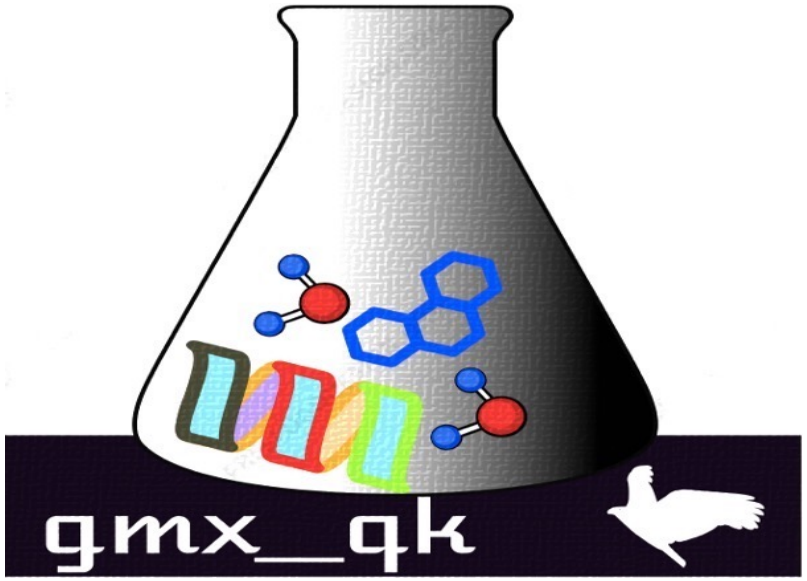

About: gmx_qk 1.0.0

The tool gmx_qk is a **Zenity, Python and Gromacs** dependent bash program. It is designed for the beginners to the