Unix introduction

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1. About this tutorial

Scientists often need to work with command line tools, organize files and move about the file system efficiently using the command line environment. This tutorial is meant to prepare command line beginners for this task. We will concentrate on learning to navigate around the file system, manage files and run programs.

2. Login

In this tutorial, we are going to use a Linux machine called "freebee.abel.uio.no". This system can be used by all UiO students and staff.

- 1. Make sure you are connected to a network. Open a command line tool on your laptop. For windows use Putty (http://www.putty.org/).
- 2. Before you log into the tutorial machine, you have to have a username and password. UiO students and staff can use their UiO credentials, others can ask the instructor for a guest account.
- 3. Log into freebee.abel.uio.no Windows:

Open Putty and type "freebee.abel.uio.no" in the host name dialog box. Press "Open". New window opens and you will be prompted for a password.



MacOS or Linux:

Use ssh command (secure shell) to log into freebee. Type "ssh <u>username@freebee.abel.uio.no</u>". You will be prompted for a password.

4. When you log in you should see the following:

```
taterim@freebee.abel.uio.no's password:
Last login: Thu Nov 7 11:33:52 2013 from malmo.uio.no
                       * FREEBEE
                       * Research Computing Services
                       * University of Oslo
                       * Freebee is part of the ABEL system
                       * URL http://uio.no/hpc/abel/
                       * Monitoring http://uio.no/hpc/abel/log
                                   http://www.abel.uio.no/ganglia/
                       * Notur http://www.notur.no
* Support hpc@usit.uio.no
                                     support-uio@notur.no
                       * See http://uio.no/hpc/abel/log/
                       * for ABEL operational messages and information
           ';:':::;:,; * Operational news:
  .+#+##++''#;:;;;;';:
 ###++#+'+#'''+;:'+;;
bash-4.1$
```

3. Command line

3.1. Shell

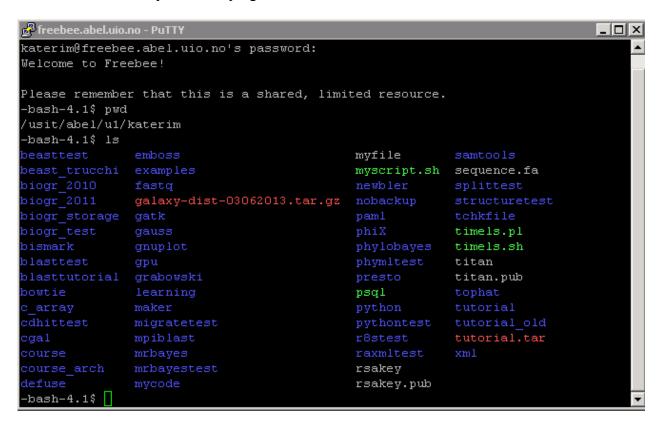
When you login into freebee, you find yourself in a "shell" (in our case the "bash shell"). Shell provides an interface between you and the operating system of the computer. The "\$" sign is the prompt and that is where you type commands. Commands are executed by pressing "Enter" at the end.

[&]quot;Command-line interfaces are often preferred by more advanced computer users, as they often provide a more concise and powerful means to control a program or operating system." Wikipedia

3.2. Directory listing

People used to graphical interfaces usually open some sort of a file manager to navigate the directories and files on their machine. In the next sections, we will learn how to do the same the command line.

To see the contents of the current directory, type "ls" (list) at the prompt. The command displays a simple list of files and directories. This output gives no details about the listed items though. The next section introduces ways to modifying the command behavior.



3.2.1. Command options

The behavior of the command ls can be changed by using options (or switches or flags). Below, you see the output of "ls -l". The option "-l" tells the list command to display each file/directory on a separate line in a "long" format. Typically, unix commands can be used with multiple flags. To learn about options available, use "man command" (e.g. for ls, type "man ls").

Note: The command "ls -l" is often shortened to "ll" for convenience.

```
bash-4.1$ ls -l
  total 265
 drwxr-xr-x
                                                                                   4 May 28 11:16 beasttest
                              2 katerim users
 drwxr-xr-x 2 katerim users
                                                                                 36 Nov 2 05:43 beast trucchi
drwxr-xr-x 23 katerim users 21 Sep 24 2012 biogr_2010
drwxr-xr-x 10 katerim users 8 Sep 24 2012 biogr_2011
                                                                              16 Sep 24 2012 biogr storage
 drwxr-xr-x 3 katerim users
drwxr-xr-x 3 katerim users
                                                                           476 Sep 24 2012 biogr test
                                                                           31 Sep 24 2012 blasttest
 drwxr-xr-x 2 katerim users

      drwxr-xr-x
      2 katerim users
      7 Sep 26 11:04 Bowtle

      drwxr-xr-x
      2 katerim users
      7 Sep 26 11:04 Bowtle

      drwxr-xr-x
      2 katerim users
      12 Sep 24 2012 c_array

      drwxr-xr-x
      2 katerim users
      8 Sep 24 2012 cdhittest

      drwxr-xr-x
      2 katerim users
      0 Apr 30 2013 cgal

      drwxr-xr-x
      4 katerim users
      26 Jun 27 16:47 course

      20 Jun 27 16:47 course
      20 Jun 27 16:47 course

 drwxr-xr-x 2 katerim users
                                                                                   7 Jun 28 12:46 blasttutorial
drwxr-xr-x 3 katerim users 239 Sep 24 2012 course arch

      drwxr-xr-x
      2 katerim users
      239 Sep 24 2012 examples

      drwxr-xr-x
      2 katerim users
      20 Aug 5 15:40 gauss

      drwxr-xr-x
      2 katerim users
      1 Sep 24 2012 gpu

      drwxr-xr-x
      2 katerim users
      7 Oct 30 11:50 grabowski

      drwxr-xr-x
      3 katerim users
      1 Sep 3 11:32 learning

      drwxr-xr-x
      4 katerim users
      26 Jun 18 15:57 migratetest
```

3.2.2. File ownership and permissions

The output of "ls –l" above produces extra information. From the left:

- permissions
- number of hard links (can be safely ignored for now)
- user name of the owner
- group that owner belongs to
- file size
- date of last modification
- file/directory name

File ownership and permissions provide control over actions performed on files and directories. In the above caption the owner is "katerim" and the group is "users". The first 10 characters on each line specify permissions (or access rights). Files (and directories) can be read (r), written into (w) or executed (x).

