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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.5**
**Lecture No.22**
**GNU Octave:**
**Introduction**

Welcome, in the next few lectures and this one we are going to be using high level interactive programming language or a software called GNU octave. GNU octave is equivalent to mat lab except that it is a free where, it is a open source free software and it is available for both windows operating system and linux operating systems. So depending on whichever computer we use it is available for you to download for free and load it on your computer and you can use it.

So we are going to use this program to do all the numerical computations related to phase fail models in this course. So it is a good idea for you to download the software and load it in the, in your computer in your laptop or your desktop whichever computer you have access to. So that as the course proceeds you can do all the class work by yourself on your computer and you will see that you are getting the results that I am showing. And later if there are some tutorials are problems that you have to solve on your own for the course then you will also be able to do them.

There are many good textbooks that are available some of them are meant for both octave and mat lab and some of them are meant for mat lab, but most of the mat lab commands work on the octave. For example, there is a good book by Prof. Rudra Pratap called introduction to mat lab. So you can use any of those books to practice for yourself.

In these lectures I am going to give a very tutorial introduction to octave so that you will be able to use it for our purposes. And if you have done any programming earlier, then it is very, very easy to follow how these programs are written and even if you have not, then with little bit of effort you will be able to pick one of the reason why I am using octave, even though any professional quality code that you would write has to be written in a programming language like FORTRAN or C.

The reason why we are using octave is to fold the one, you do not have to worry too much about the programming or syntax related issues that is a huge advantage especially when you are writing for the first time. The second reason is that octave is also a program which can plot and show things. So visualization also becomes very, very easy when you sue programming language like octave.

So the scripts that you write can not only do computation, but they can also show you pictorially what is happening. So this is the reason why I have decided to use octave, but it is not necessary that you should use only octave, if you are comfortable with python or scilab or any other program for that matter you are welcome to use. But for this course I am going to use octave to show you the example.

So if you are comfortable with some other programming language you can take these same things and you can do it for yourself in those programming language, if not it is a good idea for you to atleast learn octave along with this course. So there is also a tutorial that I have written for octave which is available as part of an NPTEL course, it is available in phase two in the metallurgy courses, it is called the computational approach to material science and engineering.

This is a course that me and one of my colleagues Prof. Prita Pant did together, so the notes for this course are available this is an online course, there is no video lectures for this NPTEL course, those are downloadable, they are available at the NPTEL site they are also available at several places online apart from the NPTEL site. So you can just look for this course and then download in the course in part two I think the third tutorial or third lecture is on GNU octave.

The third module basically is on GNU octave, we will not do everything that is there in the tutorial even though in the initial stages we will do what is there in the tutorial. Later we are going to do problems that are regulated to phase in module. So some of the material that is there, that can be done using GNU octave is if you are interested in learning more about octave and using it for your teaching, research or learning purposes.

So for now let us start with octave, so I have laptop which is running Ubuntu, I think Russian 14.04. Ubuntu is a version of linux and it is a free where and it is available for free to download. And the versions like 14.04 and 12.04 are the long term support version, they are called LPS, so 14.04 means in the year 2014 this got released and that is the version that I have. In that is the operating platform Ubuntu in that I have loaded GNU octave. There are two ways in which you can access octave, so I am going to show you now on the screen.

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As you can see on the side, so there is a symbol which, if I, you know take my mouse then it shows GNU octave.

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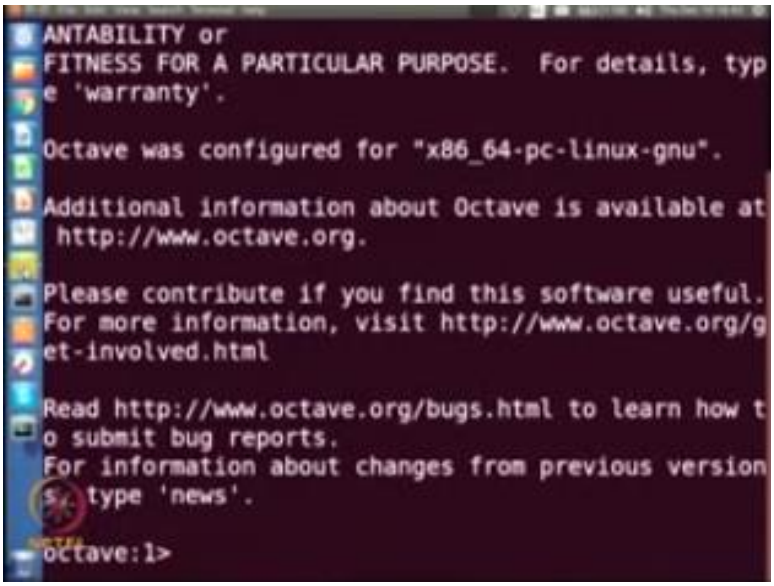


So if you double click on it, you will get GNU octave invoke for you.

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This is the same way you can also do in for example windows machines, that you will see when you load this GNU octave, you will see an icon which says GNU octave and you double click on it, you will get the GNU octave window.

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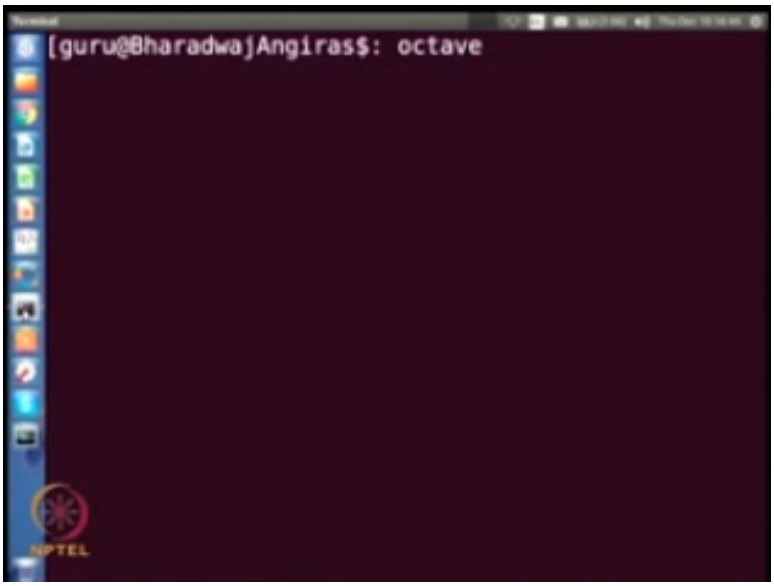


There is also another way of doing it and that is by opening a terminal okay. So I have the terminal now. In the terminal I can type octave.

