

XMGRACE Tutorial: ASESMA 2010

This tutorial covers basic 2 dimensional plotting techniques using XMGRACE. XMGRACE requires an INPUT text file, which can contain any number of columns.

Go to the directory asesma/xmgrace (to be created)

The directory contains XMGRACE-tutorial.pdf and five example files: example00.dat, example01.dat, example1.dat, example2.dat and example3.dat

1 TUTORIAL 1:

Two-column data file - Single plot

Open XMGRACE by typing xmgrace on the terminal

- READ the input file example00.dat
Data/Import/ASCII/example00.dat
- PLOT:
Choose the 1st and 2nd columns of example00.dat
- LABELS:
Label both x and y axis
- LEGENDS:
Incorporate legend in the plot
- LINES and SYMBOLS:
Change the line style and symbol type
- SIZE:
Change the size of the plot
- Exercise 1
 1. Plot the input file of *example1.dat* using column 1 and 2
 2. Label the x-axis as **Distance(Å)** and Y-axis as **Distribution**
 3. Put a legened *test-legend* on the graph
 4. Change the symbol for the data to filled square

2 TUTORIAL 2:

Three-column data file - Single plot

Open XMGRACE by typing `xmgrace` on the terminal

- READ the input file `example00.dat`
Data/Import/ASCII/example00.dat
- PLOT:
Choose the 1st and 2nd columns of `example1.dat`
Choose the 1st and 3rd columns of `example1.dat`
- LABELS:
Label both x and y axes
- LEGENDS:
Incorporate legends in the plot
- LINES and SYMBOLS:
Change the line styles and symbol types
- SIZE:
Change the size of the plot
- Exercise 2
 1. Plot the input file of *example1.dat* using column 1 and 2, and using column 1 and 3 on the same graph
 2. Label the x-axis as **Distance(Å)** and Y-axis as **Distribution**
 3. Put a legened *test-legend1* for the first data set and *test-legend2* for the second data set
 4. Make the symbol for the first data set to be filled circle and for the second data set to be open circle
 5. Make the line for the first data set to be straight with size 3 and for the second data set to be broken line with size 5

3 TUTORIAL 3:

Two-column data file with error bar - Single plot

Open XMGRACE by typing `xmgrace` on the terminal

- READ the input file example1.dat
Data/Import/ASCII/example01.dat
- PLOT:
Choose the 1st and 2nd columns of example01.dat
USE set type XYDY
- LABELS:
Label both x and y axes
- LEGENDS:
Incorporate legends in the plot
- LINES and SYMBOLS:
Change the line style and symbol type
- SIZE:
Change the size of the plot
Change the size of the error bar
- **Exercise 3**
 1. Plot the input file of *example2.dat* using column 1, 2 and 3 using **single set** option and **load** as **XYDY** set type, where the 3rd column is an error bar
 2. Label the x-axis as **Distance(Å)** and Y-axis as **Distribution**
 3. Put a legened *test-legend1*
 4. Change the color and size of the error bar

4 TUTORIAL 4:

Two-column data file - Multiple plot

Open XMGRACE by typing xmgrace on the terminal

- READ the input file example1.dat
Data/Import/ASCII/example00.dat
- MULTIPLY:
Create two graphs in one plot
Choose the 1st and 2nd columns of example00.dat and plot it on graph1
Choose the 1st and 3rd columns of example00.dat and plot it on graph2

- LABELS:
Label both x and y axes
- LEGENDS:
Incorporate legends in the plot
- LINES and SYMBOLS:
Change the line styles and symbol types
- SIZE:
Change the size of the plot
- Exercise 4
 1. Create two graphs from the input file of *example1.dat* using column 1 and 2 for the first graph and using column 1 and 3 for the second graph
 2. For the first graph, label the x-axis as **Distance(Å)** and Y-axis as **Distribution**
 3. For the second graph, label the x-axis as **Distance(Å)** and Y-axis as **Distribution²**
 4. Put a legened *test-legend1* on graph1 and *test-legend2* on graph2

5 TUTORIAL 5:

Two-column data file: Interpolation and Fitting

Open XMGRACE by typing xmgrace on the terminal

- READ the input file example00.dat
Data/Import/ASCII/example00.dat
- MULTILOT:
Choose the 1st and 2nd columns of example00.dat
- LABELS:
Label both x and y axes
- LEGENDS:
Incorporate legends in the plot
- LINES and SYMBOLS:
Change the line styles and symbol types

- SIZE:
Change the size of the plot
- INTERPOLATE:
Interpolate the data
- FITTING:
Fit the data with expression.

- **Exercise 5**

1. Plot the input file of *example1.dat* using column 1, 2
2. Label the x-axis as **Distance(Å)** and Y-axis as **Distribution**
3. Put a legened *test-legend1*
4. Fit the data and obtain an expression for the curve
5. Repeat all of the above for the data in column 1 and 3 of *example1.dat*
6. Compare the fitting expression in the two cases

6 TUTORIAL 6:

Two-column data file: Miscellaneous – Greek letters, logariitmic plot and Drawing objects

Open XMGRACE by typing xmgrace on the terminal

- READ the input file example00.dat
Data/Import/ASCII/example00.dat
- MULTILOT:
Choose the 1st and 2nd columns of example00.dat
- LABELS:
Label both x and y axes
- LEGENDS:
Incorporate legends in the plot
- LINES and SYMBOLS:
Change the line styles and symbol types
- SIZE:
Change the size of the plot

- ADDING TEXT and LINES:
Add text and lines on the graph

- **Exercise 6**

1. **Practice on input file example1.dat: add text, line and objects.**