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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.1
Lecture No.1
Tutorial – 4

The purpose of this tutorial is to show how good is the Sterling approximation so sterling approximation that we used while calculating the configuration entropy and it goes something like this. Suppose if I take a logarithm of N! I am going to approximate it as the N logarithm of N - N -N so this is what the Sterling approximation is and we said that for large N this is a very good approximation ok so we are going to do a very simple exercise now to see what is the error suppose a N is 5 how much is the error in this approximation N is 20 how much is the error and N is 100 for example how much is the error okay. So we can do that for that I am going to use octave.

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So let me write so let me do a small calculation in octave so I am going to write a function the function is basically a factorial function so let us assume that I do not give it non integers or numbers like 0 then if you give x then for I = 1 to X.

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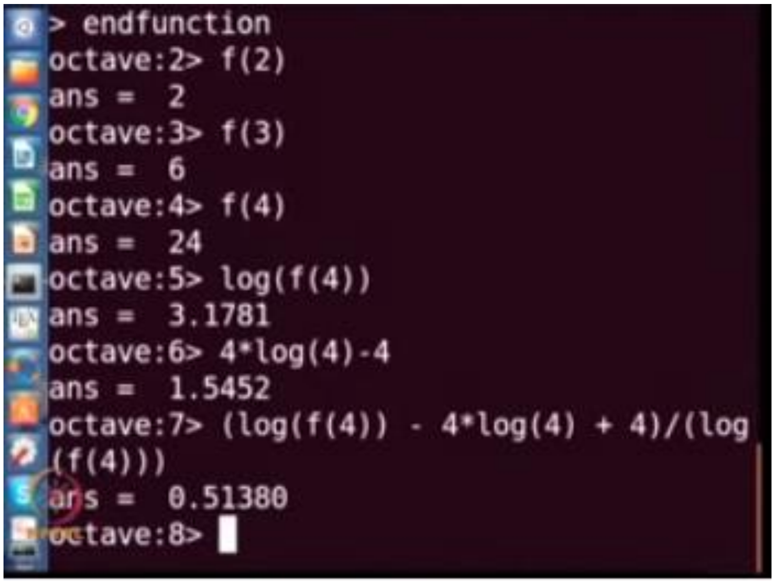

So Y okay so I need to I need to define function so I am going to first define y = 1 and then I am going to say for i = 1 to x a y = Y x I end for so this is basically the function so what does it do so if I give to then it is going to go to multiply 1 x 1 and then resultant is one that is going to multiply by 2 so it will return me 2! So if for example if I say f(2)it will give me to f (3) is basically 6 f (4) 24 and so on.

So it is basically returning mean the factorial right so logarithm of f(4) let us take is 3.17 if I calculate using the approximation which is for x log 4-4 I get 1.54 so this is half by about forty percent maybe so we can we can actually calculate that log of f(4) is the exact number minus 4x log of (4) + 4 +4 and I am going to divide this entire quantity x log of f(4) to know what is the relative error right f ( )4 so the error is like some 51%.

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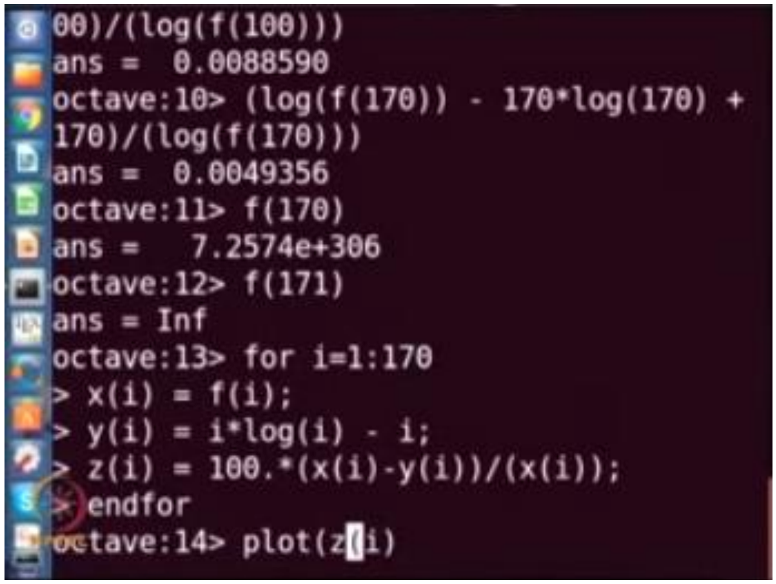

Now let us do it for a number like 20 let us see how much is the error okay so the error has dropped from 50 to 5.7% suppose if I do this 400 okay so the error has become 0.88% of course I can do for a much larger number let me do it for 170 okay so I get an error which is like 0.49% so within 0.5% for a number like 170 when we are doing the Sterling approximation we are assuming the numbers which are of the order of 10^{23} so you can see how good the this approximation is going to be okay.

