Numerical Techniques Practicum 1

Getting started with LINUX and FORTRAN:

Solving the oscillation equation.

Daan Degrauwe

October 5, 2022

Most NWP and climate models are Fortran codes working on Linux machines. For this reason, the exercises and projects for the Numerical Techniques course will be given in such an environment.

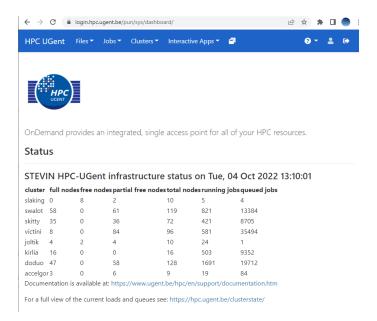
Since not all students are familiar with Linux and/or Fortran, this first practicum is conceived as a step-by-step exercise, where both Linux basics and Fortran basics are dealt with.

The goal is to write a Fortran program that calculates a numerical solution for the oscillation equation, as given by

$$\frac{d\psi}{dt} = i\kappa\psi$$

with initial condition $\psi_{t=0} = 1$. The exact solution is given by $\psi(t) = \exp(i\kappa t)$.

For this exercise, it is assumed that you work on the HPC (High-Performance Computer) infrastructure of UGENT. The first thing to do (preferably <u>before</u> the first practical session) is therefore to ask for an HPC account on https://www.ugent.be/hpc/en/access/faq/access. Afterwards, you should be able to login via https://login.hpc.ugent.be. This should give you an interface like



Different tools from this web platform will be used: the "Files" application to access files on the HPC, the "Cluster Desktop" application to enter a Linux desktop, and the "Jupyter Notebook" application for visualization of results.

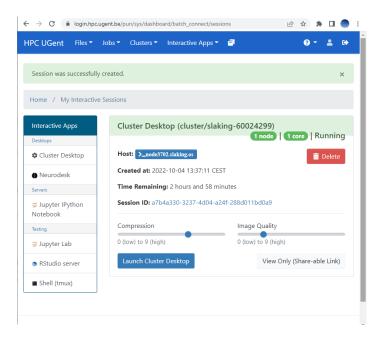
What is a bit peculiar about using HPC infrastructure is that nearly everything you do is done inside a 'job'. This means that you first have to submit/launch your job, and once it starts you can begin your work.

1 Accessing files

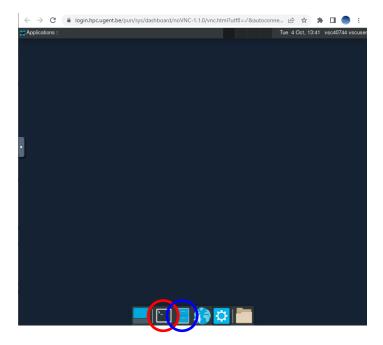
Under the "Files" application, hitting "Home Directory" should give you a graphical interface to your personal space on the HPC infrastructure. It lists all existing files and allows to download them, to upload new files, to view and edit (text) files, etc. However, in this practicum we'll work inside a Linux desktop to create/view/edit files. The Files application is mainly useful to exchange files with your local machine.

2 Linux desktop

Launching a desktop job is done under "Interactive Apps"-"Cluster Desktop". Choose an appropriate time for your job (typically a few hours), and set the clustername to "slaking". Then hit the "Launch" button at the bottom. After a few minutes, you should see something like the following under "My Interactive Sessions":



This means the job has started, and you can begin to work in it. Hit the "Launch Cluster Desktop" button to enter the desktop environment, which should look as follows:



The most important applications in this desktop environment are the Linux terminal (red circle) and the File browser (blue circle).

2.1 The file browser

This is just a convenient tool like Windows Explorer to browse and open files.

2.2 The Linux terminal

Opening a Linux terminal gives you access to what is called the *command line*. In Linux, almost everything you do is done by typing commands on the command line. For instance, try to execute the following command:

\$ date

where the \$ denotes that the command should be typed in the command line. The \$ should not be typed itself! Hitting ENTER after this command prints the current date on the screen.

Note: Linux is case-sensitive. This means that typing DATE or Date will not work.

