Tools in Scientific Computing
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Lecture - 30
PETSc – Creating Vectors and Matrices

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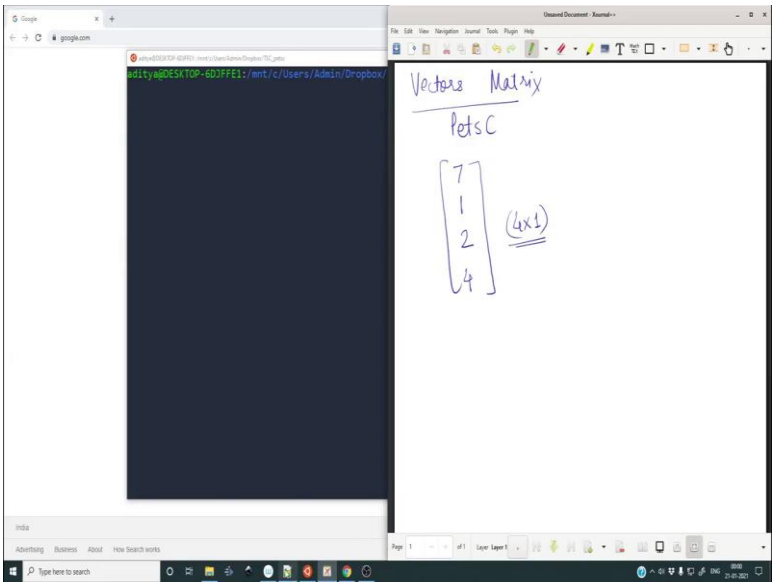

Hi everyone, in this particular lecture we are going to look at matrices and vectors in Pets C. And if time permitting we are going to solve a simple algebraic equation and see all the objects that we can access. So, in the previous class we looked at some aspects of m p i, but in this particular lecture we are going to make use of a single processor just to avoid any kind of confusion.

So, let us try to create this particular vector. [7 1 2 4]; so it is a 4×1 vector 4 rows and 1 column and yeah; so, all the elements are non zero as you can see. So, let us see how we can go up go about defining this particular vector.

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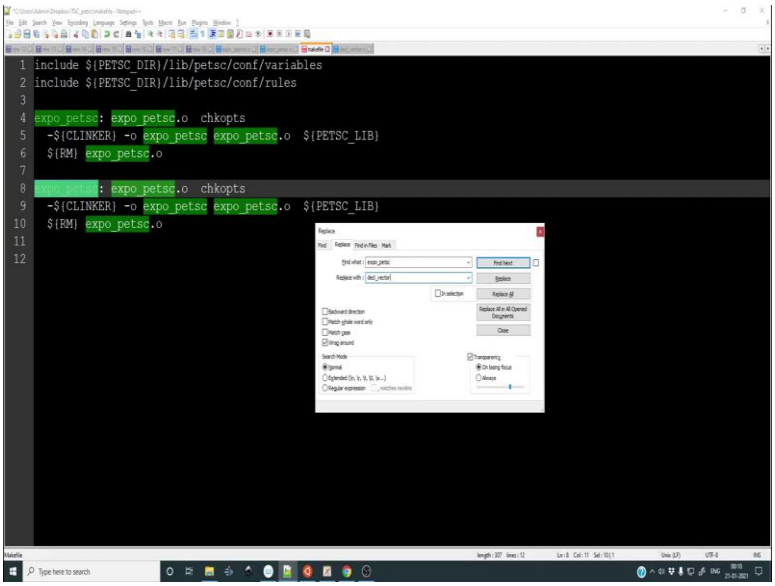

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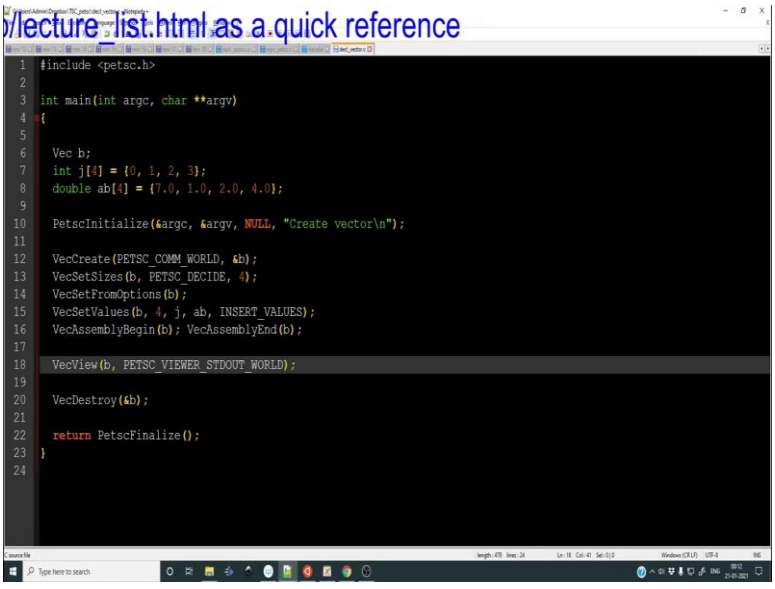

So, as usual we will create a new file and first things, first we are going to import petsc. So, hash include std not std petsc.h. Then we are going to make the main function. So, int main arg sorry int argc char star star argv and we are going to return the output of petsc finalize.

We have looked at petsc finalize. So, petsc finalize its wrapping up the code and the return value is simply the i e r r that is the error signal. So, it's going to be an integer. So,

we can return that that is the conclusion of the code. So, there are certain things that every petsc code must have right.

So, first things first there has to be a Petsc initialize. If there is a finalize, there has to be an initialize as well and the initialize takes the command line arguments and some help string alright. So, with this out of the way so we have petsc initialize and this.

So, now we must declare certain variables. So, in order to declare an array, the way to do it is to tell which elements are going to be non zero right. So, what we can do is; so, let us declare some element, some variables that we will need. So, we will need a vector, let us call it b. So, vec is a data type inside petsc and so it is a vector right. So, similar to this there are there is a data type called mat, but we will come to that later.

So, b is a vector alright. So, we will need the integers where we are going to insert values and of course, we are going to need some will be, we are going to need an array of numbers with which we are going to fill in the array b ok.

So, I mean this is a very synthetic example and over here you are not going to truly appreciate the power of petsc, but I am going to give you some pointers on how this may work out, not may work out it works out.

So, we are going to create a double array we are going to call it a b just to distinguish it from b and the a prefix I use it so that it reminds me that it is like an auxiliary array to b ok. So, let me declare this as so what did we have? 7 1 2 4. So, 7.0 1.0 2.0 and 4.0. So, this is the elements that we want to put inside b and apart from this what else are we want to need anyway. So, as we go ahead we are going to declare things as and when they come ok.

So, the way to initialize or create a vector is the following. So, first things first you must do VecCreate, you must then do VecSetSizes. So, this is a common procedure of declaring a vector. Then we must do VecSet from sizes from options, then we must so over here we must set values ok, let me save this file alright.

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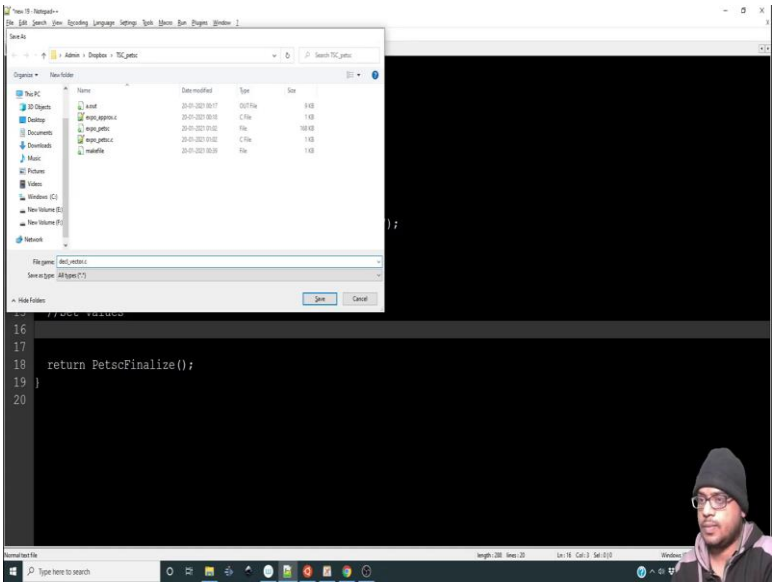

So, now we have some colors. So, there must be some code over here which will sort of assign values into this, then what do we have we must then assemble the vector. So, VecAssemblyBegin and then we must follow this particular function called by VecAssemblyEnd and it is just a idiosyncrasy of this particular library, you have to do this always.

This these two follow each other. So, I have not yet put in the arguments of this function calls, but the argument of assembly end is going to be the vector that you are going to populate and b is also going to be this; so yeah so far so good.

So, now VecCreate; so VecCreate must be done over. So, since we are using one processor. Well, it is not just a question of one processor; it is a question of making the address of b available to all the threads that you will declare. That is why you have PETSC COMM WORLD and you are giving the address of b. Now, inside set size you must tell that we must set the size for b and we must let petsc decide I will come to the syntax in a while and the size is going to be 4 alright.

So, petsc decide, this particular keyword is used to signify the fact that if you are using multiple processors so, one processor will maybe initialize these two, one processor will initialize these two. Things like this, I mean so for such a small array it does not matter right, but once it starts becoming very big, you may benefit tremendously by distributing the load over several processors alright.

So, now once we have set the size of b. So, this is the overall size and petsc decide will decide how to distribute the load alright. So now, set from options it has to be only passed to b. Now, we must set values. So, there are various ways of setting values. So, let us start with method one.

I mean rather than going with method one I will I am going to show you the easiest method which is VecSet values. And VecSet values must first accept the argument b that is the vector you want to populate, then how many entries do you want to populate that is; 4, then we must specify the indices where you want to populate.

So, we must create an integer array. So, let me call it j and we will make this j 4 and we will make it 0, 1, 2, 3 right. So, j is the address of the array which holds the indices where we want to insert these nonzero entries and I will change this and show you how it will affect the code.

So, we want to insert 4 values at the j locations. So, j is the indices where you want to insert and lastly, we want to tell what exactly we want to insert. So, we want to insert the entries inside the array a b. So, a b is the address of the array 7, 1, 2, 4 and how do you want to set the values? There are two modes; one is insert values and one is add values.

So, if there is an already existing entry for b, if you do add values you will sort of add whatever you are doing to the existing values. If you do insert values that will erase the value insert the present values alright; so far so good. So, yeah this assembles the matrix and in the end before finalizing we must do vec destroys, we must clear the variables. So, we must give the address of b and that is it. So, let us save this, let us go to our make file and create a new target.