It is going to be very, very good approximation now why stop at 170 why not check it for 10 20 23 there is a problem the problem is factorial 170 is some number 10 / 306 if I try to calculate the factorial 171 it is going to give me infinity that is because the number is so large that for the given storage that I have I will not be able to calculate for as far as the mission is concerned this number that I am getting is N already and infinity.

So that is the reason why we had to stop this at 117 of course it will be a good idea to do this calculation and plot the approximation as well as the actual function or to plot even the error so that we can do so you can say for I = 1 to 170 because that is the limit to which we can go let us say X (i) is nothing but f (i) okay so that is the factorial calculated analytically and let me say Y(i) as nothing but I x log (i) – I right this is Y(i).

So let me calculate as z(i) as the error percentage so I am going to say that is x(i) –y(i) /x(i) and I am going to multiply this number by 100 so this is my z(I) and for so I can plot z(i) okay. So why is it that I am not getting okay that is it is storing only the number is not clear to me okay so let me write it as a script okay.

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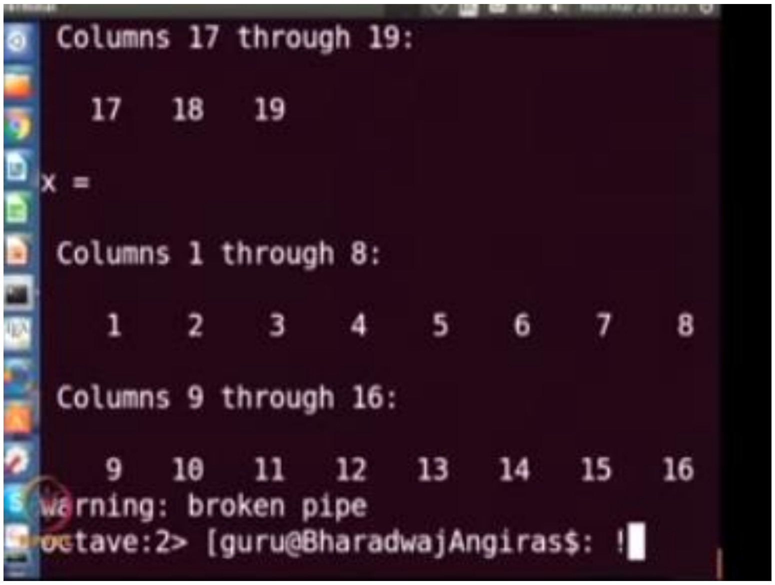

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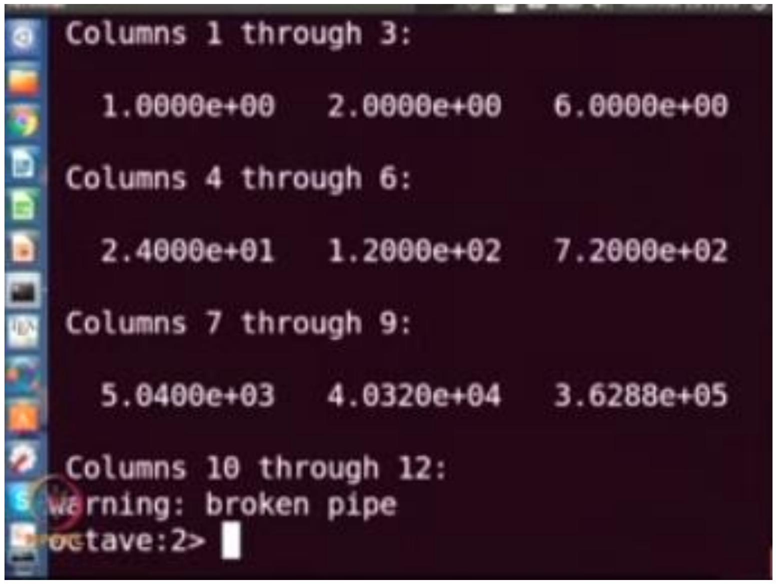

