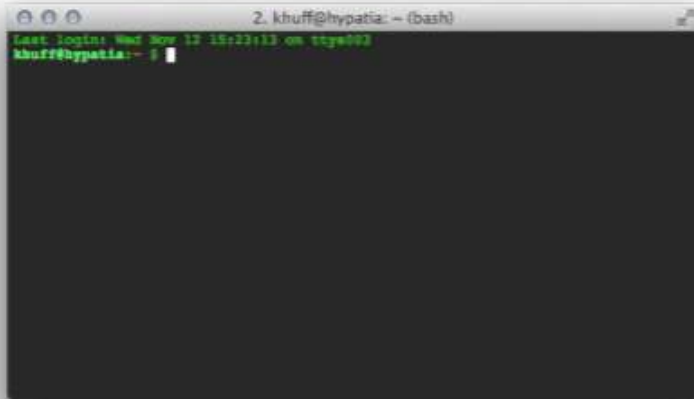


# Linux command line (the shell)



- the shell is a programming language
- it has variables and states
- uses obtuse syntax including special characters

## Terminal in Linux or OS/X

- For windows download Ubuntu (alternate bash shells)
- MobaXterm (<https://mobaxterm.mobatek.net>)
- Gitbash (<https://git-scm.com/download/win>)

if you don't have bash, install it now.

## different shells

Shell	Name	Description
sh	Bourne shell	Popular, ubiquitous shell developed in 1977, still guaranteed on all Unixes
csh	C shell	Improves on sh
ksh	Korn shell	Backward-compatible with sh, but extends and borrows from other shells
bash	Bourne again shell	Free software replacement for sh, much evolved
tcsh	Tenex C shell	Updated and extended C shell

# Warning.

---

The following lecture is *super* dry.

It contains a bunch of information that you will not remember.

# very basic shell commands (pwd, ls, and cd)

when opening a terminal you start in your “home directory” mine is /c/Users/damien, the shortcut is the tilde, ~

- (print working directory) : use **pwd** command to determine current directory.

```
27/05/2022 03:37.59 /home/mobaxterm pwd
/home/mobaxterm
```

to see output which has scrolled off-screen can typically use shift+pg up(down) to look through output buffer.

- (listing): use **ls** to show contents of current directory.

```
27/05/2022 03:38.56 /home/mobaxterm ls
CONTCAR          Untitled4.ipynb
Desktop          Untitled5.ipynb
Ener             Untitled6.ipynb
JCWZcell.ipynb   Untitled7.ipynb
LauncherFolder   Untitled8.ipynb
MyDocuments      Untitled9.ipynb
OUT              bitan_fig.ipynb
OUTCAR           data.pdf
```

\* is a wildcard.

\$ **ls Un\*** (would show any file/directory which begins with Un)

- (change directory): use **cd** to change the current directory.

```
27/05/2022 03:40.45 /home/mobaxterm cd mysrc
/home/mobaxterm/mysrc
27/05/2022 03:40.50 /home/mobaxterm/mysrc ls
file1.py file2.py
```

tab completion is nice!

```
/mysrc 03:41.54 cd di
/mysrc 03:41.54 cd dirwithlongname/
```

# directory structure and shortcuts

Syntax	Meaning
--------	---------

/	The root, or top-level, directory of the filesystem (also used for separating the names of directories in paths)
~	The home directory
.	Current working directory
..	Parent of current working directory
../..	The parent of the parent of current directory