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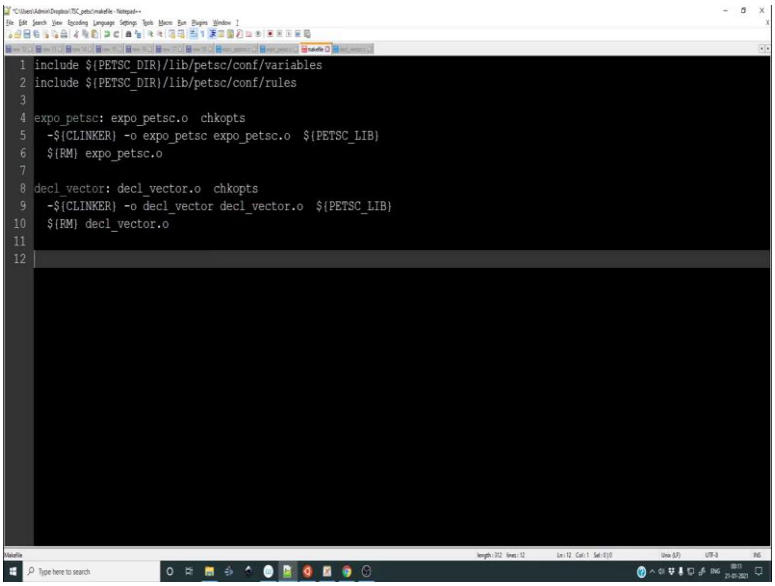

So, let me hit conrol H oops, control H and I want to replace this by declare vector ok. So, replace, replace, replace, replace, replace. So, there is no use of like rewriting this entire thing. We simply having the same variables and rules. We are just making a new target right.

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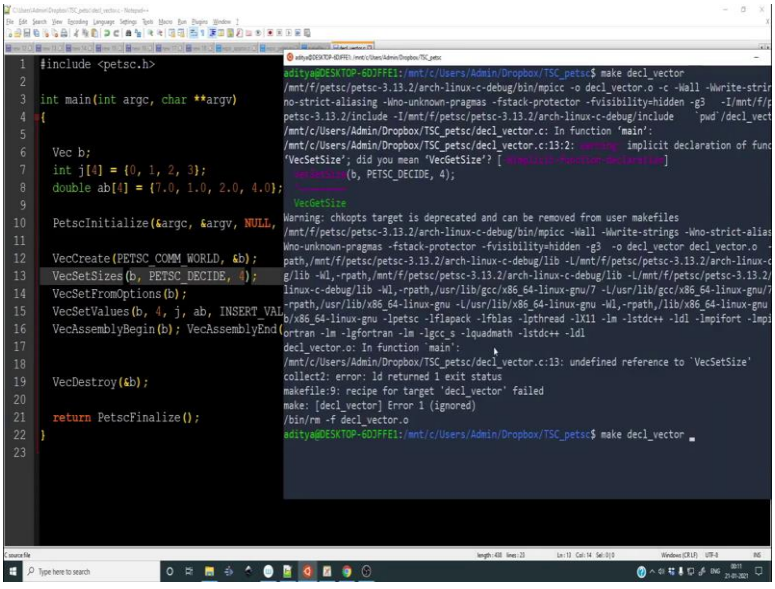

So, let us save this file. So, we have our code over here alright. So, make decl vector ok, there appears to be an error. So, let us see what the error is. So, there appears to be so, this has to be set sizes oops! Yeah, ok.

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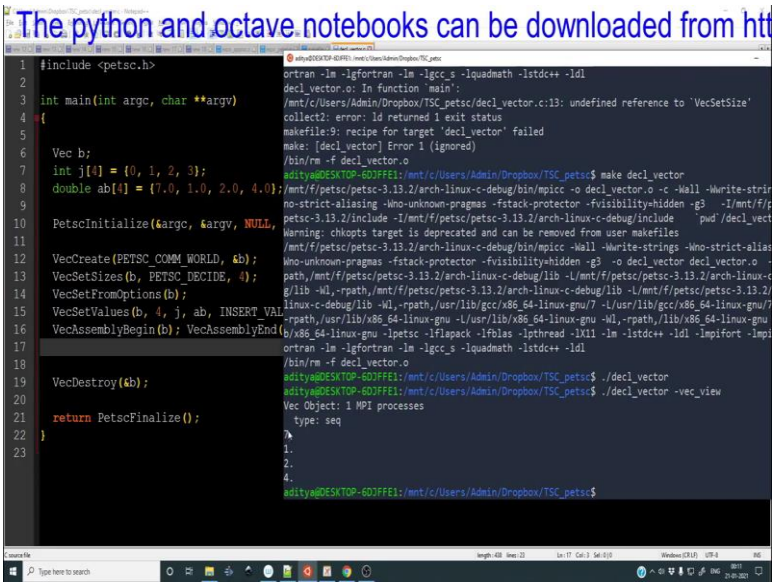

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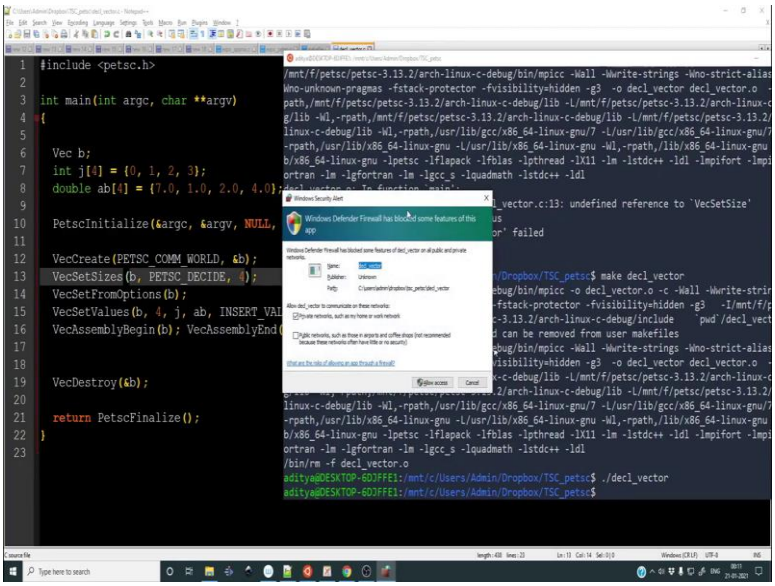

So, it compiles nice and well. So, let us just do dot slash declare vector we have to allow this ok. So, it does nothing as expected, because we have not printed anything we have not like asked it to do anything for us. But what we can do is pass this command line argument minus VecVeiw and it will show us the elements of the vector ok.

So, additionally we can insert this VecVeiw inside the code itself. So, what we can do is vec so, before destroying the vector we can do VecVeiw, we will pass b, then petsc viewer std out world, just to say that it has to run on a single process.

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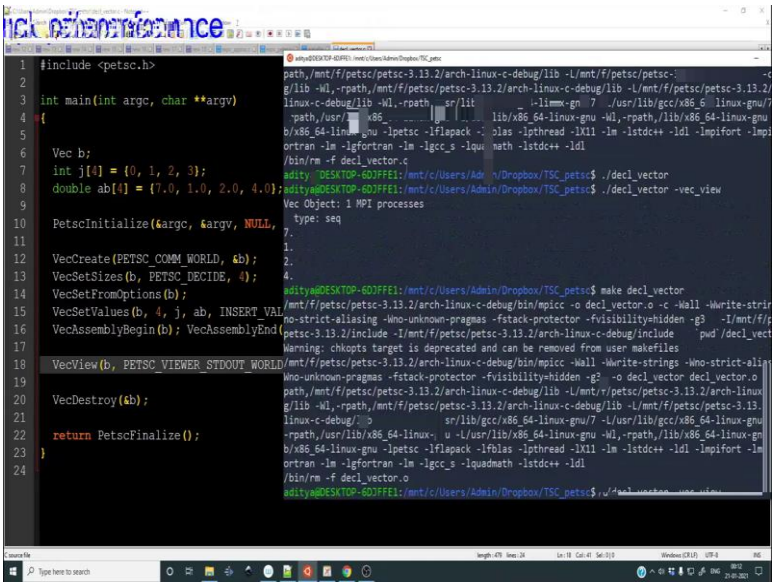

So, let us make it again, let us run it and now, it shows without having to pass the extra argument. So, without using this ok, alright so, we have now initialized this now. So, what happens? If we still make j equal to this, but we only do b as so, we only want to insert 3 values.

So, we still have the 4 indices and the 4 values, but instead we say we want to insert only 3 first indices and the first three indices the first three values. Let us see what happens.

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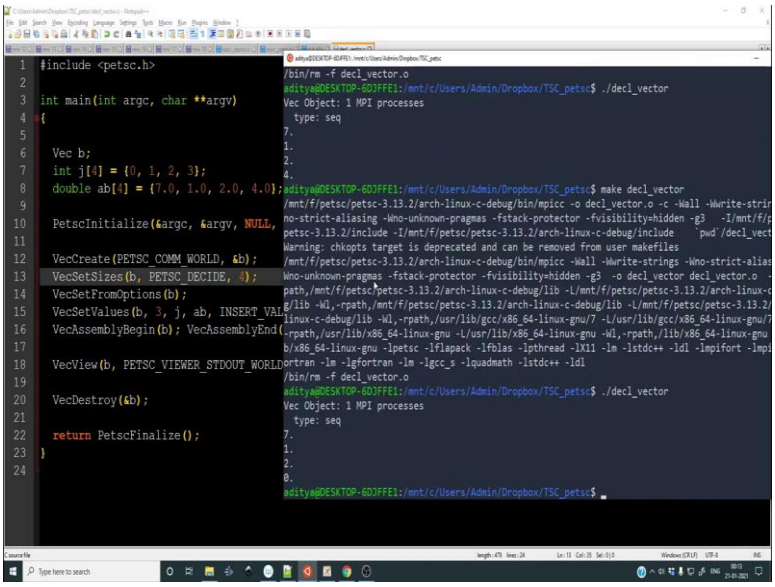

So, look its initialized it to 0 instead of getting a 4, because we have not told it to populate b with 4 values, we only told it to populate with 3 values.

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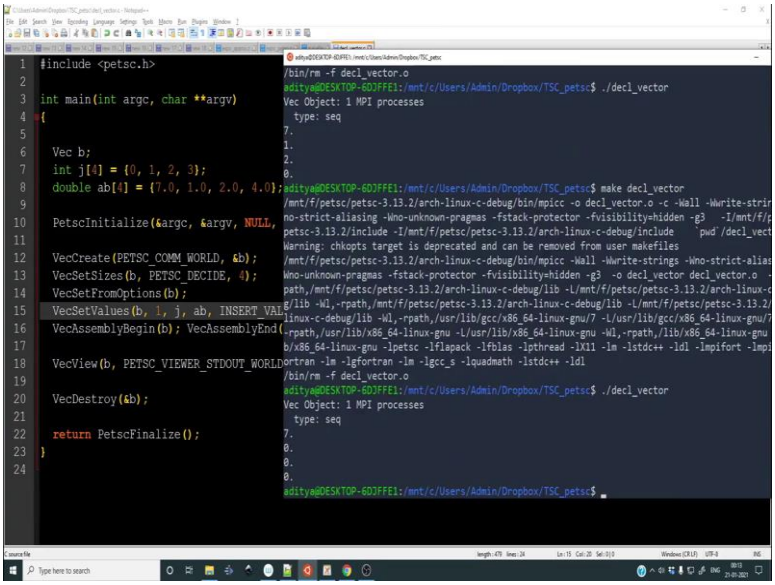

Similarly, if I do only one it will only populate the first value. Let us make it again value ok. So, it is incredibly versatile you can declare everything you want, but in the end if you want to fill partially you can choose to do that, there is nothing wrong in that. So, this is how we can declare vectors and sort of print them out. Well, there are various ways of viewing a vector as well.

