

C2110 UNIX and programming

9. lekce

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INVESTICE DO ROZVOJE VZDĚLÁVÁNÍ

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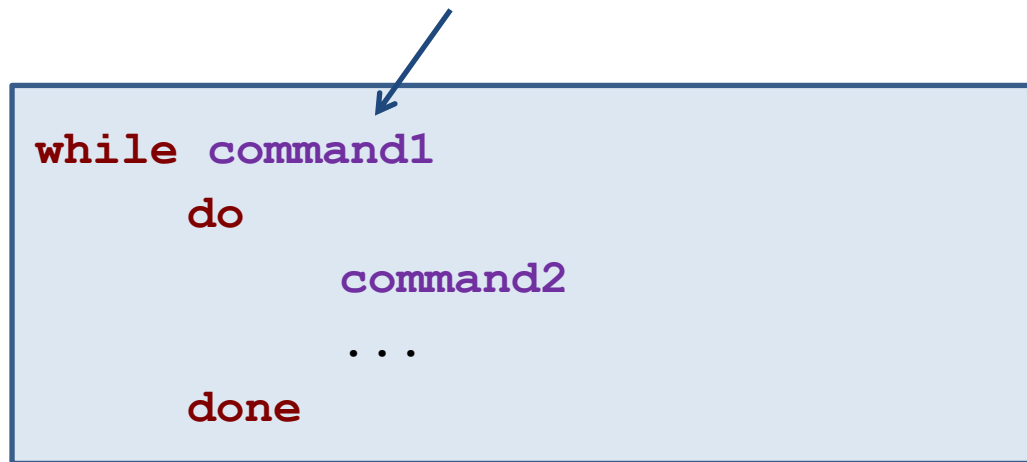
Bash

- **Cycle using while**

Cycle using while

Cycle (loop) is control structure, that repeatedly processes set of commands. Repeats are done until condition is fulfilled.

Cycle repeats **until** command1 return value is 0.



```
while command1
do
    command2
    ...
done
```

The diagram shows a light blue rectangular box containing the code for a while loop. The code is: `while command1` on the first line, `do` on the second line, `command2` on the third line, `...` on the fourth line, and `done` on the fifth line. A blue arrow points from the text above to the `command1` part of the first line.

Compact form:

```
while command1; do
    command2
    ...
done
```

Cycle using for vs. while cycle

```
for((I=1;$I <= 10;I++)); do  
    echo $I  
done
```

Done before script start
(count initialisation)

If conditions is fulfilled, then commands in
block do/done are processed


```
I=1  
while test $I -le 10; do  
    echo $I  
    I=`expr $I + 1`  
done
```

Count update after
processing commands

Redirection and pipes

Reading file per lines:


```
cat file.txt | while read A; do
    command2
    ...
done
```



A blue arrow points from the label 'roura' to the vertical pipe character in the code snippet above.

roura

```
while read A; do
    command2
    ...
done < file.txt
```




A blue arrow points from the label 'redirection' to the '<' symbol in the code snippet above.

redirection

Redirection to file:

```
for((I=1;I <= 10;I++)); do
    echo $I
done > file.txt
```




A blue arrow points from the label 'Output of all commands is redirected to file.txt.' to the '>' symbol in the code snippet above.

Output of all commands is redirected to **file.txt**.

Home work I


Explain different behavior of following scripts file.txt obsahuje pět řádků.

```
#!/bin/bash
I=0
cat data.txt | while read A; do
    I=$((I+1))
done
echo $I
```



Print number 0

```
#!/bin/bash
I=0
while read A; do
    I=$((I+1))
done < data.txt
echo $I
```




Print number 5

Home work II

File rst.out (wolf.ncbr.muni.cz:/home/kulhanek/Data/rst.out) contains results of molecular dynamics simulation. Task is to extract dependence of temperature on simulation time from file.

```
.....
NSTEP =          500    TIME (PS) =          0.500    TEMP (K) =      288.02    PRESS =          0.0
Etot   =          942.6248    EKtot   =          151.0990    EPtrot   =          791.5258
BOND   =          51.3204    ANGLE   =          292.3619    DIHED    =          176.5980
1-4 NB =          17.7099    1-4 EEL =          981.4071    VDWAALS  =          -68.3301
EELEC  =          -494.7423    EGB     =          -164.7991    RESTRAINT =          0.1822
EAMBER (non-restraint) =          791.3436
.....
```

