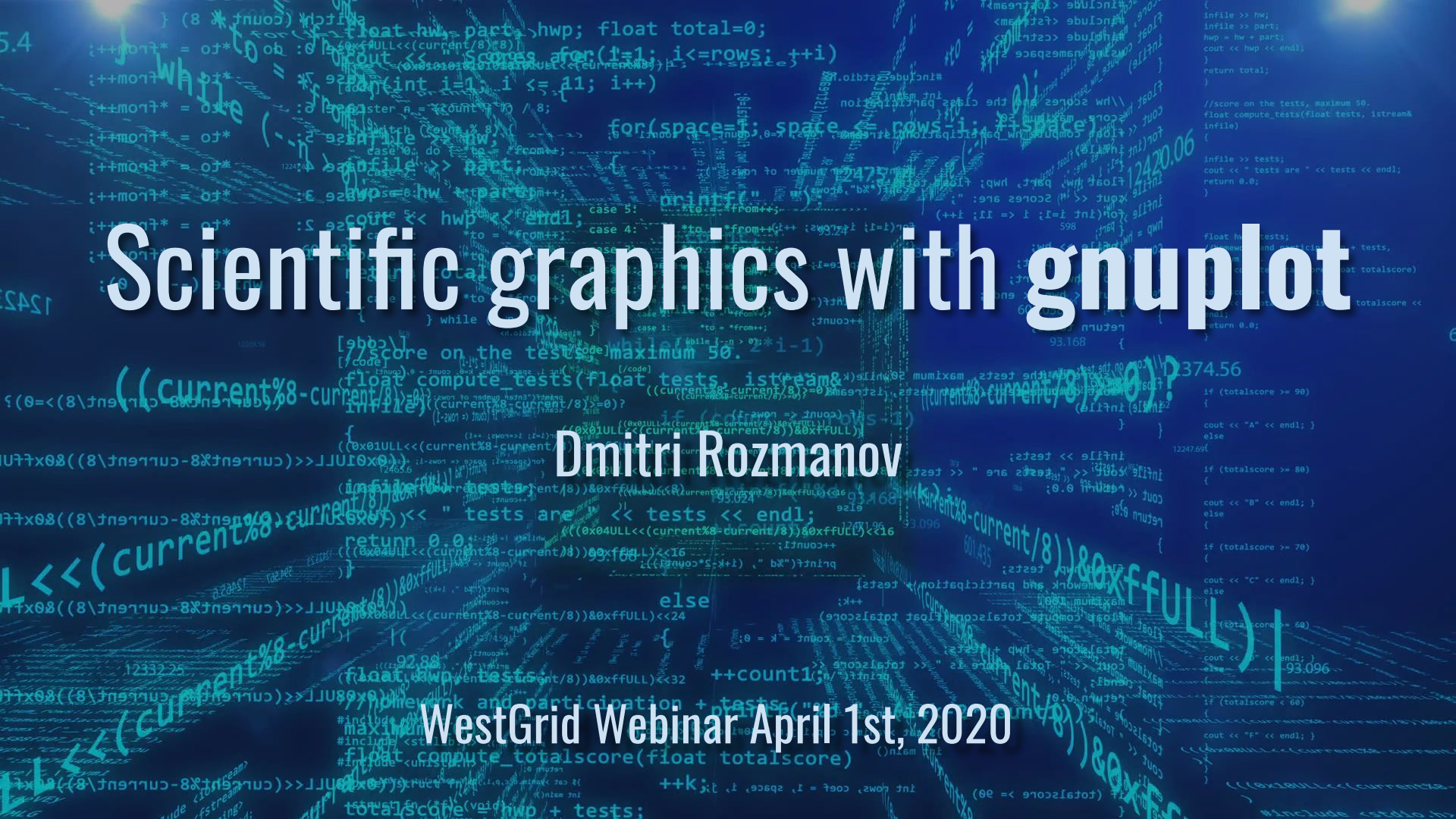

Scientific graphics with gnuplot

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Motivation

- **gnuplot** is a very **powerful graphing tool** and a function plotter.
- **gnuplot** follows the UNIX idea of doing **one thing very well**.
- **gnuplot** is **less known now** due to adoption of other options.
- I want to share my **positive experience** with **gnuplot**.
- **gnuplot** is still **relevant** and sometimes is a better option.
- It feels necessary to increase **awareness** about **gnuplot**.

Today we will

- Learn about **gnuplot**. Learn what it is and what it can do.
- See some **examples** of gnuplot graphics.
- Practice **function plotting** in 2D using various coordinates and modes.
- **Plot data**.
- **Fit models** to the data.
- Produce a **figure** suitable for scientific discussion.
- Learn gnuplot **interface** and **commands** by doing all of the above.
- Make **conclusions**.

gnuplot facts:

- It is a **portable command-line driven** graphing utility for Linux, OS/2, MS Windows, OSX, VMS, and many other platforms.
- It was **originally created** to allow scientists and students to visualize mathematical functions and data interactively,
- Despite **gnuplot**'s name, it is not named after, part of or related to the GNU Project, nor does it use the GNU General Public License.
- **GNUplot** name is **incorrect**. The real name of the program is "**gnuplot**".
- The Gnuplot history dates back to **1986**.
- Current stable version of **gnuplot** is **5.2** released in Aug. 2017.
- Current development version of **gnuplot** is **5.5**.

What does **gnuplot** offer?

- **2D data plots** in many styles.
- **Polar** and **log-scaled** axes, general nonlinear **axis mapping**, **parametric** coordinates.
- **Representations** such as heat maps, beeswarm plots, violin plots, histograms, ...
- **3D plots** of data points, lines, and surfaces in different styles (contour plot, mesh)
- **Algebraic computation** using integer, floating point, or complex arithmetic.
- **Model fitting** using Marquardt-Levenberg minimization.
- Available for **many OSs**, supports many file formats and output devices.
- On-line **help**, extensive **documentation**, and printed **books**.
- TEX-like **text formatting** for labels, titles, axes, data points.
- Interactive **command line** editing and history.

Scripting with **gnuplot**:

- Gnuplot can **read in files** containing additional commands in interactive mode.
- Gnuplot can be run in **batch mode** by piping a pre-existing file or a stream of commands to stdin.
- Gnuplot is used as a **back-end** graphics driver by higher-level mathematical packages such as Octave.
- Gnuplot can be wrapped in a **cgi script** for use as a web-driven plot generator.
- Gnuplot supports context- or data-driven **flow control** and iteration using familiar statements ***if else continue break while for***.

Getting **gnuplot**:

- The **gnuplot** website: http://www.gnuplot.info/
- It is hosted on **SourceForge**: https://sourceforge.net/projects/gnuplot/
- **GitHub** mirror is unofficial: https://github.com/gnuplot/gnuplot
- In **Linux**:

```
$ apt install gnuplot
$ yum install gnuplot
```

- Unofficial binaries for **Windows** and **MacOS**: http://www.gnuplot.info/download.html#OSX

gnuplot examples 1

nents of the molecular frame diffusion (Fig. 7). The switching of preferences for translations and rotations occurs in the same temperature range, and indicates a change in the mechanism of diffusion (as measured in the molecular frame). It is known that the melting temperature of the model is about

temperature (over the range studied) than the rotational diffusion coefficient $D^{\theta,\mathrm{WF}}$ (see Figs. 3 and 5). At the same time, it is known that according to the hydrodynamic views of the Stokes-Einstein (SE) and Stokes-Einstein-Debye (SED) relations[34] both of these diffusion coefficients are inversely

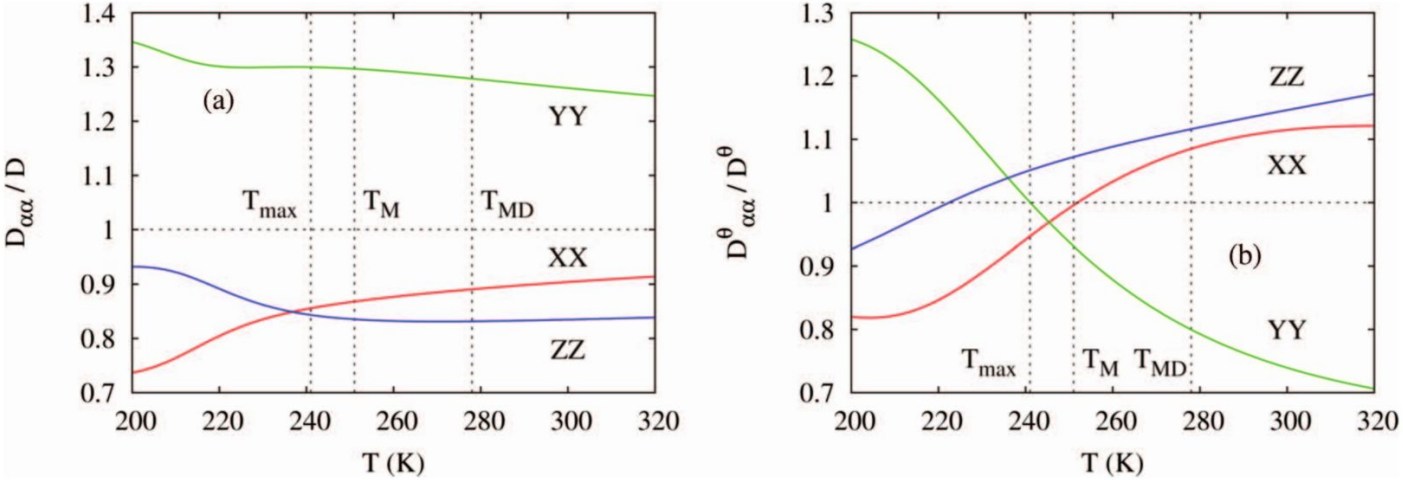


FIG. 7. Temperature dependence of of the XX, YY, and ZZ diagonal elements of the reference molecular frame diffusion of the TIP4P-2005 water model relative to their isotropic averages: (a) translational diffusion, $D^{\mathrm{MF}}_{\alpha\alpha}/D^{\mathrm{MF}}$, (b) rotational diffusion, $D^{\theta,\mathrm{MF}}_{\alpha\alpha}/D^{\theta,\mathrm{MF}}$. The corresponding fit functions were used to generate these ratios. The horizontal dashed line shows the reference value of unity, the vertical dashed lines indicate the temperature of maximum ice growth, T_{max}, the melting temperature, T_M, for this model from Ref. 24, and the temperature of maximum density, T_{MD}, from Ref. 46.