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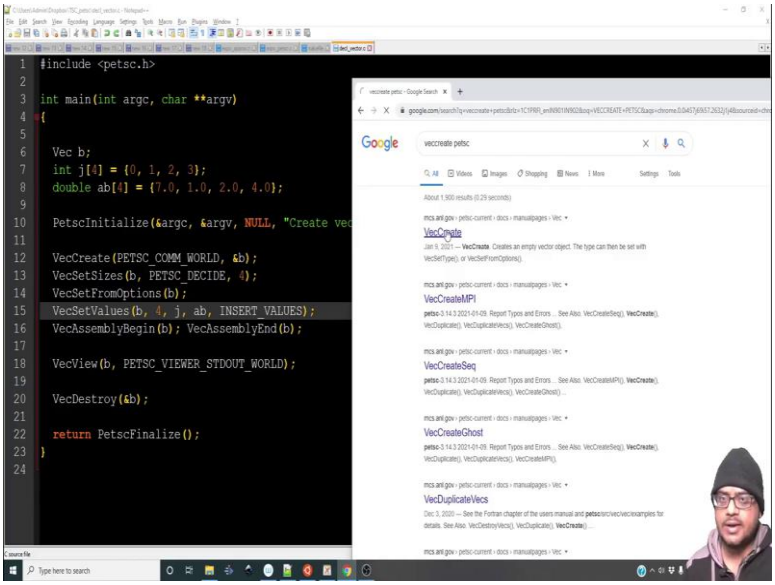

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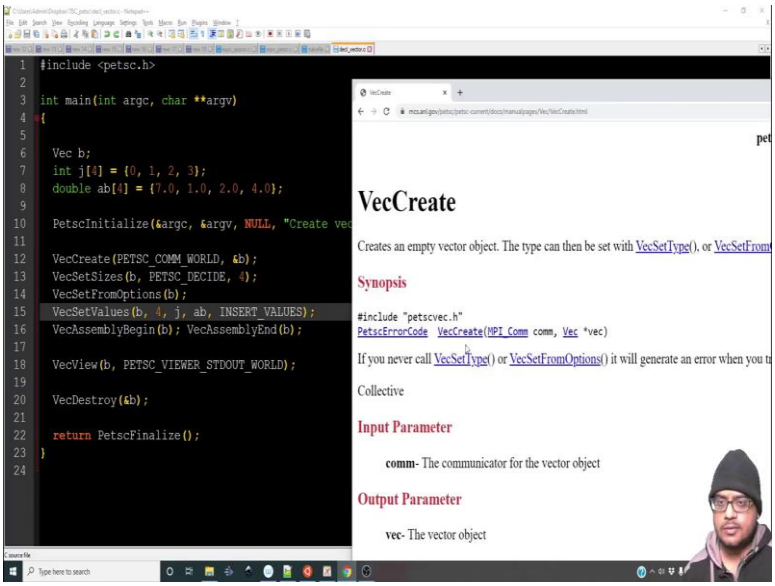

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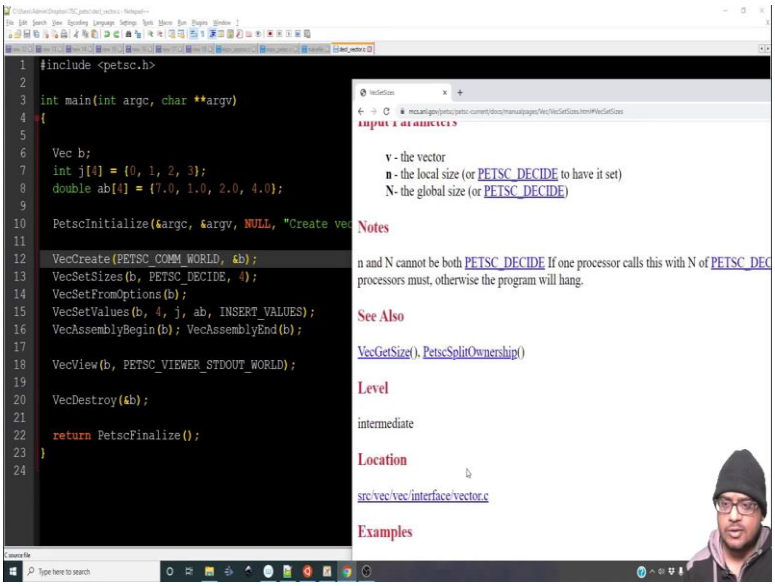

So, like I told I am going to show you the function reference. So, VecCreate so, it requires the MPI communicator which in this case is PETSC COMM WORLD and it requires the pointer to b the address of b. So, we have passed the address of b ampersand b that is standard c syntax. So, VecSetSizes so, it sets the local sizes.

So, we have to pass the vector the small n is the local size if you have multiple processors then you have to pass small n, but in this case we have let petsc decide and then the global size alright. So, the global size of our array is 4, but we have asked petsc

to decide for us the best load balancing it can do. In this case we are running it on one processor. So, it does not matter anyway alright. So, with these options it is going to initialize b over here.

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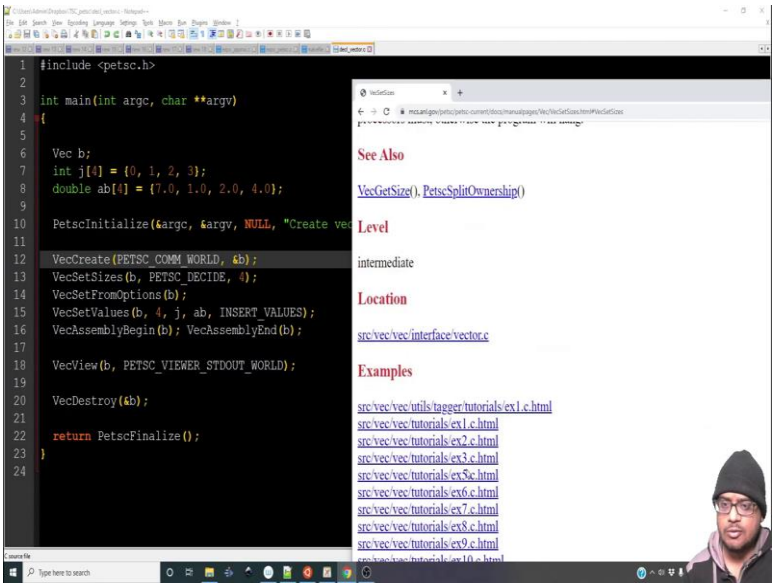

So, now VecSet Values let me go to the function reference like set values alright.

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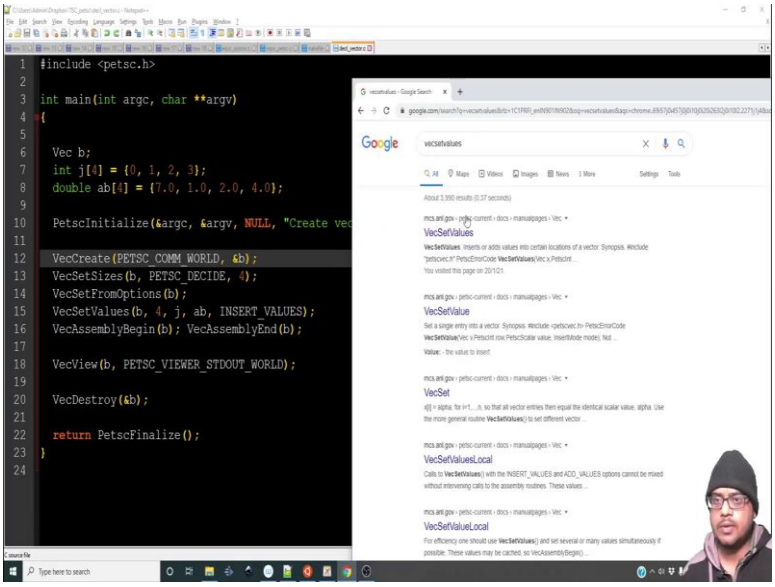

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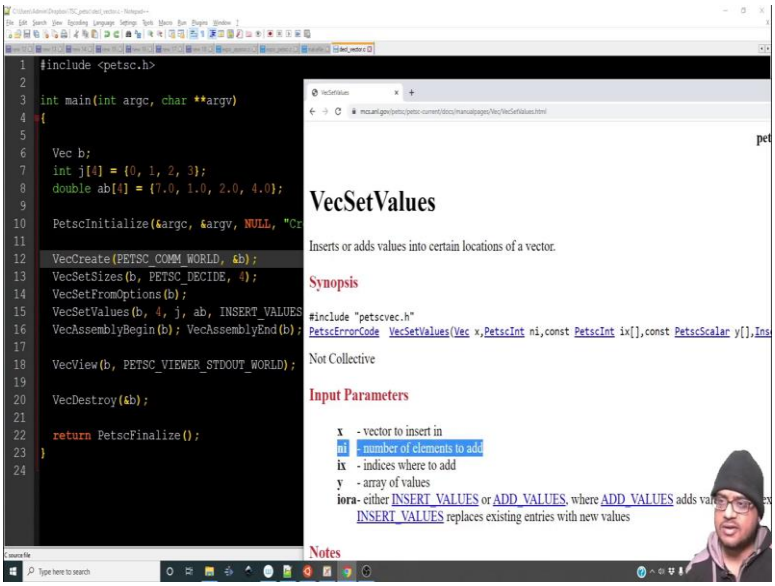

So, it requires the vector the number of elements to add look is the it is number of elements right. In this case we wanted 4 and I have showed you what happens when you reduce it.

If you increase it, it will let us see what happens when we increase it ok. Before that we must show the, we must tell what the indices of insertion are ok and we must tell what values you want to insert and you can either insert values or add values. So, it is quite simple. This is the standard syntax of creating a vector in petsc.

So, now let us increase this and see what happens let me make it 6 just to go beyond the boundary case. So, let me make this; obviously, there is not going to be an error over here, because we would not done any illegal sentence and there is an error argument out of range. So, it cannot do that, it gives a big garbage value. So, we must have this maximum 4. So, let me fix it great. So, now we will proceed to figure out how we can declare matrices in this particular way.

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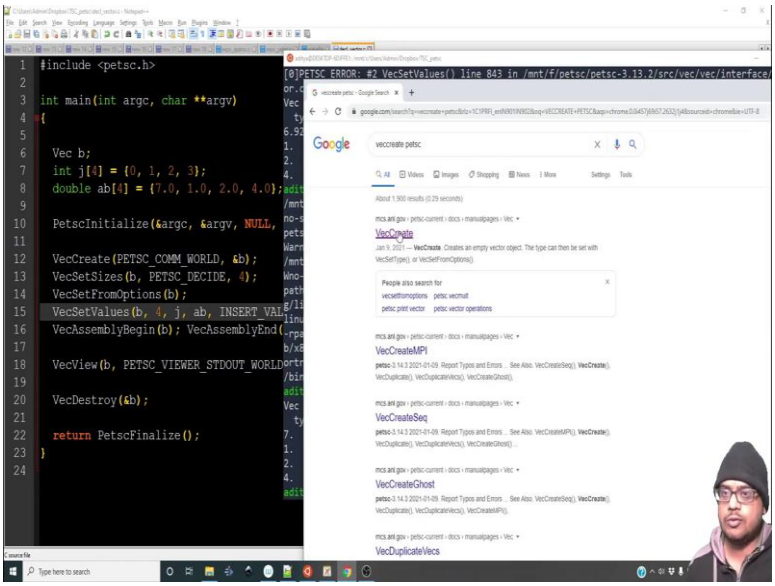