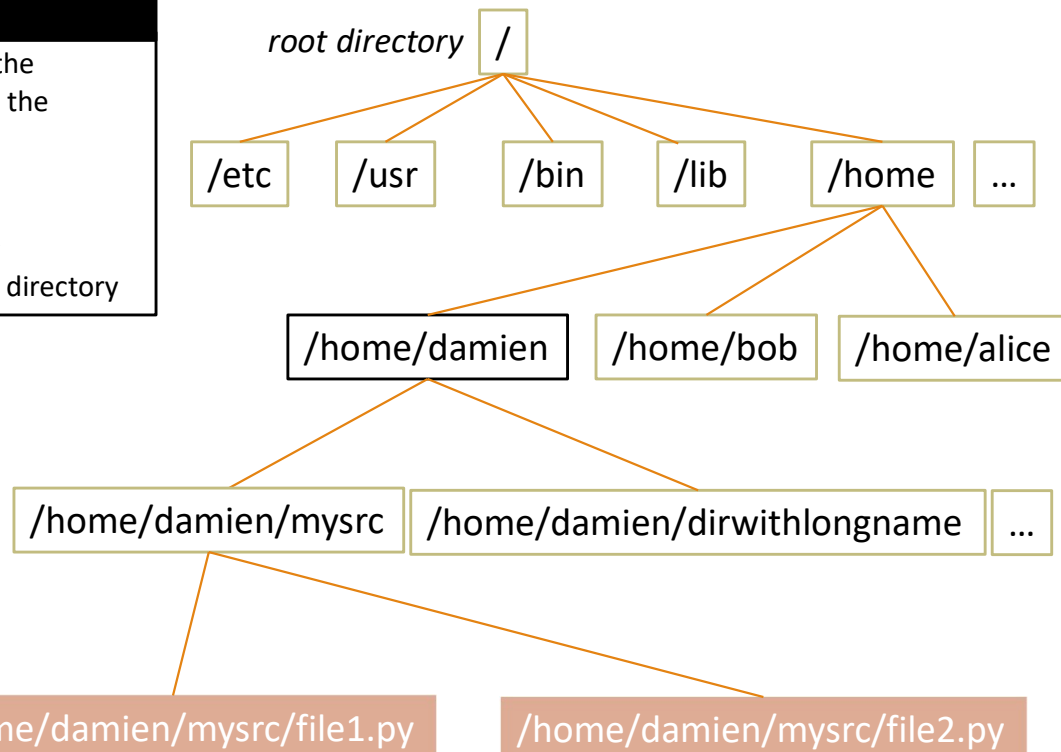
Absolute path:  
/home/damien/mysrc/file1.py

Relative path:

(if current dir is /home/damien)

./mysrc/file1.py

or ../damien/mysrc/file1.py



# continued

pwd	ls
cd	mkdir
cp	mv
man	less
echo	>

- **mkdir** *directoryname* (makes a new directory in the current directory)
- **cp** *filetocopy newfile* (makes a copy of “filetocopy” and names it “newfile”)
- **mv** *sourcefile newfile* (moves sourcefile to newfile, can be used to rename file or put in a different directory)
- **man** *command* (brings up manual on how to use command)
- **apropos** *keyword* (equivalent to **man -k**, searches the manual for commands whose descriptions contain the keyword/s) e.g. \$ apropos “text editor”
- **less** *filename* (displays text of filename to screen one page at a time, can use pg-up/down, search for expression with /*expr*, q to quit)
- **echo** “*type something*” (displays what you type to the screen)
- **>** (**redirects** the output which would go to the screen and sends it somewhere else, e.g. a file or a device.)

\$ **echo** “hello world!” > hworld.txt

(creates new file, “hworld.txt” which contains the text “hello world!”.)

command --help (usually shows usage and command line arguments)