gromacs, who would like to simulate **Protein-Ligand complex. Gmx_qk** is a fully automated program, efficiently works with gromacs version 5.0 and newer one as 2021.4. Informative widgets are supported by Zenity (GUI).

Author:

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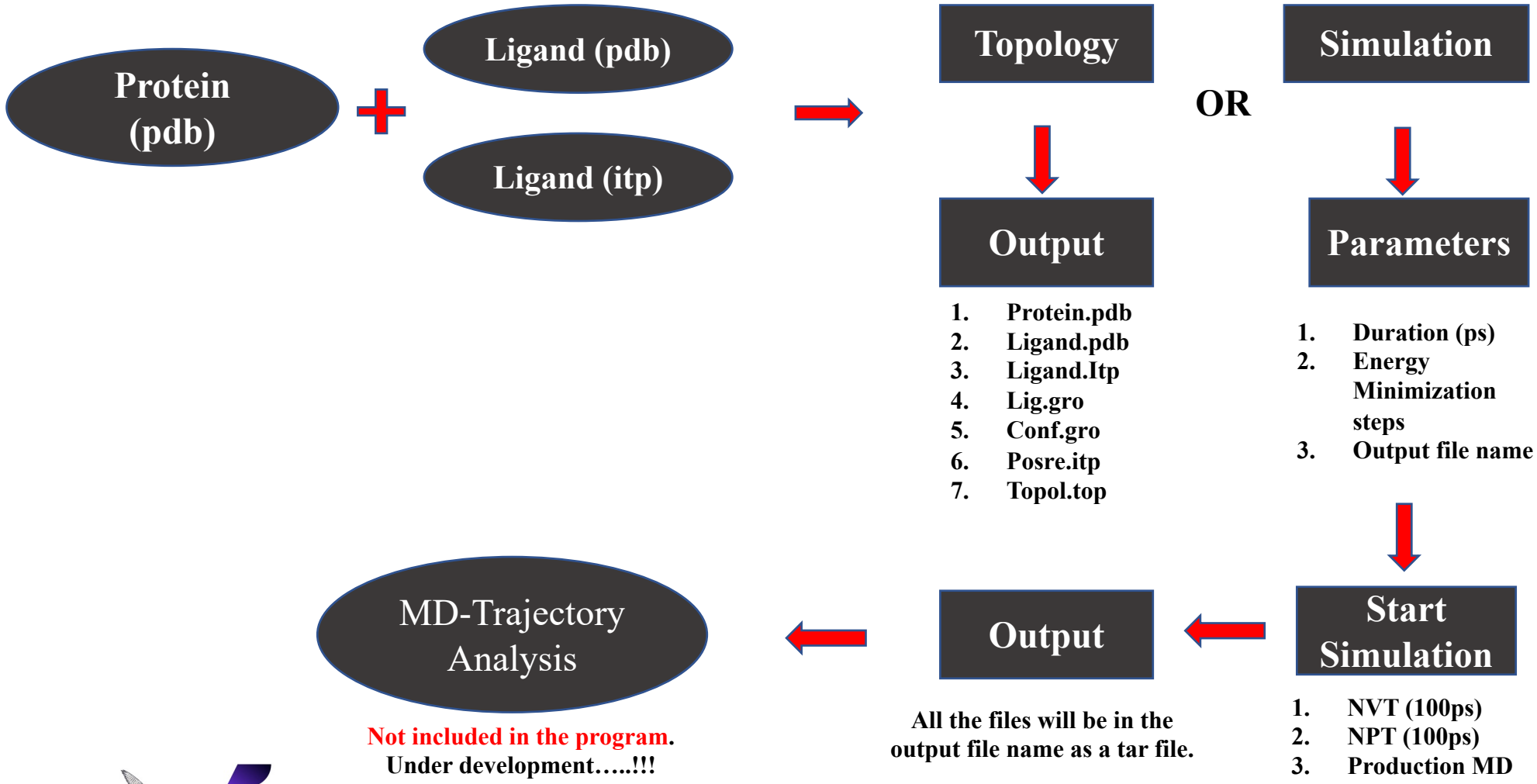
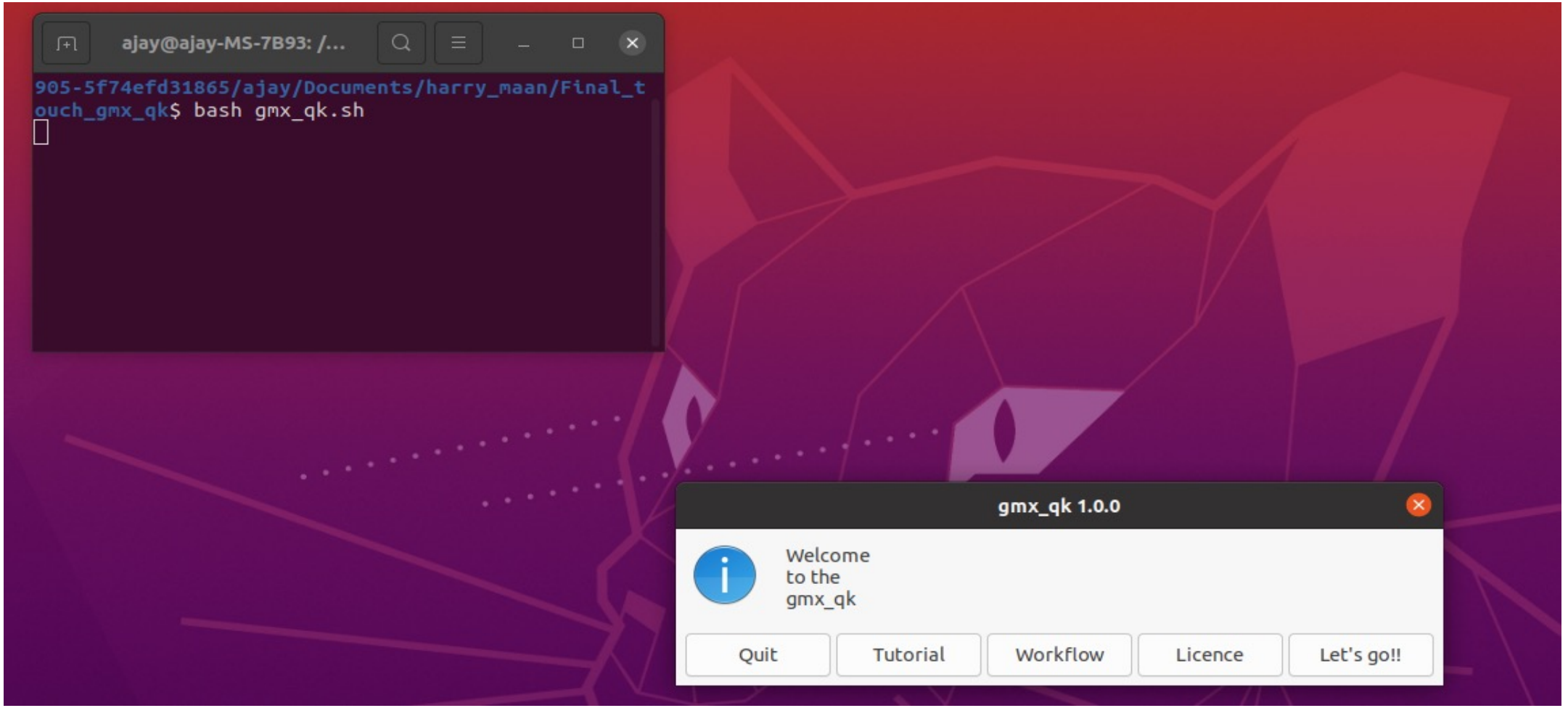