The permission statement consists of 10 positions: -rwxrwxrwx. The first position is reserved for a directory sign (d). Ordinary files have just a "-" sign. The next three rwx triads specify permissions for the owner, group and everyone else. Each triad holds rwx permissions always in the same order. For example, in –rwsrwxrwx statement all permissions are set and all users can read, write into and execute a file. In -rw------ statement, the file can only be read and written to by the owner.

3.3. Moving about in the directory tree – pwd, cd

3.3.1. Home directory

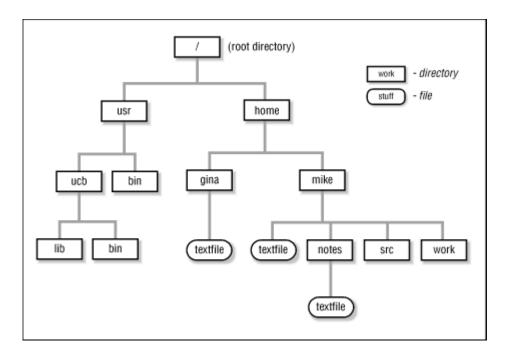
When you log into a Unix machine and open a terminal, you find yourself in your home directory. It is a place in the directory tree where you have permission to keep your directories and files. Type "pwd" (print working directory) to see your home directory. The example shows home directory belonging to the user katerim - "/usit/abel/u1/katerim".

```
-bash-4.1$ pwd
/usit/abel/u1/katerim
-bash-4.1$ [
```

3.3.2. Path

Path (e.g. - "/usit/abel/u1/katerim") specifies a position in the directory tree. There are two kinds of paths – absolute and relative.

- Absolute path always starts at at the top of the tree (at the root directory), for example "/home/username". The absolute path always starts with a "/" (root).
- The relative path is the path to the destination from your current position and it does not start with a "/".



In the figure above, you can see a simple directory tree. Let's pretend that you are Mike and when you log into the computer, you will find yourself at your home directory "/home/mike"; this directory is your current working directory.

- If you want to change working directory to directory called "work", you will type "cd work" (cd stands for change directory). By doing so you used the relative path. The way to express this operation using absolute path would be "cd /home/mike/work". In this example, using the relative paths was a more convenient way of accomplishing the task.
- Consider changing directory to the "lib" (bottom left) starting from "/home/mike". The relative path command would be "cd ../../usr/ucb/lib" while the absolute path would look like this "cd /usr/ucb/lib". Here, using the absolute path is easier.

3.3.3. Special notations

There are few special notations to remember when navigating the directories.

- Typing "cd ../" will take you one directory level up (from "/home/mike" to "/home").
- The sign "./" means current directory ("cd work" is the same as "cd ./work").
- Typing "cd" anywhere will get you to your home directory.
- You can use "~" in the path to substitute for your home directory (e.g. "cd ~/work" is the same as "cd /home/mike/work").
- Typing "cd -" will send you back where you just came from. E.g. you start at "/home/mike/src", then "cd /home/usr". When you need to go back to "/home/mike/src", type "cd -".

3.3.4. Autocompletion

Autocompletion means you do not have to type full file/directory name. If the fragment of the name you have just typed is unique, pressing TAB key will complete the name. This reduces typing and errors dramatically.

Consider that you (Mike) made a directory "/home/mike/data/results_blast_lutra". Two months later, you want to check the blast results. In your home directory, you start typing "cd data/results_blast..." and then you cannot remember the name of the experiment. Use autocompletion to see all blast directories you've made. When you have typed "cd data/results_blast" press the "Tab" key. If there is exactly one matching name, it will complete automatically. If there is more than one match, all relevant options will show when you press Tab second time.

3.3.5. Wild cards

Wildcards are symbols "*" and "?". They can be used in pattern matching. For example, "ls results_*" produces a list of items beginning with "results".

In general, "?" matches exactly one character, while "*" matches any string of any length including an empty one.

3.4. Managing your files and directories – mkdir, cp, mv, rm, rmdir

In this section, we will learn how to create, copy, move and delete directories and files. Here is the list of the key commands:

- Make a directory mkdir
- Remove directory rmdir
- Copy file cp
- Move file mv
- Delete file rm

3.4.1. Practise the commands

This section is a hands-on exercise. We'll set up a space for your tutorial and manipulate files to get comfortable with using the command line. Read the text carefully and try to replicate the highlighted commands. The screen captures demonstrate every command needed to replicate the exercise.

- 1. On freebee, make sure that you are in your home directory ("cd").
- 2. Make a directory named tutorial "mkdir tutorial" and "ls –l" to see it

```
-bash-4.1$ pwd
/usit/abel/u1/katerim
-bash-4.1$ mkdir tutorial
-bash-4.1$ ls -l
-color drwxr-xr-x 2 katerim usit 0 Nov 7 14:03 tutorial
```

3. Cd into the tutorial directory "cd tutorial" and use "pwd" to see the path. You've made a new directory for today's tutorial.

```
-bash-4.1$ cd tutorial
-bash-4.1$ pwd
/usit/abel/u1/katerim/tutorial
```

4. Place a file into the tutorial directory. The file is available elsewhere on the machine in the "/cluster/teaching/unix_tutorial" directory. You can copy this file to your tutorial directory by using "cp /cluster/teaching/unix_tutorial/sequence.fa." Note that the command ends with "a space and a dot".

The last "dot" is important because the copy command requires a source and destination path. The source is "/cluster/teaching/unix_tutorial/sequence.fa" and the destination is the current directory or ".".

