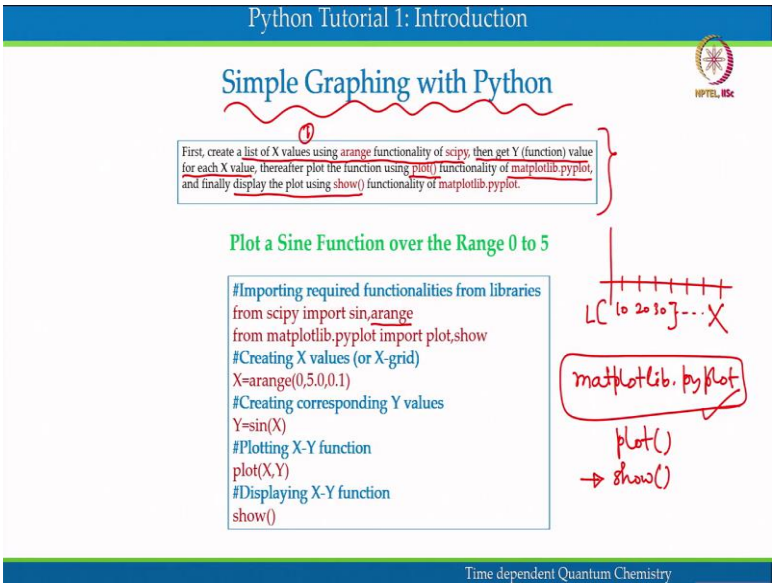
Time Dependent Quantum Chemistry
Professor. Atanu Bhattacharya
Department of Inorganic and Physical Chemistry
Indian Institute of Science, Bengaluru
Lecture No. 07
Plotting Graph with Python Programming

Welcome back to Python tutorial 1 of the course Time Dependent Quantum Chemistry. In this tutorials, Python tutorials, we are going over different techniques for scientific computing and slowly we are nudging ourselves to the computation we require to explore Time Dependent Quantum Chemistry.

(Refer Slide Time: 00:50)



So far we have gone over simple computation, different techniques of computation, simple arithmetic computation, then we have checked how to use different mathematical functions in Python and in this session, we will go over simple graphing tools. How to plot a mathematical function for our visual inspection?

So, the procedure is following. Previously, we have seen that how to create a list and that list can be used as x axis which is like we had 10, 20, 30 like this way we prepared the list and this list was prepared using Python built in list functionality as well as the list was prepared previously, with the arange functionality taken imported after importing arange functionality from scipy.

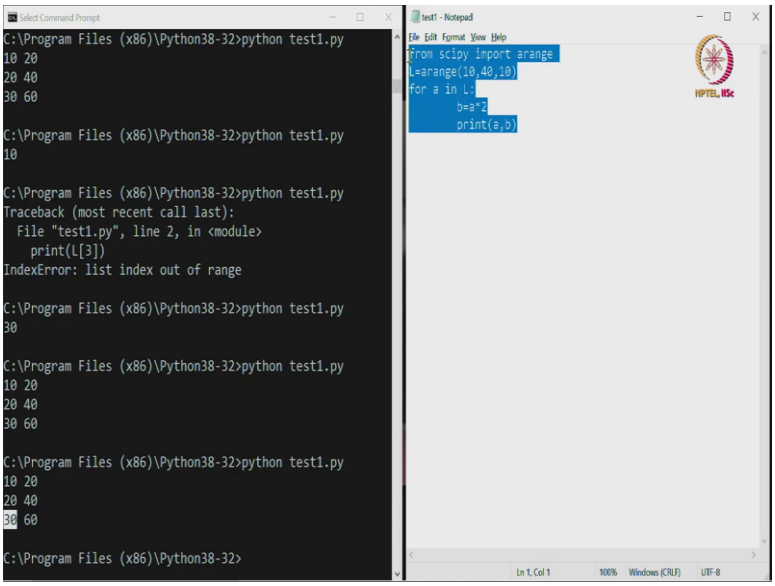
We will use arange functionality, this is very powerful functionality, because this gives me an array. Array is a matrix, we will discuss it later, but for the time being we will consider it as a list of numbers we are getting. So, first thing, what we have to do to prepare a graph is that to