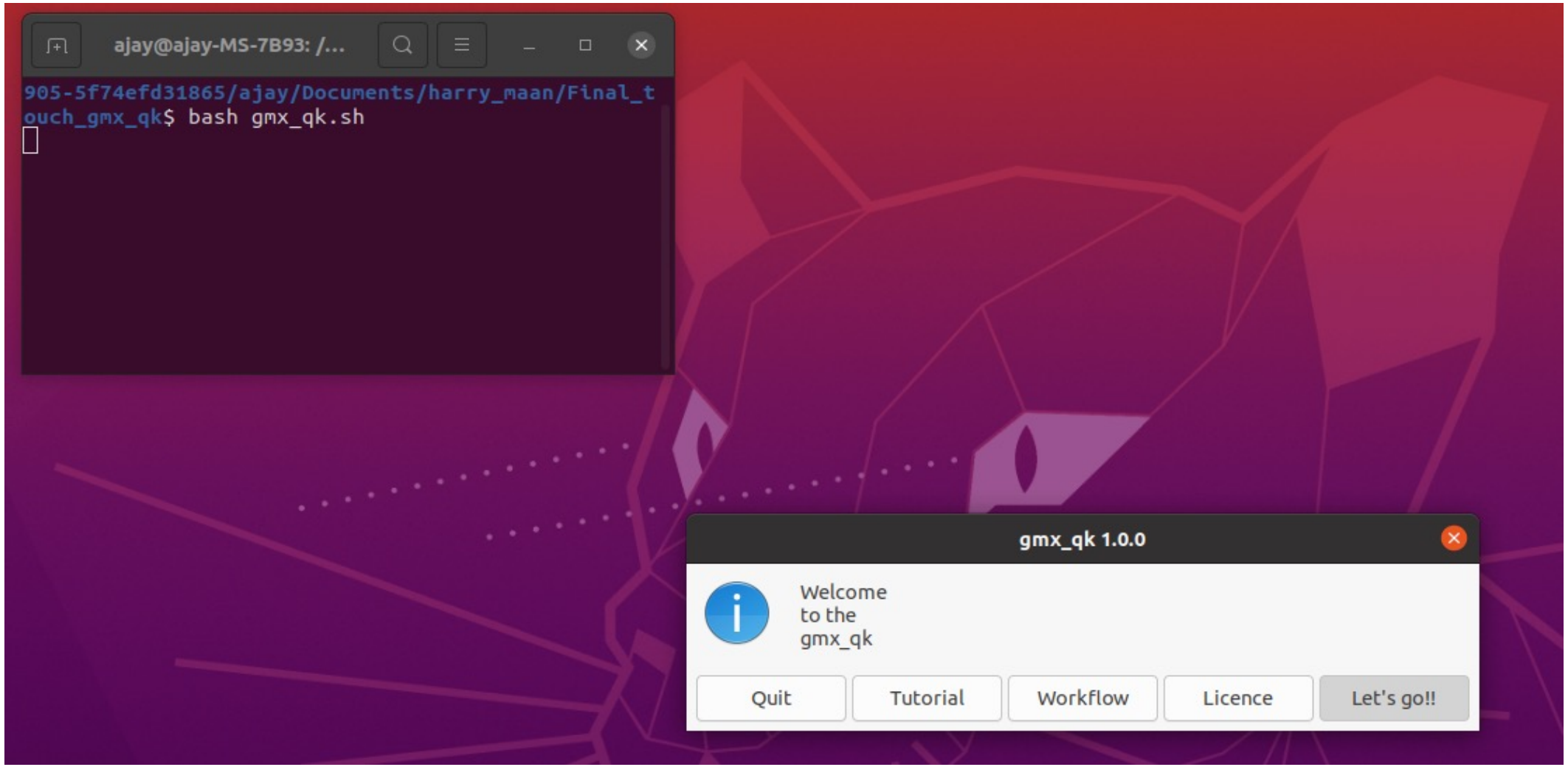
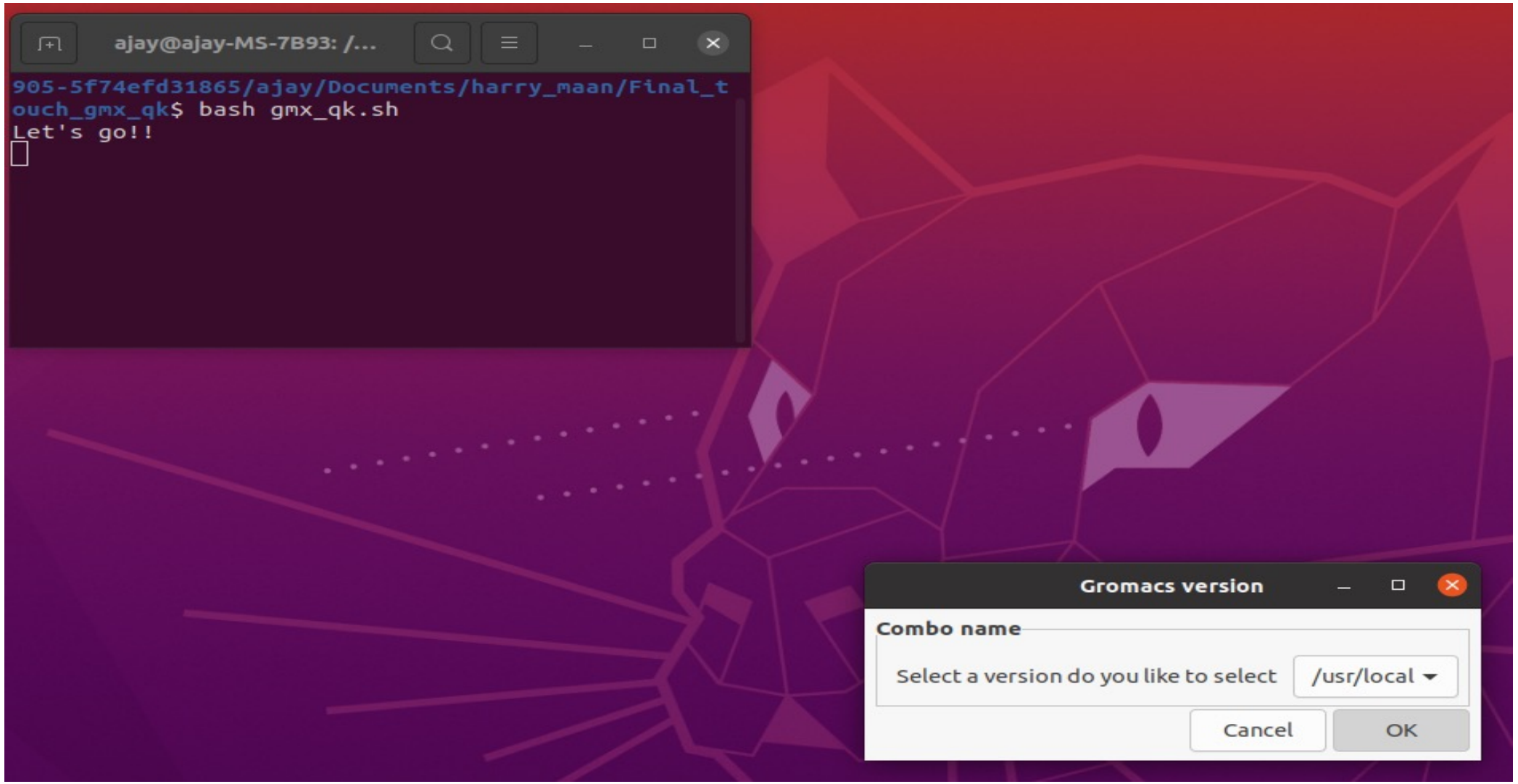
harvindermaan4@gmail.com

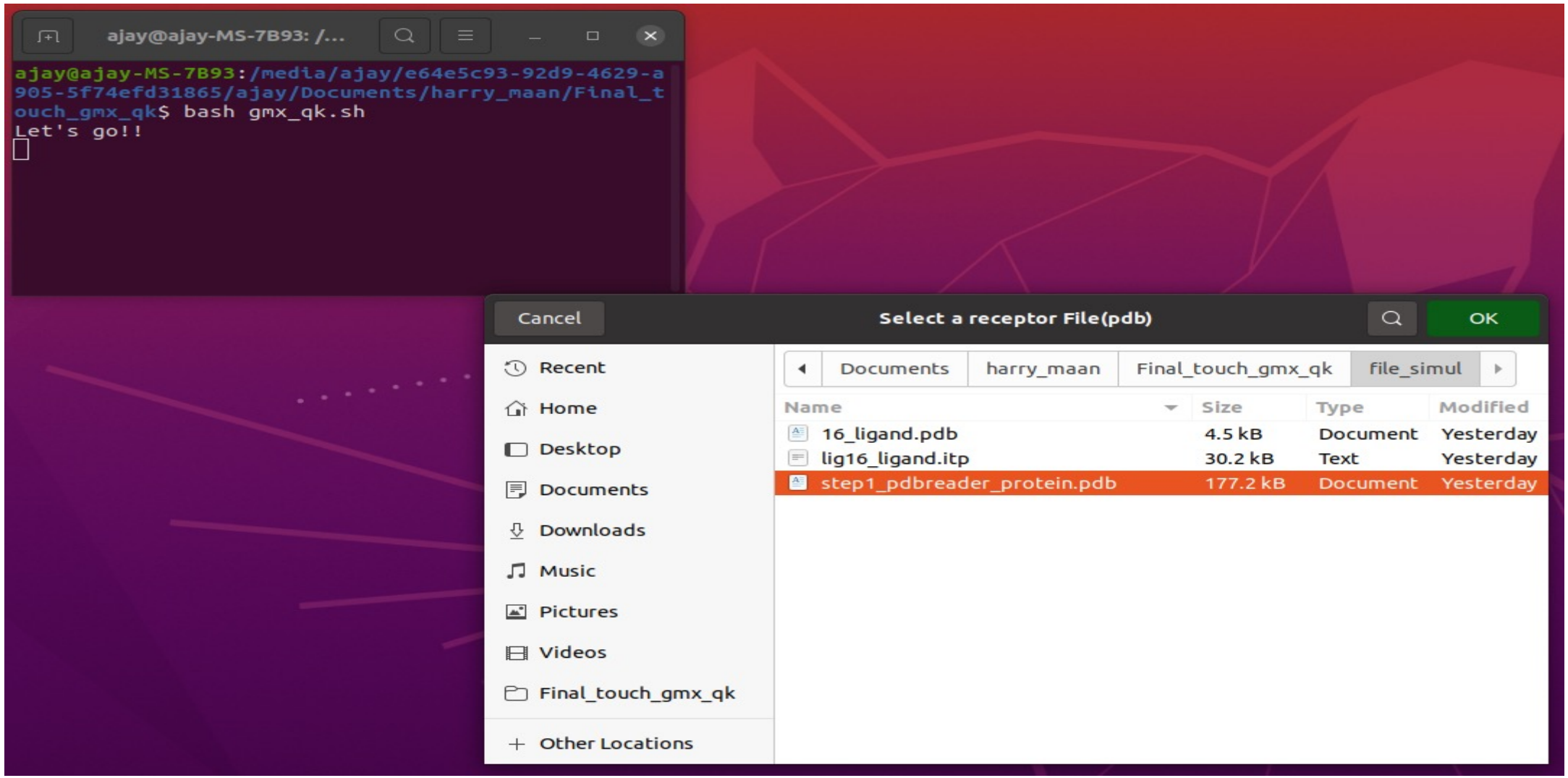
Workflow gmx_qk