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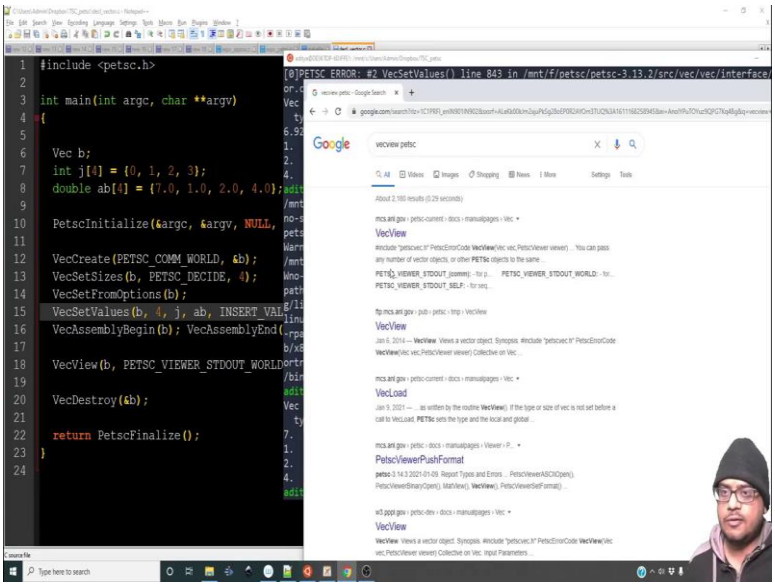

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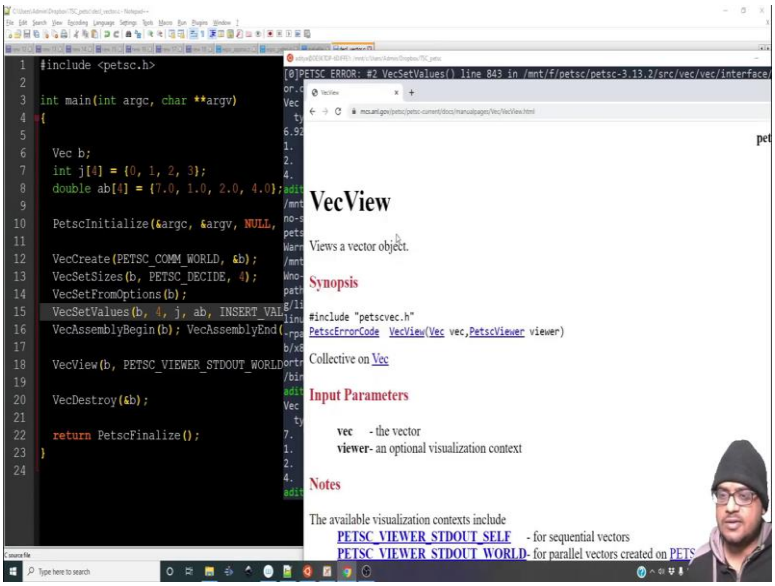

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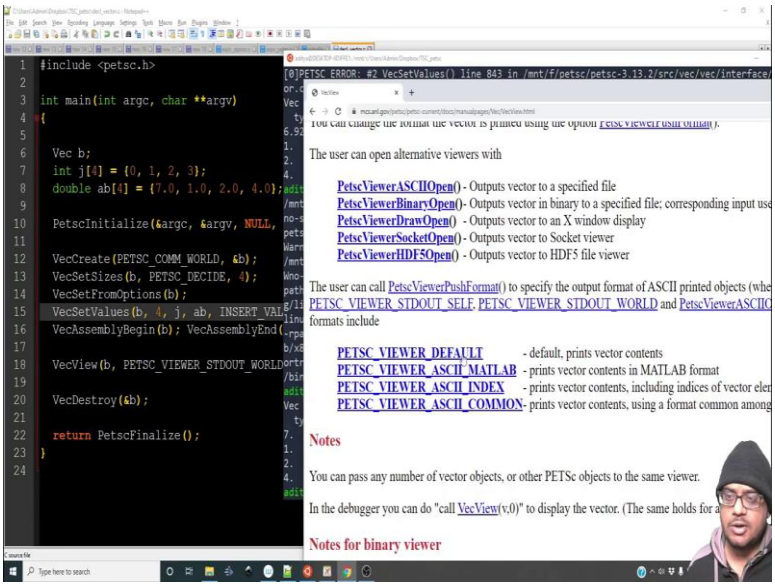

But before we go to that let us just go to VecView, because I want to show you function reference for VecVeiw. There are various kinds of viewers. So, this ASCII, binary, draw ok. So, there are various kinds of viewers that we have. So, this a PETSC VIEWER DEFAULT, PETSC VIEWER ASCII MATLAB. Let us see what happens when we do that.

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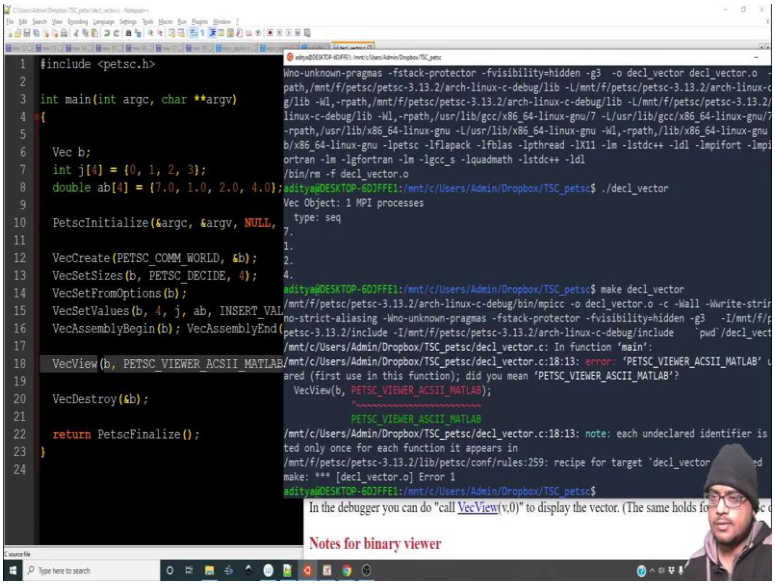

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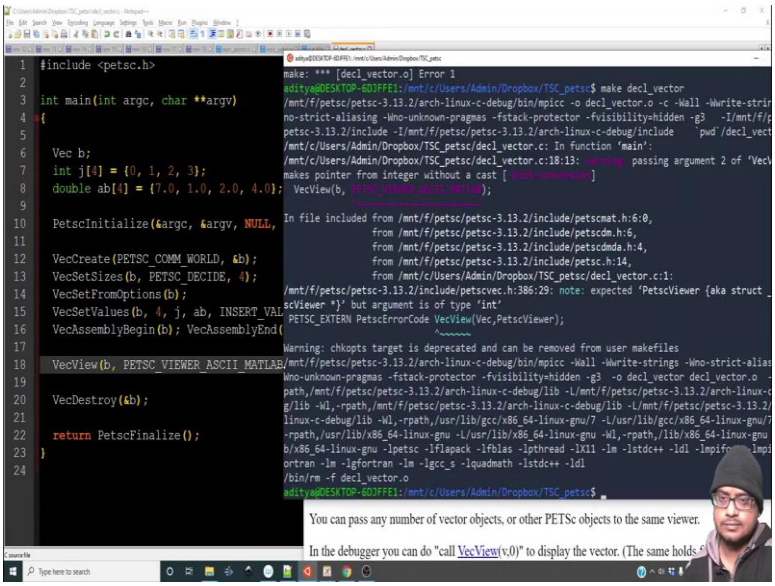

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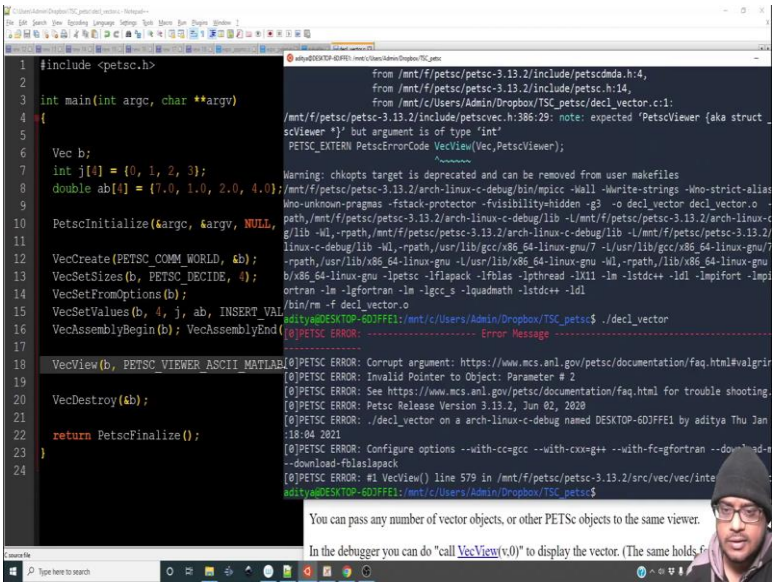

It will show us the output in MATLAB forward. This is spelling mistake, ASCII alright. Well, there is an error and it does have to do something with the viewer.

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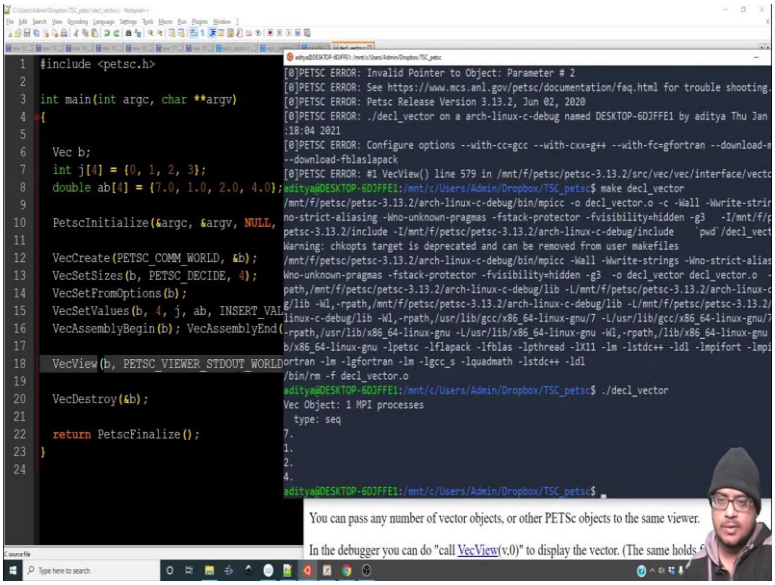

Well, for some reason it does not work on my PC, but maybe it does on your ok. So, let us see whether this should work, there is no reason for this not to work.

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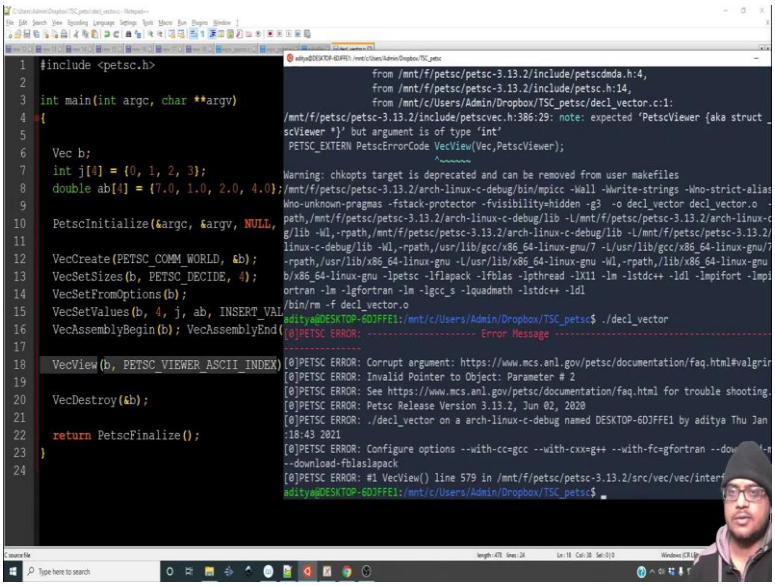

Let us see, there is some errors that is weird ok. Anyway, ok. So, I need to call this one anyway. So, forget about this, do not worry about this, is as a beginner course. We will just keep it as STDOUT _WORLD and yeah. So, do not worry about that, we can call we can push a format and then we can bring it, but you do not need to worry about all that. So, so far we have this grid. So, now let us proceed to create a matrix alright so in fact, let us modify this file itself.