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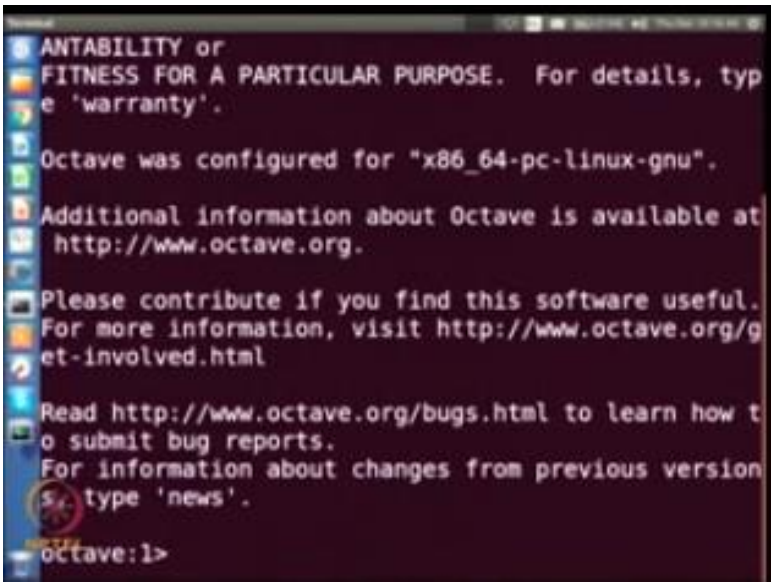


And if I enter I get the same program invoked okay. So if you see when you invoke GNU octave and you will see that.

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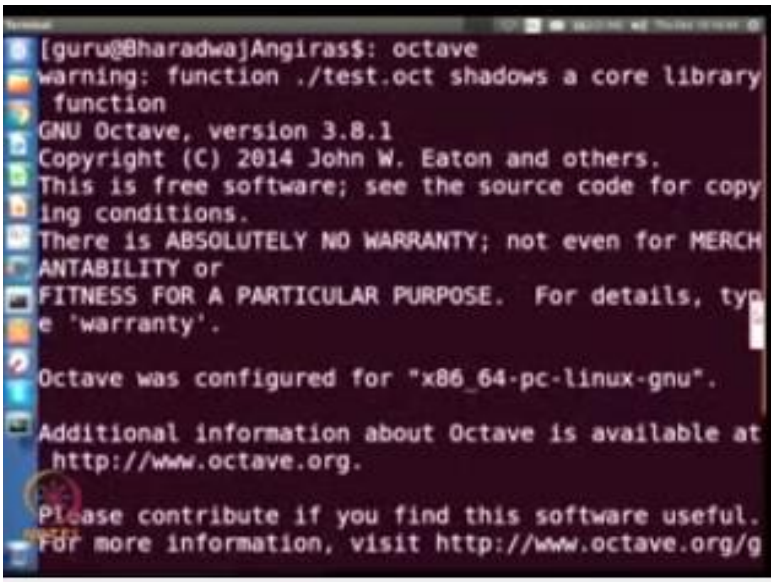


So first it says so there is some warning here, I do not understand why okay, generally it is not same, but occasionally if you see some such warning you can figure out what it is about. I certainly do not know what it is about so generally when you invoke octave first it says GNU octave and it tells the version so I recommend that you use version 3.8.1 or higher because everything that I am going to do then will work sometimes there are versions like 3.0 and they might not behavior the way my version is behaving.

So it is better for you to use a version 3.8 or above and then there is copy right information and says this is free software so see the source code for copying conditions of course there is absolutely no warranty okay so that is true for what I am going to do also.

You are welcome to use this code whatever I write is available for everybody your welcome to modify your welcome to share your welcome to use it to build the other things but finally responsible for what you do with the software so this I am using here for pedagogical purposes so I will show things I expect you to do and learn and try to explore but none of the programs that I give come with any warranty okay so that is very important so now that is clear.

So it says the octave was configured for x86_ 64 – pc – linux- gnu so I am using GNU Linux specifically this flavor is called dope into and this is a 64 bit installation that I have okay now they also give additional information about octave is available at http://www.octave.org. I strongly recommend that you go to this site and look around look at the downloads look at the manuals look at other information that is available there are plenty of information that is available online with respect to GNU octave.

There are lots of tutorials there are lots of probably videos on YouTube even though I have not explored them but probably it is available and you can try to learn so if you want to learn on your own and if you have access to the internet where you can go look up information and download then it is very easy to learn and like said there are couple of good text books pressure with a that is one I will also give you so more names of text books in the next lecture so that you can see what those text books are some of them are low prized Indian versions that are available within India.

So you can us them so this is first how to get the octave the movement you get octave suppose you do not know anything you can ask for help okay the way to ask for help is of course to type help and enter so let us see what happens if I do that.

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So if say help and enter so it says so you have to say help name okay so if you give help and some name then it will tell you the information about that command okay so this is what it says so you can see so I said help and then it gave the information that for help with individual commands and functions type help name replace name with the name of the command or function you will like to learn more about for a more detailed introduction to GNU octave please console the manual to read to manual from the prompt type doc okay so and that is that so and that is said so and then it tells you how to go.