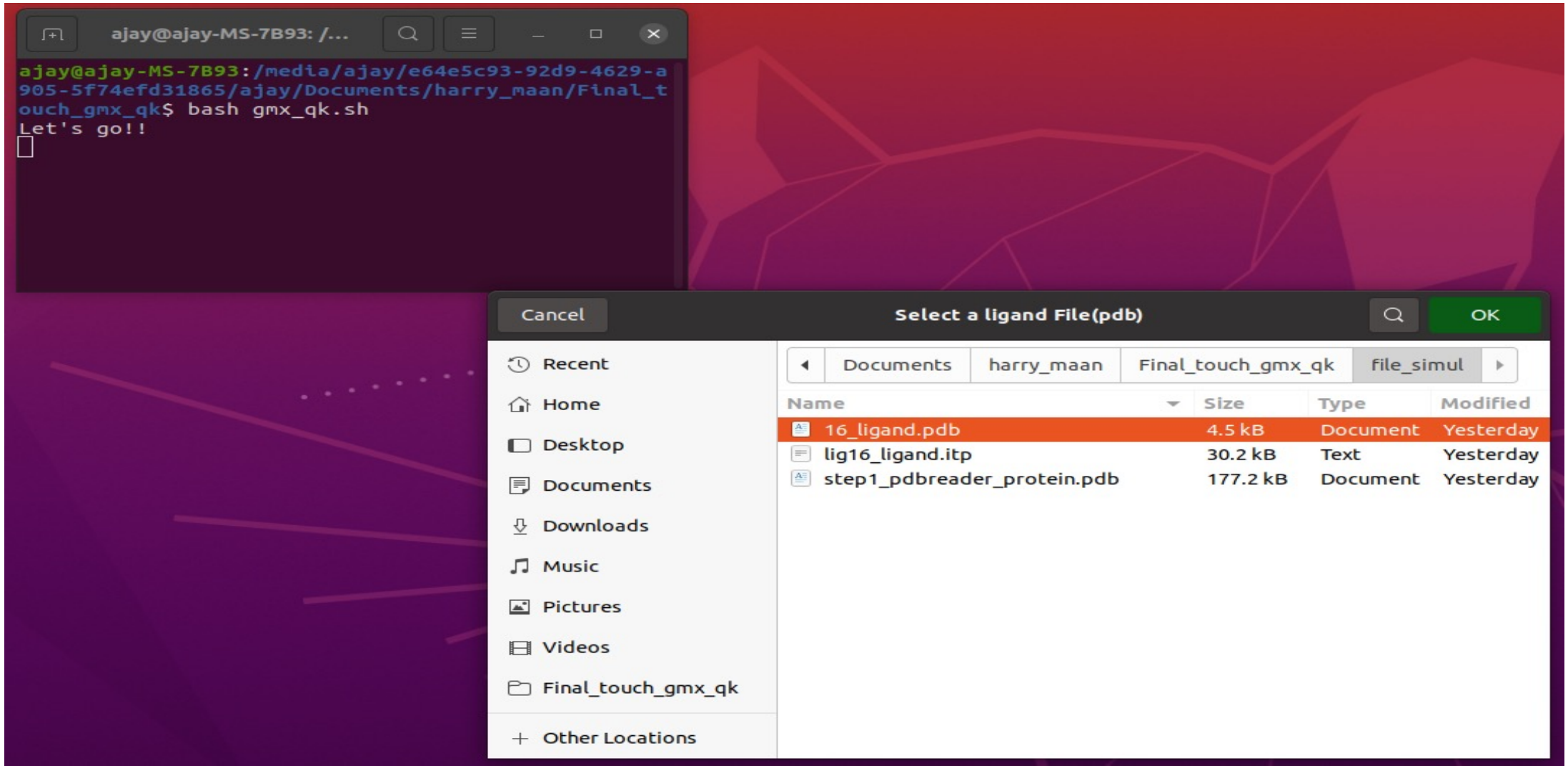


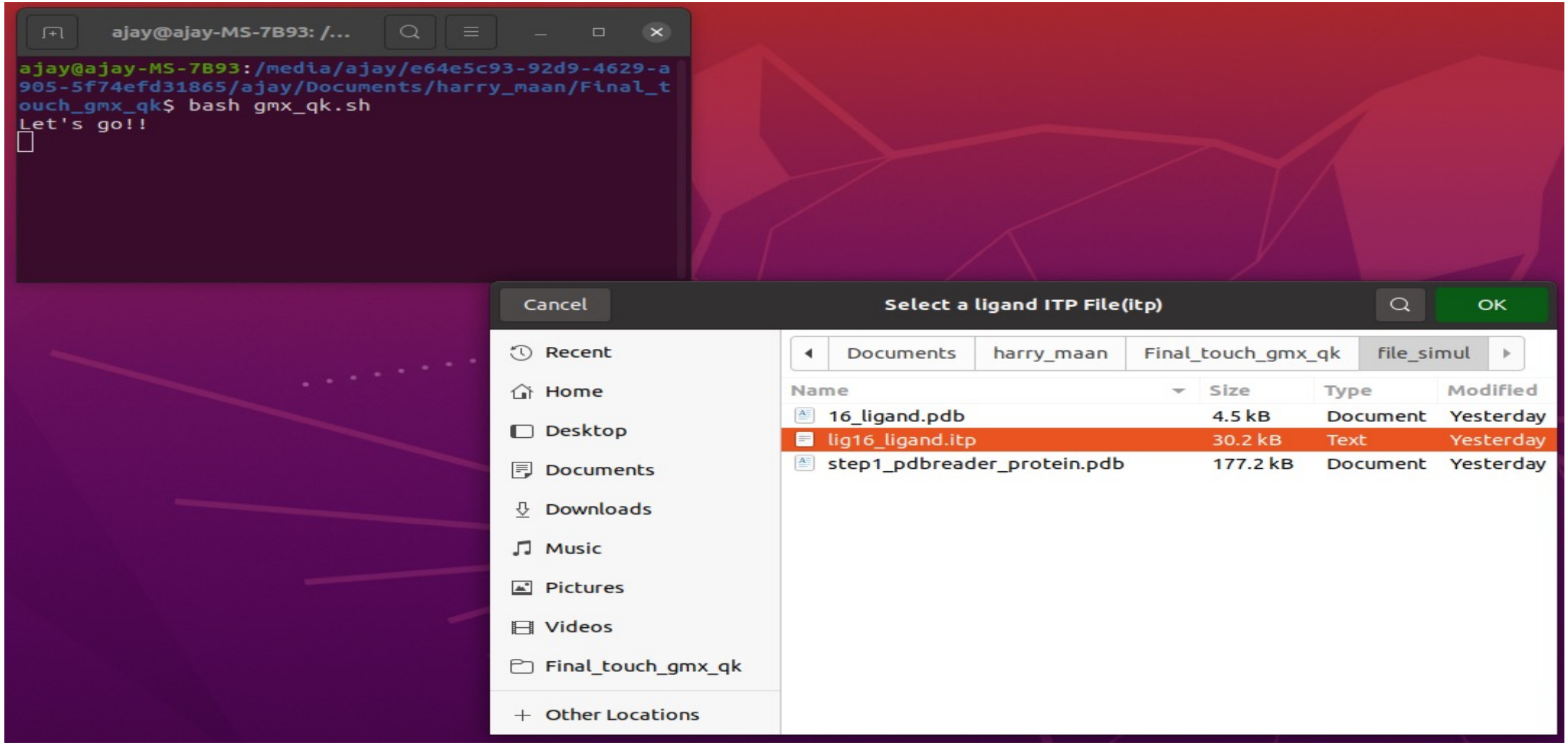

ajay@ajay-MS-7B93: /...
905-5f74efd31865/ajay/Documents/harry_maan/Final_t
ouch_gmx_qk$ bash gmx_qk.sh