note I'm just giving the simplest use cases. \$man cp (or \$scp --help)

```
damien@CHARON MINGW64 ~/mysrc
$ cp --help
Usage: cp [OPTION]... [-T] SOURCE DEST
or: cp [OPTION]... SOURCE... DIRECTORY
or: cp [OPTION]... -t DIRECTORY SOURCE...
Copy SOURCE to DEST, or multiple SOURCE(s) to DIRECTORY.

Mandatory arguments to long options are mandatory for short options too.
-a, --archive                same as -dR --preserve=all
--attributes-only            don't copy the file data, just the attributes
--backup[=CONTROL]          make a backup of each existing destination file
-b                           like --backup but does not accept an argument
--copy-contents              copy contents of special files when recursive
-d                           same as --no-dereference --preserve=links
-f, --force                  if an existing destination file cannot be
                             opened, remove it and try again (this option
                             is ignored when the -n option is also used)
-i, --interactive            prompt before overwrite (overrides a previous -n
                             option)
-H                           follow command-line symbolic links in SOURCE
-l, --link                   hard link files instead of copying
-L, --dereference            always follow symbolic links in SOURCE
-n, --no-clobber             do not overwrite an existing file (overrides
                             a previous -i option)
-P, --no-dereference         never follow symbolic links in SOURCE
-p                           same as --preserve=mode,ownership,timestamps
--preserve[=ATTR_LIST]      preserve the specified attributes (default:
                             mode,ownership,timestamps), if possible
                             additional attributes: context, links, xattr,
                             all
--no-preserve=ATTR_LIST     don't preserve the specified attributes
--parents                   use full source file name under DIRECTORY
-R, -r, --recursive         copy directories recursively
--reflink[=WHEN]            control clone/cow copies. See below
--remove-destination        remove each existing destination file before
                             attempting to open it (contrast with --force)
--sparse=WHEN               control creation of sparse files. See below
--strip-trailing-slashes     remove any trailing slashes from each SOURCE
                             argument
-s, --symbolic-link          make symbolic links instead of copying
-S, --suffix=SUFFIX         override the usual backup suffix
```

[ ] indicate something optional, ... can be more than one

```
-t, --target-directory=DIRECTORY  copy all SOURCE arguments into DIRECTORY
-T, --no-target-directory         treat DEST as a normal file
-u, --update                      copy only when the SOURCE file is newer
                                 than the destination file or when the
                                 destination file is missing
-V, --verbose                    explain what is being done
-x, --one-file-system            stay on this file system
-Z                               set SELinux security context of destination
                                file to default type
--context[=CTX]                 like -Z, or if CTX is specified then set the
                                SELinux or SMACK security context to CTX
--help                          display this help and exit
--version                       output version information and exit
```

By default, sparse SOURCE files are detected by a crude heuristic and the corresponding DEST file is made sparse as well. That is the behavior selected by --sparse=auto. Specify --sparse=always to create a sparse DEST file whenever the SOURCE file contains a long enough sequence of zero bytes. Use --sparse=never to inhibit creation of sparse files.

When --reflink[=always] is specified, perform a lightweight copy, where the data blocks are copied only when modified. If this is not possible the copy fails, or if --reflink=auto is specified, fall back to a standard copy. Use --reflink=never to ensure a standard copy is performed.

The backup suffix is '~', unless set with --suffix or SIMPLE\_BACKUP\_SUFFIX. The version control method may be selected via the --backup option or through the VERSION\_CONTROL environment variable. Here are the values:

### other common use cases

**cp -ip filetocopy newfile** (no auto-overwrite)

**cp file1 file2 file3 directory** (copy the three files to directory)

**cp f\* directory** (copy all files that start with "f" to directory)

**cp -r sourcedir newdir** (copy entire source\_dir to new\_dir)

# other useful commands

---

- **nano, vim, emacs** (terminal based text editors, nano is by far the simplest)
- **cat** (displays entire file to screen)

```
damien@CHARON MINGW64 ~/mysrc
$ cat file1.py
import numpy as np
import matplotlib.pyplot as plt

x=np.linspace(0,10,100)
y=np.sin(x)
plt.plot(x,y)
plt.show()
```

can be used on multiple files, e.g.  
\$ **cat** file1.py file2.py  
displays them one after another.

- **>** (redirect the output)

\$ **cat** file1.py file2.py > file3.py

>> will append the output to the end  
of a file instead of overwriting it.

- **grep** *expression filename* (outputs to screen lines from filename which contain expression)
- **command1 | command2** (the *pipe*. output of command1 is redirected to the input of command 2, extremely useful.)