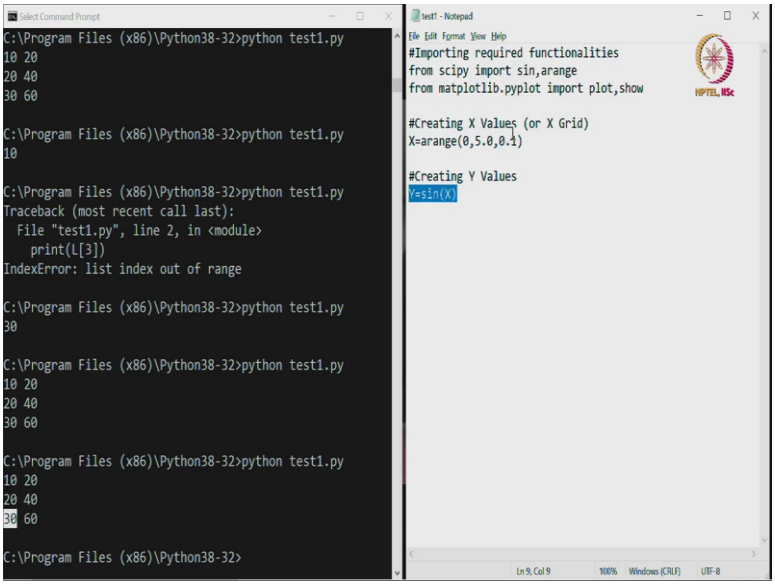
create the list of x values using arange functionality of scipy, that is the first thing we have to do.

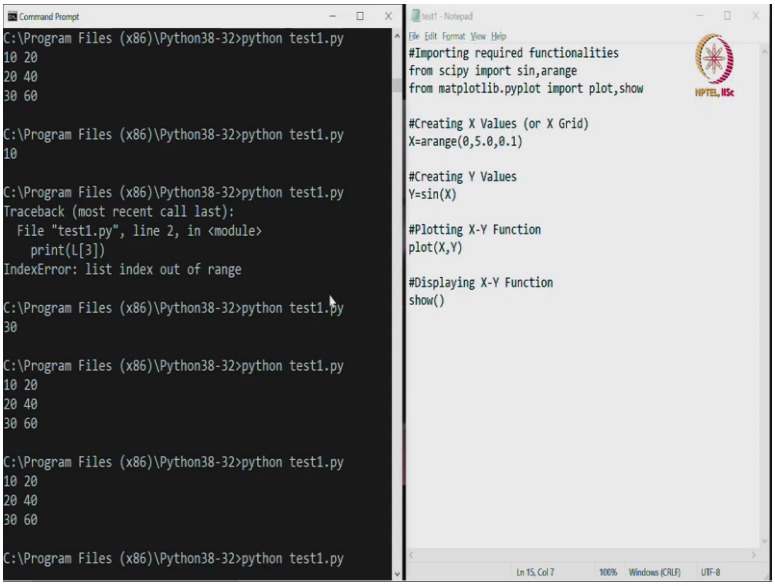
So, we prepared the x axis value first and all the numbers in the x axis value should be given. Then the y function value for each x value will be prepared. Thereafter, we have to plot the function using plot functionality of matplot library pyplot. This is another module which we will be using for plotting purpose matplotlibrary dot pyplot this is the module which we will be using in this module, there is a functionality called there is a functionality called plot functionality and we will be using this plot functionality.

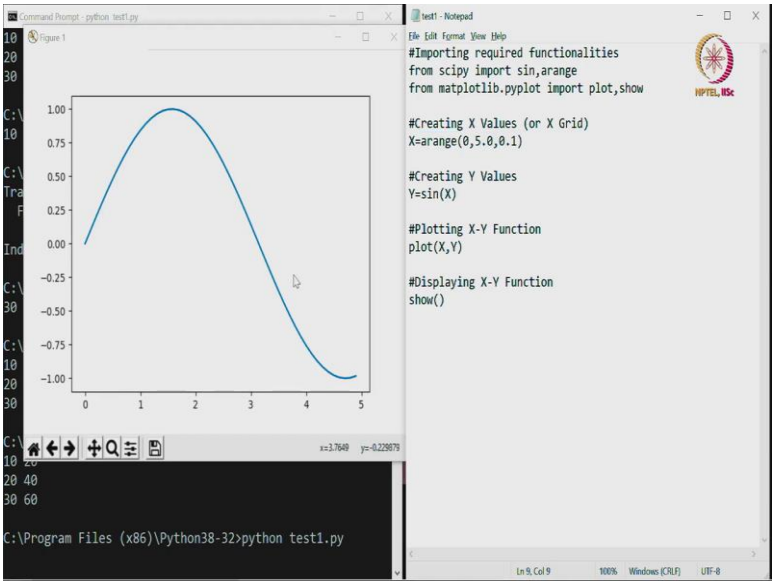
In the same module, we have another functionality to display the plot using show. Without this show functionality, we will not be able to display the graph. So, these are the following steps. These are the steps we have to follow.