gnuplot examples 2

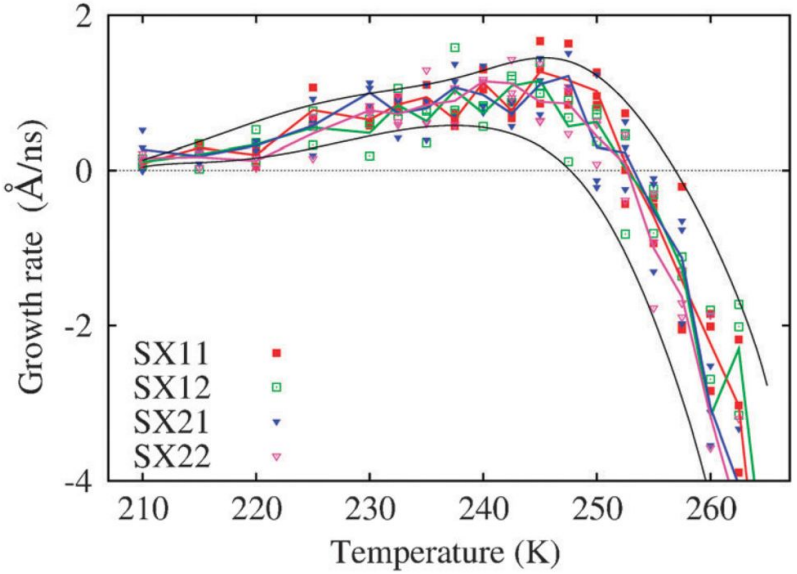


Fig. 4 Ice growth rates in the "small" system as a function of temperature. The combined set SX11, shown with filled squares, includes rates from independent sets with the same dynamical parameters (see the text and Table 1 for details): S111, S211, S311. The combined set SX12 (empty squares) includes combined data from S112, S212, and S312, the set SX21 (filled triangles) is composed of

performed to explore the p
thermostat relaxation time fr
Three temperature sets of
repeated in the "small" syste
tions of tested dynamical para
rate data of the correspondin
into the SX11, SX12, SX21,
these combined sets are show
rate variation between sets i
rate variation within one set.
all four combinations of th
apparently indistinguishable v

3.2 Ice growth rates

The temperature dependencies
systems, "small", "medium",

gnuplot examples 3

To obtain information on local structure in the system one needs to perform similar analyses on small subsets $D(z_a,z_b)$ of the total density profile, where a and b define a window over the total range of $\{z_i\}$ values. The shortest range of the density profile that can be used to distinguish ice from water in this interface detection in this work.

This detection method has been extensively tested and was found to be robust for different orientations of cubic and hexagonal ice lattices. It is expected to work well with any other lattice provided that the layering in the crystal along the

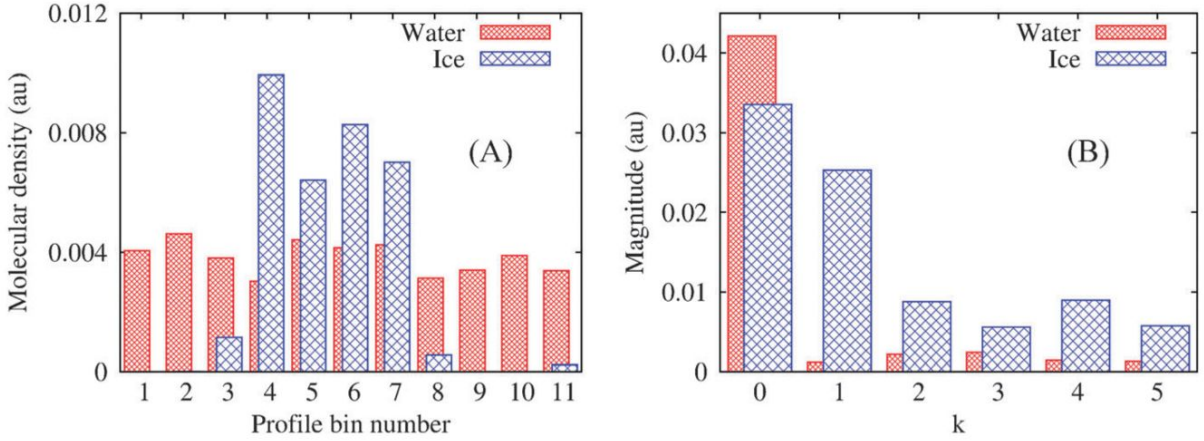
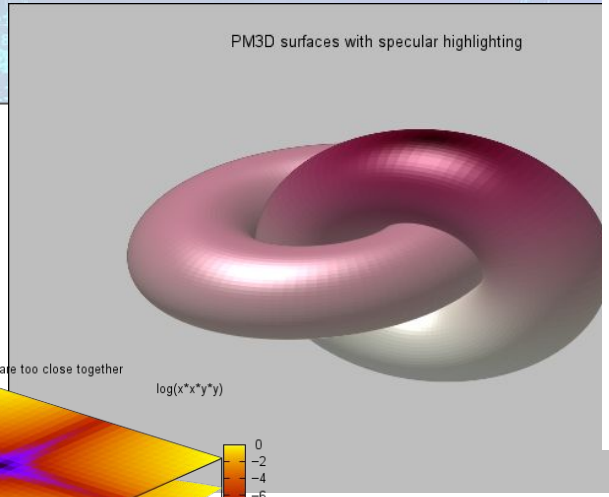
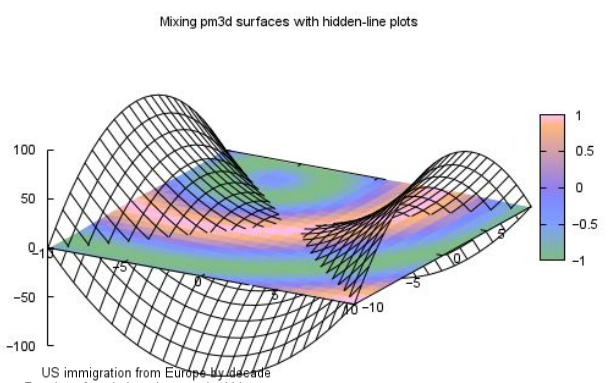
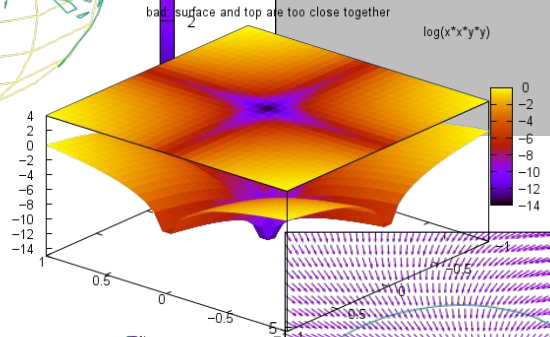


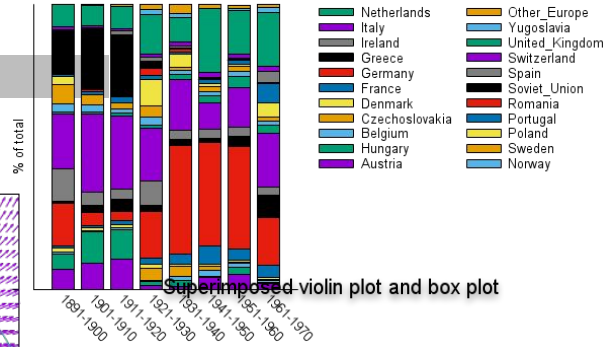
Fig. 9 Subsets of the density profile composed of 11 bins (A) from the ice phase (coarse crosshatching) and from the liquid water phase (fine crosshatching). The corresponding Fourier spectra for ice (coarse) and water (fine) are shown in (B). The ice and water subsets are respectively centered at 0.10 and 0.26 fractional Z-positions of the density profile shown in Fig. 8(A). Here k is the wave vector index.