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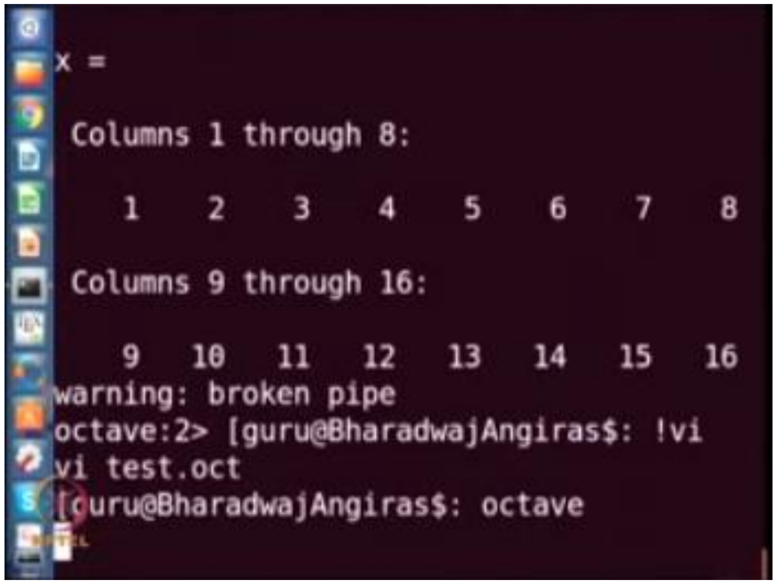

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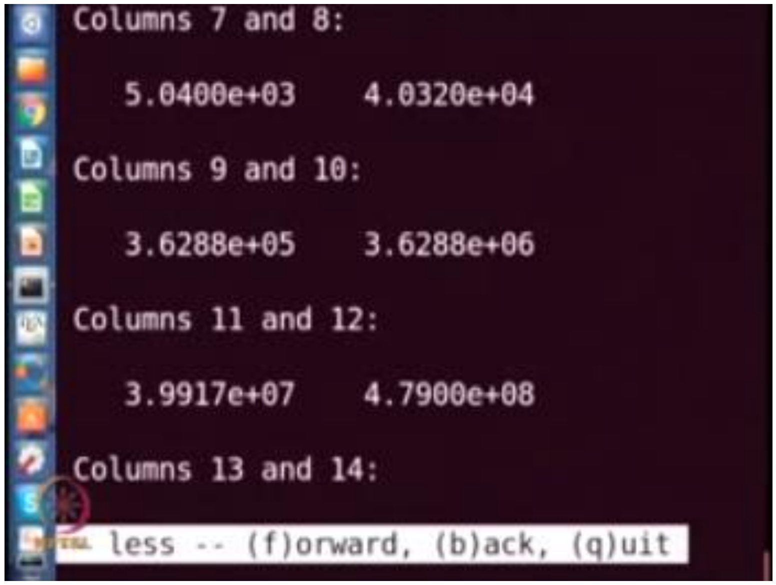

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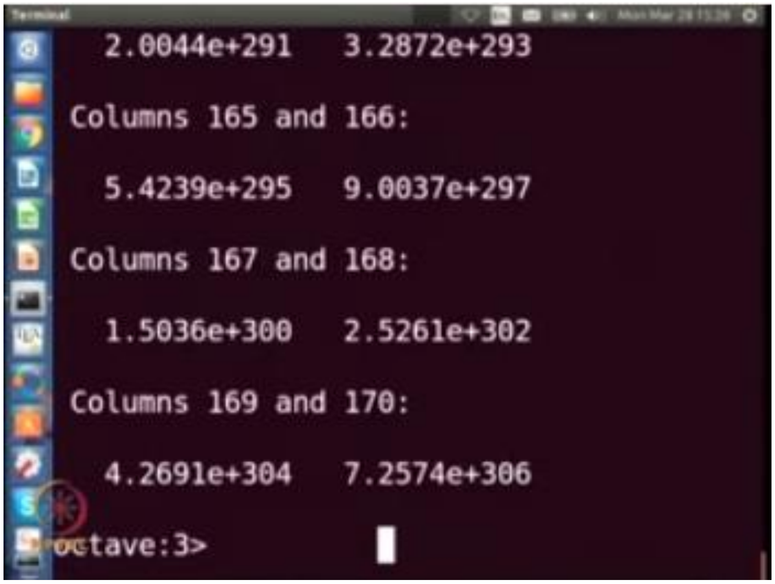

So I am going to define the function y = f (x) function and how am I going to define y = 1 for i = 1 to X Y = Y x I and for so this is the factorial function so I am going to say for i = 1 to 170 x (i) = to i and for so let me run this and see okay so if I so X is now stored.