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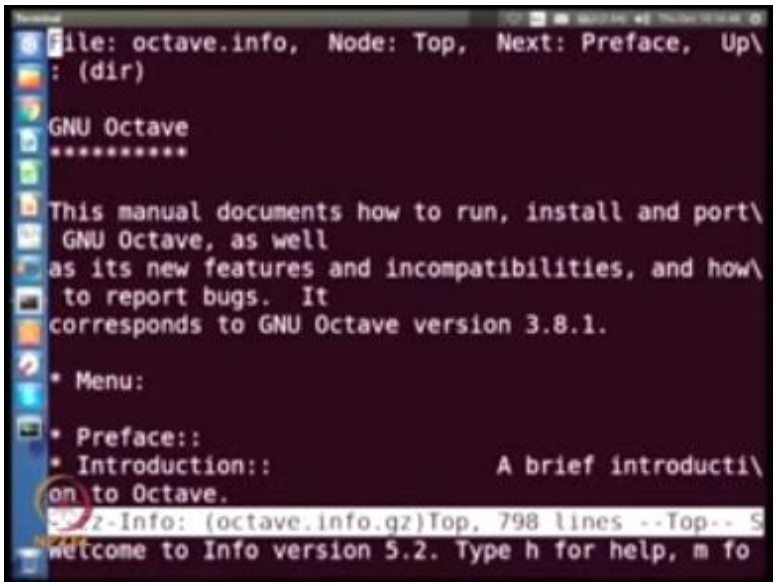


So I press the space key then comes out and it also gives commands that you can use to come out for example so it says if I type doc then it will give manual so I do know if I have the manual loaded let us try so if type doc well yes the manual is loaded okay so it as info so it as the preface introduction so you can up and down by using the up and down key arrow keys so that you can use and you can also use the space key.

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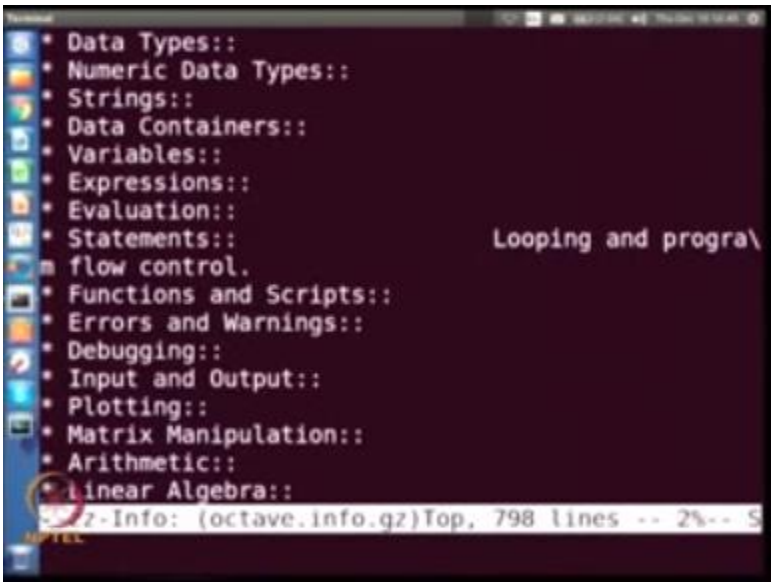


If you press space key it will go down by one page.

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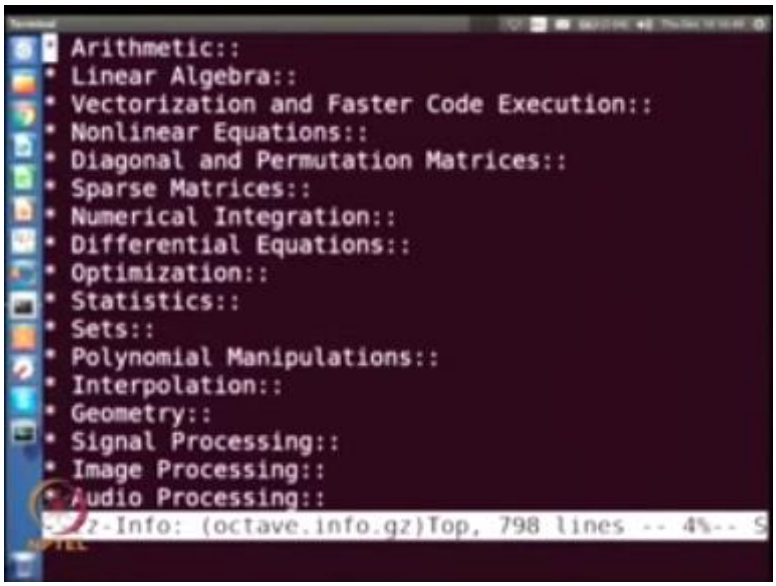

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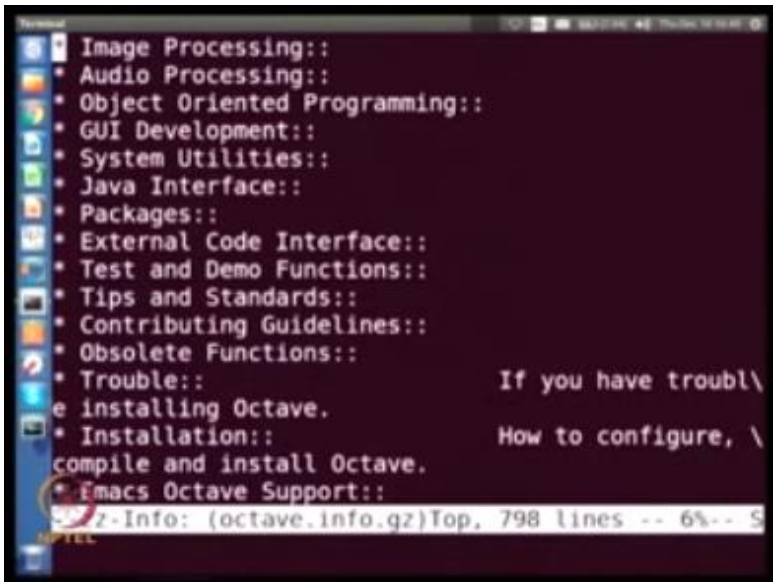


Okay 4% 6%.