- **chmod** *code filename* (changes permissions on file, who can read/write/execute.)
    - e.g, **chmod** +x filename* (make file executable)
    - chmod** -w *filename* (remove write permissions)
- 

You can make a bash script by simply by making a text file containing bash commands executable (**chmod** +x). They will be executed as if typed in terminal. Bash even supports basic loops, e.g.

## For loop in bash

<b>for i in {1..100};do echo \$i;done</b>	(displays 1 to 100 to screen)
<b>for i in {1..10};do cp file_temp file\$i;done</b>	(makes 10 copies of file_temp named: file1, file2, file3,...,and file10)
<b>for var in `cat test.txt`;do echo \$var;done</b>	(displays each space delimited string in file test.txt to screen, each on its own line)

In the above examples both i and var are variables, they are dereferenced by using \$. Variables can be created at anytime at the command line (e,g, myvar=5 or hrm="hello").

*The shell is a full-fledged programming language, with arrays, conditionals, and loops*



# Windows powershell

---

## Bash/Linux

```
ls
mv
cp
pwd
rm
cat
grep
echo
var=0
df
wc
ps
find
diff
kill
time
if [condition] then something fi
-e file
for ((i=0; i < 10; i++)) ; do echo $i ; done
```

## PowerShell

```
ls
mv
cp
pwd
rm
cat
search-string
echo
$var=0
gdr or Get-PSdrive
measure-object
ps
gci
diff
kill
measure-command
if (condition) { something }
Test-Path file
for ($i=0;$i -lt 10; $i++) { echo $i }
```

- echo, >, |, mkdir, rm, mv, ls, pwd, cd, more (common linux command similar to less) all work in the same way as in bash shell.
- grep is missing (but sls has similar functionality)
- There are also alternatives to sed and (g)awk.

# combining | with sed

- **sed** s/(stream editor, can perform text transformations on file or input from pipe. It is quite powerful, but steep learning curve)

simple search and replace:

**sed 's/texttoreplace/replacement/g'**

replace every occurrence  
on each line

replace a regular expression (regex):

**sed 's/[0-9]/replacement/g'**

matches every  
single-digit  
number

```
damien@CHARON MINGW64 ~/mysrc
$ cat example.txt
0This, is, a file, where
I 1put, in a4 55bunch of random commas.
I82 also put in 3a2 8b23un5c9h of n8umbers.

damien@CHARON MINGW64 ~/mysrc
$ cat example.txt | sed s/,//g | sed s/[0-9]//g
This is a file where
I put in a bunch of random commas.
I also put in a bunch of numbers.
```

**sed s/,//g file**

```
damien@CHARON MINGW64 ~/mysrc
$ cat example.txt
0This, is, a file, where
I 1put, in a4 55bunch of random commas.
I82 also put in 3a2 8b23un5c9h of n8umbers.

damien@CHARON MINGW64 ~/mysrc
$ cat example.txt | sed s/,//g

0This is a file where
I 1put in a4 55bunch of random commas.
I82 also put in 3a2 8b23un5c9h of n8umbers.
```

some regex examples:

a.c (will match any 3 chars that  
starts with a and ends with b,  
abc, aac, etc)

ab{2,4} ( will match abb, abbb, and  
abbbb)

ab\* (matches a,ab,abb,abbb,...)

note: sed is greedy. will match largest  
it can.

<http://www.grymoire.com/Unix/Sed.html>

<https://regexone.com> (interactive tutorial on regular expressions)

# regular expressions

<https://regexlearn.com/learn/regex101> (another tutorial)

Meta-Character	Type	Description
\		Escapes the character proceeded
.		Matches any <u>single</u> character
a z		Matches a or z
^	Anchor	Matches the beginning of a string
\$	Anchor	Matches the end of a string
*	Quantifier	0 or more of previous group or characters
+	Quantifier	1 or more of previous group or characters
?	Quantifier	0 or 1 of previous group or characters
{a,z}	Quantifier	Matches if the previous group was found between a and z times.
{a,}	Quantifier	Matches if the previous group was found at least a times.
{,z}	Quantifier	Matches if the previous group was found no more than z times.
{n}	Quantifier	Matches if the previous group was found <u>exactly</u> n times.
[abcd]	Character Class	Matches if the character in this position is either an a, b, c, or d
[^abcd]	Inverted Character Class	Matches if the character in this position is <u>not</u> an a, b, c, or d
(abcd)	Grouping	Groups the matches in the parentheses into a reference