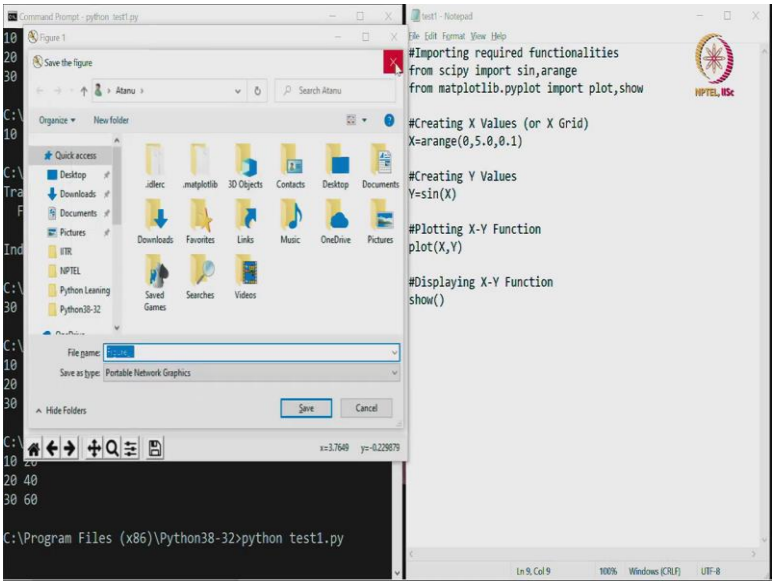
(Refer Slide Time: 03:59)




Select Command Prompt
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
10
C:\Program Files (x86)\Python38-32>python test1.py
Traceback (most recent call last):
File "test1.py", line 2, in <module>
print(L[3])
IndexError: list index out of range
C:\Program Files (x86)\Python38-32>python test1.py
30
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>
test1 - Notepad
File Edit Format View Help
#Importing required functionalities
from scipy import sin,arange
from matplotlib.pyplot import plot,show
#Creating X Values (or X Grid)
X=arange(0,5.0,0.1)
#Creating Y Values
Y=sin(X)
Ln 9, Col 9
100%
Windows (CRLF)
UTF-8


Command Prompt
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
10
C:\Program Files (x86)\Python38-32>python test1.py
Traceback (most recent call last):
File "test1.py", line 2, in <module>
print(L[3])
IndexError: list index out of range
C:\Program Files (x86)\Python38-32>python test1.py
30
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
test1 - Notepad
File Edit Format View Help
#Importing required functionalities
from scipy import sin,arange
from matplotlib.pyplot import plot,show
#Creating X Values (or X Grid)
X=arange(0,5.0,0.1)
#Creating Y Values
Y=sin(X)
#Plotting X-Y Function
plot(X,Y)
#Displaying X-Y Function
show()
Ln 15, Col 7
100%
Windows (CRLF)
UTF-8


Command Prompt - python test1.py
Figure 1
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
1
2
3
4
5
x=3.7649 y=-0.229879
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
test1 - Notepad
File Edit Format View Help
#Importing required functionalities
from scipy import sin,arange
from matplotlib.pyplot import plot,show
#Creating X Values (or X Grid)
X=arange(0,5.0,0.1)
#Creating Y Values
Y=sin(X)
#Plotting X-Y Function
plot(X,Y)
#Displaying X-Y Function
show()
Ln 9, Col 9
100%
Windows (CRLF)
UTF-8



And let us look at the, our task is to plot a sine function over the range 0 to 5. So, let us look at how to do that. We will be first importing the libraries which are required right now, from scipy, import sine function because sine function will be plotting then comma arange these are the two functionalities which will be imported from scipy. Then from matplotlibrary dot pyplot this is another module for plotting graphing, in Python.

