, but considered as an independent variable.

So this is an example of a function, there are several classic functionals, that one comes across, for example as in the so called a geodesic problem, we come across a functional and that is as follows, suppose I have a,

(Refer Slide Time: 17:25)

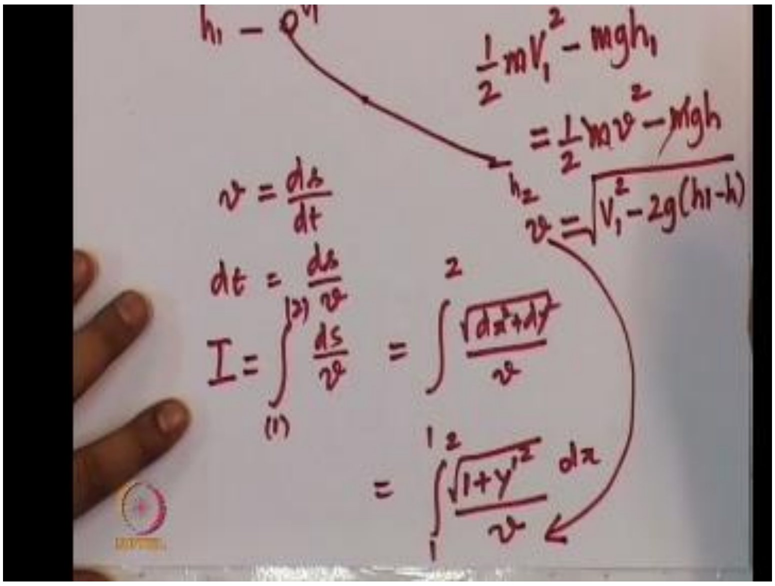


Point x1 y1 and I have another point x 2, y 2, what is the shortest line joining these two on a plane like this? We know that it is a straight line but if suppose I am looking at a globe kind of spherical surface, for example right now if I want to find out two points x1y1 and x2 y2what is the arc? which is joining these two points which will have the smallest length, arc because I am on the surface, I mean you can think of it as a rubber ball for example, if I take two points on the surface of a rubber ball and if I want to find the what is the line that is joining them which will have the shortest distance, then I have to go through this arc which it is no longer a straight line.

So this for example is the return as a functional f =i =x1 to x2 because I want to write the distance, that is the shortest distance I want so it is nothing but dx^2 + dy ^{2} and so integrated from x1 x2, so that is nothing but X 1 X2 square root of 1 + y ` ^{2} dx, right so now this in this case F is X, Y , dy $^{/}$ dx which is the slope, it so happens that this functional, an explicit function of only dy $^{/}$ dx x and y do not appear, unlike the case of action functional where t did not appear.

But both x and x dot appeared okay, but it is still in the same general form they just that this is not an explicitly x or y, dependent functional but it is a functional, all the same there is also this famous problem which is known barkiest cone problem, that is the shortest time problem and the shortest time problem is defined as follows, suppose I take two points,

(Refer Slide Time: 19:41)



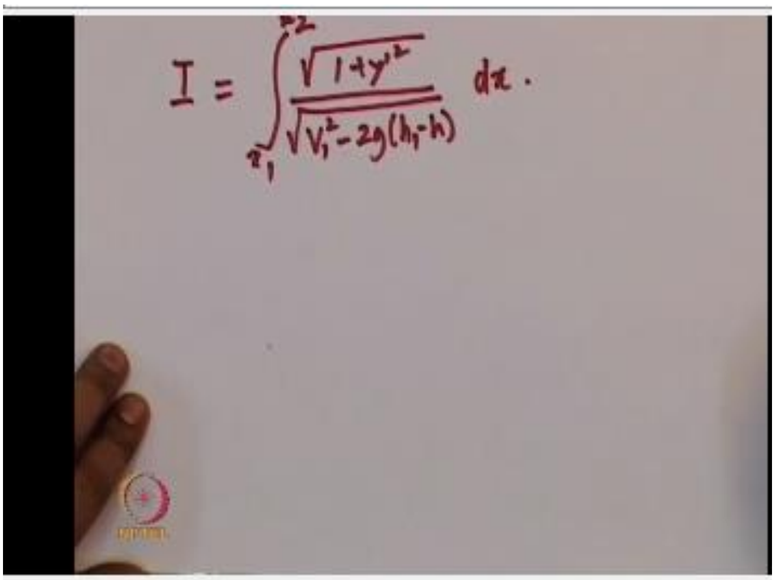
And I connect them through a chute, right and then I leave a particle here with some velocity v1, and under the gravitational field and then it reaches this point, and I want to know what is the shape of this chute, which will have the shortest time for this particle to traverse from this point to this point right, so we know that point it will have some velocity let us say that velocity is d s / dt, so I want to know the shortest time so dt is nothing but d s $^{/}$ v.