You can check if you got the file by listing the directory content (ls or ll) and you can see the file content using "cat sequence.fa" (more about cat later).

```
bash-4.1$ cp /cluster/teaching/unix tutorial/sequence.fa .
bash-4.1$ 11
total 1
-rw-r--r-- 1 katerim usit 875 Mar 20 16:04 sequence.fa
-bash-4.1$ cat sequence.fa
oqi|340011|qb|AAA61239.1| kinase=
MNKVRDIKNKFKNEDLTDELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIGRYSQAIE
ALPPDKYGQNESFARIQVRFAELKAIQEPDDARDYFQMARANCKKFAFVHISFAQFELSQGNVKKSKQLLQKAVERGAVI
LEMLEIALRNLNLQKKQLLSEEEKKNLSASTVLTAQESFSGSLGHLQNRNNSCDSRGQTTKARFLYGENMPPQDAEIGYF
NSLRQTNKTKQSCPFGRVPVNLLNSPDCDVKTDDSVVPCFMKRQTSRSECRDLVVPGSKPSGNDSCELRNLKSVQNSHFF
EPLVSDEKSSELIITDSITLKNKTESSLLAKLEETKEYQEPEVPESNQKQWQAKRKSECINQNPAASSNHWQIPELARKV
NTEQKHTTFEQPVFSVSKQSPPISTSKWFDPKSICKTPSSNTLDDYMSCFRTPVVKNDFPPACQLSTPYGQPACFQQQQH
QILATPLQNLQVLASSSANECISVKGRIYSILKQIGSGGSSKVFQVLNEKKQIYAIKYVNLEEADNQTLDSYRNEIAYLN
KLQQHSDKIIRLYDYEITDQYIYMVMECGNIDLNSWLKKKKSIDPWERKSYWKNMLEAVHTIHQHGIVHSDLKPANFLI\
DGMLKLIDFGIANQMQPDTTSVVKDSQVGTVNYMPPEAIKDMSSSRENGKSKSKISPKSDVWSLGCILYYMTYGKTPFQQ
IINQISKLHAIIDPNHEIEFPDIPEKDLQDVLKCCLKRDPKQRISIPELLAHPYVQIQTHPVNQMAKGTTEEMKYVLGQI
VGLNSPNSILKAAKTLYEHYSGGESHNSSSSKTFEKKRGKK
-bash-4.1$
```

5. To practise copy command some more, make a backup of the sequence.fa file. Type "cp sequence.fa sequence_copy.fa". List the directory content to see what happened. The contents of the original file were copied to a new one and the directory now contains two files.

```
-bash-4.1$ cp sequence.fa sequence_copy.fa
-bash-4.1$ ll
total 2
-rw-r--r-- 1 katerim usit 875 Mar 20 16:05 sequence_copy.fa
-rw-r--r-- 1 katerim usit 875 Mar 20 16:04 sequence.fa
-bash-4.1$ [
```

6. After looking at the directory listing, you decide that the sequence_copy.fa is not informative enough and you that you want to change the name. This can be done using the mv command (or move). Type "mv sequence_copy.fa sequence_orig.fa". As with the copy command, the move command requires target and destination paths.

```
-bash-4.1$ mv sequence_copy.fa sequence_orig.fa
-bash-4.1$ 11
total 2
-rw-r--r-- 1 katerim usit 875 Mar 20 16:04 sequence.fa
-rw-r--r-- 1 katerim usit 875 Mar 20 16:05 sequence_orig.fa
-bash-4.1$ [
```

7. In the tutorial directory, make a subdirectory "backup" and place your backup sequence file there. Type "mkdir backup" and "mv sequence_orig.fa backup/". Check what you did by "ll backup/". Note: this is the first time we use the list command with a path. The directory listed is the one specified by the path.

```
-bash-4.1$ mkdir backup
-bash-4.1$ mv sequence_orig.fa backup/
-bash-4.1$ ll backup/
total 1
-rw-r--r-- 1 katerim usit 875 Mar 20 16:05 sequence_orig.fa
-bash-4.1$ [
```

8. We have learned to manipulate individual files. In the next steps, we'll try to manipulate whole directories.

Let's pretend that this is not the only tutorial you are attending today and you realize that you don't want to have many tutorial directories in your home area. You want to make one directory called "learning" in your home and then move the existing tutorial directory (and all its content) into learning. We'll proceed cautiously, first we copy the files and if all is right, we delete the original ones.

Return to your home directory (remember a simple "cd" will do). Type "mkdir learning". Use the copy command to replicate the entire contents of the tutorial directory tree by typing "cp —a tutorial/ learning/". Examine your action by using the list command. Note: we used "-a" option for the copy command. The —a option turns on recursive mode and preserves all properties of the files.

```
-bash-4.1$
-bash-4.1$ cd
-bash-4.1$ mkdir learning
-bash-4.1$ cp -a tutorial/ learning/
-bash-4.1$ ll learning
total 1
drwxr-xr-x 3 katerim usit 2 Mar 20 16:08 tutorial
-bash-4.1$ ll learning/tutorial/
total 2
drwxr-xr-x 2 katerim usit 1 Mar 20 16:08 backup
-rw-r--r- 1 katerim usit 875 Mar 20 16:04 sequence.fa
-bash-4.1$ ll learning/tutorial/backup/
total 1
-rw-r--r- 1 katerim usit 875 Mar 20 16:05 sequence_orig.fa
-bash-4.1$ []
```

9. We made sure that the all files were copied properly and now we can delete the original "~/tutorial" directory and its contents. There is a fast way to do this, but for the sake of the tutorial, we start deleting in steps.

From you home directory, type "rm tutorial/backup/sequence_orig.fa" to get rid of you original sequence backup. Check the outcome by "ls –l tutorial/backup". Next, get rid of the original backup directory by "rmdir tutorial/backup/". Check the outcome by "ls –l tutorial/".

As said, it is possible to delete the whole directory subtree using one command. This is to be used with caution. Type "rm –ri tutorial/". The –r option turns on recursive mode, the tutorial directory and all its contents will be removed. As this could be dangerous, I added –i option that turns on interactive mode. See in the capture below how this works. The command asks the user to agree with each delete first.

```
-bash-4.1$ pwd
usit/abel/u1/katerim
-bash-4.1$ rm tutorial/backup/sequence orig.fa
-bash-4.1$ ll tutorial/backup/
total 0
-bash-4.1$ rmdir tutorial/backup/
-bash-4.1$ ll tutorial
total 1
-rw-r--r-- 1 katerim usit 875 Mar 20 16:04 sequence.fa
-bash-4.1$
-bash-4.1$
-bash-4.1$
-bash-4.1$ rm -ri tutorial
rm: descend into directory `tutorial'? y
rm: remove regular file `tutorial/sequence.fa'? y
rm: remove directory `tutorial'? y
-bash-4.1$
```

10. An alternative way of viewing your files and directories is using the "tree" command. Type "cd" and "tree learning" to see the whole directory tree so far.

```
-bash-4.1$ tree learning
learning
âââ tutorial
âââ backup
â Â âââ sequence_orig.fa
âââ sequence.fa

2 directories, 2 files
```

3.5. Editing your files

There are two types of files on your computer.