These are only some of the basic special chars associated with regex. They can get quite complicated pretty quickly.

```
damien@CHARON MINGW64 ~  
$ pwd  
/c/Users/damien  
  
damien@CHARON MINGW64 ~  
$ pwd | sed 's/\c/Users/damien/\c/Users/Bob/'  
/c/Users/Bob/
```

<https://regexone.com/>  
interactive tutorial for regex

Exercise 3: Matching Characters

Task

Text

Match

can



Match

man



Match

fan



Skip

dan

Skip

ran

Skip

pan

[cmf]an|

Continue >

Exercise 6: Matching Repeated Characters

Task

Text

Match

wazzzzup



Match

wazzup



Skip

wazup

waz{2,}up|

Continue >

Solve the above task to continue on to the next problem, or read the [Solution](#).

# A fairly common example

I have a big output file which is not in any conventional format and I want to generate a plot of the value of “E0”.

Things like this can be done very quickly by stringing together greps and sed or gawk.

```
[damien@matisse InSe_Sb2Te3]$ cat OUT
running on 64 total cores
distrk: each k-point on 64 cores, 1 groups
distr: one band on 8 cores, 8 groups
using from now: INCAR
vasp.5.3.3 18Dez12 (build Feb 15 2014 03:00:23) complex

POSCAR found type information on POSCAR In Sb Se Te
POSCAR found : 4 types and 30 ions
LDA part: xc-table for Pade appr. of Perdew
POSCAR, INCAR and KPOINTS ok, starting setup
WARNING: small aliasing (wrap around) errors must be expected
FFT: planning ...
WAVECAR not read
entering main loop

  N      E      dE      d eps      ncg      rms      rms(c)
DAV: 1      0.122893268265E+04      0.12289E+04      -0.58579E+04      1184      0.794E+02
DAV: 2      0.260839424513E+02      -0.12028E+04      -0.11675E+04      1248      0.245E+02
DAV: 3      -0.103492601378E+03      -0.12958E+03      -0.12735E+03      1376      0.990E+01
DAV: 4      -0.108937420232E+03      -0.54448E+01      -0.53977E+01      1424      0.201E+01
DAV: 5      -0.109151827079E+03      -0.21441E+00      -0.21425E+00      1632      0.370E+00      0.249E+01
DAV: 6      -0.105520432222E+03      0.36314E+01      -0.59424E+00      1616      0.136E+01      0.159E+01
DAV: 7      -0.105752132894E+03      -0.23170E+00      -0.91480E+00      1392      0.833E+00      0.402E+00
DAV: 8      -0.105572757757E+03      0.17938E+00      -0.62217E+00      1448      0.543E+00      0.221E+00
DAV: 9      -0.105437745690E+03      0.13501E+00      -0.22599E+00      1344      0.296E+00      0.139E+00
DAV: 10     -0.105420835044E+03      0.16911E-01      -0.17833E-01      1368      0.111E+00      0.848E-01
DAV: 11     -0.105419334362E+03      0.15007E-02      -0.39570E-02      1408      0.550E-01      0.387E-01
DAV: 12     -0.105419352913E+03      -0.18551E-04      -0.86087E-03      1424      0.277E-01      0.371E-01
DAV: 13     -0.105419244079E+03      0.10883E-03      -0.13707E-03      1408      0.126E-01      0.276E-01
DAV: 14     -0.105418777803E+03      0.46628E-03      -0.79038E-04      1168      0.870E-02      0.695E-02
DAV: 15     -0.105418674467E+03      0.10313E-03      -0.27561E-04      896      0.675E-02      0.734E-02
DAV: 16     -0.105418638479E+03      0.36197E-04      -0.10010E-04      640      0.324E-02

  1 F= -.11678187E+03 E0= -.11677904E+03 d E =-.116782E+03