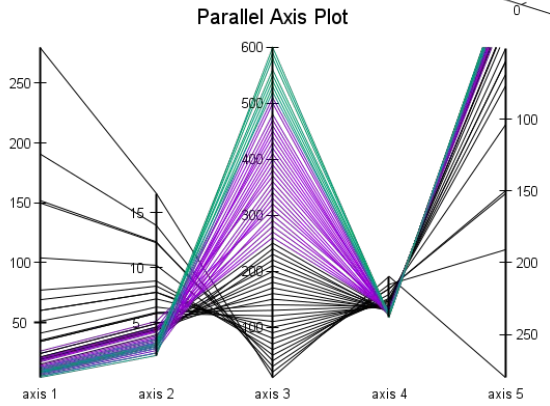
gnuplot examples 4

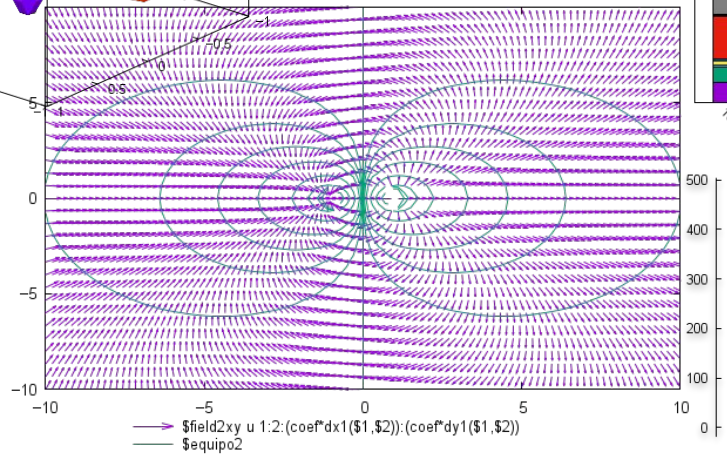


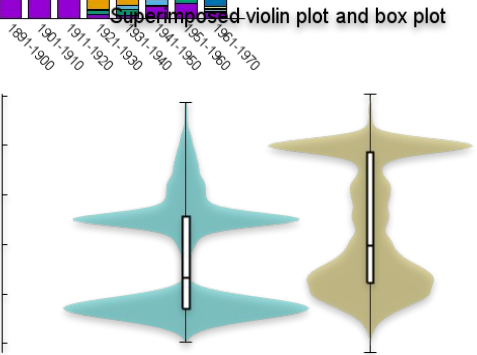




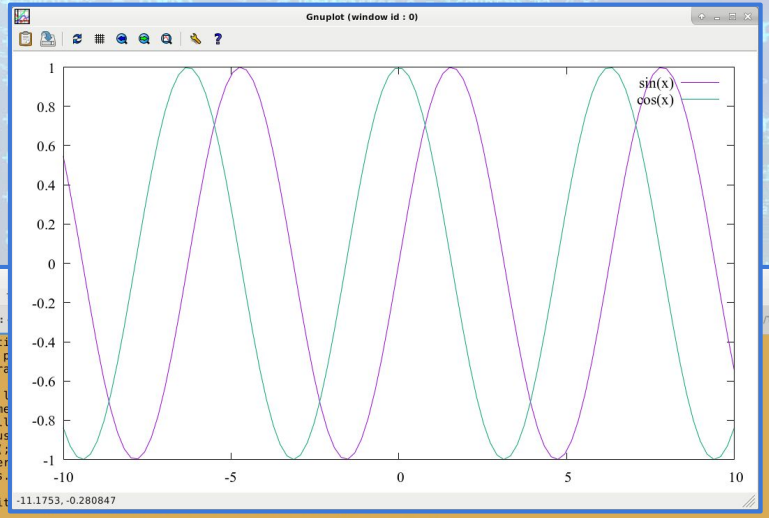




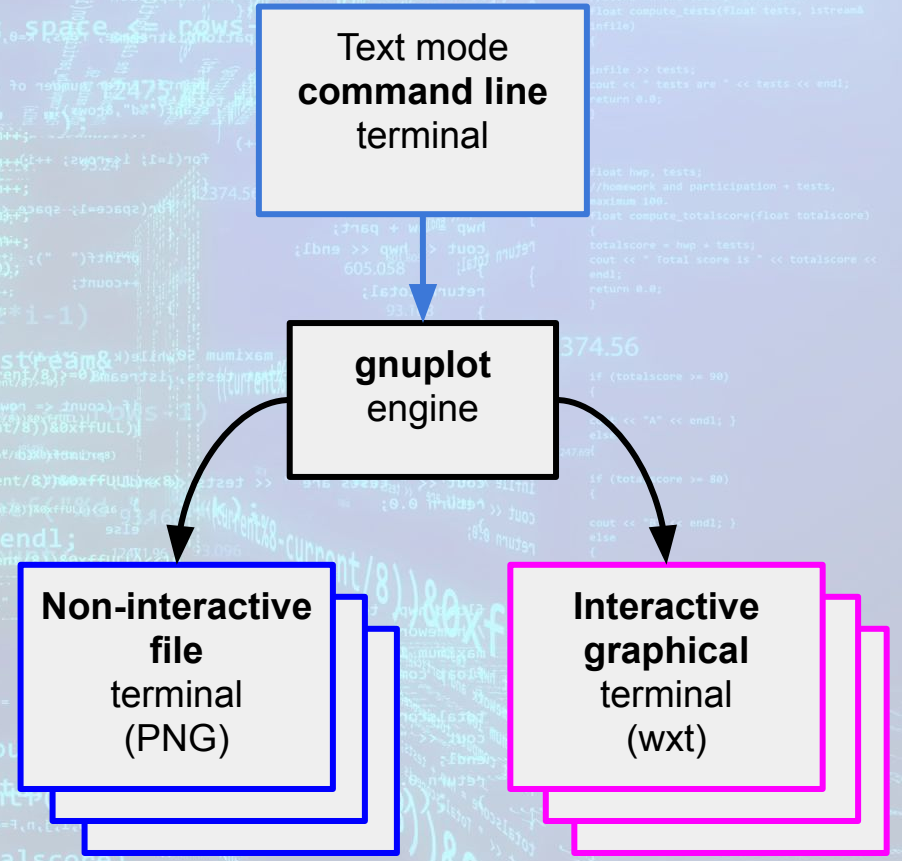




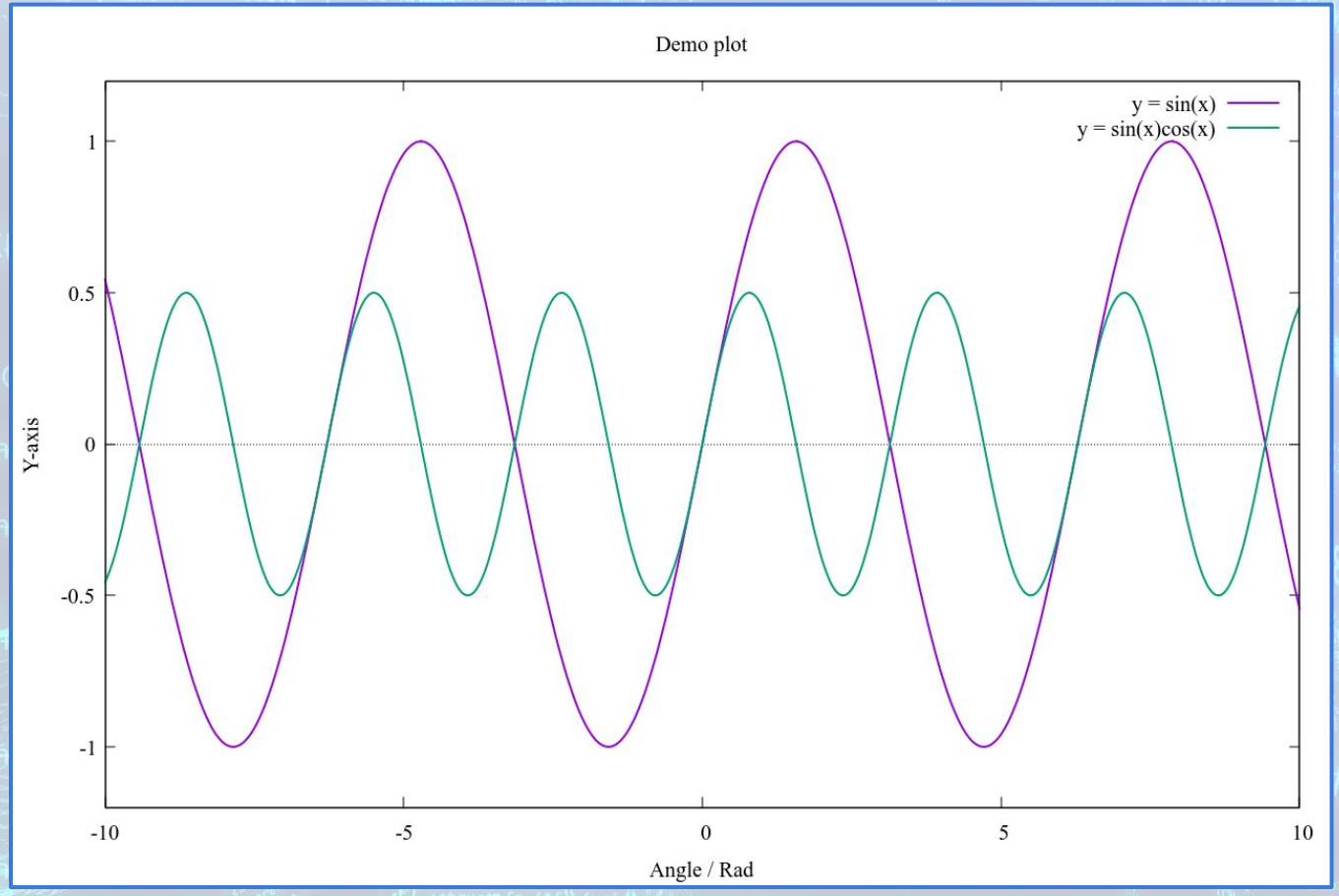
gnuplot. How does it work?




```
File  Edit  View
dima@goblin:
Recent additi
on multiple p
can be genera

The command l
function name
capitals. All
not ambiguous
semicolons (;
although ther
more details.

      set tit

  Commands may extend over several input lines by ending each line but the last
  with a backslash (\).  The backslash must be the _last_ character on each
  line.  The effect is as if the backslash and newline were not there.  That
  is, no white space is implied, nor is a comment terminated.  Therefore,
  commenting out a continued line comments out the entire command
  (see `comments`).  But note that if an error occurs somewhere on a multi-line
  command, the parser may not be able to locate precisely where the error is
  and in that case will not necessarily point to the correct line.

Help topic:
gnuplot> ^D
dima@goblin:~/ownCloud/Teaching/2020-WG-gnuplot$ gnuplot

        G N U P L O T
        Version 5.0 patchlevel 5    last modified 2016-10-02

        Copyright (C) 1986-1993, 1998, 2004, 2007-2016
        Thomas Williams, Colin Kelley and many others

        gnuplot home:     http://www.gnuplot.info
        faq, bugs, etc:   type "help FAQ"
        immediate help:   type "help"  (plot window: hit 'h')

Terminal type set to 'wxt'
gnuplot> plot sin(x), cos(x)
gnuplot> replot
gnuplot>
```



Plotting functions: y = y(x)