Time Temperature



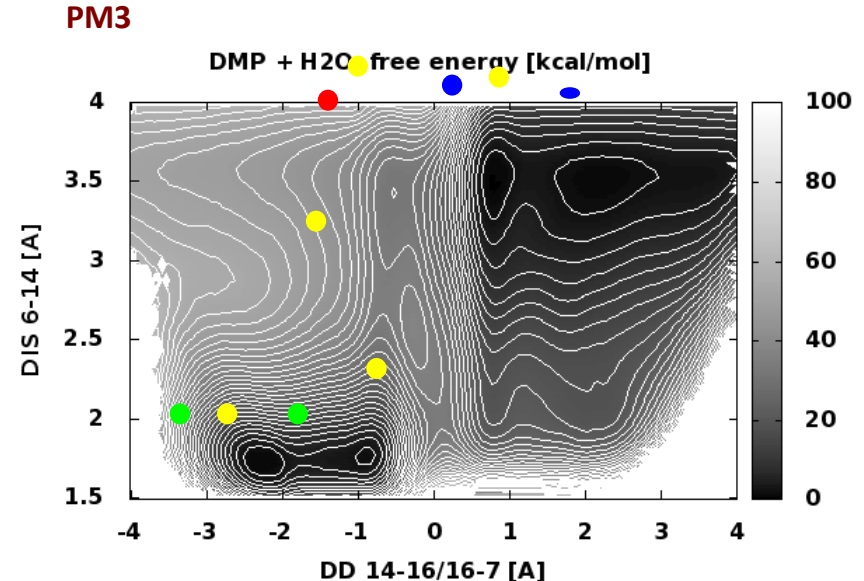
WARNING: Script must not contain commands `grep`, `awk` and their variants. Use command `read` and `while`.