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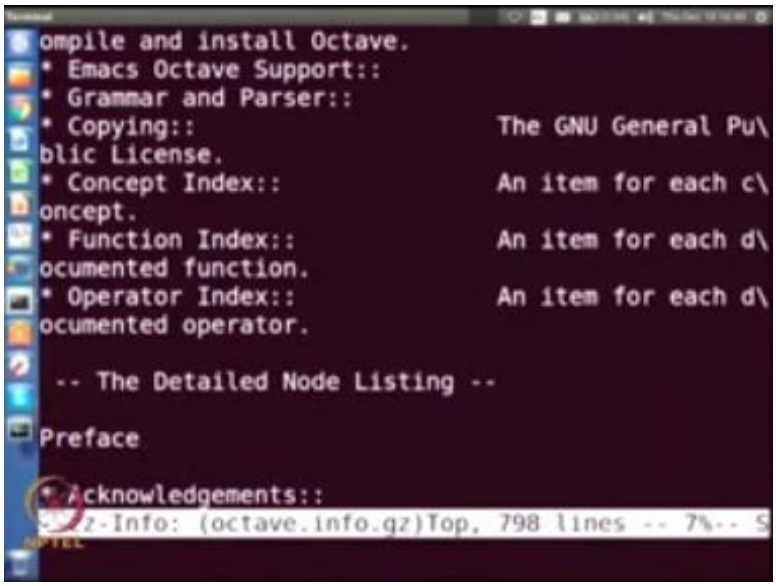


So it is going on and you can see all the type of information you have right.

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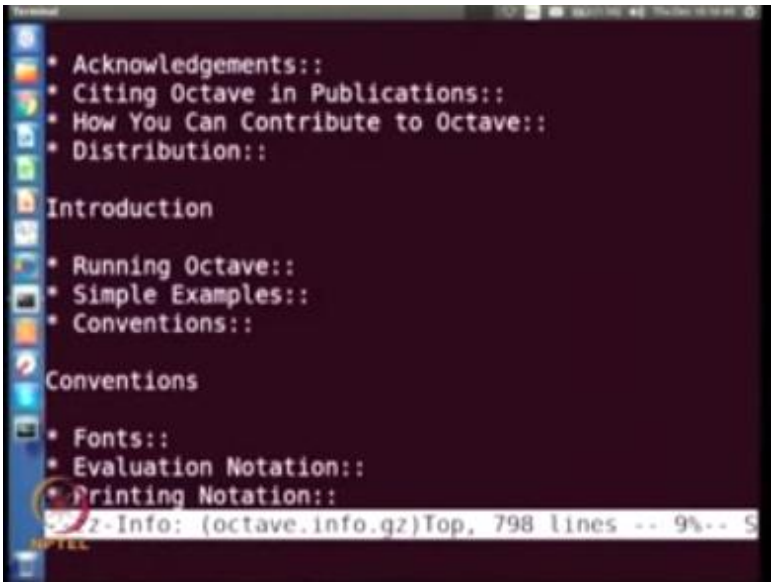


So you can also use page up page down to go back and forth.

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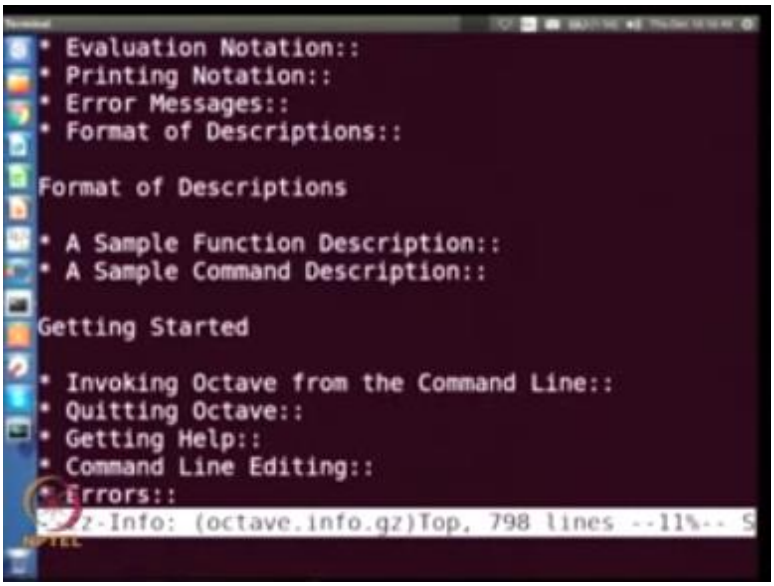


So I am using now page down I can use page up so it says all the kind of things that octave can do right and if you keep going down then you will get information on each one of these thing and you can try to find out more information.

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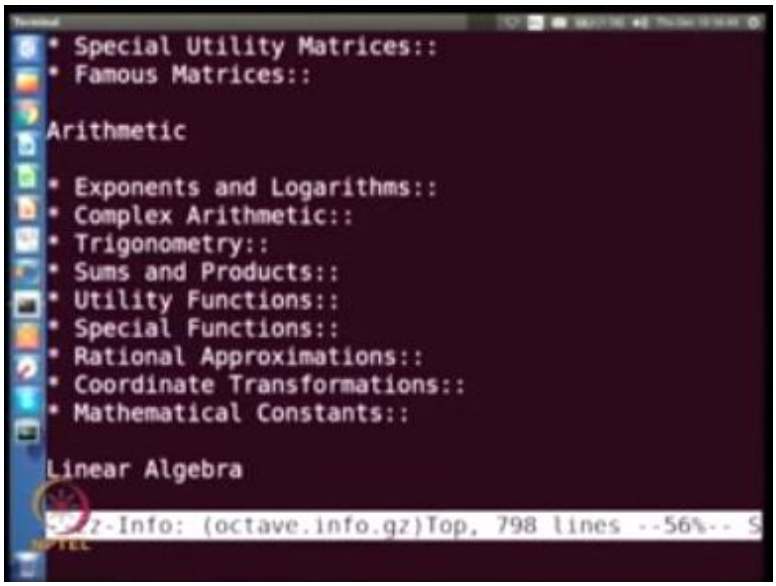


So this is full document as you can see it can do lots of things arithmetic.