- text files that are human-readable (e.g. FASTA sequences)
- binary files that contain many more special characters and not easily readable (e.g. a computer program)

The command "file" returns information about the file type. Type "file learning/tutorial/sequence.fa" to see an output for a text file. Type "file /bin/ls" to find the type of the list command to see an executable or binary type.

```
-bash-4.1$
-bash-4.1$ file learning/tutorial/sequence.fa
learning/tutorial/sequence.fa: ASCII text, with very long lines
-bash-4.1$
-bash-4.1$
-bash-4.1$ file /bin/ls
/bin/ls: ELF 64-bit LSB executable, x86-64, version 1 (SYSV), dynamically linked
(uses shared libs), for GNU/Linux 2.6.18, stripped
-bash-4.1$
```

3.5.1. Display a contents of a text file – cat, more, less

There are several commands for displaying the content of a file:

- cat
- less
- more

Use all three to view the contents of sequence.fa file by typing "cd learning/tutorial", "more sequence.fa" and "cat sequence.fa". You will notice that the less command behaves differently than the others. In case of larger files, it allows scrolling up and down. Most importantly it allows searching. Type "q" to quit the less command.

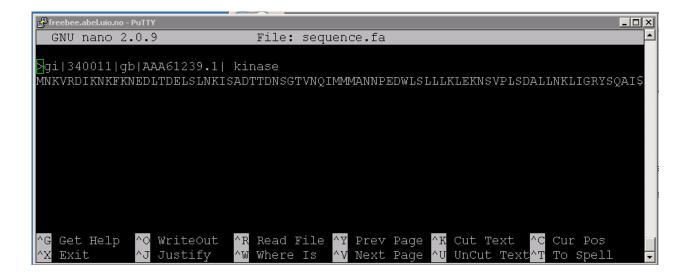
```
-bash-4.1$
-bash-4.1$ cat learning/tutorial/sequence.fa
>gi|340011|gb|AAA61239.1| kinase
MNKVRDIKNKFKNEDLTDELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIGRYSQAIE
ALPPDKYGQNESFARIQVRFAELKAIQEPDDARDYFQMARANCKKFAFVHISFAQFELSQGNVKKSKQLLQKAVERGAVP
LEMLEIALRNLNLQKKQLLSEEEKKNLSASTVLTAQESFSGSLGHLQNRNNSCDSRGQTTKARFLYGENMPPQDAEIGYR
NSLRQTNKTKQSCPFGRVPVNLLNSPDCDVKTDDSVVPCFMKRQTSRSECRDLVVPGSKPSGNDSCELRNLKSVQNSHFK
EPLVSDEKSSELIITDSITLKNKTESSLLAKLEETKEYQEPEVPESNQKQWQAKRKSECINQNPAASSNHWQIPELARKV
NTEQKHTTFEQPVFSVSKQSPPISTSKWFDPKSICKTPSSNTLDDYMSCFRTPVVKNDFPPACQLSTPYGQPACFQQQQH
QILATPLQNLQVLASSSANECISVKGRIYSILKQIGSGGSSKVFQVLNEKKQIYAIKYVNLEEADNQTLDSYRNEIAYLN
KLQQHSDKIIRLYDYEITDQYIYMVMECGNIDLNSWLKKKKSIDPWERKSYWKNMLEAVHTIHQHGIVHSDLKPANFLIV
DGMLKLIDFGIANQMQPDTTSVVKDSQVGTVNYMPPEAIKDMSSSRENGKSKSKISPKSDVWSLGCILYYMTYGKTPFQQ
IINQISKLHAIIDPNHEIEFPDIPEKDLQDVLKCCLKRDPKQRISIPELLAHPYVQIQTHPVNQMAKGTTEEMKYVLGQL
VGLNSPNSILKAAKTLYEHYSGGESHNSSSSKTFEKKRGKK
-bash-4.15
```

If you have a very large file and only want to check a part of it, use "head" and "tail" command. These commands accept an option that specifies a number of lines to be displayed.

3.5.2. Edit a file - nano

Today we'll use a simple text editor called nano. Change directory to ~/learning/tutorial and start a simple text editor by typing "nano sequence.fa". You will see the file contents and also menu options on the bottom. You can navigate the text using arrow keys. The basic operations are "ctrl O" to save and "ctrl X" to quit the editor. When saving or exiting, you are asked to confirm the operation with "Enter". Open the editor and try out the basic operations |(listed below). As an exercise, add some mock text (preferable protein sequences) at the end of the file. Here is an example:

>gi|1111|gb|AA2322|liase DELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIG >gi|2222|gb|AA5657|dehydrogenase LKLEKNSVPLSDALLNKLIGRYSQA



Help

^G Nano help (^X to return to edit mode)

Navigation

- ^A move to beginning of line
- ^E move to end of line
- **^Y** move down a page
- **^V** move up a page
- ^_ move to a specific line (^_^V moves to the top of the file, ^_^Y to the bottom)
- ^C find out what line the cursor is currently on
- **^W** search for some text.

Saving and Exiting

- ^O save contents without exiting (you will be prompted for a file to save to)
- ^X exit nano (you will be prompted to save your file if you haven't)
- ^T when saving a file, opens a browser that allows you to select a file name from a list of files and directories

(source http://mintaka.sdsu.edu/reu/nano.html)