curvature: 0.00 expect dE= 0.000E+00 dE for cont linesearch 0.000E+00
trial: gam= 0.00000 g(F)= 0.180E-01 g(S)= 0.000E+00 ort = 0.000E+00 (trialstep = 0.100E+01)
search vector abs. value= 0.180E-01
bond charge predicted
  N      E      dE      d eps      ncg      rms      rms(c)
DAV: 1      -0.105437350929E+03      -0.18676E-01      -0.88572E-03      1136      0.186E-01      0.633E-02
DAV: 2      -0.105437328287E+03      0.22643E-04      -0.49615E-04      1328      0.503E-02

  2 F= -.11679964E+03 E0= -.11679680E+03 d E =-.177745E-01
ZBRENT: can't locate minimum, use default step
trial-energy change: -0.017774 1.order -0.017895 -0.018049 -0.017742
step: 4.0000(harm= 58.7000) dis= 0.00661 next Energy= -117.311612 (dE=-0.530E+00)
bond charge predicted
  N      E      dE      d eps      ncg      rms      rms(c)
DAV: 1      -0.105491571579E+03      -0.54221E-01      -0.78624E-02      1136      0.552E-01      0.165E-01
DAV: 2      -0.105491742579E+03      -0.17100E-03      -0.43446E-03      1288      0.141E-01      0.827E-02
DAV: 3      -0.105491729921E+03      0.12658E-04      -0.34209E-04      1152      0.425E-02

  3 F= -.11685132E+03 E0= -.11684840E+03 d E =-.694487E-01
curvature: -2.97 expect dE= 0.464E-01 dE for cont linesearch -0.464E-01
ZBRENT: increasing interval
opt : 10.0000 next Energy= -116.946294 (dE=-0.164E+00)
bond charge predicted
  N      E      dE      d eps      ncg      rms      rms(c)
DAV: 1      -0.105591328921E+03      -0.99586E-01      -0.31497E-01      1136      0.110E+00      0.321E-01
DAV: 2      -0.105592067524E+03      -0.73860E-03      -0.16816E-02      1288      0.279E-01      0.162E-01
DAV: 3      -0.105592113945E+03      -0.46422E-04      -0.12702E-03      1360      0.776E-02      0.127E-01
DAV: 4      -0.105592091761E+03      0.22184E-04      -0.68618E-05      736      0.263E-02

  4 F= -.11694632E+03 E0= -.11694339E+03 d E =-.164452E+00
curvature: -6.08 expect dE= 0.754E-01 dE for cont linesearch -0.751E-01
```



\$grep E0 OUT

We can use **sed**

. \* is a wildcard for sed which will match anything

\$ grep E0 OUT | sed s/.\*E0=//|sed s/d.\*//

But **gawk** is the better tool here.

value is in 5<sup>th</sup> column

\$ grep E0 OUT | gawk '{print \$5}'

can also output multiple columns and perform some basic math on them. e.g,

\$ grep E0 OUT | gawk '{print \$1" "\$3-\$5}'

```
[damien@matisse InSe_Sb2Te3]$ grep E0 OUT|gawk '{print $1" "$3-$5}'
1 0.00283
2 0.00284
3 0.00292
4 0.00293
5 0.00299
6 0.00306
7 0.00281
8 0.00307
9 0.00299
10 0.0027
11 0.00235
```

```
-.11677904E+03
-.11679680E+03
-.11684840E+03
-.11694339E+03
-.11710027E+03
-.11728515E+03
-.11717763E+03
-.11731700E+03
-.11733686E+03
-.11739084E+03
-.11747260E+03
-.11753657E+03
-.11758777E+03
-.11764067E+03
-.11767466E+03
-.11773262E+03
-.11773813E+03
-.11776158E+03
-.11782072E+03
-.11788565E+03
-.11789223E+03
-.11794968E+03
-.11798444E+03
-.11798810E+03
-.11804272E+03
-.11808044E+03
-.11811290E+03
-.11811346E+03
-.11812743E+03
-.11812816E+03
-.11813491E+03
-.11813585E+03
-.11814133E+03
-.11814525E+03
-.11815374E+03
-.11815921E+03
-.11817105E+03
-.11817529E+03
-.11817658E+03
-.11818476E+03
-.11819587E+03
-.11820239E+03
```