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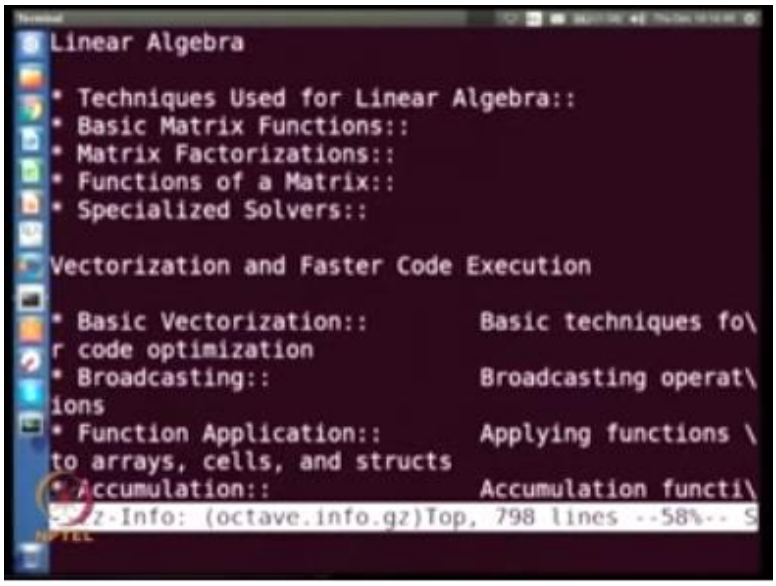


Linear algebra.

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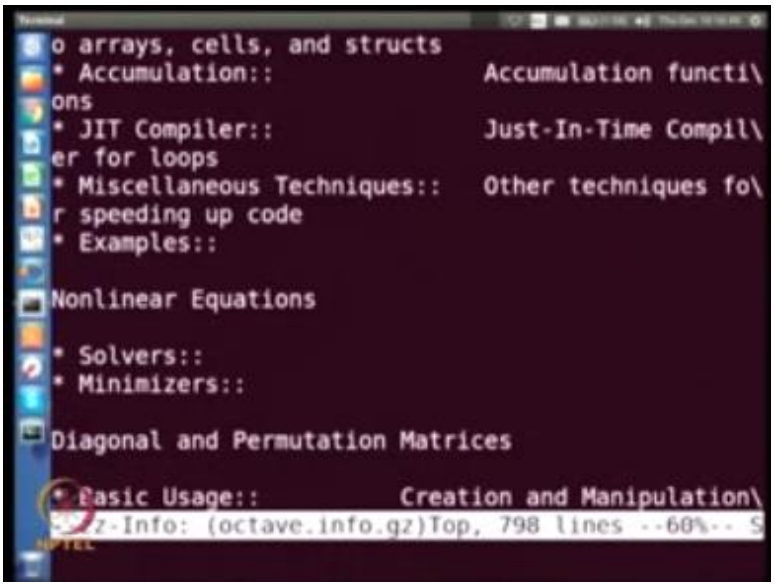


Vectorization non linear equation and optimization and plenty of other stuff okay the numerical integration differential equation.

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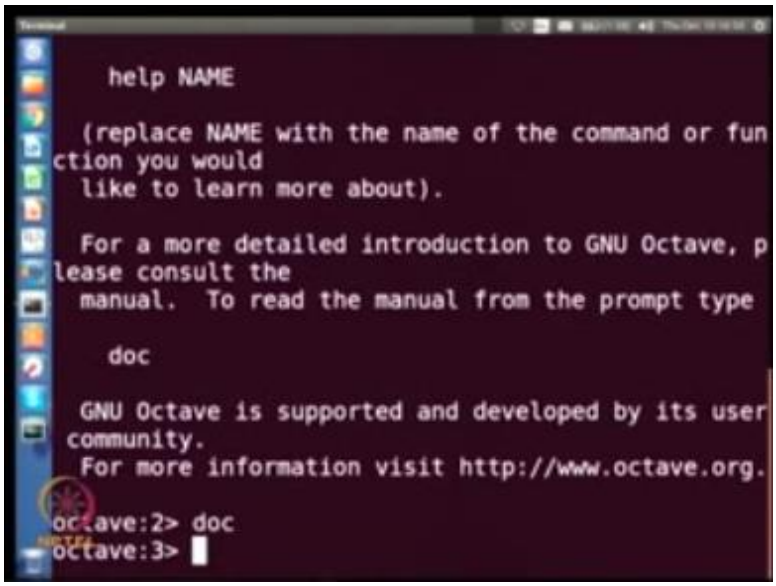


So you can see that it is basically so if you want to quite from this screen you just type q and that quits q is for quit okay so q is for quite so if you type that it will come out so the octave program even though we are going to use all the furthers that are available is pretty power full you can do plenty of stuff with it but for our purposes we are just going to use it two solve some piratical differential equations like the once that I have been showing you diffusion equations the Cahn Hilliard equation and things like that and we are going to do it one dimensions and two dimensions 3D you can do but I do not think using octave two solve 3D problems is a good idea.

Mat lab or octave or not meant for scaling up like that unless you have lots of resources so it is better write programs which are very intensive in programming language like Fortran or C but for our purposes up to 2D we will sue in this course to solve and we will use octave to do that okay so this is the first step you have to load octave of course I have not told you how to do that I am assuming that you will able to go online look up information on loading software depending on which operating system you are using open to Linux or windows and then corresponding version you have to download sometimes you may to compile sometimes it might just be an executable that you click and then it gets installed.

In either case there will be in the case of windows you will sew an icon which you can double click and get to octave in the case of open to also you will get an icon and just that in my case as we can see on my screen.