The Linux commands that are needed for this lesson will be explained during the course of the exercise. Appendix A gives an overview of some of the most common Linux commands. At this point, you get following tricks for free:

- Linux stores a history of commands you entered. To repeat a previous command, hit the UP arrow.
- Hitting the TAB key autocompletes. For example, if you type dat, and then hit TAB, it will autocomplete to date. This also works for files and directories. If multiple options exist for autocompletion, you can hit TAB twice, to see the options. For instance, if you type cat, and then hit TAB twice, you should see that cat, catman and catchsegv are possible commands.

When working on a Linux command line, it is important to note that one works in a specific directory. Normally, this directory is visible before the \$ symbol. \sim denotes the home directory. You can also use the pwd command to print the working directory.

2.3 Creating and modifying a text file

Creating and modifying text files is very important for the rest of this exercise (and the remainder of the course).

On the command line, execute the following commands:

- \$ mkdir \${HOME}/numtech
- \$ cd \${HOME}/numtech
- \$ touch test.txt

Some explanation:

- mkdir creates a new directory
- with cd, you go to this directory
- touch creates a (empty) file

To check if the file was indeed created, you can open the file browser and navigate to the newly created numtech directory, where the test.txt file should be visible. You can also check the contents of a directory from the command line with

\$ ls

To modify a (text) file, select it in the file browser and double-click or hit Enter. This should launch a text editor (Geany) where you can modify the file as desired. Make sure to save a file after making modifications!

Next, you can check the contents of a file with the following command in the command line:

\$ cat test.txt

which should show you the text you entered in Geany. Finally, remove the test file with

\$ rm test.txt

3 My first Fortran program

3.1 The Fortran code

First, create a directory for this program, and create an empty file osceq.F90:

- \$ mkdir \${HOME}/numtech/osceq
- \$ cd \${HOME}/numtech/osceq/
- \$ touch osceq.F90

Open this file in Geany, and put the following Fortran code inside:

PROGRAM OSCEQ

! a program to solve the oscillation equation

WRITE (*,*) "Welcome to the Oscillation Equation Solver."

END PROGRAM OSCEQ

Some explanations:

- PROGRAM and END PROGRAM statements indicate the start and end of our program
- Text after a ! denotes a comment. Use comments abundantly to make notes on the code.
- The WRITE statement is used to print text on the screen, or to write text to a file (see later). The argument (*,*) means that writing should be done to screen, in default formatting.
- Fortran is not case sensitive. This means it doesn't matter whether you write PROGRAM or program or PrOgRaM.

3.2 Compiling

Before being able to execute Fortran code, it must be *compiled*. This is the process of transforming a code that's readable to humans (Fortran) into a code that's readable to computers (executable files). For this, we use a *compiler*.

Compilation is quite easy (as long as your code doesn't contain any mistakes). We will use the gfortran compiler. To convert the Fortran code into an executable program, type the following in the command line:

\$ gfortran osceq.F90 -o osceq

This command tells gfortran the following: take the file osceq.F90, convert it to an executable program, and put the result in the file osceq.

If all goes well, you should now have two files in the directory: osceq. F90 and osceq. You can check this with the Linux 1s command. If you don't see the file osceq, the compilation failed, most probably due to a coding mistake in the Fortran file. If you encounter errors during the compilation, try to understand what went wrong. Always look at the first error (later errors may be consequence of the first error). Ask for help if necessary: don't lose too much time on practicalities. You can use comments to indicate where you made a mistake in your program, in order to avoid such mistakes in the future.

Remark: make sure to recompile the program after every modification of the Fortran file!

3.3 Running

To execute the program, type the following on the command line:

\$./osceq

This will print some text to screen.

3.4 Automating tasks with Linux scripts

You may have noticed that recompiling and running often go together. It is therefore useful to create a Linux script that automates these two tasks. First create a file run.sh:

- \$ touch run.sh
- \$ chmod +x run.sh

Where the chmod command marks the file as an executable script.

Next, open this file in Geany, and put the following text in it:

```
# Script to compile and run the oscillation equation program

# remove executable file
rm osceq

# Compile
echo "Compiling"
gfortran -o osceq osceq.F90

# Run
echo "Running"
./osceq
```

Some explanations:

- Comments in Linux scripts are indicated by a #.
- The rm command removes the existing executable.
- The echo command prints text to the screen.

Running the script is done with

\$./run.sh

4 Defining and using variables in Fortran

Let us now introduce some variables in our Fortran program. However, before making further modifications, it is good practice to take a copy of the current directory:

```
$ cd ..
$ cp -r osceq/ osceq_v1
$ cd osceq/
```

With the first command, we move one directory up (so to \${HOME}/numtech/). The cp command takes a copy; to copy directories, the additional argument -r is required.