# connecting to other computers (ssh and scp)

---

## Open a terminal on a Remote Computer

(secure shell): use **ssh username@remotehostname** to connect to a remote host. After password authentication you should have a remote shell.

## Copy a file from a Remote Computer to your own computer

(secure copy): **scp [optional arguments] source\_file destination\_file**

- if one of the files is remote, it should be specified as username@remotehostname:/path/to/file

for example,

**scp** damien@komodo.phys.rpi.edu:~/myfile.txt coolfile.txt

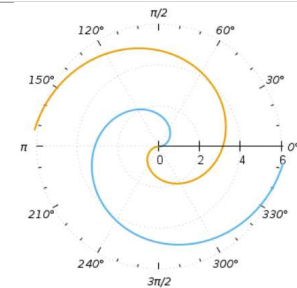
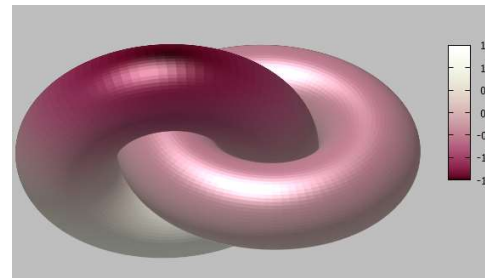
username on remote computer	remote computer name	full path to file on remote computer	name you want to give copied file on your computer
--------------------------------	----------------------	---	---

copies file “myfile.txt” from my home directory at komodo.phys.rpi.edu to my current working directory on my local computer and gives it the name “coolfile.txt”.

# gnuplot

<http://gnuplot.sourceforge.net/demo/>

```
# set terminal pngcairo transparent enhanced font "arial,10" fontsize 1.0 size 600, 400
# set output 'pm3d_lighting.2.png'
unset border
set style fill solid 1.00 noborder
set dummy u, v
unset key
set style increment default
set object 1 rect from screen 0, 0 to screen 1, 1
set object 1 behind clip lw 1.0 dashtype solid fc rgb "gray" fillstyle solid 1.00 border lt -1
set parametric
set view 236, 339, 1.245, 1
set isosamples 75, 75
unset xtics
unset ytics
unset ztics
set title "PM3D surfaces with specular highlighting"
set urange [-3.14159 : 3.14159] noreverse nowriteback
set vrange [-3.14159 : 3.14159] noreverse nowriteback
set xrange [* : *] noreverse writeback
set x2range [* : *] noreverse writeback
set yrange [* : *] noreverse writeback
set y2range [* : *] noreverse writeback
set zrange [* : *] noreverse writeback
set cbrange [* : *] noreverse writeback
set rrange [* : *] noreverse writeback
set pm3d depthorder
set pm3d lighting primary 0.5 specular 0.6
set palette rgbformulae 8, 9, 7
slice(x,y) = (x**2+y**2 < 10.0) ? 1.0 : (x**2+y**2 > 300.0) ? NaN : sin(abs(atan2(x,y)))
sinc2(x,y) = sin(sqrt(x**2+y**2))/sqrt(x**2+y**2)
flatten(x,y) = sqrt(x**2+y**2)/5.
F(x,y) = sinc2(x,y) * slice(x,y) * flatten(x,y)
## Last datafile plotted: "+"
splot cos(u)+.5*cos(u)*cos(v),sin(u)+.5*sin(u)*cos(v),.5*sin(v) with pm3d, 1*cos(u)+.5*cos(u)*cos(v),.5*sin(v),sin(u)+.5*sin(u)*cos(v) with pm3d
```