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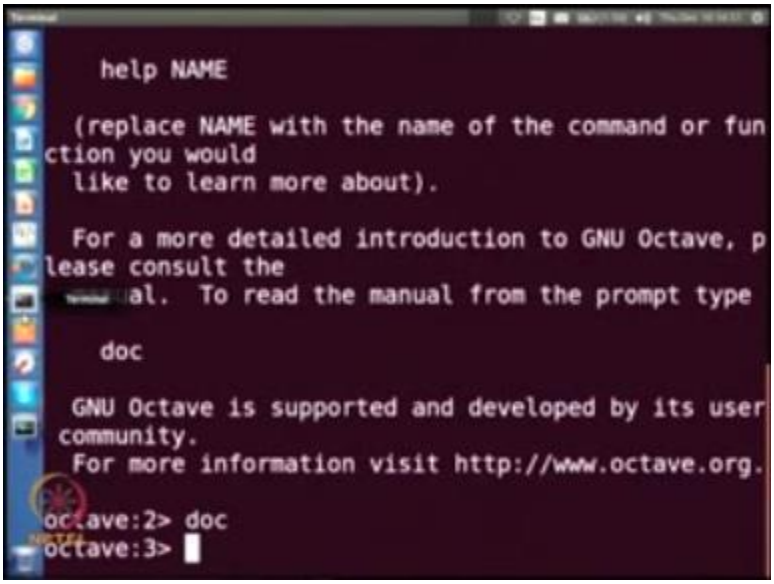


All my icons or lined up on the left hand side okay so you can see some browser and some file manager and octave and lots of other stuff you can see Skype and then you can see system load this thing and terminal and so all the icons are here in which there is one icon which is made for GNU octave so you can double click on that and you will get the octave window and in that terminal then you can do start. One of the things that you can do is that you can use octave like a calculator if you have a computer and if it is switch turn you do not need a calculator to do calculations, okay.

Well, what type of calculation you can give anything you want any if you have done programming you know how to give the symbols for multiplication, division extra and those symbols work. For example, I can multiply 281/16, right.

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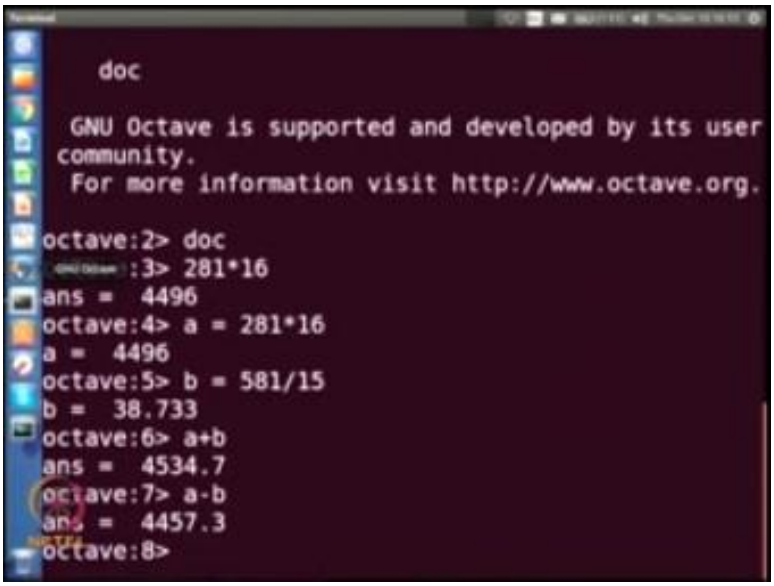


So how do I do that I will show you so you take 281 then you multiply this is * symbol 16 and enter it will give you the answer, okay. You can do a little bit more than this, for example I can say a=281*16 sorry, okay so the value of 4496 is now stored in a, if you do not give any variable it is just strode in answer and that answer will be written when you ask the next question. Now am I task okay, b is some 581/15 okay, right I can now ask what is a+b it will give you the answer and you can ask what is a-b it will give you the answer, so simple algebra arithmetic you can do of course this is very nice.

However, suppose I want to do another small calculation that is a little bit involved, the calculation is something like that.

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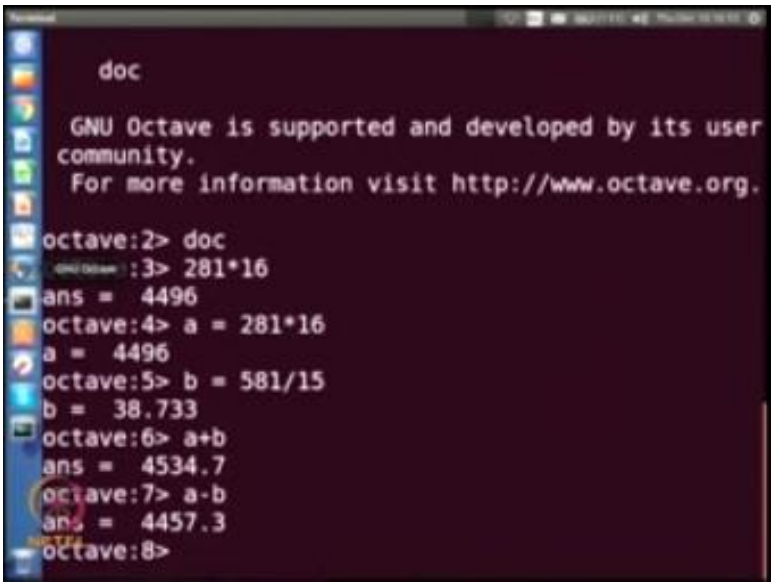


I know that the vacancy concentration so I am going to write down the expression for vacancy concentration.

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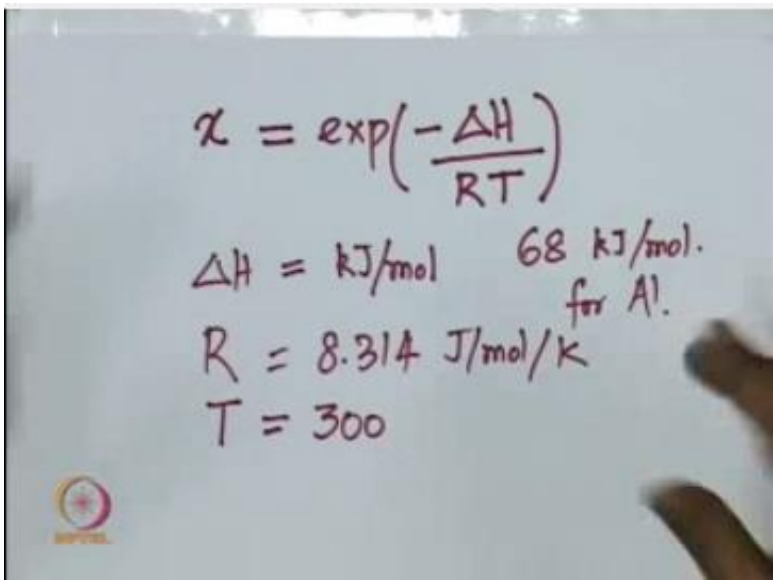


The vacancy concentration in a material is given by exp -ΔH for vacancy formation divided by RT where ΔH is given in kJ/mol and say, let us say that this is 68 I think kJ/mol in the case of for aluminum, okay. R is the universal gas constant so it is 8.314 J/mol/K, okay and T so this is J/mol/K, T is the temperature in the absolute scale that is, let us say that I want to know what is the vacancy concentration in aluminum given that it is 68 kJ/mol is the ΔH vacancy for aluminum and 300 K which is near about room temperature, okay.