Now we have stored a backup, we can proceed with modifying the source code. In Geany, change the file osceq.F90 as follows:

```
PROGRAM OSCEQ
! a program to solve the oscillation equation
IMPLICIT NONE
                    ! safety to make sure all variables are declared
! declarations
REAL :: KAPPA
                    ! parameter kappa in the oscillation equation (frequency)
REAT.
       :: DT
                    ! timestep
INTEGER :: NT
                    ! number of timesteps
COMPLEX :: PSIO
                    ! initial condition
WRITE (*,*) "Welcome to the Oscillation Equation Solver."
! initialize parameters
```

```
KAPPA = 0.5
DT = 1.0
NT = 20
PSIO = COMPLEX(1.0,0.0) ! complex number 1.0 + 0.0 * i

WRITE (*,*) 'Total integration time = ',NT*DT
WRITE (*,*) 'Courant number = ',KAPPA*DT
END PROGRAM OSCEQ
```

Compile and run this program by running the run.sh script.

The program contains the following new ingredients:

- The statement IMPLICIT NONE is a safety. It's good practice to put it in all your Fortran programs. It means that all variables should be declared explicitly.
- The statements REAL, INTEGER and COMPLEX are used to *declare* variables. Declaration is where you tell the compiler what kind a certain variable is. Besides REAL, INTEGER and COMPLEX, Fortran also knows CHARACTER and LOGICAL types.
- The variables are *assigned* their values with the = operator.
- The variables can then be used in calculations as shown in the WRITE statements

It is important to be aware of the types of variables. For instance, the numbers 2 and 5 are of type INTEGER. This means that 5/2 will take value 2, because dividing two variables of type INTEGER results in another INTEGER! To correctly perform divisions, make sure that one of the numbers is of type REAL. For example, 5.0/2 will give you the desired 2.5.

It should be mentioned that the organization of a Fortran program is quite strict: *all* declarations should come before the executable statements. If you want to introduce a new variable, it should be declared at the beginning of the program, even if you only use it somewhere at the end.

5 Loops

Now we get to the actual purpose of our program: the time integration. We will do this with the forward scheme, for which

$$\phi^{n+1} = (1 + i\kappa \Delta t)\phi^n$$

The time integration is a repetitive task: given the solution at the current timestep (ϕ^n) , the solution at the next timestep (ϕ^{n+1}) is calculated. A repetitive task is implemented in Fortran with a D0-loop.

First, store a copy of your program with

```
$ cd ..
$ cp -r osceq/ osceq_v2
$ cd osceq/
```

Then, modify the file osceq.F90 as follows:

```
PROGRAM OSCEQ
! a program to solve the oscillation equation
IMPLICIT NONE
                    ! safety to make sure all variables are declared
! declarations
REAL
        :: KAPPA
                    ! parameter kappa in the oscillation equation (frequency)
R.F.A.T.
        :: DT
                    ! timestep
INTEGER :: NT
                    ! number of timesteps
INTEGER :: IT
                    ! current timestep
COMPLEX :: PSIO
                    ! initial condition
COMPLEX :: PSI, PHI ! exact and numerical time-solution
COMPLEX :: II
                    ! imaginary unit
! initialize parameters
```

```
KAPPA = 0.5
    = 1.0
      = 20
PSIO = COMPLEX(1.,0.)
     = COMPLEX(0.,1.)
! set initial conditions
TT=0
PSI=PSI0
PHI=PSI0
! show values at zero'th timestep
WRITE (*,*) 't = ',IT*DT,'; PSI = ',REAL(PSI),'; PHI = ',REAL(PHI)
! start loop over timesteps
DO IT = 1,NT
  ! exact solution
 PSI = EXP(II*KAPPA*DT)*PSI
  ! numerical solution: forward scheme
 PHI = (1+II*KAPPA*DT)*PHI
  ! show values at current timestep
 WRITE (*,*) 't = ',IT*DT,'; PSI = ',REAL(PSI),'; PHI = ',REAL(PHI)
ENDDO
END PROGRAM OSCEQ
```

New ingredients are:

- \bullet The functions REAL() and EXP(), which respectively take the real part of a complex number, and the exponential function
- The statements DO IT=1,NT and ENDDO denoting the start and end of a *loop*. The enumerator IT takes the initial value of 1, and augments every timestep by 1, until it gets larger than NT.