So the shortest time will be obtained by looking at this functional, which goes from 0 point 1 to point 2 d s / v, and that is nothing but 0 point 1 to point 2 D s is nothing but square root of dx ^{2} + dy $^{2\ /}$ v and again you can use the same trick, when it goes from point 1 to 2, 1+ y ` ^{2} the square root dx $^{/}$ v, and energy conservation can be used to identify this instantaneous v, and replace it how does that work.

So you have this 1/2m v1 ^{2} which is the initial velocity - whatever potential energy suppose that is at some height h, so you have mgh and is equal to so, let us call that as h1 so let this be some h 1 with respect to some references and this should be some h2 so that will be equal to at suppose I am at some height h, here than 1/2 m ^{2} at that point will be equal to mgh.

So you can cancel all m, and you can get an expression for v which is nothing but, so all m goes away, and you have to multiplied so it will be v1 ^{2} - 2 gh 1 and this - will go there so it will become + h, so - h - into -, so you can come and replace this v here, and that gives the functional for the so called brackets cone problem okay. So if you write the functional for the bracket cone problem, substituting all that you get this functional, so what is the functional now?

(Refer Slide Time: 22:34)



It is =∫ 1 to 2 so you are integrating, in dx so it is x 1 to x 2, if you want to put it that way square root of 1 + y ` ^{2} / √ $v1^2$ - 2 g h 1 - h dx right, so if you integrate like that and the h1 h are basically the excess, you are going in the height then you minimize this function you will find the shortest time, so the solution of this will give me shape of the chute for a particle which is left with velocity V1on top attached one position true come to h2 at the shortest possible time.

So this is known as a brackets cone problem, and there is some interesting story about this problem, told that how this problem came not to be a which you can look up and find out our interest, is in trying to find out like we said, suppose if I have a function I know what is the necessary and sufficiency condition for that function to have an extremum, which is a minimum or a maximum at any given point, can we have a similar concept which tells me, for example what is the necessary condition? For a functional to have a minimum, because all as you have noticed all functional problems have been posed as a minimization or maximization.

We notice that geodesic problem is the problem of finding the shortest path and brackets cone problem, is a problem of finding the shortest time required for traversing some distance and, action is also defined in classical mechanics and there is a principle of least direction okay so the action which is the functional that we wrote should be minimized.

So this is what in classical mechanics, one comes across so we will see a similar thing we will see it in a thermodynamic setting we will write free energy, and we will demand that free energy should be optimized, so being a free energy it has to be minimized, and we will see that the free energy that we write is actually a functional, not a function and that is where this necessary condition for a functional to achieve minimum or maximum becomes very important.

So which is what I want to do in the next part of this lecture, how do we find out? What is the optimum or minimum or maximum for a given function? How do we get this condition in the case of simple function it is just that the first derivative should be 0, at that point where extra members achieve how it works in the case of a functional, we will look at it in the second part of this lecture thank you.

NPTEL
Principal Investigator
IIT Bombay

Prof. R.K Shevgaonkar

Head CDEEP

Prof. V.M Gadre

Producer

Arun Kalwankar

Digital Video Cameraman

&Graphics Designer

Amin B Shaikh

Online Editor

&Digital Video Editor

Tushar Deshpande

Jr. Technical Assistant

Vijay Kedare

Teaching Assistants

Arijit Roy

G Kamalakshi

Sr. Web Designer

Bharati Sakpal

Research Assistant

Riya Surange

Sr. Web Designer

Bharati M. Sarang

Web Designer

Nisha Thakur

Project Attendant

Ravi Paswan

Vinayak Raut

NATIONAL PROGRAMME ON TECHNOLOGY

ENHANCED LEARNING

(NPTEL)