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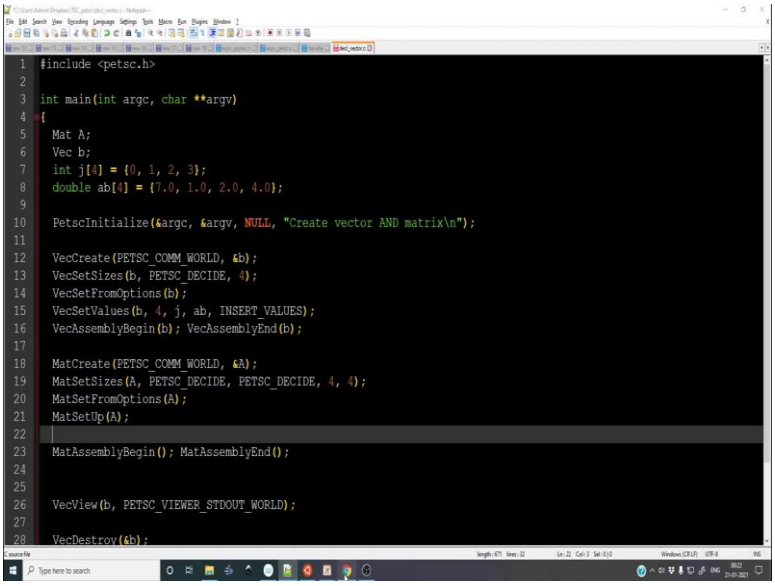

So, yeah similar to this there will be a sequence which will follow exactly this vector creation sequence. So, there will be a MatCreate, then there will be a MatSetSizes, then there will be a MatSet from options then we will have MatSetUp it is to and this is different from the vector, but you need to set up the matrix, then there has to be insertion of values lastly, there has to be an assembly and so, for that there will be two steps; so, MatAssemblyBegin followed by MatAssemblyEnd.

So, unlike the vector, the assembly has to have a certain key word additional, but first let us declare the matrix. So, Mat A alright. So, we have declared a matrix A and let us create the matrix A. So, A will also be 4×4 suppose. So, in order to create once again we have to pass this and the address of A that is common, set sizes again. So, for vector you need to only declare one dimension, but for matrices you need to declare two dimensions.

So, A, PETSC DECIDE comma PETS; PETSC DECIDE, because we have two dimensions and the processor load has to be balanced in two directions and the size of the matrix. It is pretty straightforward. Set from options it is simply going to have the variable A, after this we are going to set up A. Now, we have to insert values. Well, there are again various ways of inserting values, but the most common is the Compressed Storage Row format, the CSR format Compressed Sparse Row format ok.

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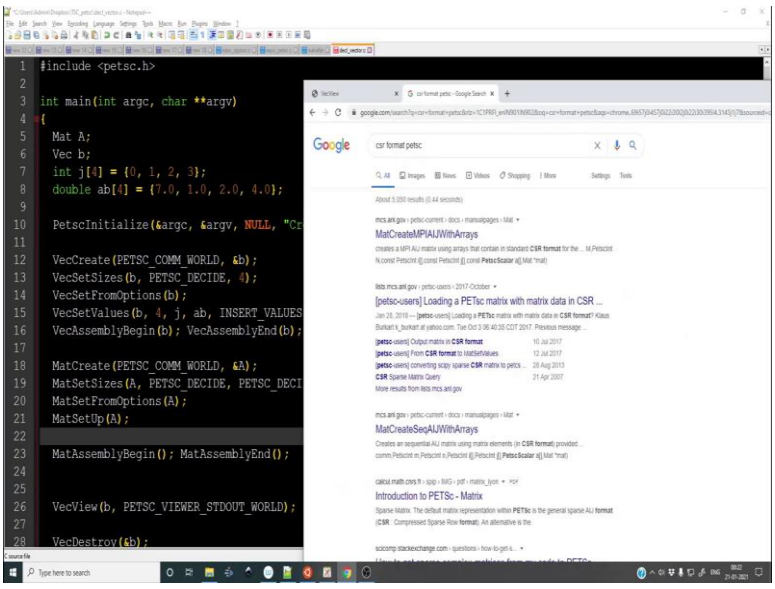

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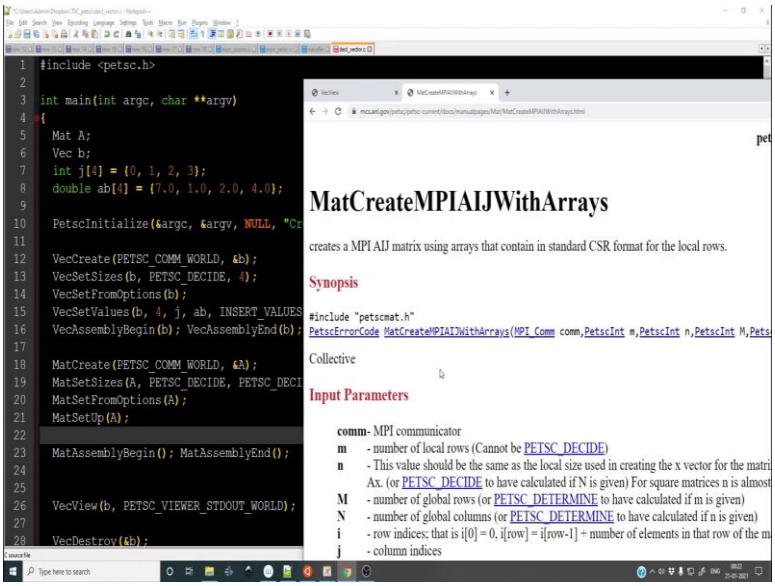

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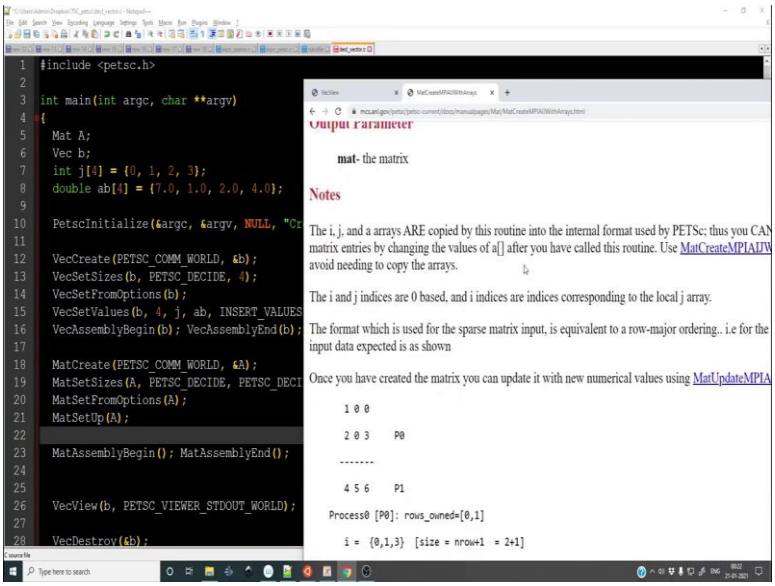

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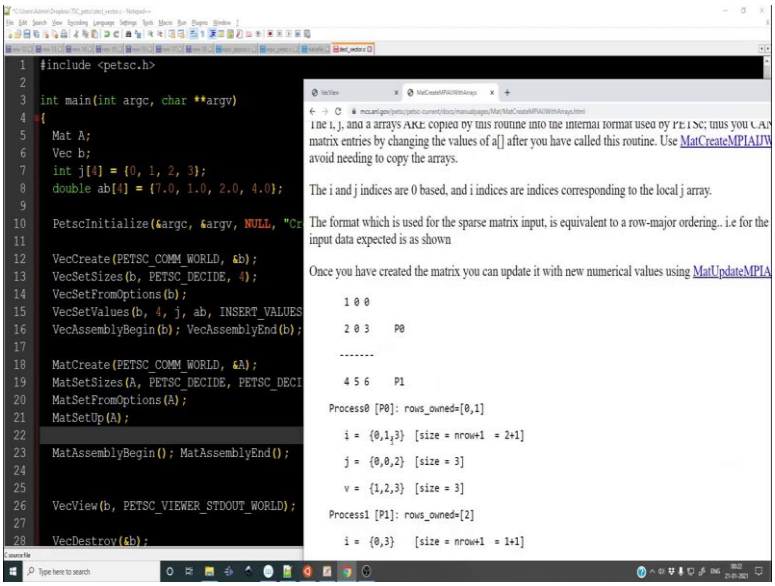

Let us so, in the standard CSR format you are going to create a MPIAIJ matrix. So, what it does is, it is going to; it is going to store what nonzero entries you have right in a single row. It is going to store the column number and the corresponding value; ok this is what it is alright.

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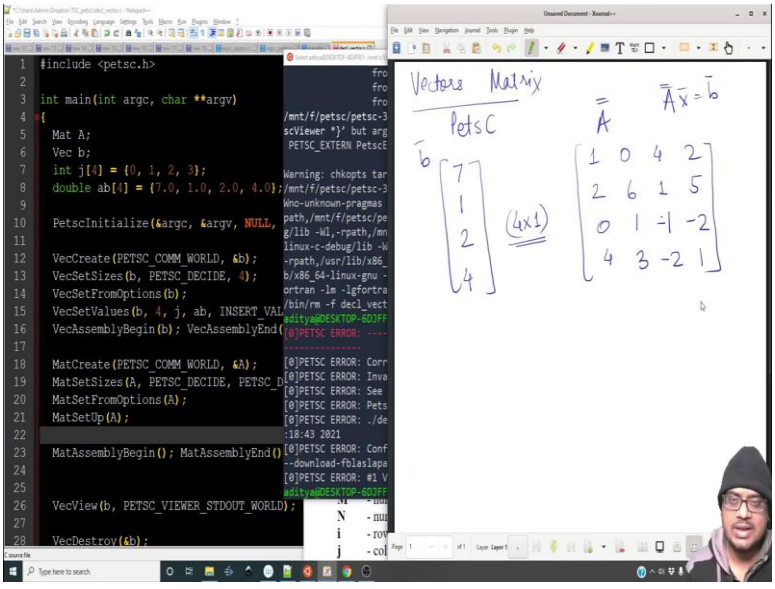

So, so far we have not decided what the matrix should be. So, first we have to decide what the matrix has to be or let us create something 1 0 4 2 2 6 1 5 0 1 -1 -2 and 4 3 -2 1, I am hoping the determinant is an 0, because later we may be tempted to solve. So, if this

is A this is b we will tempted to solve A x = b. Anyway, let us declare the matrix b like this. So, let me yeah got it, ok.