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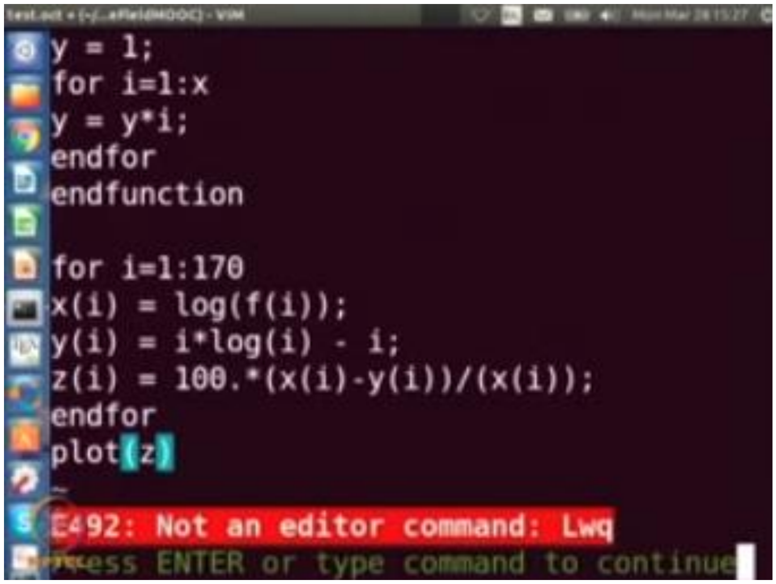

So now I am going to write Y (I) okay so I have to take x(i) as logarithm of factorial and Y (i) as I x logarithm of i, I think that was a mistake I made earlier Y(i) so Z(i) is basically this logarithm of F(i) sorry x(i) –y(i)/ the total thing is multiplied by 100 to make it a percentage so plot z.

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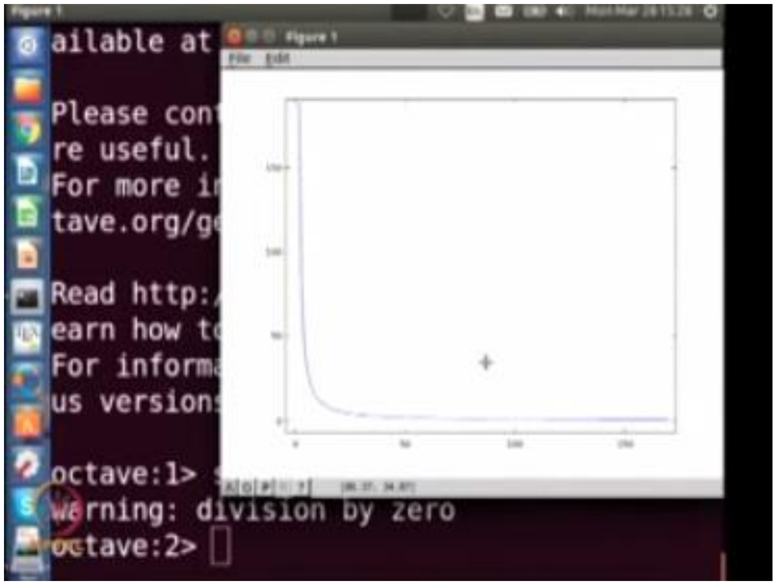

So this is how the error goes as you can see so the error is very high it is more than 170 180 % and as the number increases it falls so somewhere around 50 we are already down to about 2% and when we get to 150 we are already down to about 0.8% or something and as we go to 170 we are down 2.5 % so this shows how good is the Sterling approximation and we have only reached hundred and seventy so the numbers that we are going to consider is at least 21 orders of magnitude larger than this.

So the Sterling approximation is going to be very good for such very large numbers and if you take a look at a book like cry sick there is another form of this approximation it is also called sterling approximation in the probability and statistics chapter that you can look at and probably do the same exercise with that approximation also again to see how good is this approximation as the numbers become larger and larger okay. Thank you.

NPTEL
Principal Investigator
IIT Bombay

Prof. R.K Shevgaonkar

Head CDEEP

Prof. V.M Gadre

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