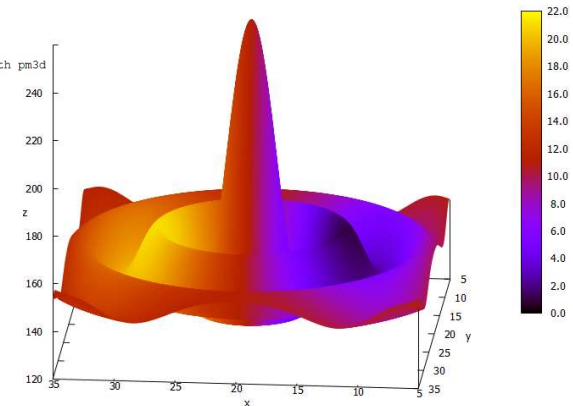
4D data (3D Heat Map)  
Independent value color-mapped onto 3D surface

4 data columns x/y/z/color

gnuplot has its own scripting language for producing high quality plots.

widely used in physics.

we will just only touch on it here.



# quick plot in gnuplot

help	exit
plot	replot
set	unset

can plot a function or data from file.

## plot a function:

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

## plot data:

```
gnuplot> plot "data.txt" (default is ugly)
```

```
gnuplot> plot "data.txt" pointtype 7 (better)
```

```
gnuplot> plot "data.txt" with lines
```

## Things you can set

```
set xrange [-pi:pi]
```

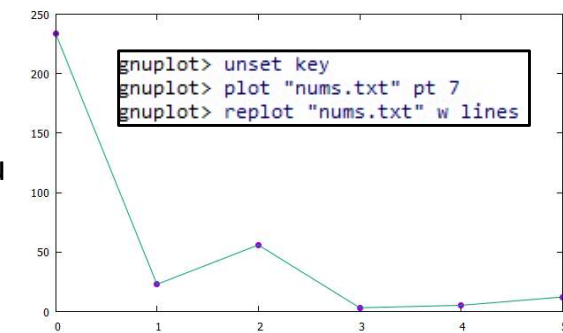
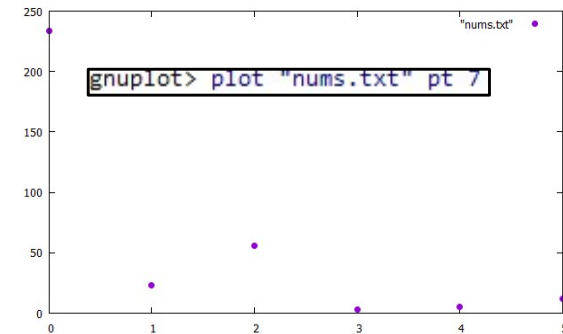
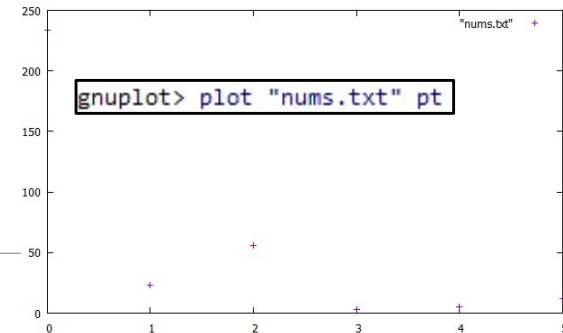
```
set yrange [-2:2.5]
```

```
set gridlines
```

```
set xtics <start>,<incr>,<end>
```

```
set terminal ... lots more
```

use **replot** to plot more than one thing, or after you have changed a setting.





# gnuplot> test terminal

different terminal  
types have formatted  
output.

set term pdf

replot will display pdf  
code to screen.

To **output to file:**

```
set term pdf
set output "out.pdf"
replot
```