When running the program, it should become clear that the forward scheme is unstable.

6 Conditions

Conditional branching in Fortran is done with the IF statement. For instance, we could introduce the following piece of code to check for an unstable scheme:

```
PROGRAM OSCEQ
! a program to solve the oscillation equation
... (see previous version of the program)
! start loop over timesteps
DO IT = 1,NT
! numerical solution: forward scheme
PHI = (1+II*KAPPA*DT)*PHI
! warning if unstable
IF ( ABS(PHI) > 10.0 ) THEN
WRITE (*,*) 'WARNING: unstable behaviour detected'
ENDIF

ENDDO

END PROGRAM OSCEQ
```

When running long enough (NT ≥ 21), you should see a warning in the output.

More advanced conditions are achieved with .AND., .OR. and .NOT.. If you want to execute some code when the condition is not fulfilled, use the ELSE statement.

7 Arrays

Arrays are collections of numbers. In this program, they allow to store the solution for the full time-range. Consider the following program:

```
PROGRAM OSCEO
! a program to solve the oscillation equation
IMPLICIT NONE
                    ! safety to make sure all variables are declared
! declarations
REAL :: KAPPA ! parameter kappa in the oscillation equation (frequency)
REAL
      :: DT ! timestep
                 ! number of timesteps
INTEGER :: NT
INTEGER :: IT
                  ! current timestep
COMPLEX :: PSIO ! initial condition
COMPLEX :: II ! imaginary unit
                    ! imaginary unit
COMPLEX, ALLOCATABLE :: PSI(:), PHI(:) ! arrays of exact and numerical solution
! initialize parameters
KAPPA = 0.5
DT
     = 1.0
     = 100
NT
PSIO = COMPLEX(1.,0.)
     = COMPLEX(0.,1.)
! allocate memory for arrays
ALLOCATE(PSI(0:NT),PHI(0:NT))
! set initial conditions
IT=0
PSI(IT)=PSI0
PHI(IT)=PSIO
! start loop over timesteps
DO IT = 1,NT
 ! exact solution
 PSI(IT) = EXP(II*KAPPA*DT)*PSI(IT-1)
 ! numerical solution: forward scheme
 PHI(IT) = (1+II*KAPPA*DT)*PHI(IT-1)
ENDDO
! show values
WRITE (*,*) 'PSI = ',REAL(PSI)
WRITE (*,*) 'PHI = ',REAL(PHI)
! release memory
DEALLOCATE (PSI, PHI)
END PROGRAM OSCEQ
```

Working with arrays requires the following:

- During the declaration, you should add the ALLOCATABLE attribute, and specify the number of dimensions. In this program, one-dimensional arrays are used, hence the (:). Two-dimensional arrays would be declared with (:,:)
- The ALLOCATE statement tells the compiler what the size of the array should be, and makes sure the necessary memory is reserved for this array

- A single element of an array is accessed with the () construct. For instance, we calculate PHI(IT) from PHI(IT-1)
- At the end, the reserved memory should be released with the DEALLOCATE statement.

Quite important to remember when working with arrays is that you shouldn't exceed the limits of the array. For example, using PHI(NT+1) in our program would lead to erroneous results or a crash of the program, because PHI was allocated with an upper bound of NT. You can tell the compiler to detect such out-of-bound errors by compiling with the switch -fbounds-check:

\$ gfortran -fbounds-check osceq.F90 -o osceq

8 Subroutines and modules

For larger computer programs (NWP and climate models often contain millions of lines of code), it becomes necessary to organize the code in a structured way. This is achieved with *subroutines*. A subroutine is a piece of code that can be called from somewhere else in the code.

In principle, variables that are declared in the main part of the program are not known in the subroutine. Two mechanisms exist to transfer information to and from subroutines. Either by using *arguments*, or by using *global variables*. Global variables are implemented in Fortran by putting them in a *module*.

It is common practice to put all subroutines and modules in separate files.

Let's organize our oscillation equation program in the following pieces:

- a module CONSTANTS containing all constant variables;
- a subroutine SETUP_CONSTANTS to setup the values of these constant variables;
- a subroutine TIMELOOP to perform the time-loop;
- a subroutine WRITE_RESULT to write the results to a file;
- the main program, making calls to the other routines.