3.5.3. Manipulate file content - diff, grep, sort, uniq

"Diff" is used for comparing file contents (text and binary). Type "diff sequence.fa backup/sequence_orig.fa"; this compares the sequence file and the backup that you made earlier. All modifications that you introduced using nano (and saved) will show.

```
-bash-4.1$ cat sequence.fa
>gi|340011|gb|AAA61239.1| kinase
MNKVRDIKNKFKNEDLTDELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIGRYSQAIE
ALPPDKYGQNESFARIQVRFAELKAIQEPDDARDYFQMARANCKKFAFVHISFAQFELSQGNVKKSKQLLQKAVERGAVF
LEMLEIALRNLNLQKKQLLSEEEKKNLSASTVLTAQESFSGSLGHLQNRNNSCDSRGQTTKARFLYGENMPPQDAEIGYF
NSLRQTNKTKQSCPFGRVPVNLLNSPDCDVKTDDSVVPCFMKRQTSRSECRDLVVPGSKPSGNDSCELRNLKSVQNSHFF
EPLVSDEKSSELIITDSITLKNKTESSLLAKLEETKEYQEPEVPESNQKQWQAKRKSECINQNPAASSNHWQIPELARKV
NTEQKHTTFEQPVFSVSKQSPPISTSKWFDPKSICKTPSSNTLDDYMSCFRTPVVKNDFPPACQLSTPYGQPACFQQQQF
QILAT PLQNLQVLASSSANECISVKGRIYSILKQIGSGGSSKVFQVLNEKKQIYAIKYVNLEEADNQTLDSYRNEIAYLN
KLQQHSDKIIRLYDYEITDQYIYMVMECGNIDLNSWLKKKKSIDPWERKSYWKNMLEAVHTIHQHGIVHSDLKPANFLI\
DGMLKLIDFGIANQMQPDTTSVVKDSQVGTVNYMPPEAIKDMSSSRENGKSKSKISPKSDVWSLGCILYYMTYGKTPFQQ
IINQISKLHAIIDPNHEIEF PDI PEKDLQDVLKCCLKRDPKQRISI PELLAHPYVQIQTHPVNQMAKGTTEEMKYVLGQI
VGLNSPNSILKAAKTLYEHYSGGESHNSSSSKTFEKKRGKK
>gi|1111|gb|AA2322|liase
DELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIG
>gi|2222|gb|AA5657|dehydrogenase
LKLEKNSVPLSDALLNKLIGRYSQA
bash-4.1$
bash-4.1$
bash-4.1$
bash-4.1$ diff sequence.fa backup/sequence 1211.fa
 >gi|340011|gb|AAA61239.1| kinase
  >gi|340011|gb|AAA61239.1| kinase
 >gi|1111|gb|AA2322|liase
 DELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIG
 >gi|2222|gb|AA5657|dehydrogenase
 LKLEKNSVPLSDALLNKLIGRYSQA
-bash-4.1$
```

"Grep" is used to find a pattern in a file. Type "grep "LIGR" sequence.fa" and if the pattern is found, the whole line from the target file is shown in the output.

Note: if the pattern does not contain any white space or special characters, you can skip the quotes. Grep has many useful options, for example "–i" turns on text insensitive mode ("grep –i ligr sequence.fa") produces the same result as "grep LIGR sequence.fa").

```
-bash-4.1$ grep --color LIGR sequence.fa

MNKVRDIKNKFKNEDLTDELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIGRYSQAIE
ALPPDKYGQNESFARIQVRFAELKAIQEPDDARDYFQMARANCKKFAFVHISFAQFELSQGNVKKSKQLLQKAVERGAVP
LEMLEIALRNLNLQKKQLLSEEKKNLSASTVLTAQESFSGSLGHLQNRNNSCDSRGQTTKARFLYGENMPPQDAEIGYR
NSLRQTNKTKQSCPFGRVPVNLLNSPDCDVKTDDSVVPCFMKRQTSRSECRDLVVPGSKPSGNDSCELRNLKSVQNSHFK
EPLVSDEKSSELIITDSITLKNKTESSLLAKLEETKEYQEPEVPESNQKQWQAKRKSECINQNPAASSNHWQIPELARKV
NTEQKHTTFEQPVFSVSKQSPPISTSKWFDPKSICKTPSSNTLDDYMSCFRTPVVKNDFPPACQLSTPYGQPACFQQQQH
QILATPLQNLQVLASSSANECISVKGRIYSILKQIGSGGSSKVFQVLNEKKQIYAIKYVNLEEADNQTLDSYRNEIAYLN
KLQQHSDKIIRLYDYEITDQYIYMVMECGNIDLNSWLKKKKSIDPWERKSYWKNMLEAVHTIHQHGIVHSDLKPANFLIV
DGMLKLIDFGIANQMQPDTTSVVKDSQVGTVNYMPPEAIKDMSSSRENGKSKSKISPKSDVWSLGCILYYMTYGKTPFQQ
IINQISKLHAIIDPNHEIEFPDIPEKDLQDVLKCCLKRDPKQRISIPELLAHPYVQIQTHPVNQMAKGTTEEMKYVLGQL
VGLNSPNSILKAAKTLYEHYSGGESHNSSSSKTFEKKRGKK
LKLEKNSVPLSDALLNKLIGRYSQA
-bash-4.1$
```

Sorting of the file content is done using the "sort" command. Type "sort sequence.fa". Examine the output, as expected the sequence was sorted alphabetically by lines. Note: -n option enables numerical sorting, sorting by column (and much more) is also possible

```
-bash-4.1$ sort sequence.fa
DELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIG
gi|1111|gb|AA2322|liase
>gi|2222|gb|AA5657|dehydrogenase
>gi|340011|gb|AAA61239.1| kinase
LKLEKNSVPLSDALLNKLIGRYSQA
MNKVRDIKNKFKNEDLTDELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIGRYSQAIE
<u>ALPPDKYGQNESFARIQVRFAELKAIQEPDDARDYFQMARANCKKFAFVHISFAQFELSQGNVKKSKQLLQKAVERGAV</u>
LEMLEIALRNLNLQKKQLLSEEEKKNLSASTVLTAQESFSGSLGHLQNRNNSCDSRGQTTKARFLYGENMPPQDAEIGYF
NSLRQTNKTKQSCPFGRVPVNLLNSPDCDVKTDDSVVPCFMKRQTSRSECRDLVVPGSKPSGNDSCELRNLKSVQNSHFK
EPLVSDEKSSELIITDSITLKNKTESSLLAKLEETKEYQEPEVPESNQKQWQAKRKSECINQNPAASSNHWQIPELARKV
NTEQKHTTFEQPVFSVSKQSPPISTSKWFDPKSICKTPSSNTLDDYMSCFRTPVVKNDFPPACQLSTPYGQPACFQQQQH
QILATPLQNLQVLASSSANECISVKGRIYSILKQIGSGGSSKVFQVLNEKKQIYAIKYVNLEEADNQTLDSYRNEIAYLN
KLQQHSDKIIRLYDYEITDQYIYMVMECGNIDLNSWLKKKKSIDPWERKSYWKNMLEAVHTIHQHGIVHSDLKPANFLIV
DGMLKLIDFGIANQMQPDTTSVVKDSQVGTVNYMPPBAIKDMSSSRENGKSKSKISPKSDVWSLGCILYYMTYGKTPFQQ
IINQISKLHAIIDPNHEIEFPDIPEKDLQDVLKCCLKRDPKQRISIPELLAHPYVQIQTHPVNQMAKGTTEEMKYVLGQI
/GLNSPNSILKAAKTLYEHYSGGESHNSSSSKTFEKKRGKK
bash-4.1$
```