Import plot and show. These are the two functionalities which will be imported. So, first thing we are doing is importing required functionalities, we have given this instruction with a hash sign, so it will not be executed when you are running the programme. Now we will be creating X values or X grid in computation in computational language, it is also called grid.

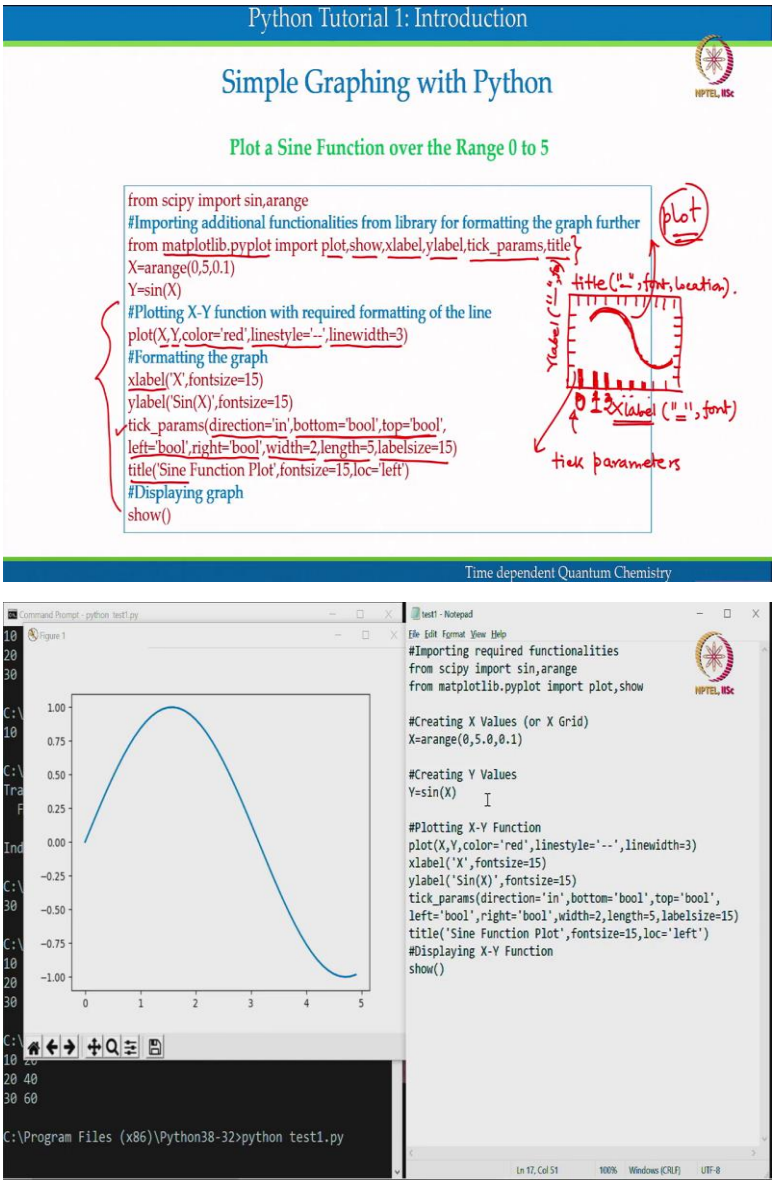
We will discuss this grid later. So, we are creating the X values now, and note how I am writing the instruction for my own benefit for future reading and for anybody who can easily go through the programme. I can give space here to separate each section. So, now I am going to define X value, X equals arange and I am going to prepare a starting from 0 ending up to 5.0 and then step size I am taking considering 0.1. This is the X value, so it will create a list of X values, then I am going to create Y values and this is simply if I write down Y equals sine of X. If I do that, then X is a list.