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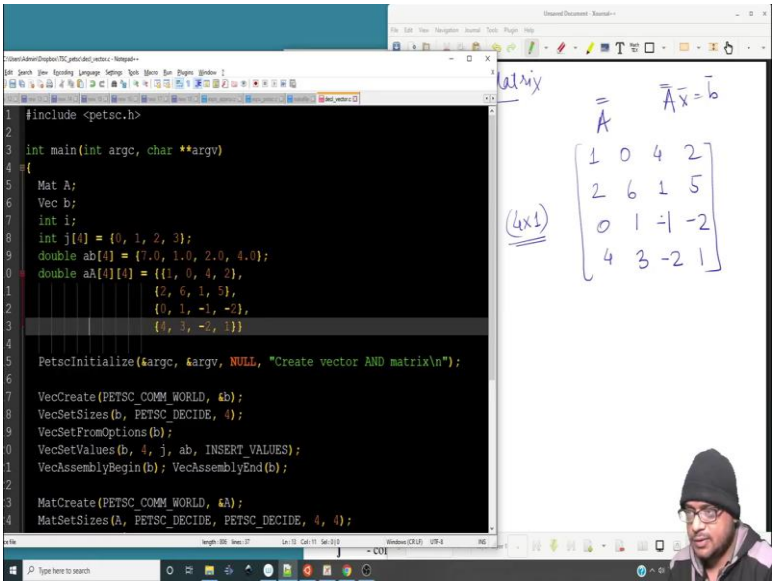

So, now what we can do is create a double matrix. So, a A and size will be 4 × 4 and we can actually declare the entire array over here as well. So, what is this going to be 1 0 4 2 and we have 2 6 1 5 , and 0 1. Well, we are doing it the hard way, because it is so, small we can do it non-programmatically. Later on you will find tremendous benefit in doing it programmatically meaning; you run everything in a loop.

There is a distinct logic behind how these matrices will be set up, but in this case not no such thing exists. So, if the world so, we have defined the double array and yeah so, we need an integer to loop over 1 to 4 ok. So, we have an integer over here.

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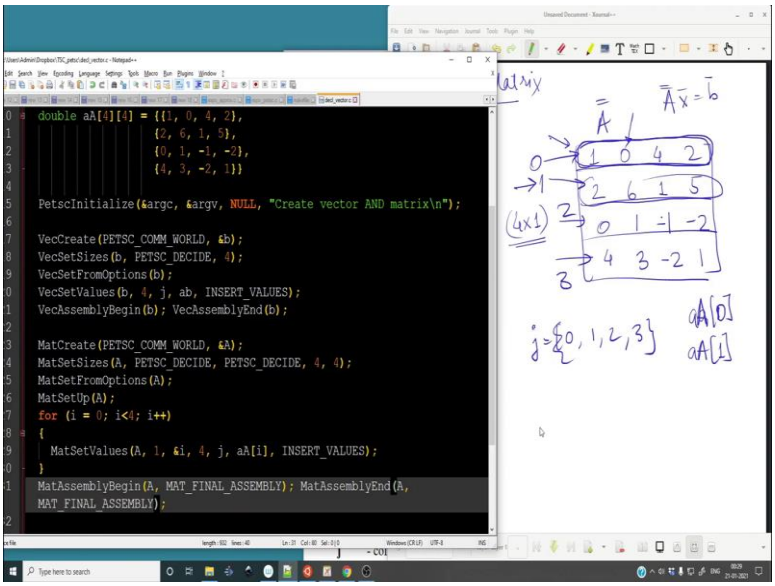

So, what we can do over here in order to do this, so for i = 0 i < 4 i ++. Now, we can insert the elements into the matrix. So, the way to do it is MatSetValues into A. So, we are we doing it row by row the fact that I am using; the fact that I am using a loop I, is to loop over 1, 2 so, rather 0, 1, 2, 3. So, I am looping over 0, 1, 2, 3 through this particular for loop and in doing so, I am going to insert these particular values into this.

So, since we are doing it in a dense form, we are not really bothering about this 0 over here. It is a dense matrix. So, we are going to do j equal to 0 1 0, 1, 2, 3 which it already is. So, it already is 0, 1, 2, 3. So, we are going to take each row of this double array, a double pointer. So, we are going to take each row, insert it as column 0, 1, 2, 3, then take the first row insert 0, 1, 2, 3, second row insert 0, 1, 2, 3, third row insert 0, 1, 2, 3.

So, once I write it will be clear what I mean. So, I have, I am going to insert one row, I am going to pass the address of the row index that I want to insert. So, ampersand i means; the address of the current row index then I want to insert four values, I want to insert values into 0, 1, 2, 3. So, j is already an address. So, j so, thing is because i is an integer % i is the address, but because j is a j is an array rather j 4 is an array, j is the address, you do not need to pass an ampersand for the array alright.

So, these are some things which you pick up in C programming and lastly, we must pass the address of these fellows; this row, then this row, then this row, then this row, one by one and so, it is aA and it is simply going to be i and all is implied over here. So, in

python you would have done this, but not over here that is implied. So, the address aA i holds these four elements. So, it is a double pointer so if the two square brackets, the two sets of square brackets means; there is a set of pointers which holds another set of point and which holds pointers to these rows ok.

So, meaning there is a pointer which holds these arrays and what holds this array? It is aA 1 rather aA 0; what holds this? aA 1 and so on. So, we are passing the address of those rows ok. So, this is how so, lastly we must tell insert values alright. So, yeah that is pretty much it with the help of this loop after. So, we have sort of set up what to insert and what where to insert.

So, now we must begin the matrix assembly. So, it is A ,MAT FINAL ASSEMBLY and you have to end also A, MAT FINAL ASSEMBLY alright. So, now you must be wondering why Final Assembly? Because there can be a sub matrix assembly as well.

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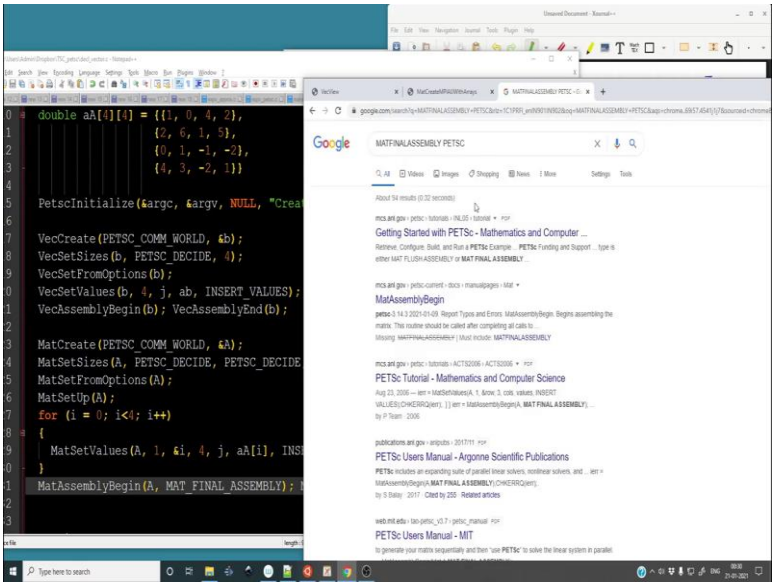

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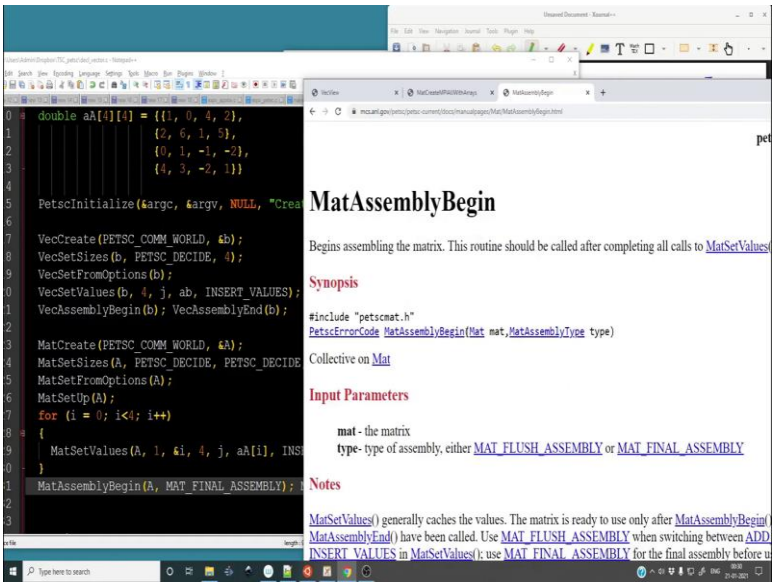

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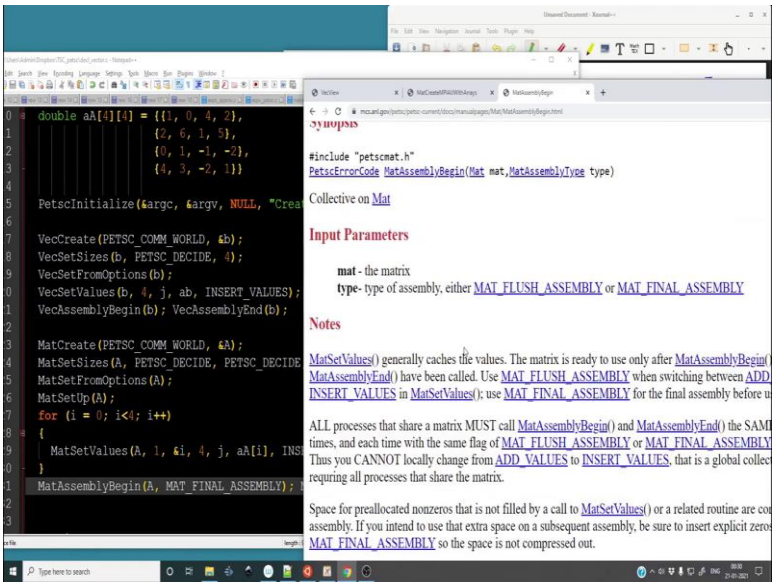

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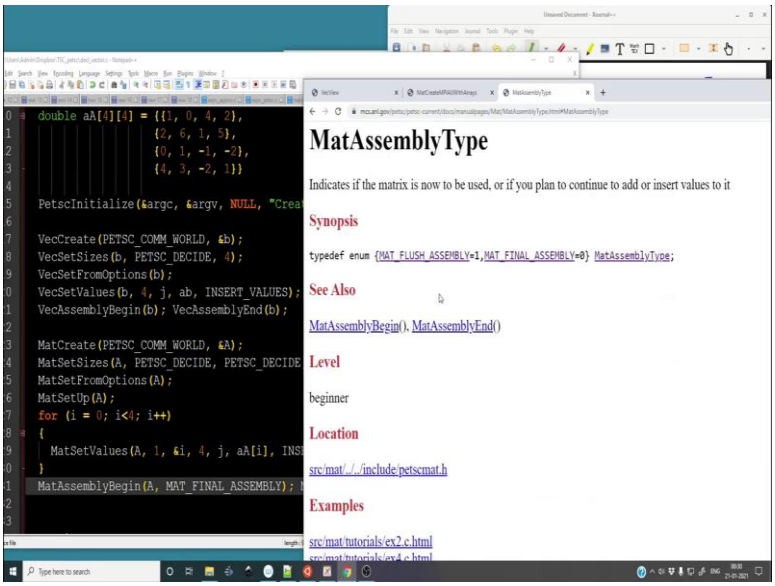

So, you so, it can be either flush assembly or final assembly ok, but in this particular examples, we just need to bother with final assembly alright.

