Plotting with GNUPLOT

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# To plot
plot "data.dat"

# To remove default key
unset key

# To re-plot with the changes made:
gnuplot> replot

# To give a title(t) to plot, you use the option "title"
# Ensure that you have the "key" set so that title can show
gnuplot> plot "potential.dat" title "Potential energy vrs time"

# Changing the line types
# 'linetype(lt)' changes type of line
# 'linecolor(lc)' changes color of line
gnuplot> plot "potential.dat" title "Potential energy vrs time" linetype 7 linecolor 0

# 'test' gives

# Connect the datapoints with lines or linespoints
plot "potential.dat" title "Potential energy vrs time" linetype 7 linecolor 0 with linespoints

# You can use shorter version of plot-related keywords
# 'linetype = lt ' changes type of line
# 'linecolor = lc' changes color of line
# 'linepoints = lp' connects datapoints with line
gnuplot> plot "potential.dat" title "Potential energy vrs time" lt 7 lc 0 w lp

# You can also connect datapoints with just lines
gnuplot> plot "potential.dat" title "Potential energy vrs time" lt 7 lc 0 w lines

#You can plot multiple curves on the same plot.
#You simply choose a new data file and add other properties or parameters to it.
gnuplot> plot "potential.dat" title "Berendsen vrs time" lt 7 lc 0 w lp, "potential_noose.dat" title
"Noose-H Pot" lt 8 lc 12 w lines


# Specifying columns to plot:
gnuplot> plot "potential.dat" using 1:2 title "Potential energy vrs time" lt 7 lc 0 w lines

# Specifying columns to plot for multiple plots:
gnuplot> plot "potential_berend_noose.dat" using 1:2 title "Berendsen vrs time" lt 7 lc 0 w
lines, ''  using 1:3 title "Noose" lt 8 lc 12 w lp
```

#You can also plot functions

You can set the range of the X-axis
gnuplot> set xrange [lowerbound:uppoerbound]
gnuplot> set xrange [0:75]

Axes Labelling
gnuplot> set xlabel "Time(ps)"
gnuplot> set ylabel "Pot Energy(kJ/mol)"

Saving chart
Set output file type
gnuplot> set terminal png size 800,600
Name file output
gnuplot> set output "outputFileName.png"