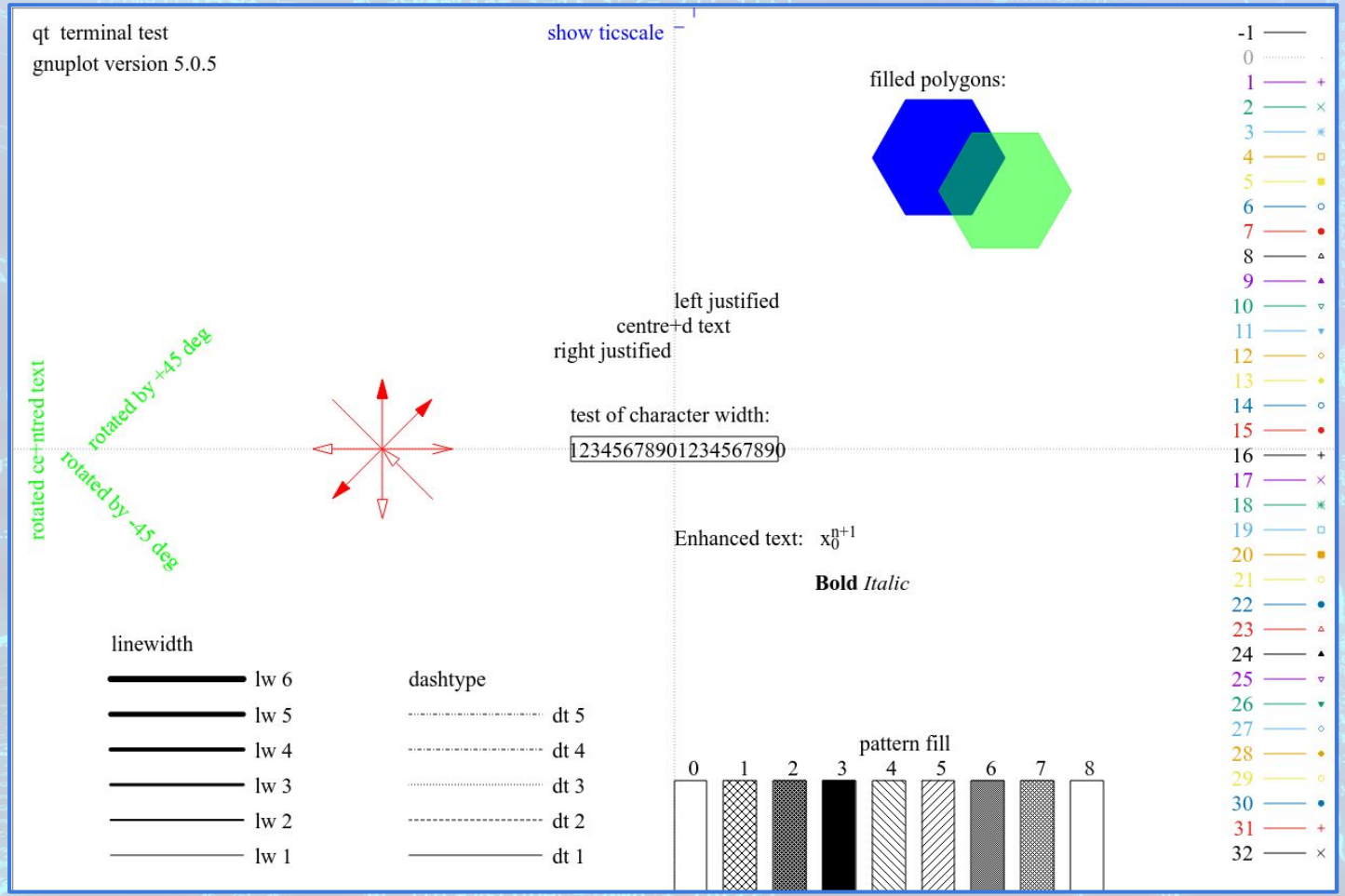
Commands

- plot / replot
- set xrange / yrange
- set title
- set xlabel / ylabel
- set xzeroaxis
- plot … with lines

- … linewidth / lw

- help plot
- help with
- help linewidth

Gnuplot terminals



Terminals:

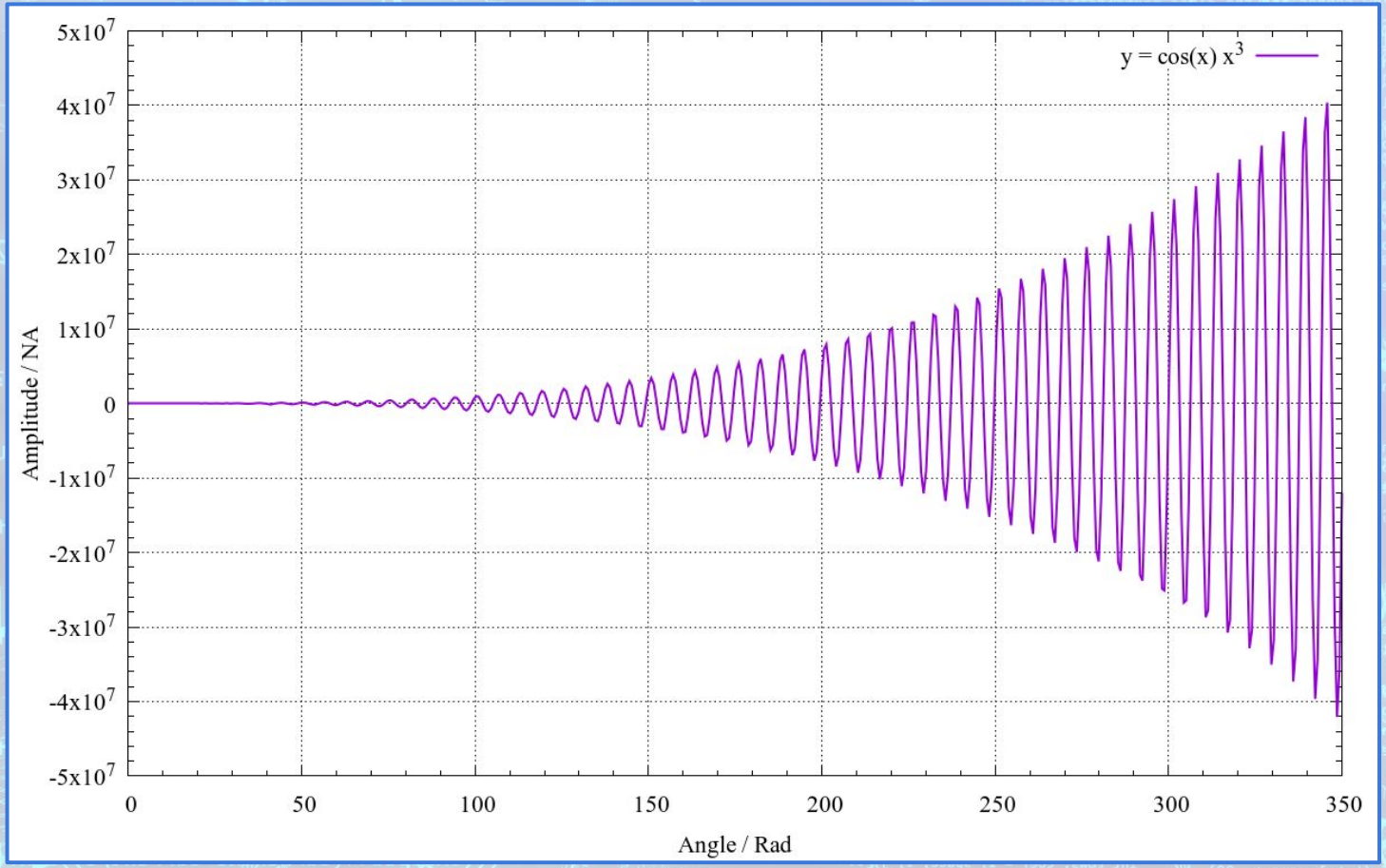
- show terminal
- set terminal
- set output "..."

Interactive

- wxt
- aqua (MacOS)
- qt
- x11
- dumb (text)

- help terminal
- help output

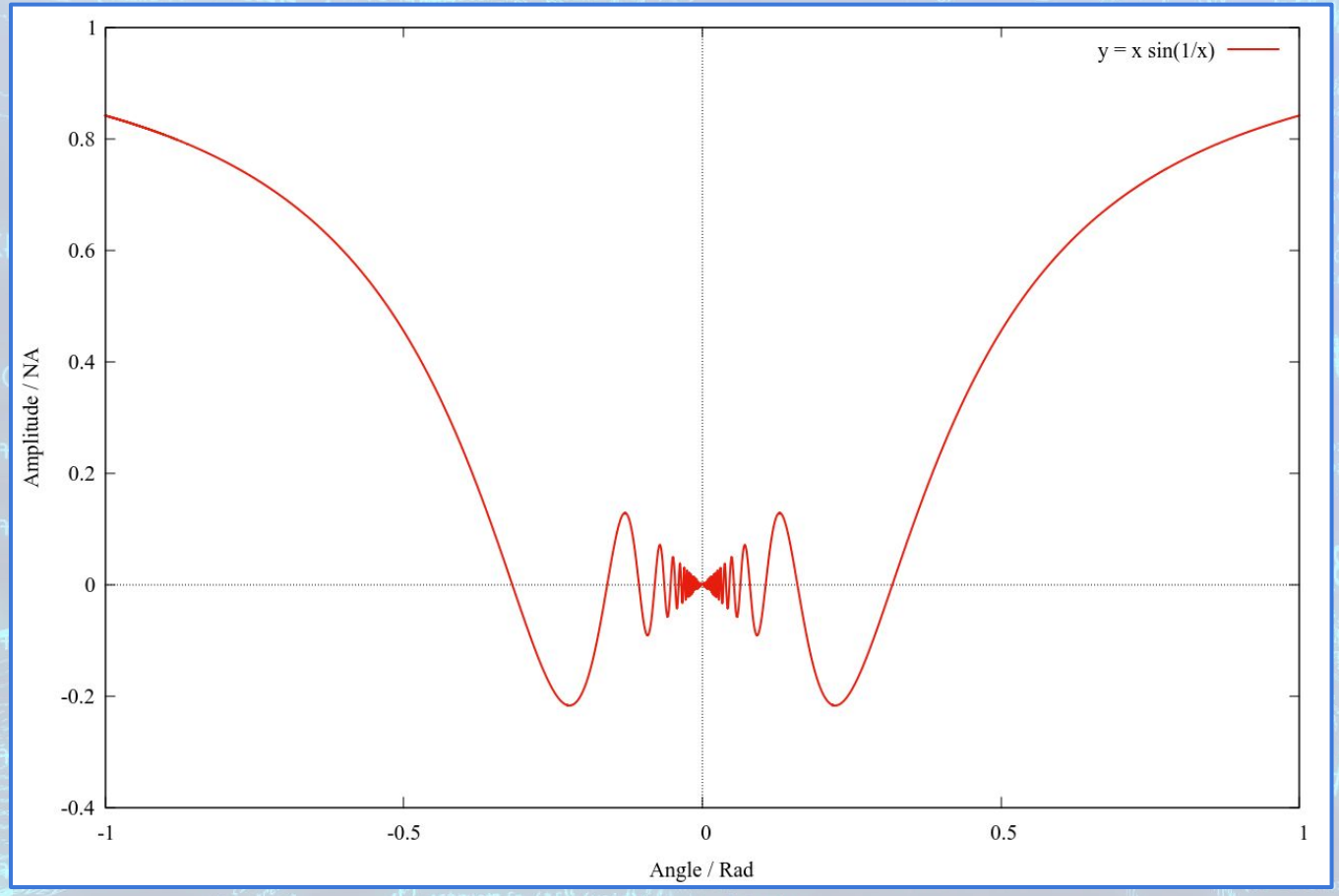
Making figures. Grid, tics, samples, superscript



Commands:

- plot … title “...”
- set grid
- set mxtics / mytics
- set samples
- superscript: x^{super}
- subscript: x_{sub}
- help grid
- help tics
- help mxtics

Making figures. Zero axes.