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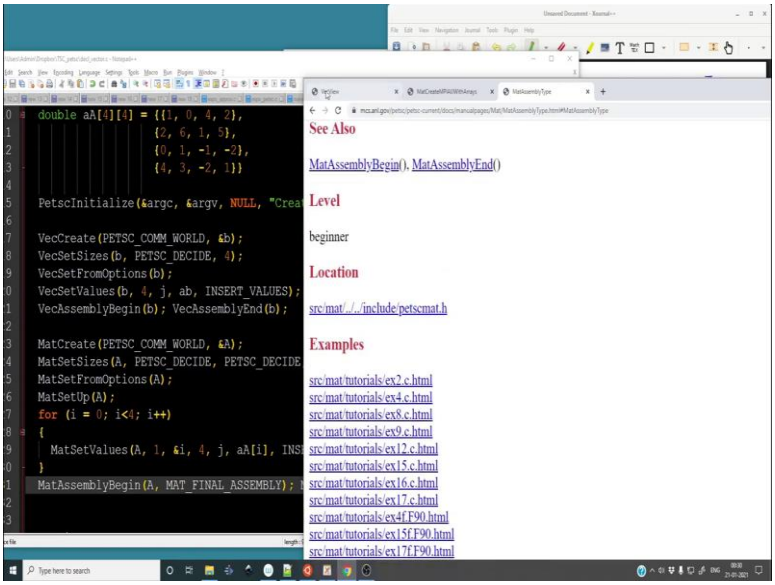

So, we can have a look at the function reference, we will figure it out. You can try various things, but yeah this is the general syntax for assembling a matrix.

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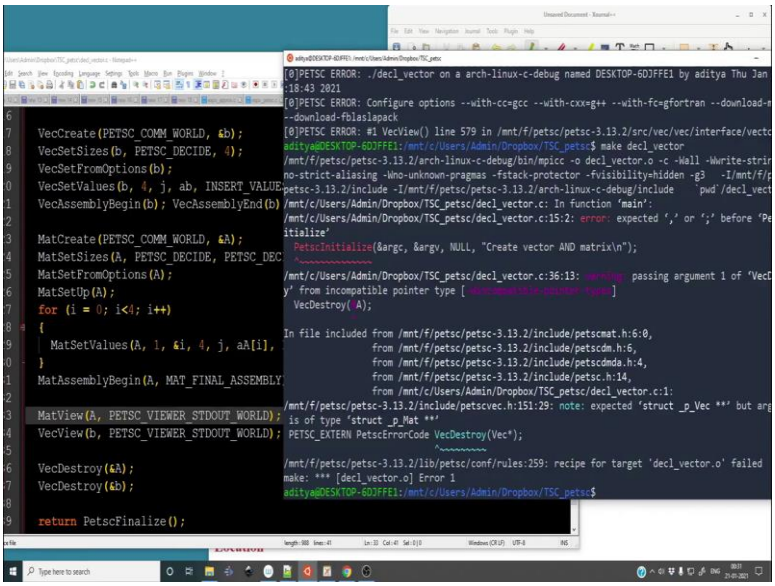

So, once we have done this we must keep in mind that we must also destroy eventually, the pointer. So, the memory has to be cleared. So, we will simply pass the address of A and we can put a viewer over here as well. So, MatView A and we can use simply the STDOUT that is the terminal for visualizing the matrix ok.

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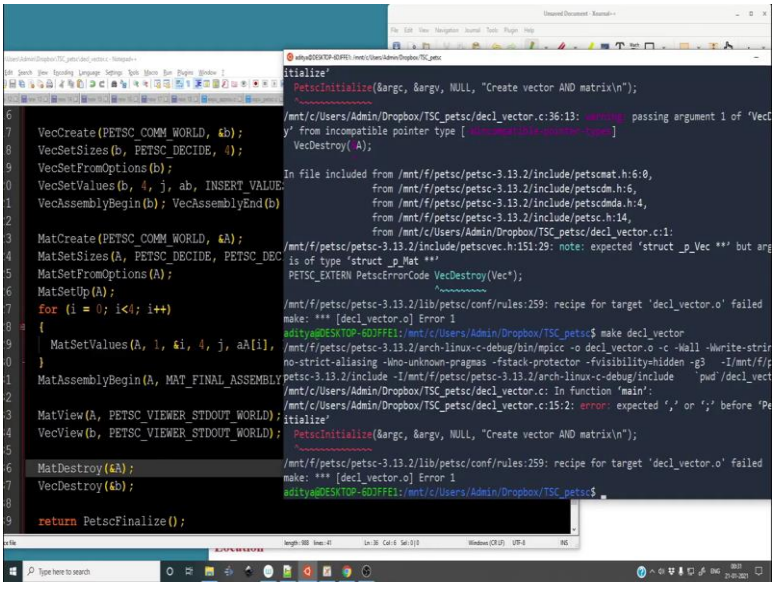

There appears to be an there is it is not like destroy, but rather it has to be MatDestroy. There is a data type error ok. Let us make it ok, there is an error. Let us see what the error is. Have I missed a semicolon somewhere? We missed a semicolon over here ok.

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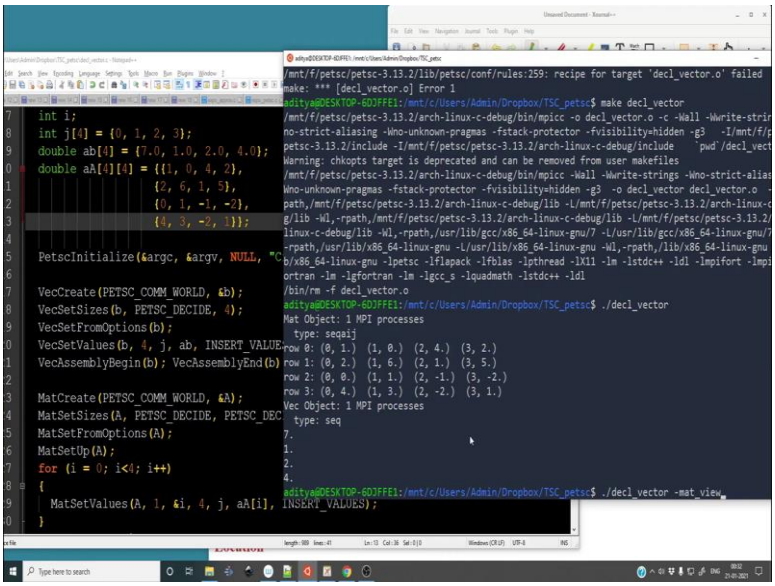

It is unforgiving in that sense, but yeah it is incredibly flexible ok. So, there you go so in row 0 the first row contains 1. So, it is CSR format so in row zeroth zeroth column has 1, first column has 0, second column has 4, third column has 2. So, the indexing; obviously, starts with 0 and similarly, you have all the other values. So, we can verify this. Now, what we can do is; we can print it over here as well.

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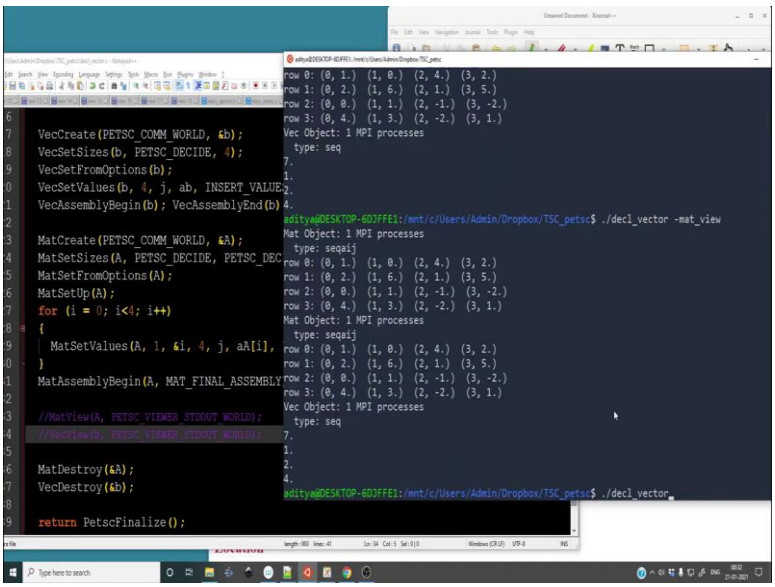

So, you can; so you can comment out these lines and print out by passing the command line argument.

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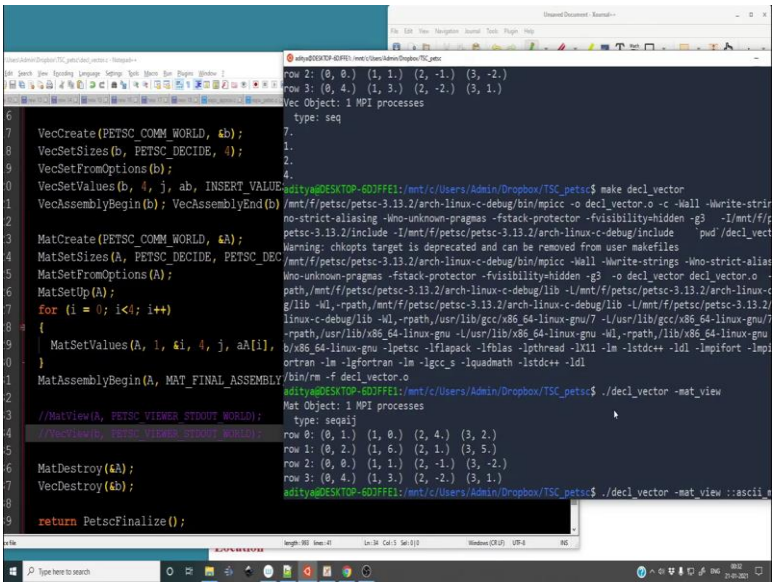

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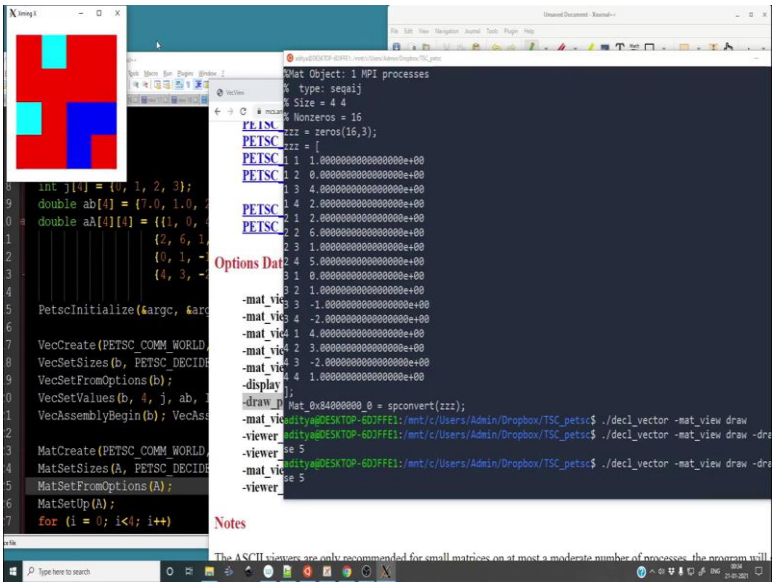

So, let us save this, let us recompile and let us call it with this. So, you can simply print the MatView, we can print it as ascii matlab this is the MATLAB way of writing it ok. So, MATLAB indexing starts from 1 1 , 1 is value 1. So, let us see 1 , 1 value is 1, 1 0 4 2 2 6 1 5 and so on. So, this is how MATLAB would represent it. There is also a way of visualizing this entire thing.