To use the "uniq" command that removes repeated lines from a file. To demonstrate this, we have to edit the sequence.fa file. Open the file in nano and add some lines, make sure that some of the lines are the same (they do not have to be very long). Type "sort sequence.fa | uniq" and examine the content. The repeated lines have been omitted.

```
-bash-4.1$ cat sequence.fa
>gi|340011|gb|AAA61239.1| kinase
MNKVRDIKNKFKNEDLTDELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIGRYSQAIE
ALPPDKYGQNESFARIQVRFAELKAIQEPDDARDYFQMARANCKKFAFVHISFAQFELSQGNVKKSKQLLQKAVERGAVF
LEMLEIALRNLNLQKKQLLSEEEKKNLSASTVLTAQESFSGSLGHLQNRNNSCDSRGQTTKARFLYGENMPPQDAEIGYF
NSLRQTNKTKQSCPFGRVPVNLLNSPDCDVKTDDSVVPCFMKRQTSRSECRDLVVPGSKPSGNDSCELRNLKSVQNSHFF
EPLVSDEKSSELIITDSITLKNKTESSLLAKLEETKEYQEPEVPESNQKQWQAKRKSECINQNPAASSNHWQIPELARKV
NTEQKHTTFEQPVFSVSKQSPPISTSKWFDPKSICKTPSSNTLDDYMSCFRTPVVKNDFPPACQLSTPYGQPACFQQQQF
QILAT PLONLQVLASSSANECISVKGRIYSILKQIGSGGSSKVFQVLNEKKQIYAIKYVNLEEADNQTLDSYRNEIAYLN
KLQQHSDKIIRLYDYEITDQYIYMVMECGNIDLNSWLKKKKSIDPWERKSYWKNMLEAVHTIHQHGIVHSDLKPANFLI\
DGMLKLIDFGIANQMQPDTTSVVKDSQVGTVNYMPPEAIKDMSSSRENGKSKSKISPKSDVWSLGCILYYMTYGKTPFQÇ
IINQISKLHAIIDPNHEIEFPDIPEKDLQDVLKCCLKRDPKQRISIPELLAHPYVQIQTHPVNQMAKGTTEEMKYVLGQI
VGLNSPNSILKAAKTLYEHYSGGESHNSSSSKTFEKKRGKK
gi|1111|gb|AA2322|liase
DELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIG
gi|2222|gb|AA5657|dehydrogenase
LKLEKNSVPLSDALLNKLIGRYSQA
gi|1111|gb|AA2322|liase
DELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIG
 bash-4.1$
```

```
bash-4.1$ sort sequence.fa | uniq
DELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIG
gi|1111|gb|AA2322|liase
gi|2222|gb|AA5657|dehydrogenase
gi|340011|gb|AAA61239.1| kinase
LKLEKNSVPLSDALLNKLIGRYSQA
MNKVRDIKNKFKNEDLTDELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIGRYSQAIE
ALPPDKYGQNESFARIQVRFAELKAIQEPDDARDYFQMARANCKKFAFVHISFAQFELSQGNVKKSKQLLQKAVERGAVI
LEMLEIALRNLNLQKKQLLSEEEKKNLSASTVLTAQESFSGSLGHLQNRNNSCDSRGQTTKARFLYGENMPPQDAEIGYF
NSLRQTNKTKQSCPFGRVPVNLLNSPDCDVKTDDSVVPCFMKRQTSRSECRDLVVPGSKPSGNDSCELRNLKSVQNSHFF
EPLVSDEKSSELIITDSITLKNKTESSLLAKLEETKEYQEPEVPESNQKQWQAKRKSECINQNPAASSNHWQIPELARK\
NTEQKHTTFEQPVFSVSKQSPPISTSKWFDPKSICKTPSSNTLDDYMSCFRTPVVKNDFPPACQLSTPYGQPACFQQQQH
QILATPLQNLQVLASSSANECISVKGRIYSILKQIGSGGSSKVFQVLNEKKQIYAIKYVNLEEADNQTLDSYRNEIAYLN
KLQQHSDKIIRLYDYBITDQYIYMVMBCGNIDLNSWLKKKKSIDPWERKSYWKNMLEAVHTIHQHGIVHSDLKPANFLI\
DGMLKLIDFGIANQMQPDTTSVVKDSQVGTVNYMPPEAIKDMSSSRENGKSKSKISPKSDVWSLGCILYYMTYGKTPFQÇ
IINQISKLHAIIDPNHEIEF PDI PEKDLQDVLKCCLKRDPKQRISI PELLAHPYVQIQTHPVNQMAKGTTBEMKYVLGQI
/GLNSPNSILKAAKTLYEHYSGGESHNSSSSKTFEKKRGKK
bash-4.1$
```

3.6. Little extra - get your bearings

This section is for the more curious of you. When you log into a new machine, it might be useful to get some basic information about this computer.

- What is the name of the machine? Type "hostname".
- What operating system is this? Type "uname -a".
- To find out what is your user name type "whoami".
- The information about the cpus and memory is stored in /proc/cpuinf and /proc/meminfo respectively.

The tutorial machines is called freebee.abel.uio.no, it is a Linux machine and has 32 cpus and 64GB or RAM.

4. Programs and parameters

4.1. Computer program

A computer program is sequence of instructions written to perform a specified task. Computer programs can be separated into the system software and application software. System software is responsible for running your computer while application packages are used, for example, for data analysis.

Each program consists of a source code written in a programming language. Some languages (C or Fortran) require compilation to produce an executable binary program. Scripting languages (such as Python or Perl) are executed using an interpreter during the run-time.

4.2. New program?

When you download a program, read instructions carefully to see if you have a binary code, source code that requires compilation or perhaps a script that requires an interpreter.