Gnuplot

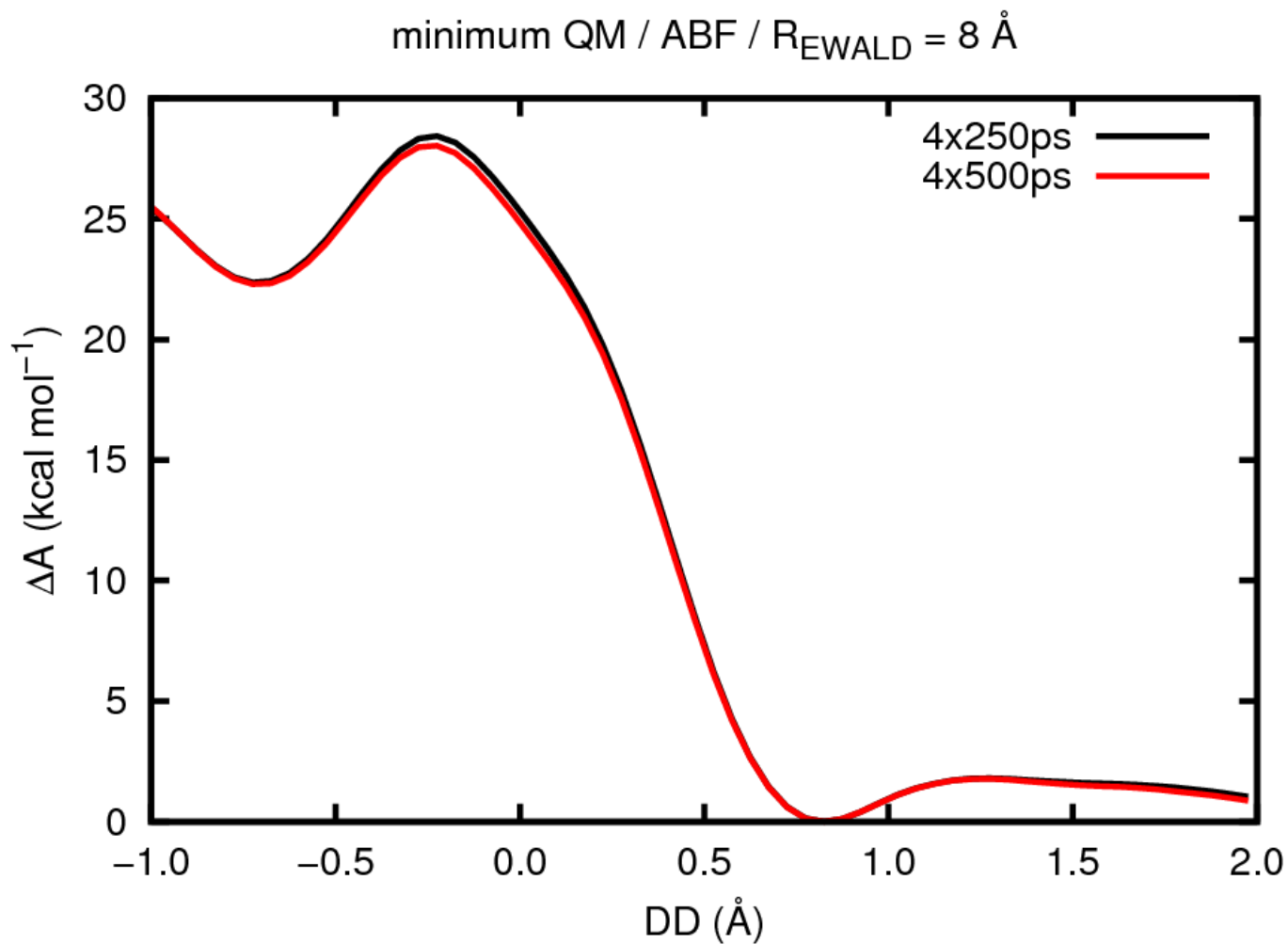
- (Non)Interactive run
- Command plot
- Terminals
- Showcases