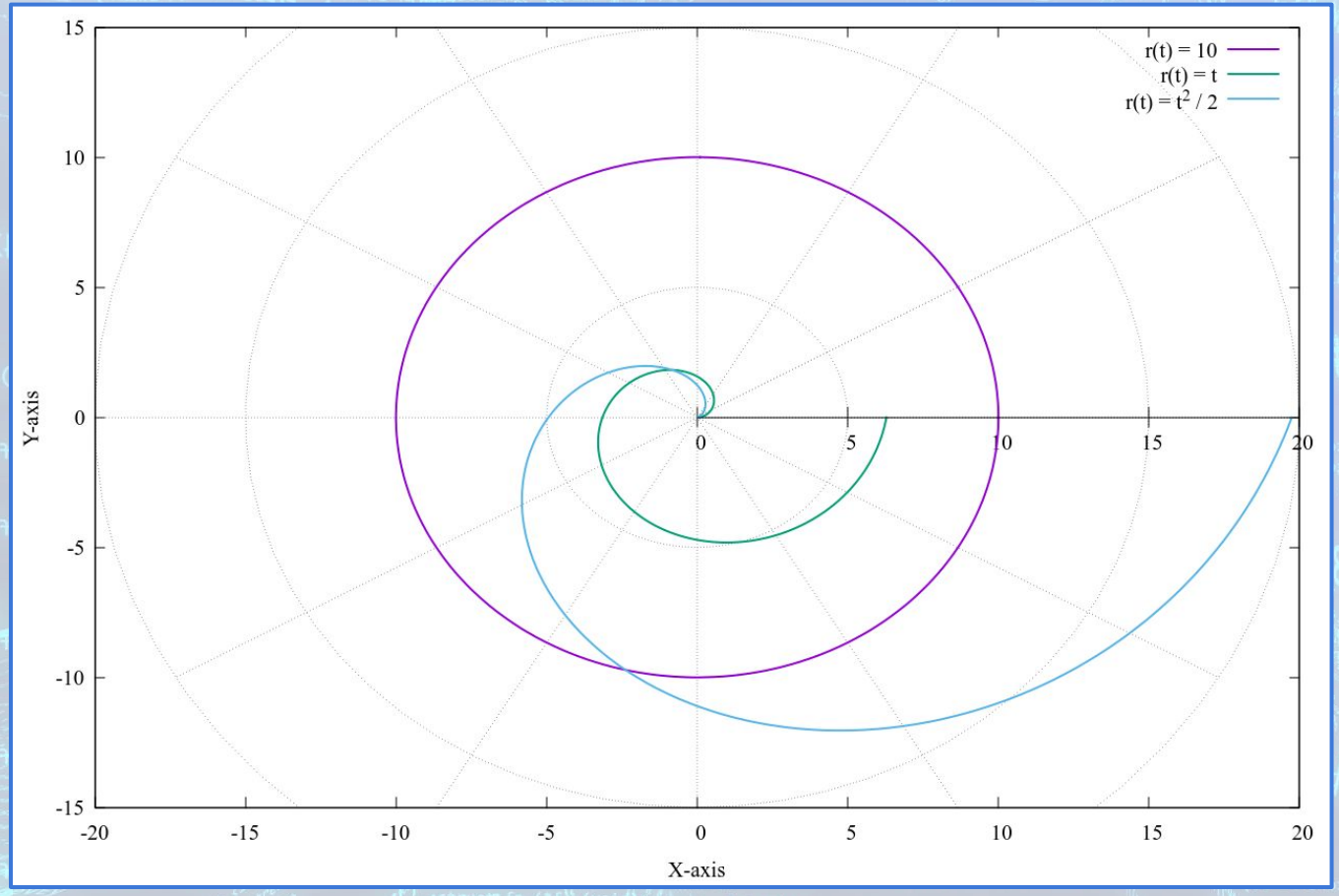
Commands:

- set yzeroaxis
- show samples
- set samples

- … linetype / lt
- … linecolor / lc

- help linetype
- help linecolor
- help zeroaxis

Polar coordinates. r = r(t)



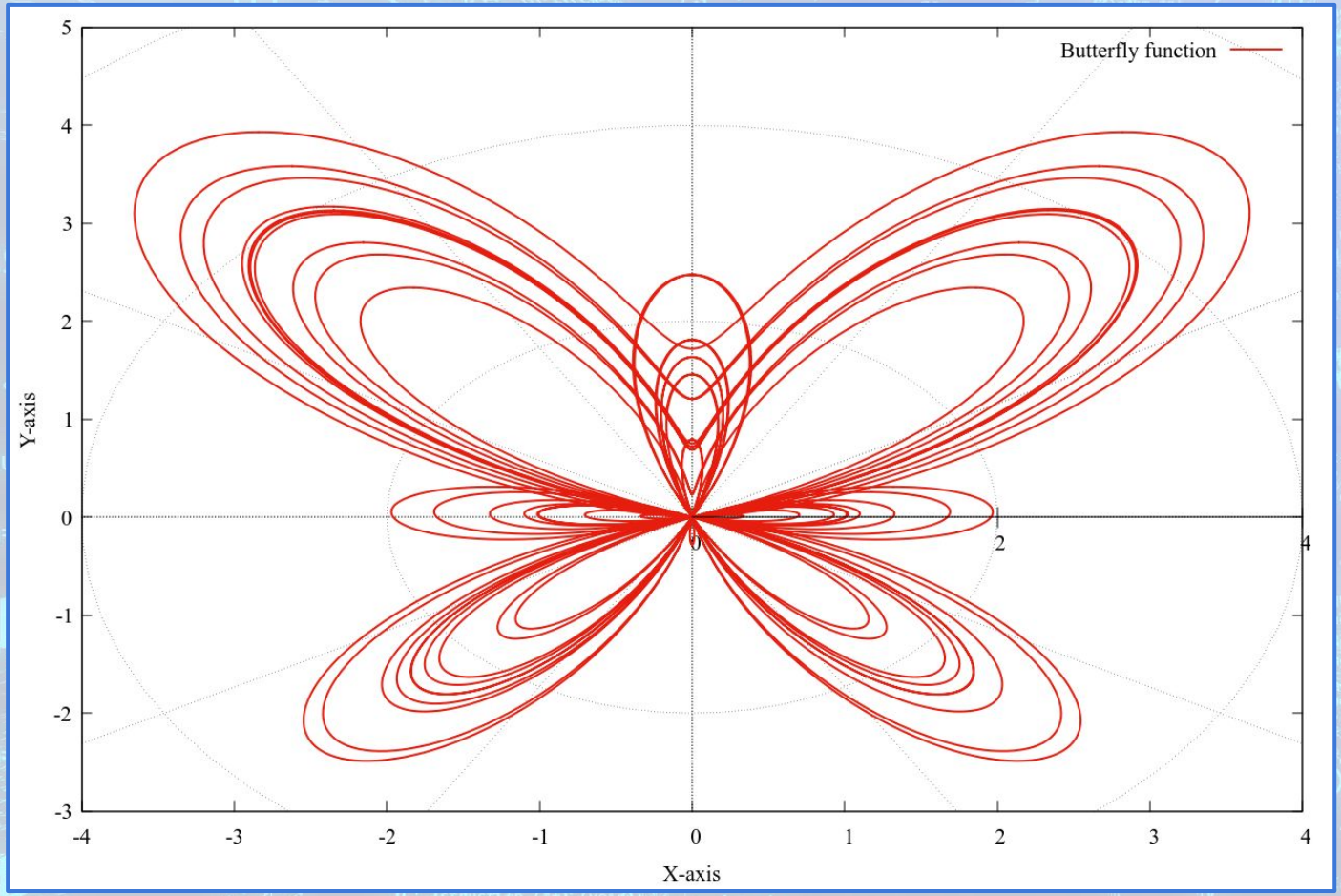
Commands:

- set polar (unset)
- set grid polar
- set trange [...]