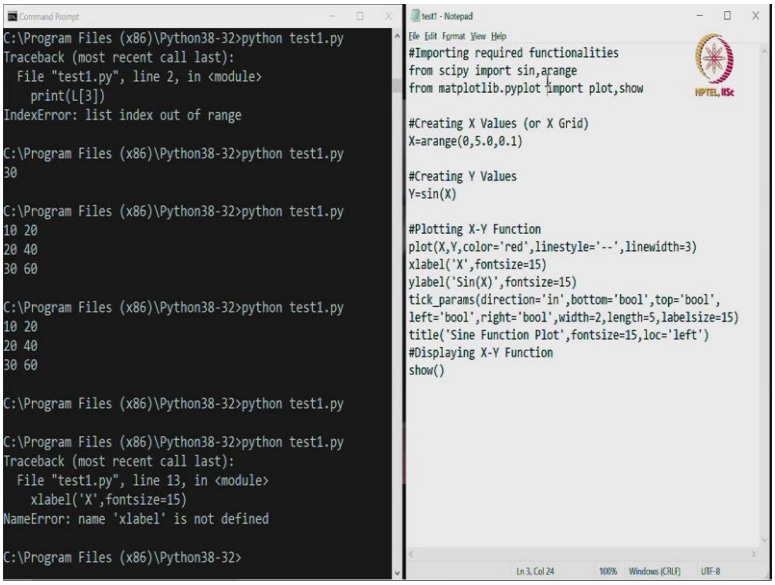
Similarly, Y will be a list of the sine value corresponding to each X value. So, it will automatically do that. For each one I do not need to prepare Y list is prepared directly. So, sine can sine functionality can accept the list as a variable. Then I am plotting X-Y function, note that we are using capital letter you can also use a small letter, but if you are using capital letter use capital always otherwise you will get syntax error and then after plotting, we have to display, displaying X-Y function.

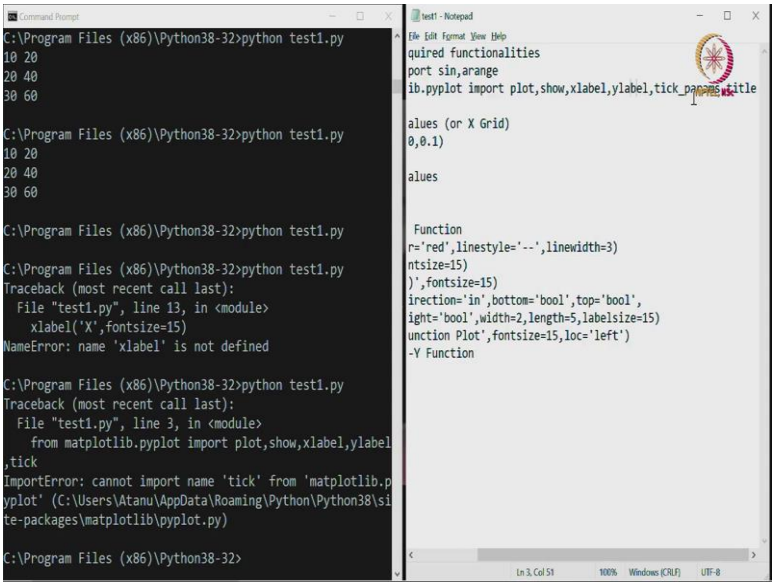
It will show up all the curves I am plotting. So now, I am going to run this programme. If I run the programme, immediately I get back the sine function which is starting from 0 ending not to 5, but the previous point in the list and the previous point is going to be 4.9, 5 here will be excluded as I mentioned that if you use arrange, arange functionality from scipy, it will not take the endpoint in the list.

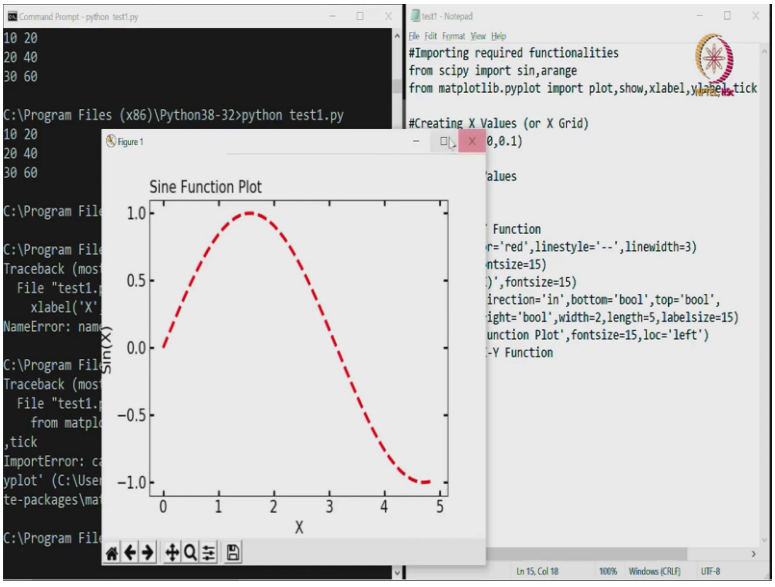
So, I have been able to plot it one can save the plot accordingly. So, this is the technique to plot the sine function. But if we look at the plot, the plot itself requires a lot of editing, editing requires because we would like to place a title in this plot, we would like to place 1 x axis, y axis then we would like to name it and we would like to change the font size there are many editing which is required right now.