So I want to know what this value is, so what does it involve it involves calculating exp(-68000/8.314x300) now you know how to do this, because that is what we did just now. But how do I get exponential, right you might guess that exponential the command would be exp, so you can directly write for example I am going to show you how to ask for help. So you can say help exp, okay

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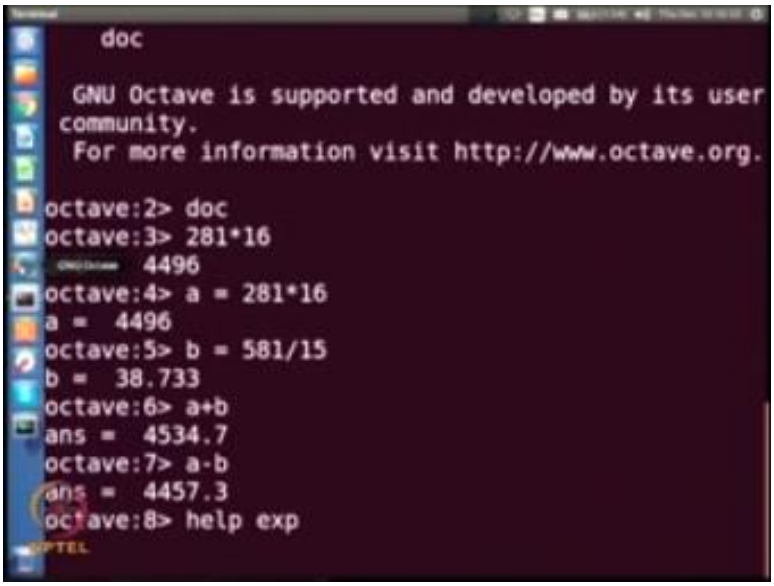

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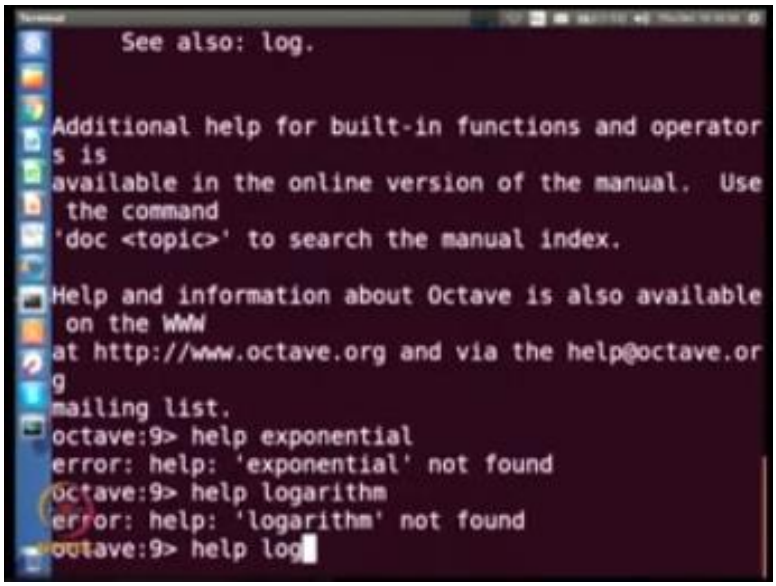


Nothing is happening on my screen well, okay so it took some time so it is giving you the information. So you can see that when I ask for help exponential , so it said mapping function, okay so it says exponential x compute $e^x$ for each element of the x, okay it is saying each element of x because the x that I give could be vector, okay we will come to that we will see why it is important and how it is important. But for now this x could be just a number you can give a number and you can give, and see it is also telling you see also log, okay that is because the natural logarithm is called log in octave it is not called a long or ln or something.

So log if you generally say it will actually calculate natural logarithm, okay so and then it if you see more information about additional help where you can get, okay so it is possible. What happens if I say help exponential, right sometimes you might not know that it is exp so if I say help exponential the exponential not found, okay. So you need to know some information for example help logarithm let us see if there is any information help logarithm not found, okay. but help log.

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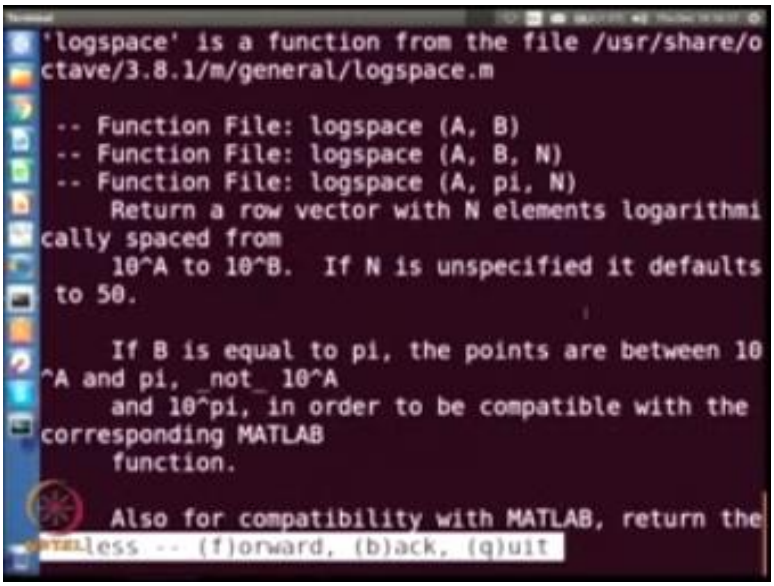


Well, yes I find help log but when I look at log then it gives all the information it gives the information on exponential and $\log_2$, $\log_{10}$ and lots of stuff, what is this log space I do not know what it is so we can find out what it is by saying help log space, right so it says is a function and written a row vector with n elements logarithmically spaced from $10^A$ to $10^B$, okay so I do not know what it is.