- pi constant

- help polar
- help grid
- help trange

Plotting in polar coordinates



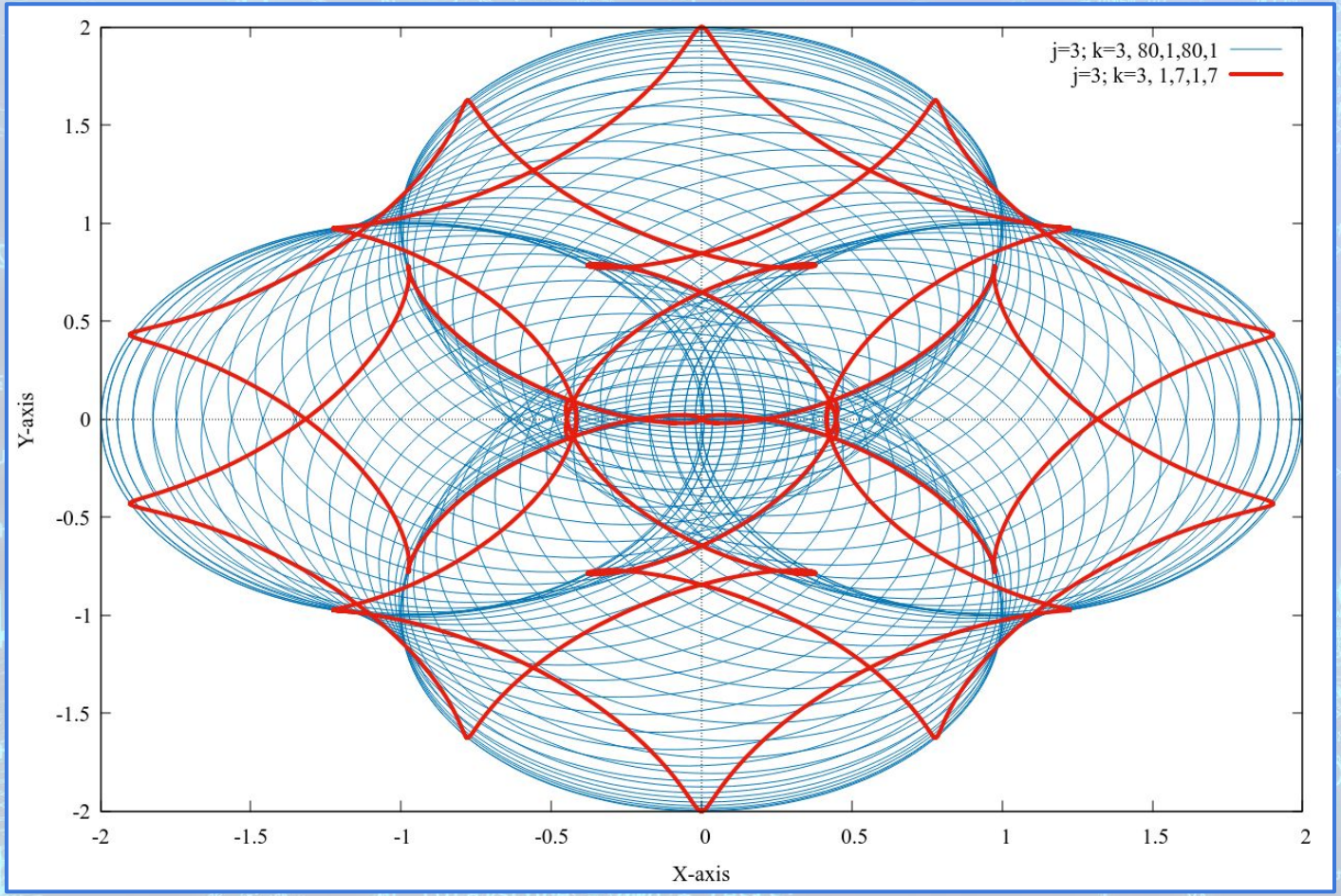
Commands:

- save “file.gp”
- load “file.gp”

- help save
- help load
- help call

- help function
- help user-defined
- help expressions functions

Parametric plots: x = x(t), y = y(t)

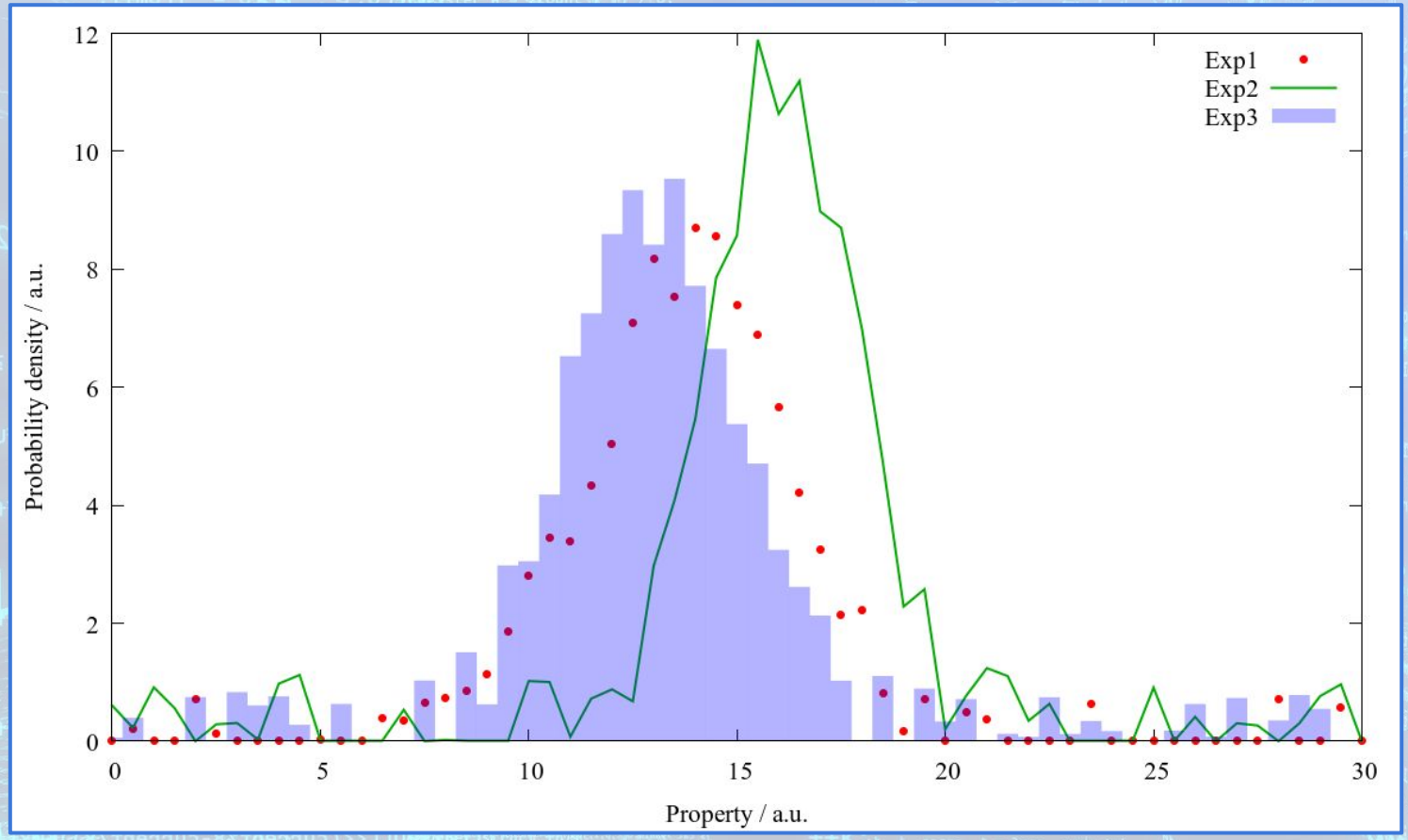


Commands:

- set parametric (unset)
- pause

- help parametric
- help pause

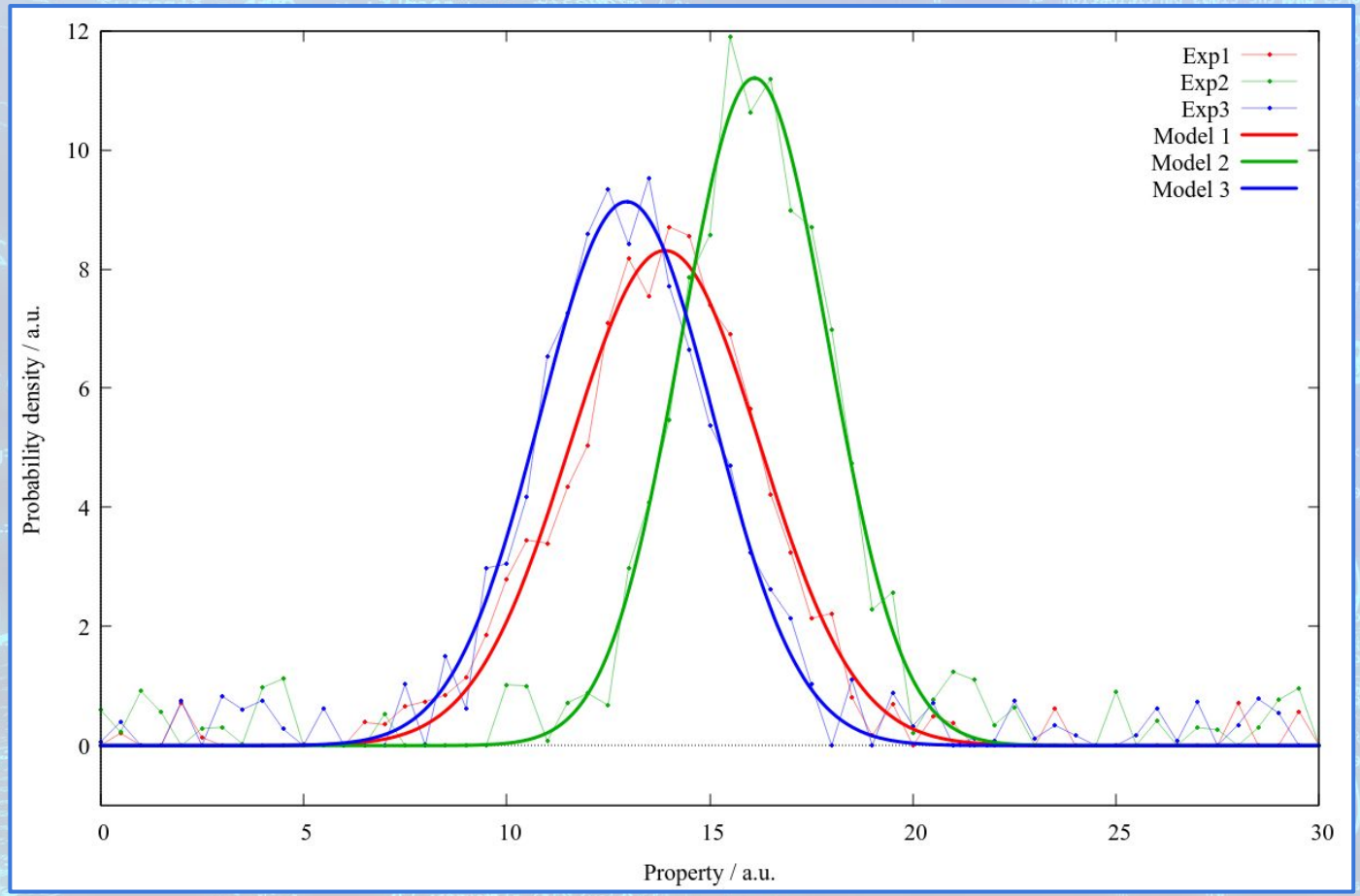
gnuplot. Plotting data



Commands:

- plot “data.dat”
- … using ...
- ... with points
- … with lines
- … with boxes
- pointsize / ps
- help data
- help using
- help with
- help points
- help pointsize
- help boxes

Fitting models to data

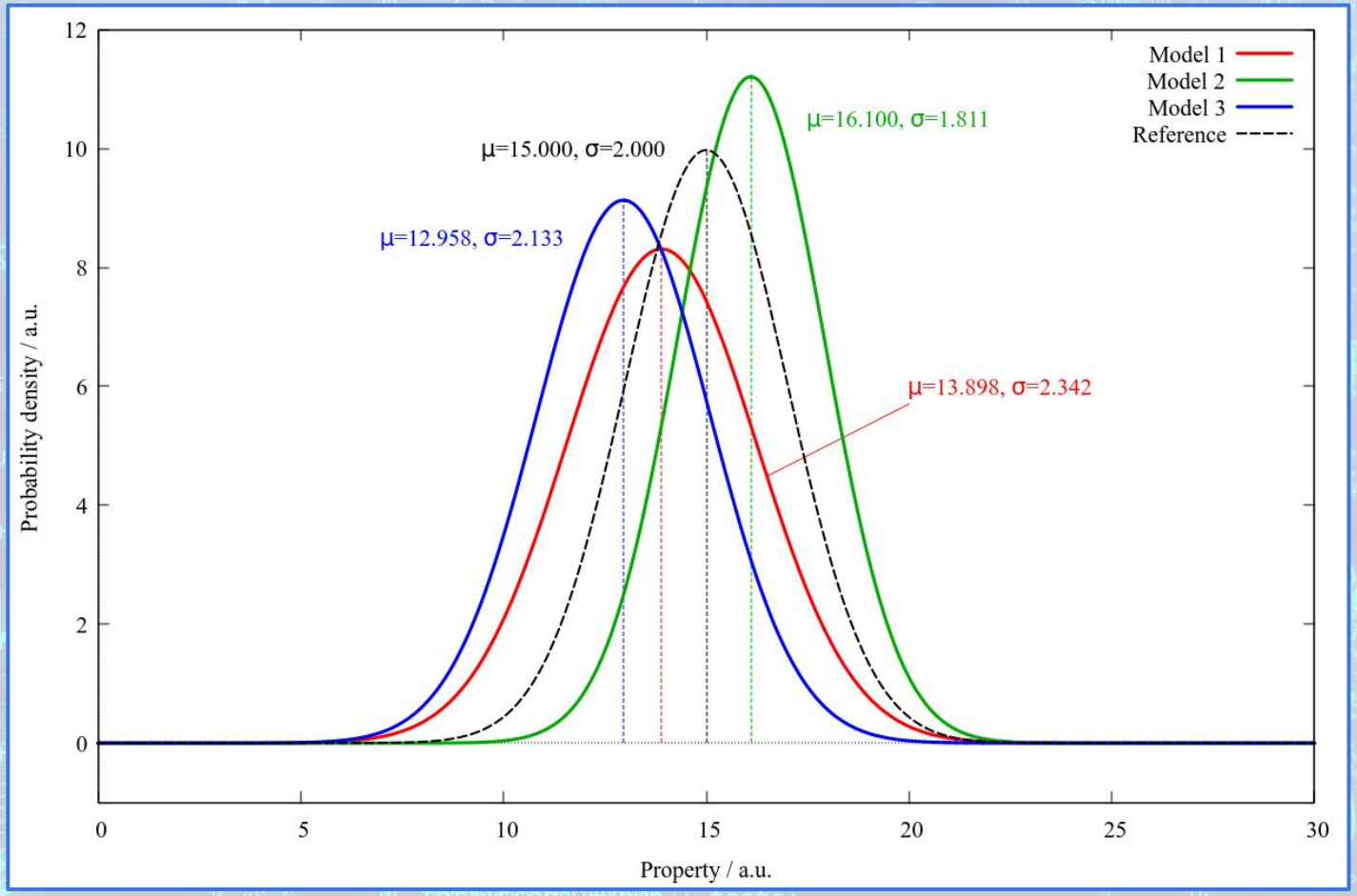


Commands:

- fit f(x) “..” … via…
- … with linespoints
- print “..”, var1

- help fit
- help variable
- help linespoints
- help print

Arrows and labels:

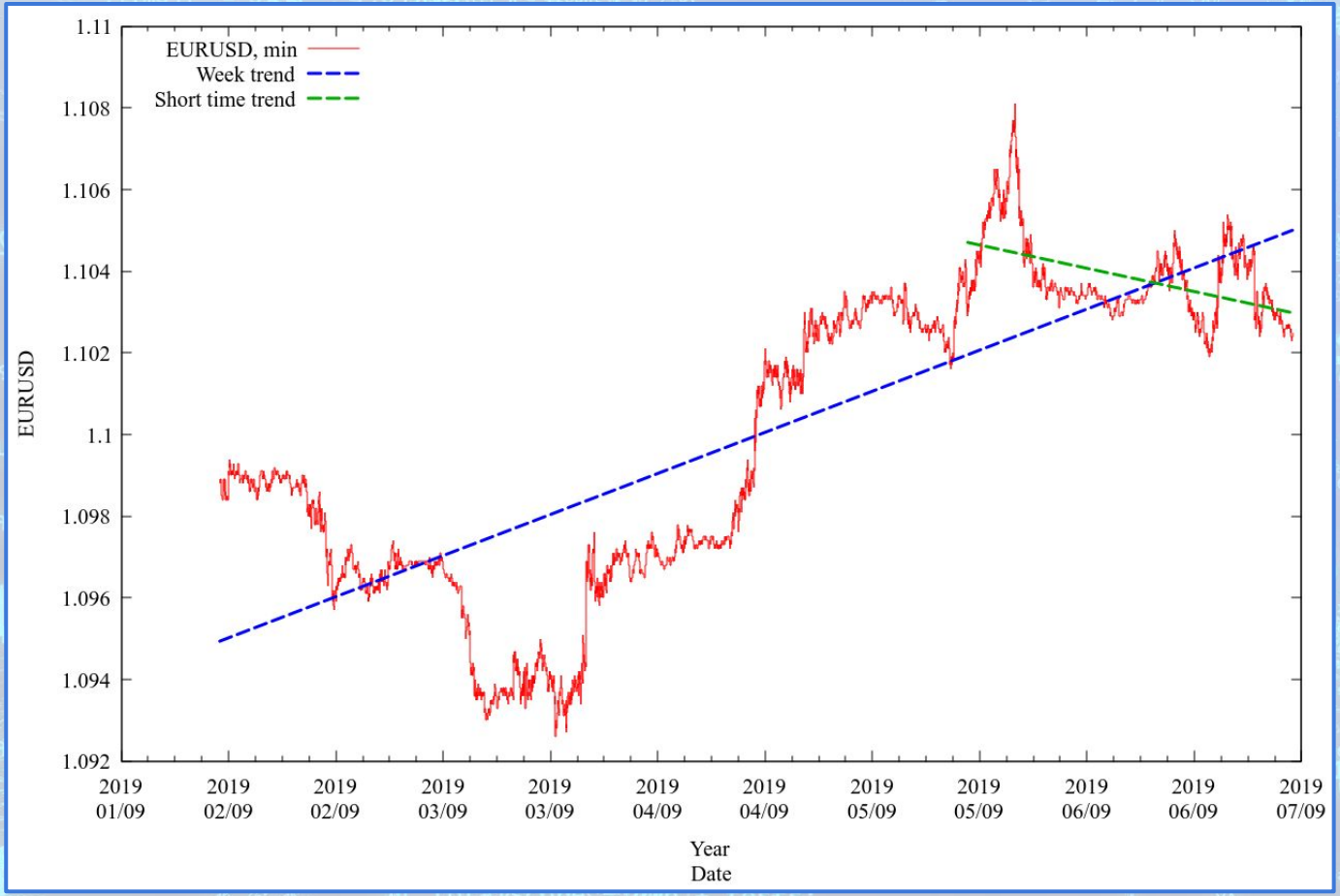


Commands:

- … dashtype / dt
- set arrow
- set label
- Symbols:
  “{/Symbol m}”
  “{/Symbol s}”

- help dashtype
- help arrow
- help label
- help sprintf
- help gprintf
- help string

Time series and trends:

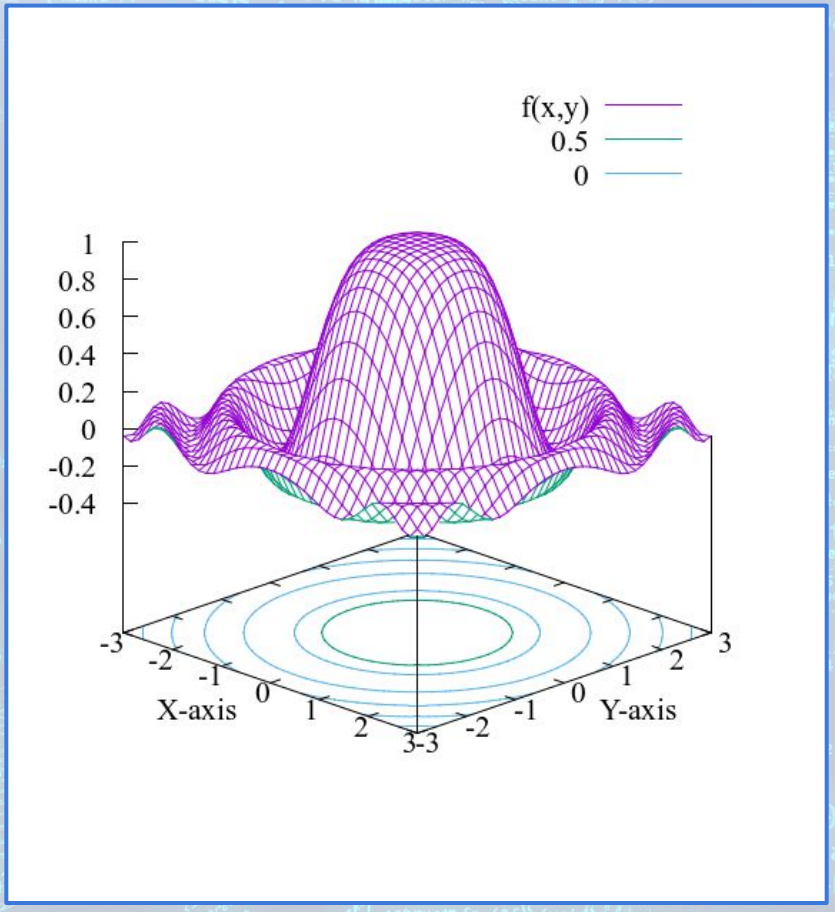


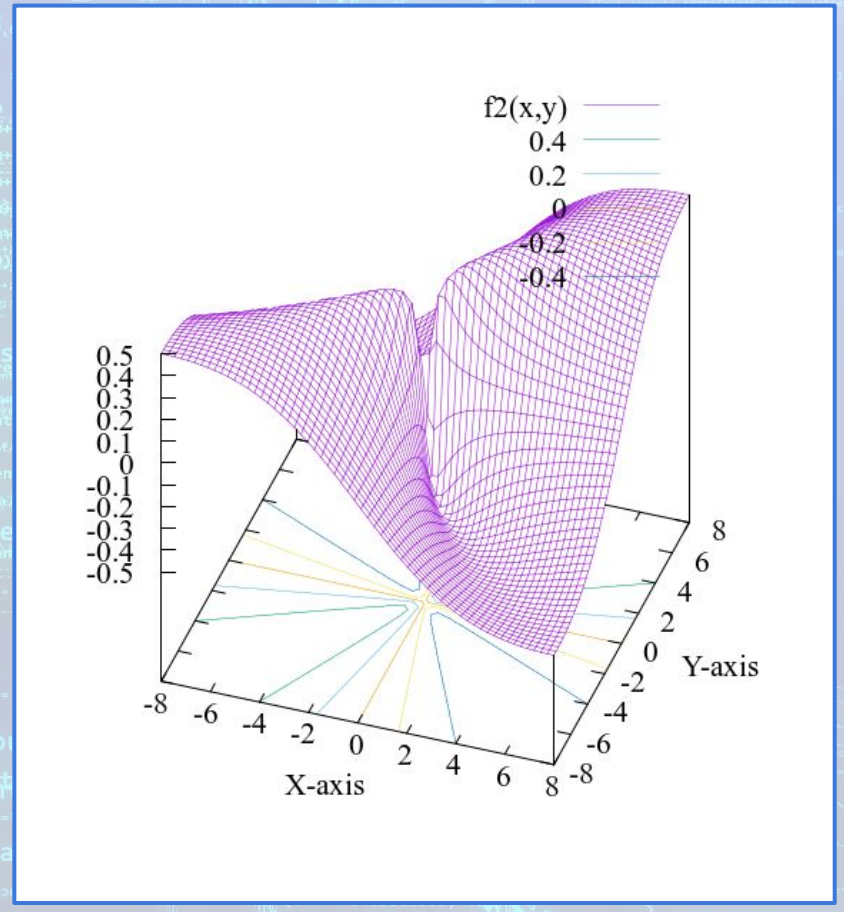
Commands:

- set timefmt
- set xdata time
- set format x
- fit [range] f(x) “file”
- replot [range] f(x)
- set key top left

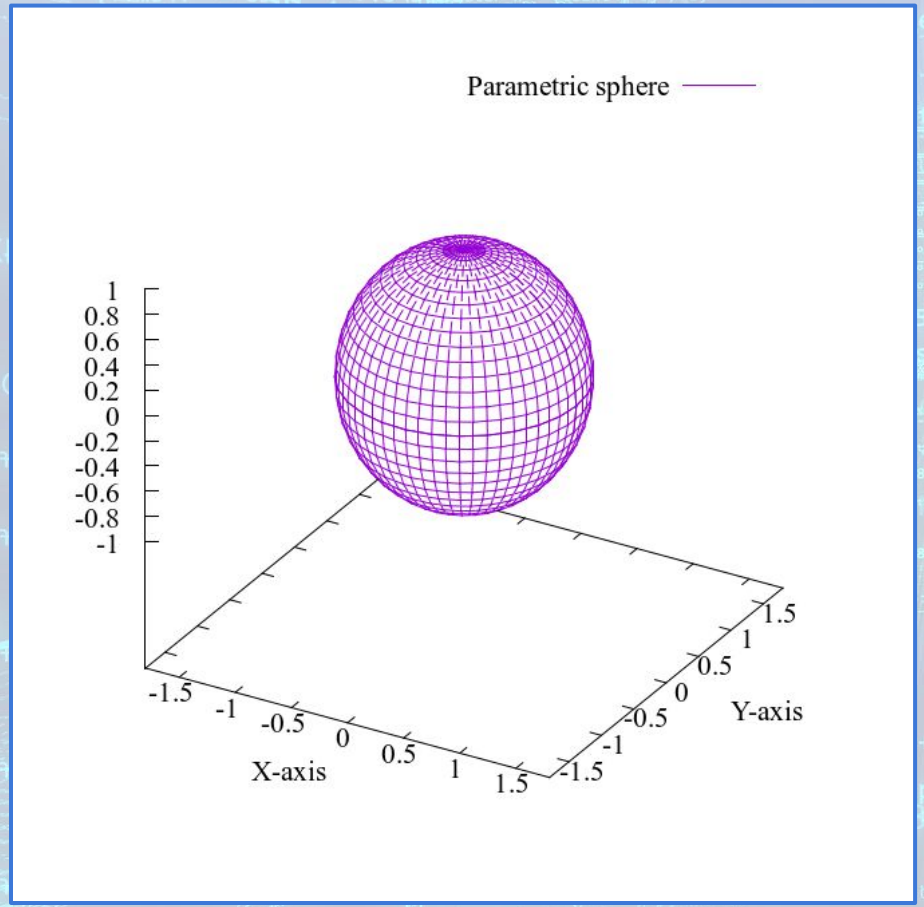
- help time
- help key
- help xdata
- help timefmt
- help format

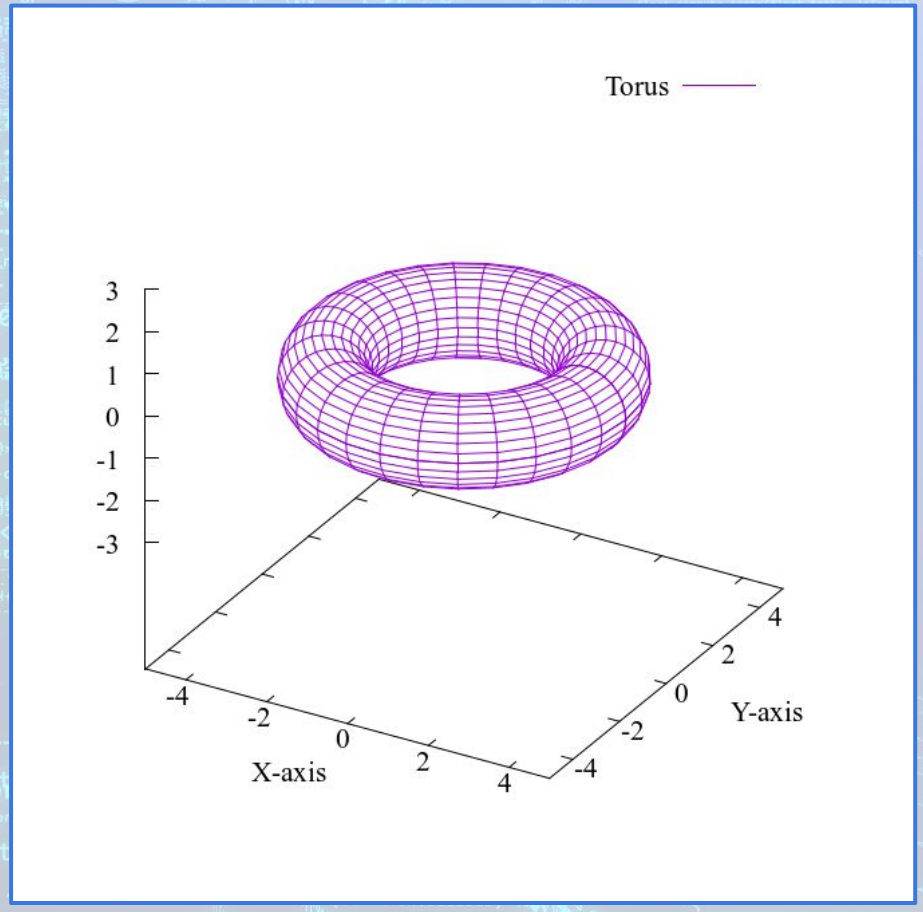
3D plots: z(x,y) (splot, view, hidden3d, contour, isosamples)





Parametrics 3D plots: x(u,v), y(u,v), z(u,v)





Conclusions:

Gnuplot

- is a powerful **plotter** and **grapher**.
- is great when you have your **data ready**.
- is **self sufficient** and does not require python or other dependencies.
- has great **documentation**: built-in, on-line, PDF.
- has a long history and is going to be a **good investment**.

Finding information:

- **gnuplot homepage**, the main resource and source: http://www.gnuplot.info/
- **Gnuplotting.org**, web site by Dr. Hagen Wierstorf: http://www.gnuplotting.org/
- **Google it**:
  “How to fit a model in **gnuplot**?”
  “How to use loops in **gnuplot**?”
  “How to do what I want in **gnuplot**?”
- There are **printed books** available (https://www.amazon.ca).

Thank you.

Questions?