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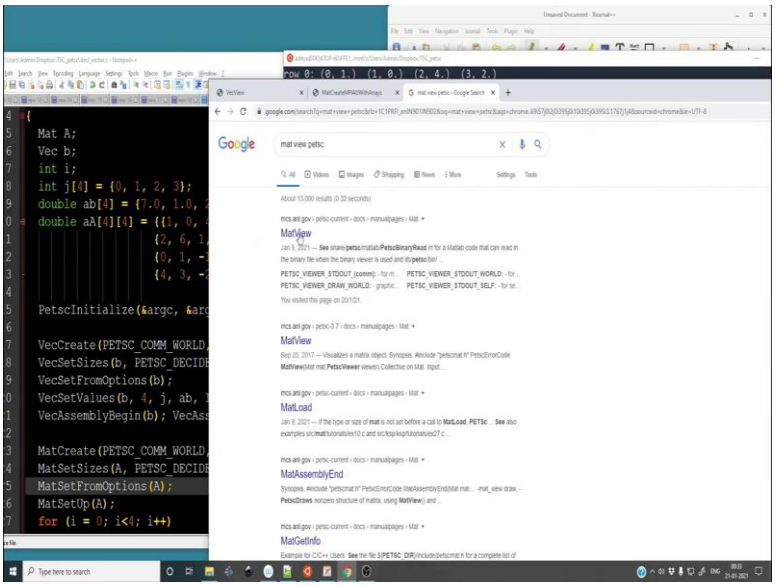

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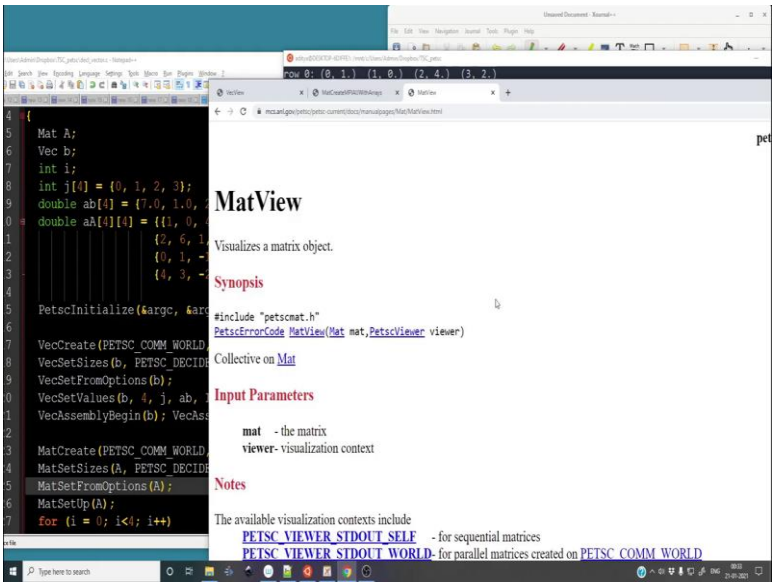

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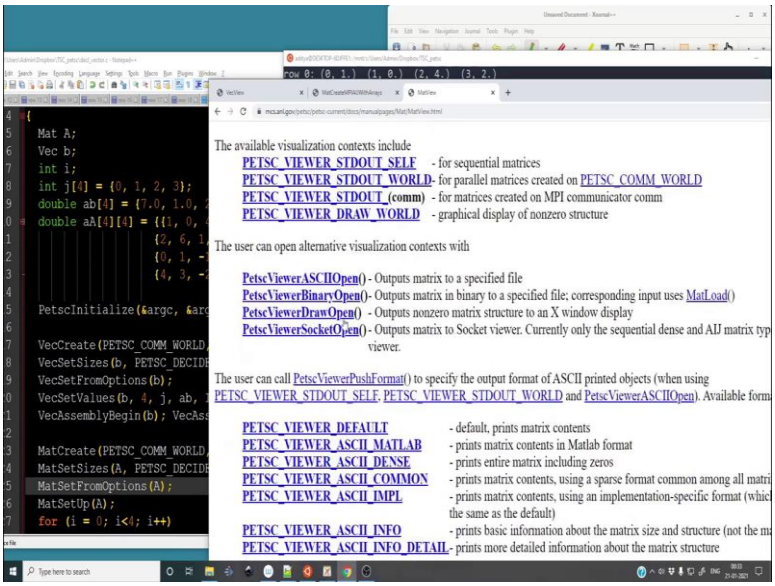

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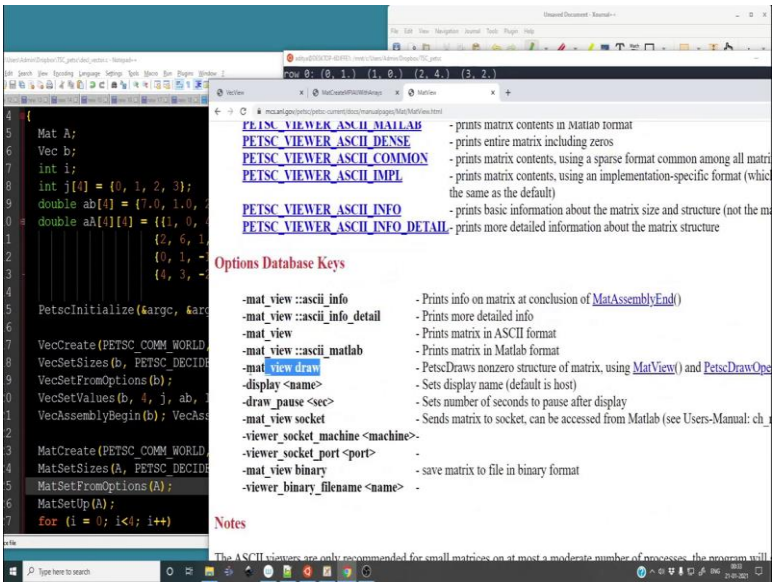

So, let me go to the function reference for mat view ok. So, what do we have? Let us see we will draw a world ok, but we can we can do this mat view draw. So, what we can do is mat view draw, quickly we came and went away. So, we must have a draw pause as well. So, look there is a draw pause as well which we need to do. So, draw pause of 5 seconds ok. So, this is how it looks.

So, the 0 is cyan, positive values are red, the negative values are blue. I will do it again in case you want to see, great. So, we have seen how to create a vector, how to create a

matrix, how to assemble it. There are many ways of doing it and in the coming lectures you will see some other ways of doing it as well. In general you will see a programmatic way of doing it. One last thing I want to point out the graphics that you just saw, for that you need to install some kind of X 11 forwarder.

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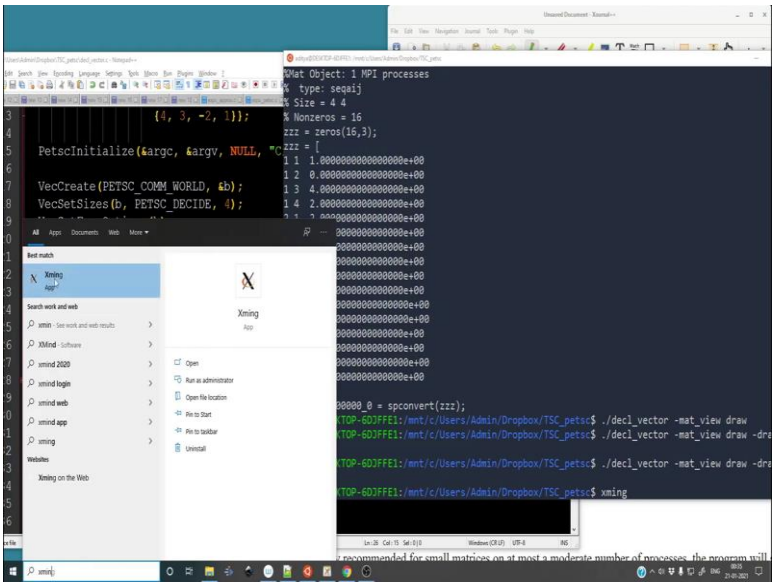

So, because we are using sort of a virtualization of Linux, you need to install something like Xming or something whatever you like you have to open it up. So, Xming Xming I have it installed. So, you have to open this, then launch the or you can launch ubuntu, then launch Xming and how to test whether Xming is installed you just say xeyes.

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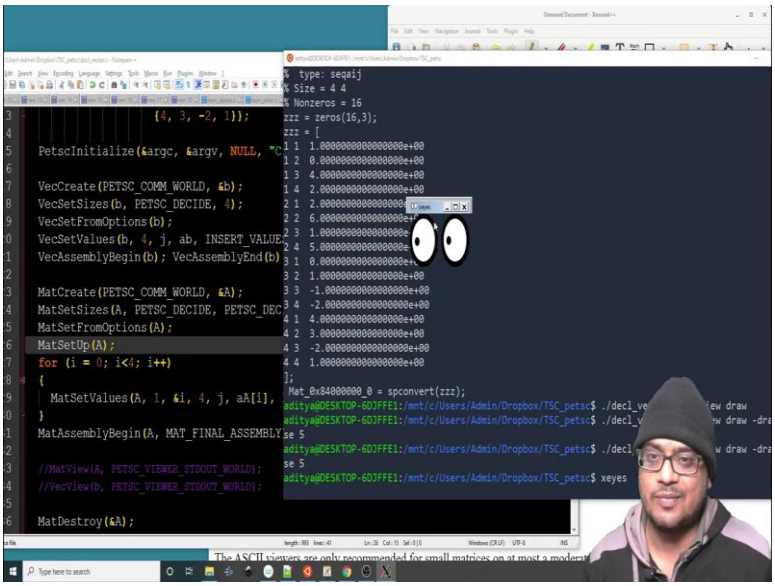

And you will have this funny X 11 application in Linux, if this works everything is fine, if this does not work then you will not be able to visualize things natively from this. But for those of you who are working natively in Linux all these things would not matter. And I am too lazy to install the whole thing the petsc library is natively in windows. So, that is why I went for virtualization.

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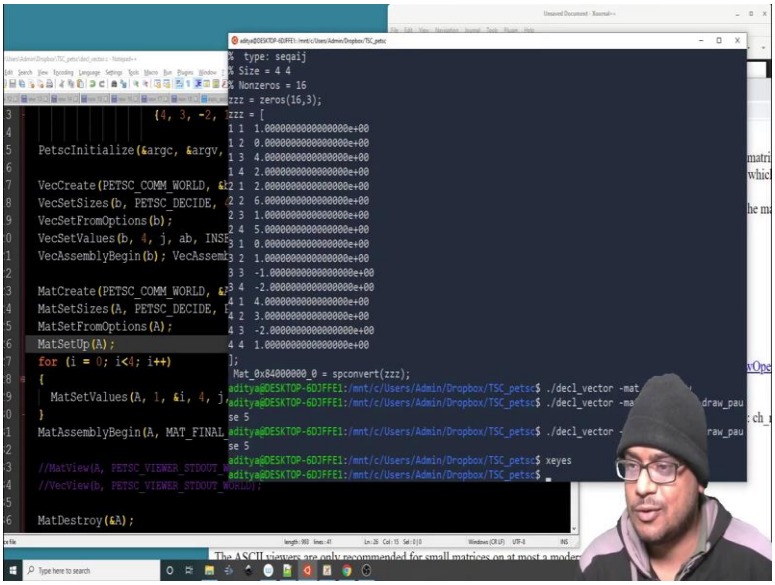

Anyway; so, I hope you will find whatever I have shown useful and practice makes you perfect. So, just go ahead and do various kinds of matrices that you like. In the next

class, we will see how to make a simple solver and we will proceed with a 1D problem. With this, I will see you next time until then, good bye.