Each of these pieces is put in a separate Fortran file. The file constants.F90 contains

```
MODULE CONSTANTS
  ! a module contains global variables.
  ! These are accessible from all subroutines and from the main program
  IMPLICIT NONE
  ! universal constants
 COMPLEX :: II
                     ! imaginary unit
  ! oscillation equation parameters
        :: KAPPA
                     ! parameter kappa in the oscillation equation (frequency)
  COMPLEX :: PSIO
                     ! initial condition
  ! discretization variables
 REAL :: DT ! timestep
  INTEGER :: NT
                     ! number of timesteps
END MODULE CONSTANTS
```

The file setup_constants.F90 contains

```
SUBROUTINE SETUP_CONSTANTS
! subroutine to assign constants appropriate values

USE CONSTANTS
! all variables from this module are now known in this subroutine

IMPLICIT NONE
```

```
= COMPLEX(0.,1.)
   KAPPA = 0.5
   PSIO = COMPLEX(1.,0.)
   DT
         = 1.0
   NT
         = 100
 END SUBROUTINE SETUP_CONSTANTS
The file timeloop.F90 contains
 SUBROUTINE TIMELOOP
   USE CONSTANTS
   IMPLICIT NONE
   ! declare local variables
   INTEGER
                :: IT
                                           ! current timestep
   COMPLEX, ALLOCATABLE :: PSI(:), PHI(:) ! arrays of exact and numerical solution
   ! allocate memory for arrays
   ALLOCATE(PSI(0:NT),PHI(0:NT))
    ! set initial conditions
   IT=0
   PSI(IT)=PSI0
   PHI(IT)=PSI0
    ! start loop over timesteps
   DO IT = 1,NT
      ! exact solution
     PSI(IT) = EXP(II*KAPPA*DT)*PSI(IT-1)
     ! numerical solution: forward scheme
     PHI(IT) = (1+II*KAPPA*DT)*PHI(IT-1)
   ENDDO
    ! write the result
   CALL WRITE_RESULT(PSI,PHI)
    ! free memory
   DEALLOCATE (PSI, PHI)
 END SUBROUTINE TIMELOOP
The file write_result.F90 contains
 SUBROUTINE WRITE_RESULT(PSI,PHI)
    ! write the result to a file
   USE CONSTANTS
   IMPLICIT NONE
    ! arguments
   COMPLEX, INTENT(IN) :: PSI(0:NT), PHI(0:NT)
    ! auxiliary results
   INTEGER :: IT
                  ! timestep
    ! open a file
   OPEN(FILE='output.dat',UNIT=20)
```

```
! write heading
WRITE (20,'(A6,A16,A16)') 'time','exact','numerical'
! write solutions at all timesteps to the file
DO IT=0,NT
   WRITE (20,'(F6.2,E16.8,E16.8)') IT*DT, REAL(PSI(IT)), REAL(PHI(IT))
ENDDO
! close the file
CLOSE(UNIT=20)
END SUBROUTINE WRITE_RESULT
```

And finally, the file osceq.F90 contains

```
PROGRAM OSCEQ
! a program to solve the oscillation equation

IMPLICIT NONE
! initialize constant parameters
CALL SETUP_CONSTANTS()
! time loop
CALL TIMELOOP()

END PROGRAM OSCEQ
```

The compilation of multiple files is done as follows:

- \$ gfortran constants.F90 setup_constants.F90 timeloop.F90 write_result.F90 osceq.F90 -o osceq Remarks and new concepts:
 - One can hardly say that our program became simpler by reorganizing into subroutines. However, each of the building blocks is quite simple in itself. It's much easier to find your way through the program now.
 - Calling a subroutine is done with the CALL statement.
 - Arguments have an INTENT attribute, which specifies whether it's an input (IN) or an output argument (OUT).
 - It's very important that the argument declaration in the subroutine matches the argument that is passed in the CALL statement! You will get strange behaviour if this is not the case. 'Matching' means that the type (COMPLEX, ...) should be the same, as well as the dimension if it's an array.
 - To make global variables accessible in a subroutine, the USE statement should be used.
 - Writing to a file is done in three steps:
 - 1. open the file with the OPEN statement. The filename is specified, and a *unit* number is assigned. You can freely choose this unit, as long as it is not in use for another file. You also shouldn't take 0, 1 or 6 as unit number.
 - 2. write stuff to the file with the WRITE statement. Specify the unit number of the file you want to write to, as well as the *format*. The code shows how to specify the formats for character strings and for floating point real numbers.
 - 3. close the file with the CLOSE statement.
 - for the compilation, it's important to put the Fortran files containing modules (in our case constants.F90) before the Fortran files using these modules.