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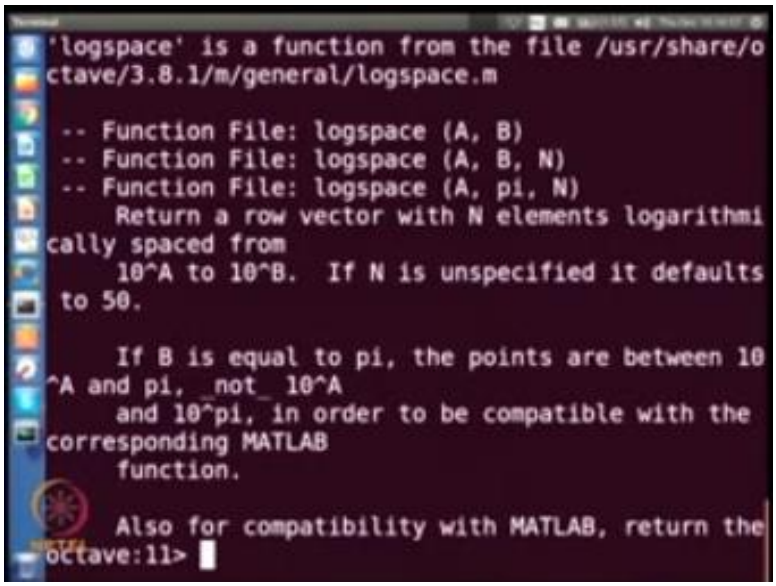


But the idea is that you can look up help you can find out not only information on that command but related commands you are expected to have some idea about how this commands are called and they are generally called by the same names in almost all programming languages, if you have done C programming for example you will know that exp log earned all that are available there those are functions calls math function calls. Okay, so this is how you invoke octave and you use it like calculator so let us calculate the vacancy concentration at 300K in aluminum what does it require.

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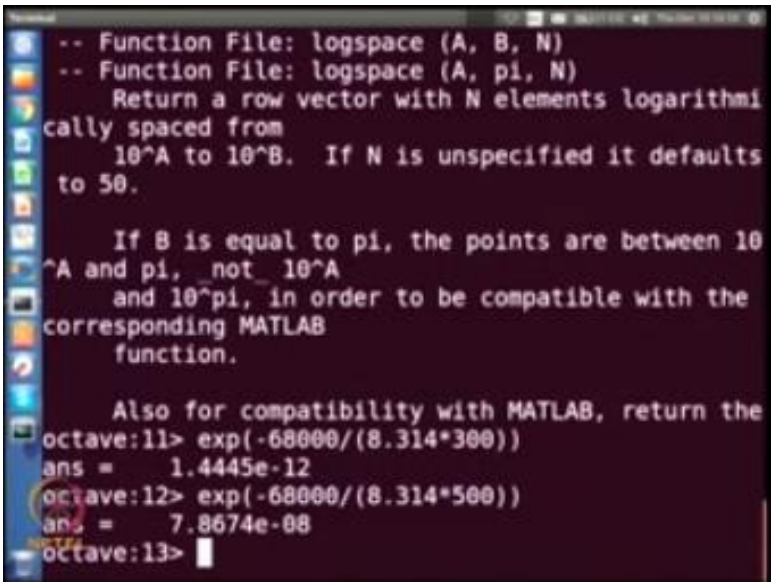


It requires me to calculate exponential, okay -68000 because remember it is 68kJ/mol/K/RT but this parenthesis is important because RT has to be calculated and that is what should divide 68000, R is 8.314 so let me calculate times T is 300, okay. So you get 1.4445 into $10^{12}$ this is the vacancy concentration at 300K in aluminum you can calculate this vacancy concentration at 500K in aluminum, okay let us say 5, so how did I get the previous command I just use the up key, okay so you can use the up key you can get the pervious command which you can then edit and you will get the answer, okay.

So when you went to 500K the vacancy concentration skipped from -12 to -8 so for order of magnitude it has increased, okay.

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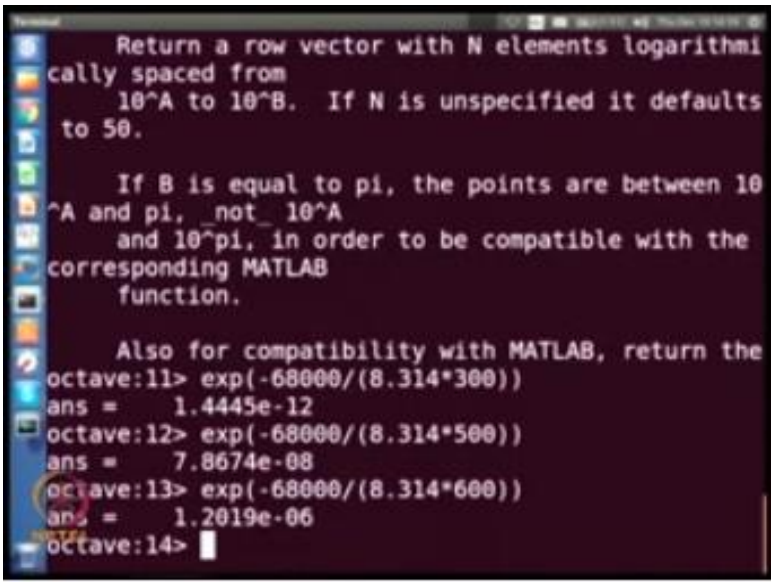


So let us calculate this quantity at 600K, okay it has become $10^{-6}$, now you might want to calculate suppose I told that from 300 to 600K I want to calculate the vacancy concentration for every 10K and I want to plot it as a function of temperature, okay. How to do that, that is what we will do in the next 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**
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**Sr. Web Designer**
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**Research Assistant**
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Nisha Thakur

**Project Attendant**
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