gmx_qk 1.0.0
Welcome
to the
gmx_qk
Quit
Tutorial
Workflow
Licence
Let's go!!

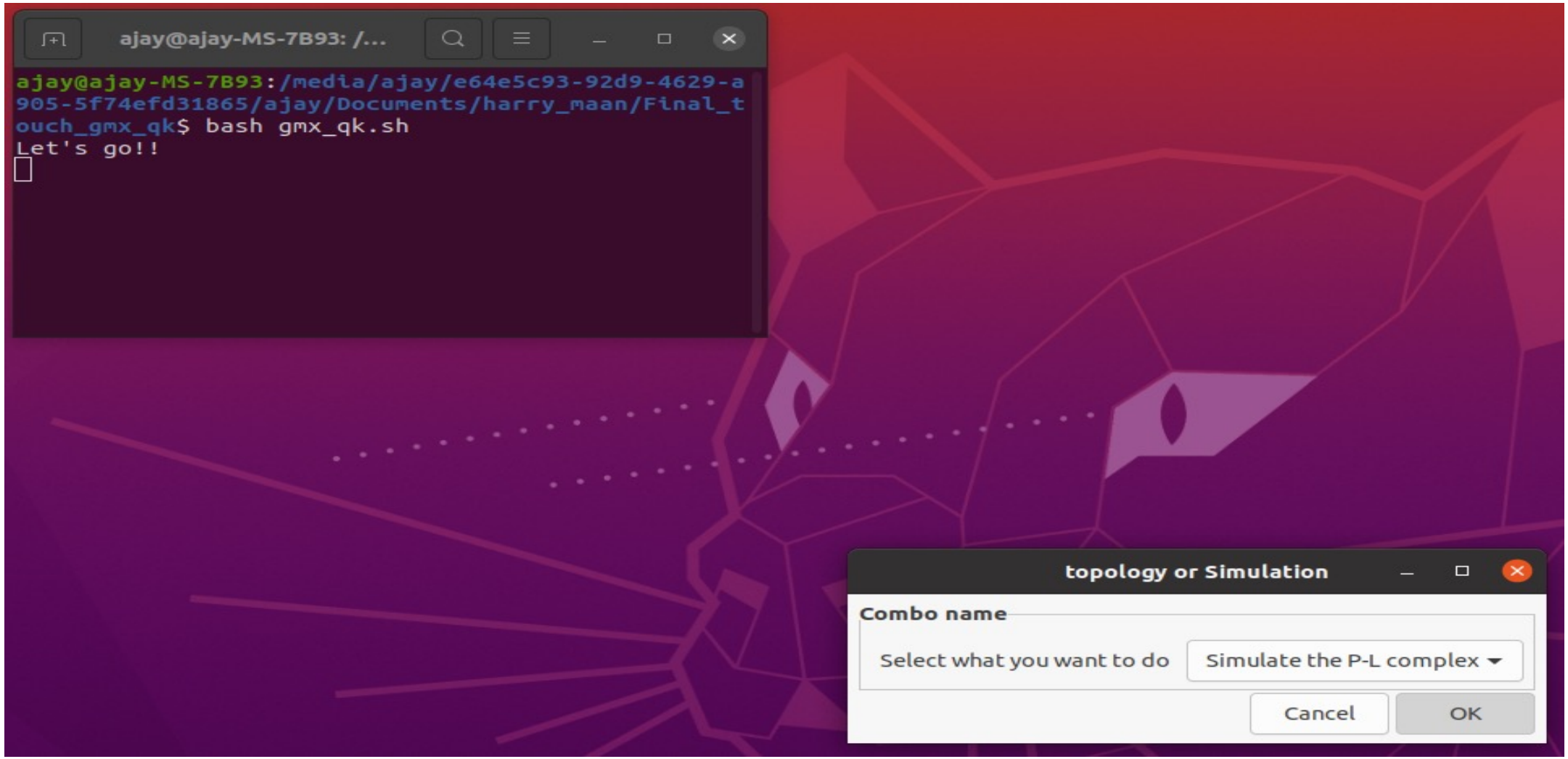

ajay@ajay-MS-7B93: /...
905-5f74efd31865/ajay/Documents/harry_maan/Final_t