<http://www.gnuplot.info/>

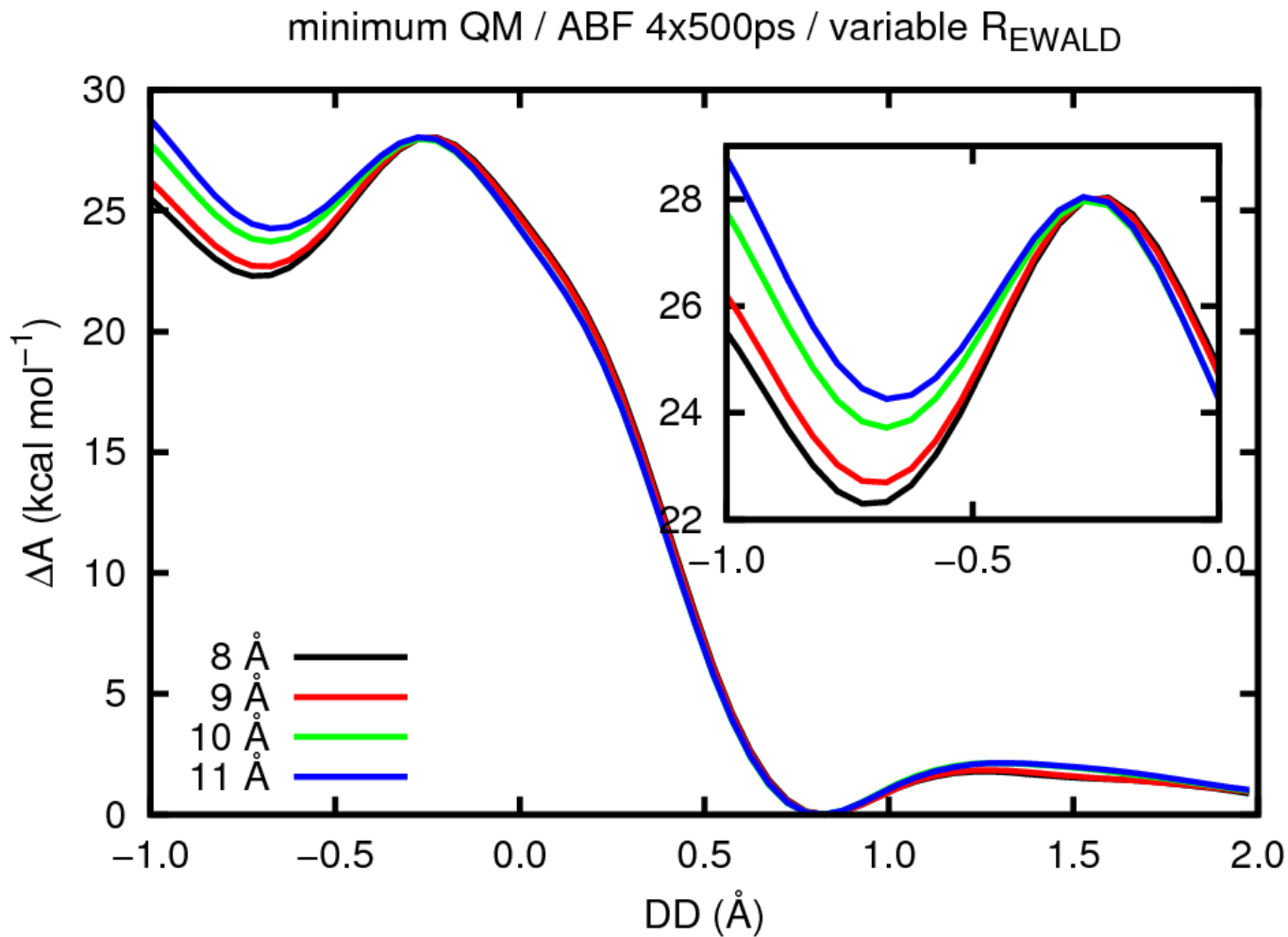
(documentation, tutorials, source codes)



Showcase



Showcase



Interactive run

Gnuplot is dedicated to draw 2D and 3D graphs, through interactive and scripting mode as well.

Interactive mode

```
[kulhanek@wolf ~]$ gnuplot
```

```
GNUPLOT
Version 4.4 patchlevel 3
last modified March 2011
System: Linux 3.2.0-31-generic
```

```
Copyright (C) 1986-1993, 1998, 2004, 2007-2010
Thomas Williams, Colin Kelley and many others
```

```
gnuplot home:      http://www.gnuplot.info
faq, bugs, etc:   type "help seeking-assistance"
immediate help:   type "help"
plot window:      hit 'h'
```

```
Terminal type set to 'wxt'
gnuplot>
```

Shell BASH command line



gnuplot command line



Noninteractive run

1) Un-direct running

We run interpreter and as its argument we put script name.

```
$ gnuplot my_gnuplot_script
```

Scripts **does not need** permission **x** (executable).

2) Direct running

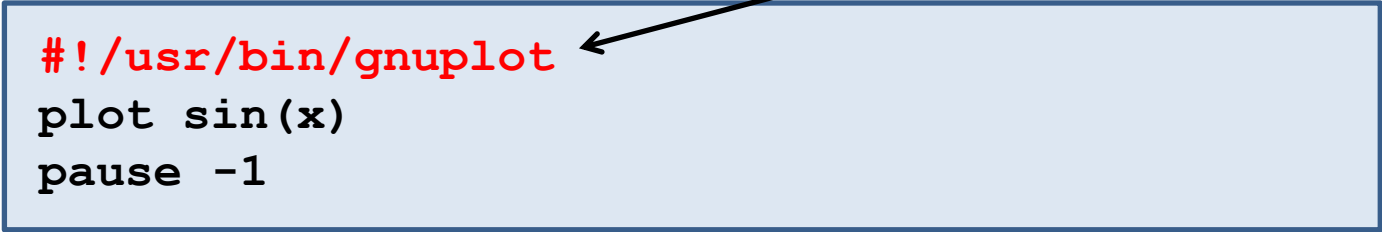
We run directly script (shell automatically start interpreter).

```
$ chmod u+x my_gnuplot_script
```

```
$ ./my_gnuplot_script
```