(Refer Slide Time: 09:26)




Command Prompt
C:\Program Files (x86)\Python38-32>python test1.py
Traceback (most recent call last):
File "test1.py", line 2, in <module>
print(L[3])
IndexError: list index out of range
C:\Program Files (x86)\Python38-32>python test1.py
30
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
C:\Program Files (x86)\Python38-32>python test1.py
Traceback (most recent call last):
File "test1.py", line 13, in <module>
xlabel('X',fontsize=15)
NameError: name 'xlabel' is not defined
C:\Program Files (x86)\Python38-32>
test1 - Notepad
File Edit Format View Help
#Importing required functionalities
from scipy import sin,arange
from matplotlib.pyplot import plot,show
#Creating X Values (or X Grid)
X=arange(0,5.0,0.1)
#Creating Y Values
Y=sin(X)
#Plotting X-Y Function
plot(X,Y,color='red',linestyle='--',linewidth=3)
xlabel('X',fontsize=15)
ylabel('Sin(X)',fontsize=15)
tick_params(direction='in',bottom='bool',top='bool',
left='bool',right='bool',width=2,length=5,labelsize=15)
title('Sine Function Plot',fontsize=15,loc='left')
#Displaying X-Y Function
show()
Ln 3, Col 24
100%
Windows (CRLF)
UTF-8


Command Prompt
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
C:\Program Files (x86)\Python38-32>python test1.py
Traceback (most recent call last):
File "test1.py", line 13, in <module>
xlabel('X',fontsize=15)
NameError: name 'xlabel' is not defined
C:\Program Files (x86)\Python38-32>python test1.py
Traceback (most recent call last):
File "test1.py", line 3, in <module>
from matplotlib.pyplot import plot,show,xlabel,ylabel
,tick
ImportError: cannot import name 'tick' from 'matplotlib.p
yplot' (C:\Users\Atanu\AppData\Roaming\Python\Python38\si
te-packages\matplotlib\pyplot.py)
C:\Program Files (x86)\Python38-32>
test1 - Notepad
File Edit Format View Help
quired functionalities
port sin,arange
ib.pyplot import plot,show,xlabel,ylabel,tick_params,title
alues (or X Grid)
0,0.1)
alues
Function
r='red',linestyle='--',linewidth=3)
ntsize=15)
)',fontsize=15)
irection='in',bottom='bool',top='bool',
ight='bool',width=2,length=5,labelsize=15)
unction Plot',fontsize=15,loc='left')
-Y Function
Ln 3, Col 51
100%
Windows (CRLF)
UTF-8


Command Prompt - python test1.py
10 20
20 40
30 60
C:\Program Files (x86)\Python38-32>python test1.py
10 20
20 40
30 60
Figure 1
Sine Function Plot
1.0
0.5
0.0
−0.5
−1.0
Sin(X)
0
1
2
3
4
5
X
test1 - Notepad
File Edit Format View Help
#Importing required functionalities
from scipy import sin,arange
from matplotlib.pyplot import plot,show,xlabel,ylabel,tick
#Creating X Values (or X Grid)
0,0.1)
alues
Function
r='red',linestyle='--',linewidth=3)
ntsize=15)
)',fontsize=15)
irection='in',bottom='bool',top='bool',
ight='bool',width=2,length=5,labelsize=15)
unction Plot',fontsize=15,loc='left')
-Y Function
Ln 15, Col 18
100%
Windows (CRLF)
UTF-8

And the editing can be also done and for each editing I have to import the functionality. So, as you can remember that from matplotlibrary.pyplot module sub module, I have previously imported plot and show functionalities now I am going to plot import xlabel, ylabel, tick parameters and title. All this needs to be imported and remaining part is the same is just the formatting part is here.