- In case of a binary code, it is essential that you get a package that was compiled on the same computer platform as you intend to use. Binaries differ for different flavors of Unix and also for different versions of Windows and MacOS. It is customary to offer various platform binaries when a package is distributed in this manner.
- When you download a source code, you have to compile it. Compilation in general requires a compiler, the open source versions are called gcc, g++ and g95 (for C, C++ and Fortran respectively). Proprietary compilers are produced e.g. by Intel. Before you compile, look for instructions in the source code (or online).
- Programs written in a scripting language require an interpreter/program such "perl" or "python" (open source and easily installed on various platforms). No compilation is required, the source code is executed through an interpreter.

4.3. Executing a program

Check the permissions associated with the file that holds your program. No program will run without the executable ("x") permission being set. The program is made executable using "chmod a+x" command (this make the program executable for all users). Executable program is executed by typing its name including the absolute or relative path. Path has to be specified even in the case when the program is in your current directory, then you call your program with "./program_name".

You can call your program from any directory on your machine using just its name and no path (similarly to Linux system commands) when the system knows where to find it. The system will always find the program if it is installed in a directory that is included in the "PATH" variable.

4.4. PATH

PATH is an environment variable. Environment variables are part of your shell environment and they might include information about your home directory, mail program, temporary files location, shell type etc.

PATH holds a list of directories that are checked every time a command is used without a full path. Type "echo \$PATH" to see which directories are in your path.

```
-bash-4.1$ echo $PATH
/usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sb
in:/opt/bin
-bash-4.1$ [
```

To find out if a command is in a path, type "which". For example, you want to compile a C program and are wondering if you have a C compiler (gcc). Type "which gcc" to find out. The compiler is installed in "/usr/bin" directory.

```
-bash-4.1$ which gcc
/usr/bin/gcc
-bash-4.1$ [
```

If there is no gcc compiler in the path, you have two options. You can look for it on your computer (e.g. using the find command) or you can install it.

When you know the location of the gcc command, add it to the PATH. Let's pretend that you installed the compiler to the "/home/katerim/sbin" directory. Type "export PATH=\$PATH:/home/katerim/sbin" to edit your PATH. This command appends new value to the existing PATH variable. Check the value of PATH using "echo \$PATH" before and after the operation.

```
-bash 4.1$ echo $PATH
/usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sb
in:/opt/bin
-bash-4.1$ export PATH=$PATH:/usit/abel/u1/katerim/sbin
-bash-4.1$ echo $PATH
/usr/lib64/qt-3.3/bin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sb
in:/opt/bin:/usit/abel/u1/katerim/sbin
-bash-4.1$
```

4.5. Program options

As we have seen with Unix commands, options modify the program behavior. Most of the software packages have available options. Sometimes, options require arguments (or values).

The program might be called with a command line such as this: "command –i infile –o outfile –b T –a 5".

- "-i" option takes input file as argument
- "-o" option takes output file as argument
- "-b" accepts Boolean argument (True or False)
- "-a" accepts integer arguments

Knowing the options (and the type of arguments) is necessary to constructing a command that will execute the program. Often, typing "-h" or "--help" after the command shows the available options and expected arguments.

On freebee (and on the computer cluster Abel) you can use a module command to manage you path. Use "module load blast+" to modify your path so the blast+ program is available.

```
-bash-4.15 echo $PATH
/usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sb
in:/opt/bin
```

```
-bash-4.1$ module load blast+
-bash-4.1$ echo $PATH
/cluster/software/VERSIONS/blast+-2.2.26/bin:/usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/bin:/usr/bin:/usit/abel/u1/katerim/sbin
-bash-4.1$ 
\begin{align*}
\text{\left}
```

Type "blastp -h" (a program from the blast+ suite) to see what options are available for the blastp program.

```
-bash-4.1$ blastp -h
USAGE
  blastp [-h] [-help] [-import_search_strategy filename]
     [-export_search_strategy filename] [-task task_name] [-db database_name]
     [-dbsize num_letters] [-gilist filename] [-seqidlist filename]
     [-negative_gilist filename] [-entrez_query entrez_query]
     [-negative_gilist filename] [-entrez_query entrez_query]
[-db_soft_mask filtering_algorithm] [-db_hard_mask filtering_algorithm]
[-subject subject_input_file] [-subject_loc range] [-query input_file]
[-out output_file] [-evalue evalue] [-word_size int_value]
[-gapopen open_penalty] [-gapextend extend_penalty]
[-xdrop_ungap float_value] [-xdrop_gap float_value]
[-xdrop_gap_final float_value] [-searchsp int_value]
[-max_hsps_per_subject int_value] [-seg SEG_options]
     [-soft_masking soft_masking] [-matrix matrix_name]
     [-threshold float_value] [-culling_limit int_value]
     [-best_hit_overhang float_value] [-best_hit_score_edge float_value]
     [-window size int value] [-lcase masking] [-query loc range]
     [-parse deflines] [-outfmt format] [-show qis]
     [-num descriptions int_value] [-num_alignments int_value] [-html]
     [-max target seqs num sequences] [-num threads int value] [-ungapped]
     [-remote] [-comp based stats compo] [-use sw tback] [-version]
DESCRIPTION
   Protein-Protein BLAST 2.2.26+
Use '-help' to print detailed descriptions of command line arquments
```

4.6. Managing command output

Unless specified by a program option, results are shown onto the screen (a.k.a standard output). When the output is large or needs to be saved, this is not very useful. This section deals with redirecting the program output.

4.6.1. Paging though output

If you want to see the output on the screen but it is too large to fit, use "command | less" construct. The first page of the command output appears and the scrolling stops. Use the arrow keys to move up and down the output. Type "blastp -help | less" to try this out.