Scripts **needs** permission **x** (executable) and **interpreter** (part of script).

```
#!/usr/bin/gnuplot  
plot sin(x)  
pause -1
```



Command - plot

```
> plot function/file [plot_setup] [, fce/file ...]
```

Shows XY graph of function or data from file.

Examples:

lines, points, linespoints, dots

Line color

```
> plot sin(x)
```

```
> plot cos(5.7*x+3.4) with points linecolor rgb "red" \  
      linewidth 2 title "cos"
```

Data file name

Line thickness

legend

```
> plot "input.txt" using 1:2 with lines
```

Second column are y-axis values.

First column are x-axis values.

```
> plot sin(x) , cos(x)
```

Plots functions sin and cos to one graph.

Exercise

1. Plot function graph of $y=x^2$
2. Plot function from task 1 again, but with blue line.
3. Plot graph of temperature dependency on time from data file **/home/kulhanek/Data/temp.txt** Time is in first column, temperature is in second column.
4. Plot graph of function $\sin(x)$ using red line and function $\cos(x)$ using orange line with points.

Do all tasks in interactive mode.

Other commands

- > `set title "title"` # Graph header
- > `set xrange [min_value:max_value]` # sets range of x axis
- `set xlabel "title"` # sets title of x axis
- > `set yrange [min_value:max_value]` # sets range of y axis
- > `set ylabel "title"` # sets title of y axis
- > `set nokey` # disables key for data in plot
- > `pause -1` # wait for key press

Exercise

1. Write script, that plots function $y=x^2$ in range 0-10 for x axis. Run script un-directly using gnuplot interpreter.
2. Write script, that plots dependence of temperature on time from data in file **/home/kulhanek/Data/temp.txt** . Add axis labels including units. Time is in picoseconds, temperature in kelvin.

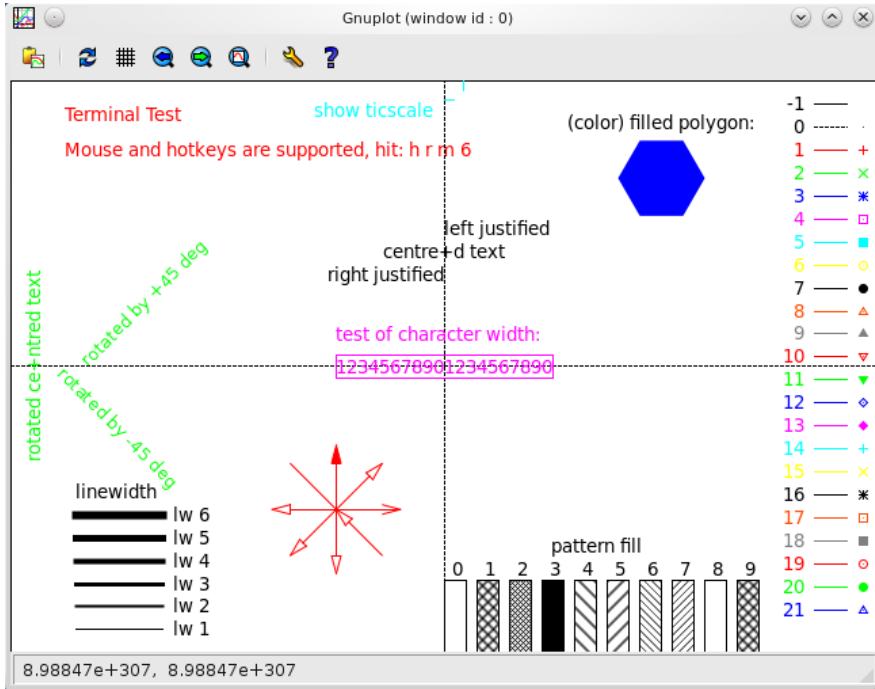
Terminals

Terminal determines output form.