So, if we look at plotting X-Y function with required formatting of the line, so the line formatting, so if I have one graph and if I have a plot like this, then this is going to be, this is called plot what I am plotting, the curve, and for that, I need x and y value previous do we have given x y value, plot X-Y. This time, we are going to specify the colour of the plot, line style of the plot, there are many line styles which can be used for this.

And line width also, I am going to define, what is the width of this line, that also I am going to define. So, this is called plot and different formattings are given here. One can change these numbers, line style and colour of the plot. Now, going back to the formatting the graph xlabel what I am writing here this is called xlabel and in the xlabel, within quote, I will write down the string which will be written here and associated font size that is the way xlabel will be defined. ylabel will be defined like this way here ylabel.

Similarly, I have a text specifying the ylabel and font. These are the xlabel and ylabel. Tick parameters, tick parameters, what are them? There are ticks which will be used here to show the and this can be some value let us say 0, then this is probably 1, this will be 2 like this way, this is just an example and in the tick parameters, so these are tick parameters.

In the tick parameters, what we have written direction equals in, it means these lines, tick lines will be inside the graph, if it is out, then it would be like this. This is going to be out direction and what we have shown here is in direction. Then this whole part, left, right, all these are shown to show the tick in every direction, bottom, top, side, every direction. Then the width, width is how wide each tick lines should be, that is the width. Length, how long is going to be each tick, that is the length and label size, this size of the label.

So, it would be bigger if we increase the label size. Then title, title comes here and within title again I have quoted string which will be written and font size and location where it is so these are the formats we are going to use. Let us look at the laptop and change the formatting. So, I have x and Y values then first we will be formatting the plot, plot will be formatted by different colour, colour equals red then line style equals line width equals 3.

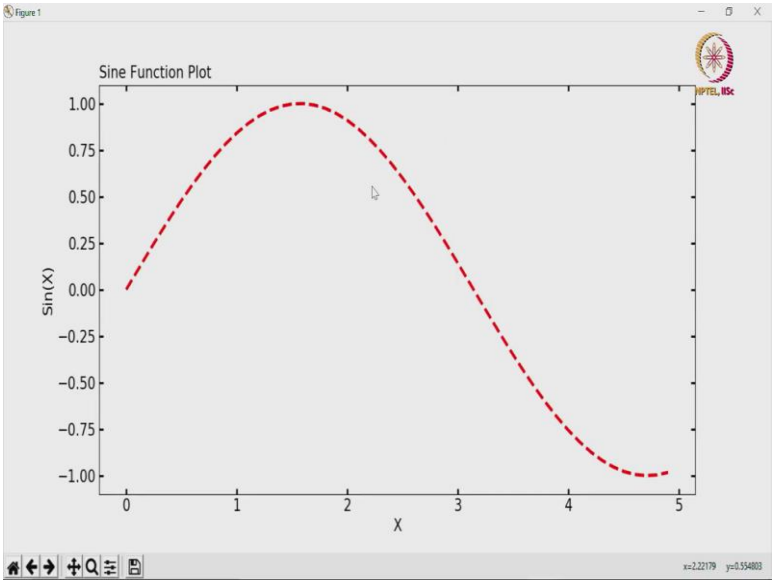
So, these are the formatting for the plot then we have some other formatting xlabel. In the xlabel we have we have to write X that is a string which will show up and font size equals 15. One can change it according to the convenience similarly, we will use ylabel as sine X font size 15 and then tick parameter, tick param, tick parameters direction equals in bottom equals Boolean.

Top left and right with length equals so, I have selected these numbers because I know this is convenient for me but this the same numbers may not be convenient for others you can change these numbers and then finally title, title again one string, with the font size 15 and location left. So, now I rerun the programme and I have an error because. Why I am getting error?

Because all these functionalities which I have used ylabel, xlabel, tick parameters then title none of this has been imported from matplotlibrary dot pyplot sub module so, we have to import it xlabel, ylabel, tick params, title. So, we have now imported tick param, params, title, tick params, ylabel, xlabel.