ouch_gmx_qk$ bash gmx_qk.sh
gmx_qk 1.0.0
Welcome
to the
gmx_qk
Quit
Tutorial
Workflow
Licence
Let's go!!

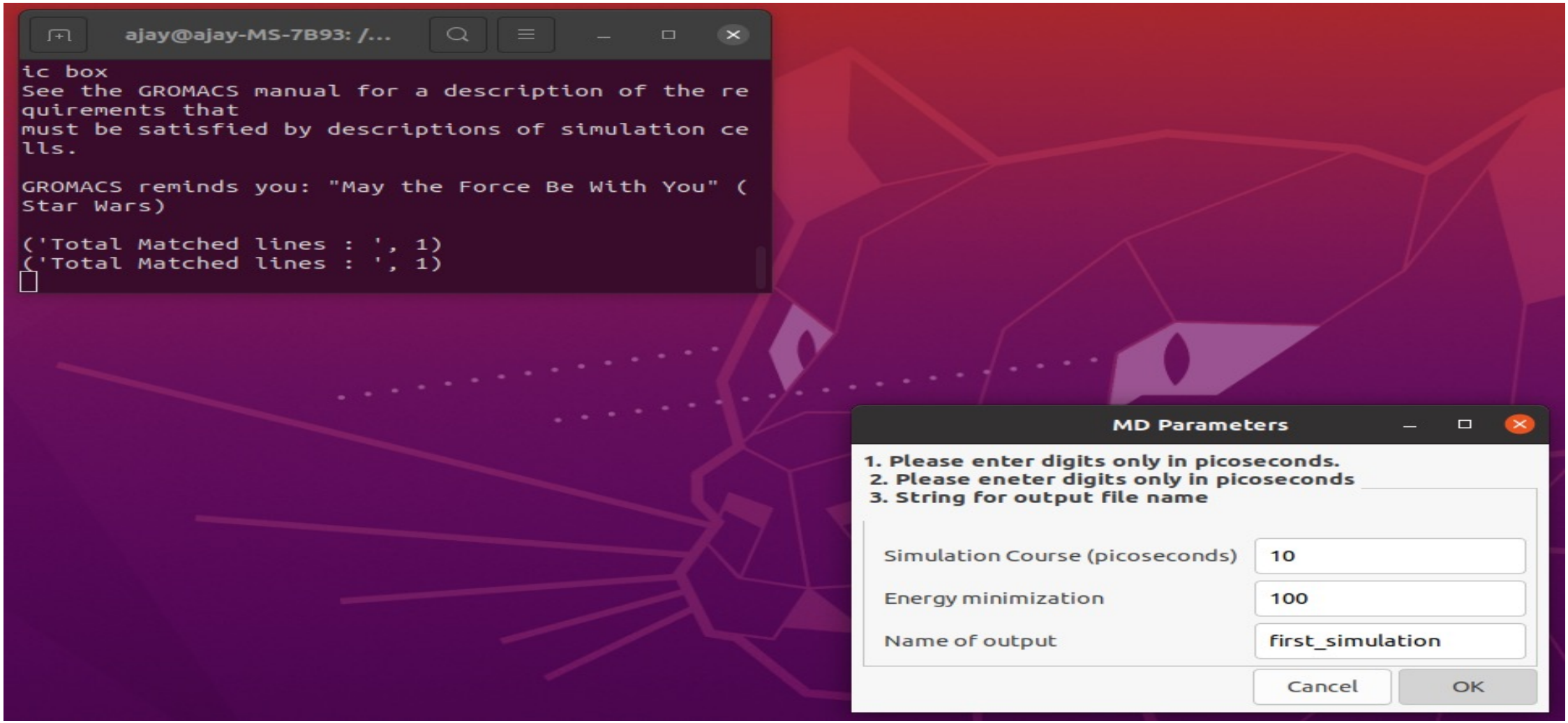

ajay@ajay-MS-7B93: /...