4.6.2. Pipeline

Pipeline utility takes an output of a command and passes it to a second command as an input. This is accomplished using the "|" pipe sign between commands. This utility can be used to string together several commands. We will illustrate this on our sequence fa file. If you have not done so earlier, edit the sequence fa file using nano and add another imaginary sequence entry (including the sequence description line that starts with ">gi"). The figure below shows an example.

```
_ | _ | × |
 -bash-4.1$ cat sequence.fa
 gi|340011|gb|AAA61239.1| kinase
 MNKVRDIKNKFKNEDLTDELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIGRYSQAIE
ALPPDKYGQNESFARIQVRFAELKAIQEPDDARDYFQMARANCKKFAFVHISFAQFELSQGNVKKSKQLLQKAVERGAVF
LEMLEIALRNLNLQKKQLLSEEEKKNLSASTVLTAQESFSGSLGHLQNRNNSCDSRGQTTKARFLYGENMPPQDAEIGYF
NSLRQTNKTKQSCPFGRVPVNLLNSPDCDVKTDDSVVPCFMKRQTSRSECRDLVVPGSKPSGNDSCELRNLKSVQNSHFK
EPLVSDEKSSELIITDSITLKNKTESSLLAKLEETKEYQEPEVPESNQKQWQAKRKSECINQNPAASSNHWQIPELARKV
NTEQKHTTFEQPVFSVSKQSPPISTSKWFDPKSICKTPSSNTLDDYMSCFRTPVVKNDFPPACQLSTPYGQPACFQQQQH
QILATPLQNLQVLASSSANECISVKGRIYSILKQIGSGGSSKVFQVLNEKKQIYAIKYVNLEEADNQTLDSYRNEIAYLN
KLQQHSDKIIRLYDYEITDQYIYMVMECGNIDLNSWLKKKKSIDPWERKSYWKNMLEAVHTIHQHGIVHSDLKPANFLIV
DGMLKLIDFGIANQMQPDTTSVVKDSQVGTVNYMPPEAIKDMSSSRENGKSKSKISPKSDVWSLGCILYYMTYGKTPFQQ
IINQISKLHAIIDPNHEIEFPDIPEKDLQDVLKCCLKRDPKQRISIPELLAHPYVQIQTHPVNQMAKGTTEEMKYVLGQI
VGLNSPNSILKAAKTLYEHYSGGESHNSSSSKTFEKKRGKK
>gi|23433|gb|RTTT5656|ligase
old 	imes 	imes
 >gi|6575|gb|RESDD666|dehydrogenase
 LKLEKNSVPLSDALLNKLIGRY
```

Type "diff sequence.fa backup/sequence_1211.fa | grep ">gi"". What happened? The first command takes a difference between two files. The second command grabs the output of diff and filters out only the lines starting with ">gi" or definition lines. This simple operation can be quite useful for a scientist who wants to compare two biological sequence files without having to look through long sequences.

```
-bash-4.1$ diff sequence.fa backup/sequence_1211.fa | grep ">gi"
< >gi|1111|gb|AA2322|liase
< >gi|2222|gb|AA5657|dehydrogenase
< >gi|1111|gb|AA2322|liase
-bash-4.1$ [
```

4.6.3. Redirecting standard output

Often, we want to capture the output of a computation into a file. If your software does not provide an option for storing results in a file and prints to the screen, use greater than sign ">" to redirect the output to a file. The statement "command > file name" stores the command output in a file.

As an example, use grep on the sequence file to find a sequence pattern. Type "grep SEEEK sequence.fa" and the output shows on the screen. Type "grep SEEEK sequence.fa > seeek.txt" to capture output to a file named seeek.txt.

```
-bash-4.1$ grep SEEEK sequence.fa > seeek.txt

-bash-4.1$ cat seeek.txt

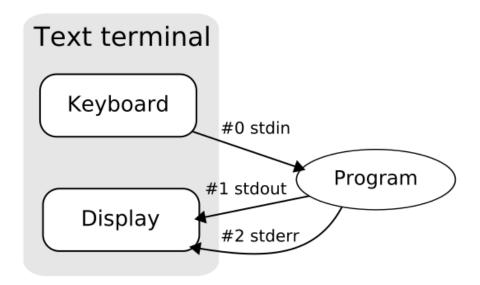
MNKVRDIKNKFKNEDLTDELSLNKISADTTDNSGTVNQIMMMANNPEDWLSLLLKLEKNSVPLSDALLNKLIGRYSQAIE
ALPPDKYGQNESFARIQVRFAELKAIQEPDDARDYFQMARANCKKFAFVHISFAQFELSQGNVKKSKQLLQKAVERGAVP
LEMLEIALRNLNLQKKQLLSEEEKKNLSASTVLTAQESFSGSLGHLQNRNNSCDSRGQTTKARFLYGENMPPQDAEIGYR
NSLRQTNKTKQSCPFGRVPVNLLNSPDCDVKTDDSVVPCFMKRQTSRSECRDLVVPGSKPSGNDSCELRNLKSVQNSHFK
EPLVSDEKSSELIITDSITLKNKTESSLLAKLEETKEYQEPEVPESNQKQWQAKRKSECINQNPAASSNHWQIPELARKV
NTEQKHTTFEQPVFSVSKQSPPISTSKWFDPKSICKTPSSNTLDDYMSCFRTPVVKNDFPPACQLSTPYGQPACFQQQQH
QILATPLQNLQVLASSSANECISVKGRIYSILKQIGSGGSSKVFQVLNEKKQIYAIKYVNLEEADNQTLDSYRNEIAYLN
KLQQHSDKIIRLYDYEITDQYIYMVMECGNIDLNSWLKKKKSIDPWERKSYWKNMLEAVHTIHQHGIVHSDLKPANFLIV
DGMLKLIDFGIANQMQPDTTSVVKDSQVGTVNYMPPEAIKDMSSSRENGKSKSKISPKSDVWSLGCILYYMTYGKTPFQQ
IINQISKLHAIIDPNHEIEFPDIPEKDLQDVLKCCLKRDPKQRISIPELLAHPYVQIQTHPVNQMAKGTTEEMKYVLGQL
VGLNSPNSILKAAKTLYEHYSGGESHNSSSSKTFEKKRGKK
-bash-4.1$
```

4.6.4. Redirecting standard input

One can provide an input to a command with less than "<" sign. The construct "command < infile" executes the command on the infile. The construct "command < infile > outfile" combines both methods. The command is executed on infile and the output captured to outfile.

4.6.5. Standard streams

Standard input and output are so-called standard streams. These are predefined channels of communication between a program and its environment. The figure from Wikipedia illustrates the concept. Stdandard input (stdin) comes from the keyboard while stdout is streamed to the diplay by default. The third standard stream is standard error - stderr. Some programs stream error messages there to separate them from data output.



You might have seen constructs like "command $> \log 2 > \&1$ ". What does this mean? On the command line, one can use "&0" to refer to stdin, "&1" to stdout and "&2" to stderr. Using this notation, the above expression redirects the program output to the "log" file. The "2 > &1" at the end of the expression redirects the standard error (&2) to standard output (&1). This way the log file contains the program output as well as possible errors.