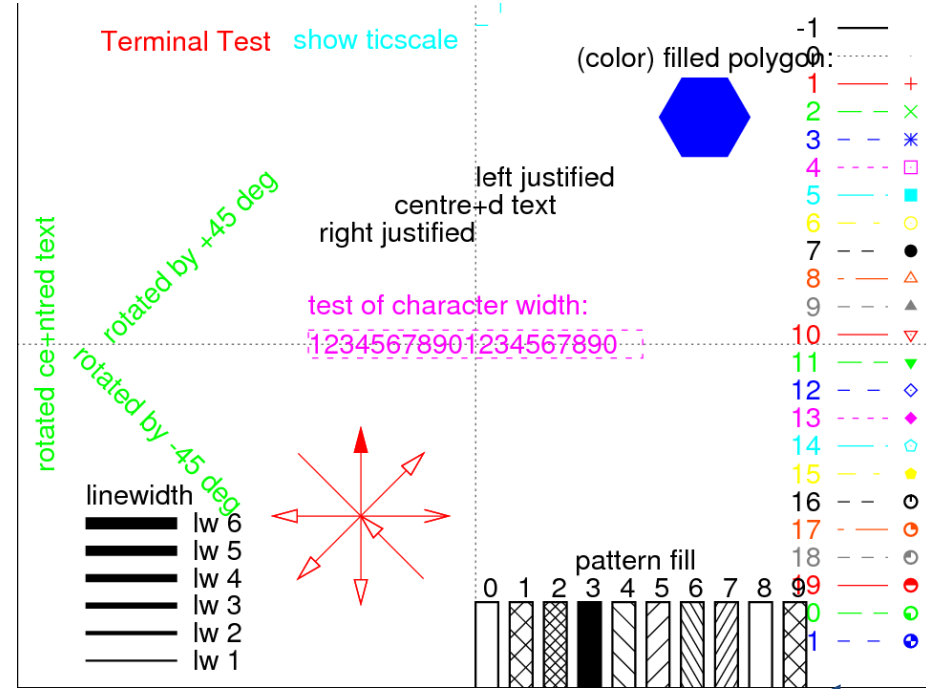
- > **set term x11** # output is shown in window
- > **set term wxt** # output is shown in advanced window
- > **set term png size 800,600**
output is plot as a picture in png format
- > **set output "output.png"** # output will be saved to file output.png
- > **test** # prints page with terminal features, terminals does have different abilities

Sample terminal outputs

wxt



postscript/eps



Supports dotted lines



Exercise

1. What possibilities offer terminals `x11` and `wxt`. Work in interactive mode and use command **test**.
2. Write script, that plots graph of function $y=5x^3 + 6x^2 - 7$ in range -10 to 5 on x axis. Run script directly with interpreter in script header.
3. Change previous script to plot graph to format png. Picture size will be 640x480. Show picture using command **display**.
4. View result of command **test** for terminal png and postscript.
5. What terminals gnuplot supports (set terminal with no argument)?

Command - splot

To plot function of two variables, command `splot` may be used.

```
> splot functionkce/file [plot_setup] [, fce/file ...]
```

Shows **XYZ** graph of function or data from file.

View point is set by command `set view a,b`, where **a** and **b** are view angles. View from top is set by `set view map`

Sampling of density for x and y axis is set by command `set isosamples a,b`, where **a** and **b** gives number of samples in given direction.

To highlight surface by its function value `pm3d` command may be used, for example:

```
> splot x*x+y*y with pm3d
```

Exercise

1. Plot function x^2+y^2
2. Set top view (**set view**)
3. Unset current view (**unset view**)
4. Raise density of points for function plot (**set isosamples**). Use values 10,20; 20,10 and 20,20
5. Use view **pm3d**
6. Set top view (**set view**)

Do all tasks in interactive mode.