9 Visualizing the output in a Jupyter Notebook

Fortran is a programming language that's intended to perform calculations. Visualizing results is commonly done with other programs, such as Matlab, R, gnuplot, python, etc. All of these programs are capable of reading numerical data from a file (like the one created by our program). For this course, we will use a Jupyter Notebook to postprocess (visualize and inspect) the results of our calculations.

9.1 Launching a Jupyter Notebook

- 1. Head back to https://login.hpc.ugent.be/
- 2. Under "Interactive Apps", select "Jupyter IPython Notebook"
- 3. Select slaking as the cluster, and select "7.15.0 foss 2020a Python 3.8.2" as the IPython version. Then hit the "Launch" button.
- 4. After a few minutes, the Jupyter Notebook session should appear in your "My Interactive Sessions" panel. Then hit the "Connect to Jupyter Notebook" button, which should launch the Jupyter browser in a new tab.
- 5. Browse to the numtech/osceq directory that you've been working in so far, and hit "New"—"Python 3" to create a new notebook.
- 6. Rename the notebook from the default 'Untitled' to something more appropriate, e.g. 'osceq'.

9.2 Working in a Jupyter Notebook

A notebook is organized in 'cells', which are pieces of python code that can be executed by hitting Shift+Enter. After modifying the content of a cell, make sure to rerun it.

In the first cell, we'll load some necessary libraries:

```
# load some libraries
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
```

In the following cell, we'll load the data from the output.dat file

```
# read the output data
filename='output.dat'
data=np.loadtxt(filename,skiprows=1)
# select columns
t=data[:,0]
y_exact=data[:,1]
y_numerical=data[:,2]
```

Next, we can visualize the results in the next cell with

```
# open a figure
fig, ax = plt.subplots(figsize=(12,8))
# plot exact and numerical result
plt.plot(t,y_exact,label='exact')
plt.plot(t,y_numerical,label='numerical')
# add legend
plt.legend();
```

10 Exercises

1. Implement the backward and the trapezium schemes. What about their stability and phase error?

$$\phi^{n+1} = \frac{1}{1 - i\kappa \Delta t} \phi^n$$
 (backward)
$$\phi^{n+1} = \frac{1 + 0.5i\kappa \Delta t}{1 - 0.5i\kappa \Delta t} \phi^n$$
 (trapezium)

2. Implement the Matsuno scheme, and check the damping as a function of $\kappa \Delta t$. Is it accelerating or decelerating?

$$\tilde{\phi} = (1 + i\kappa \Delta t)\phi^{n}$$
$$\phi^{n+1} = \phi^{n} + i\kappa \Delta t\tilde{\phi}$$

3. Implement the Leapfrog scheme.

$$\phi^{n+1} = \phi^{n-1} + 2i\kappa\Delta t\phi^n$$

Use the forward scheme during the first timestep:

$$\phi^1 = (1 + i\kappa \Delta t)\phi^0$$

- 4. Try to excite the computational mode in the Leapfrog scheme (by sabotaging the first timestep).
- 5. Implement the Robert-Asselin filter to damp the computational mode.

$$\begin{split} \phi^{n+1} &= \overline{\phi^{n-1}} + 2i\kappa\Delta t\phi^n \\ \overline{\phi^n} &= \phi^n + \gamma\left(\overline{\phi^{n-1}} - 2\phi^n + \phi^{n+1}\right) \end{split}$$

A Linux commands

Getting help

 $man \qquad \qquad \text{show manual pages for a command (exit with } q)$

e.g. man date

help show help

e.g. help cd

--help show help info

e.g. date --help

Navigation

cd change directory

e.g. cd /files/\${USER}/home/numtech/

cd .. go one directory up
pwd show current directory
ls list contents of directory

mkdir create a directory

e.g. mkdir testdir

File manipulation

touch create empty file

e.g. touch test.txt

cp copy a file

e.g. cp test.txt test2.txt

cp -r copy a directory

 ${
m e.g.}$ cp -r testdir/ testdir2

rm remove a file

e.g. rm test2.txt

rm -r remove a directory

e.g. rm -r testdir2

mv move (rename) a file or directory

e.g. mv test.txt test2.txt

File contents

show file contents

e.g. cat test.txt

less show file contents (exit with q)

e.g. less test.txt

diff show difference between two (text) files

e.g. diff test.txt test2.txt