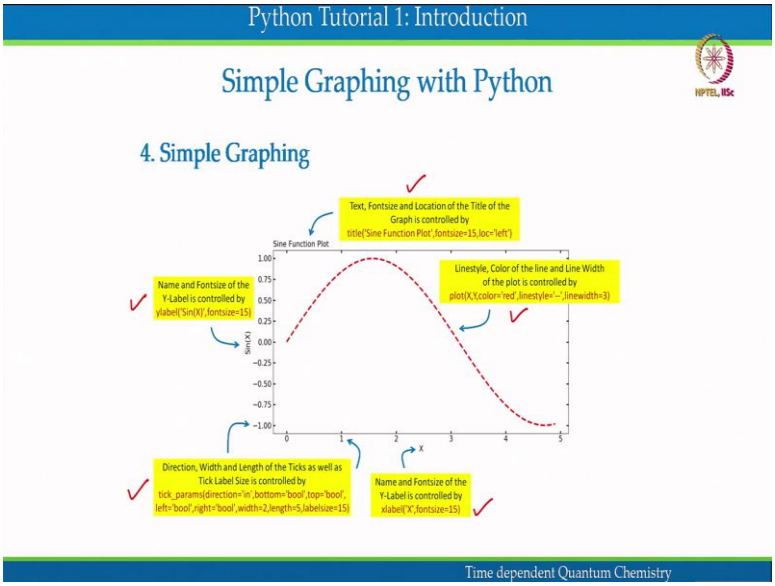
So, now we have everything as you can see the title location has been selected to be left for the title and it is showing up on the left hand side you can keep it in the centre as well on the right hand side but title will be placed here then tick parameters as you can see, the parameters are conveniently selected, size of the these values 0, 1, 2 are conveniently selected, they are in inward direction then xlabel, ylabel has been selected.

(Refer Slide Time: 20:16)



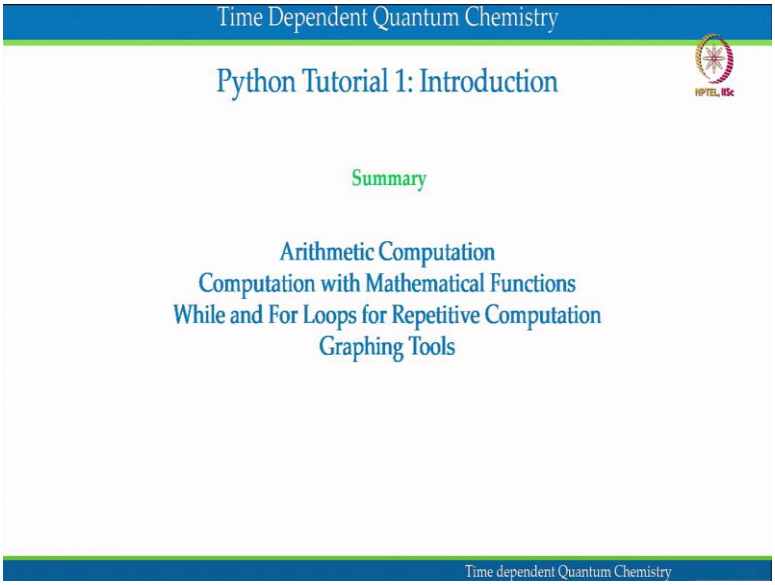
And this this is a plot which can be used for publication. So, these are the parameters which we use all the time.

(Refer Slide Time: 20:31)



In this, this is a summary of what we have just mentioned. So, far the plot style has been controlled by these parameters, then xlabel has been controlled by these parameters, then tick parameters has been controlled by this and the ylabel has been controlled by this, title has been controlled by this. So, give some time take a look at it, there are so many information given to them in the entire tutorial.

(Refer Slide Time: 21:07)



And my suggestion is that take your time go through each functionality which has been introduced today, in this module and try to solve some simple equation for an example, you can convert eV or Atomic Unit to eV using the programme or you can plot a Gaussian function with the help of this matplotlibrary that can be easily done.

We have come to the end of this session in this session. In this Python tutorial session, what we have learned? We have learned how to install Python? Then how to run a Python programme? And we have gone over simple computation, arithmetic computation, then using mathematical expression.

And finally, we have gone over how one technique we have learned how to plot the graph. There are many techniques which can be used in Python, but we have used one technique right now, and which can be commonly used in plotting one graph. We will end this session and we will meet again.