

A decorative graphic on the left side of the slide consists of a network of light blue lines and small circles, resembling a circuit board or a molecular structure. The lines are of varying thickness and connect to small open circles at various points, creating a complex, branching pattern that extends from the top to the bottom of the frame.

COMPUTATIONAL CHEMISTRY

SPRING 2022

Let's go to the course directory

```
> cd /afs/cad/courses/chem/s23/chem/737/102/UCID
```

Gnuplot the graphical interface for plotting graphs

```
>: gnuplot
```

You are inside the interface

```
> plot sin(x) with lines
```

```
> plot sin(x) with points
```

```
> p sin(x) w l
```

You can use abbreviations

```
> p sin(x) w p
```

```
> p sin(x) w lp
```

lp means line-points

```
> p sin(x) w p pt 1 ps 1
```

Default, pt pointtype, ps pointsize

```
> p sin(x) w p pt 2 ps 2
```

Try different numbers to see how many types there are.

```
> p sin(x) w l lw 2 lc 3, cos(x) w l lw 2 lc 5
```

Two graphs together

```
> q
```

quit

The important usage of gnuplot though is to make us able to plot the data that we obtain from our own calculations.

```
>: ls
```

```
>: vi test.dat
```

commenting out
the line

# X	Y1	Y2	Y3
-1.0000	0.0000	0.0000	1.0000
-0.9000	0.5700	1.1769	0.7150
-0.8000	1.0800	1.4400	0.4600
-0.7000	1.5300	1.4997	0.2350
-0.6000	1.9200	1.4400	0.0400
-0.5000	2.2500	1.2990	-0.1250
-0.4000	2.5200	1.0998	-0.2600
-0.3000	2.7300	0.8585	-0.3650
-0.2000	2.8800	0.5879	-0.4400
-0.1000	2.9700	0.2985	-0.4850
0.0000	3.0000	-0.0000	-0.5000
0.1000	2.9700	-0.2985	-0.4850
0.2000	2.8800	-0.5879	-0.4400
0.3000	2.7300	-0.8585	-0.3650
0.4000	2.5200	-1.0998	-0.2600
0.5000	2.2500	-1.2990	-0.1250
0.6000	1.9200	-1.4400	0.0400
0.7000	1.5300	-1.4997	0.2350
0.8000	1.0800	-1.4400	0.4600
0.9000	0.5700	-1.1769	0.7150
1.0000	0.0000	-0.0000	1.0000

```
>: gnuplot
```

```
> p "test.dat" u 1:2 w l
```

using

```
> p "test.dat" u 1:2 w l, "test.dat" u 1:3 w l, "test.dat" u 1:4 w l
```

Other important aspect is that we want to have high-quality figures to present in our papers/posters.

```
# The set encoding command selects a character encoding, iso_8859_1 tells gnuplot to use the most common Western European font used by many Unix workstations and by MS-Windows.
```

```
set encoding iso_8859_1
```

```
# Set the labels, their font and font size for the x and y axis.
```

```
set ylabel "{/Helvetica=28 Y axis}"
```

```
set xlabel "{/Helvetica=28 X axis}"
```

```
# Set the font for the key.
```

```
set term postscript eps colour enhanced 'Helvetica' 20
```

```
# Set the name and type of output file
```

```
set output "test.eps"
```

```
# Set the ranges for x and y axis.
```

```
#set xr [3:10]
```

```
#set yr [0:20]
```

```
# Set the separation between tics on x and y axis.
```

```
#set ytics 0.01
```

```
#set xtics 10
```

```
# Plot graphs
```

```
p 'test.dat' u 1:2 w l lt 1 lw 2 lc rgb "#ff0000" title "Y1",\
```

```
'test.dat' u 1:3 w l lt 1 lw 2 lc rgb "#00ffff" title "Y2",\
```

```
'test.dat' u 1:4 w l lt 1 lw 2 lc rgb "#8b008b" title "Y3"
```

```
quit
```

> scp |

HOMEWORK

- Please follow the whole slides and upload a file to the canvas containing:

1. The plot created from test.dat file using the plot.in script.
2. Snapshot of a gnuplot script to create a plot of a Gaussian function with x-axis range from -3 to +3 and y-axis range from 0 to 1.2.

Hint: $f(x) = Ae^{-\frac{(x-b)^2}{2a^2}} \Rightarrow f(x) \approx e^{-x^2}$

3. The plot of three Gaussian functions with incremental width and different colors using the script in point 2.

Connecting to the lab machines outside of class:

- Connect to VPN.
- Open your terminal
- Type the following

```
>: ssh -XY <UCID>@oslN.njit.edu
```

- Here, N=1-30
- Answer Yes to the prompt question and enter your email password
- Type the following

```
>: pwd
```

Display the path of current directory

- Let's go to the directory of our course by typing

```
>: cd /afs/cad/courses/chem/s23/chem/737/102/<UCID>
```

- You are going to save all your data in this directory