905-5f74efd31865/ajay/Documents/harry_maan/Final_touch_gmx_qk$ bash gmx_qk.sh
Let's go!!
Gromacs version
Combo name
Select a version do you like to select
/usr/local
Cancel
OK

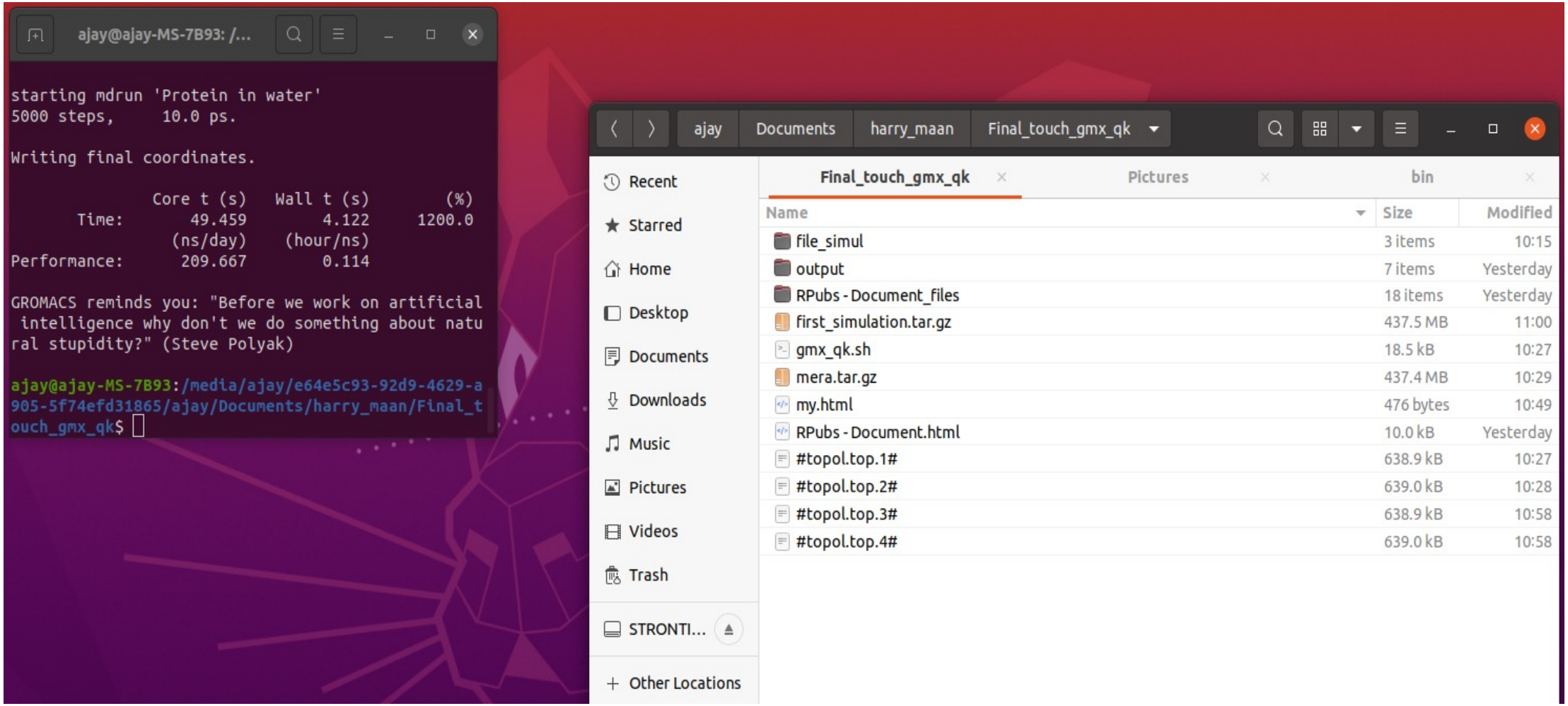

ajay@ajay-MS-7B93: /...
ajay@ajay-MS-7B93:/media/ajay/e64e5c93-92d9-4629-a905-5f74efd31865/ajay/Documents/harry_maan/Final_touch_gmx_qk$ bash gmx_qk.sh
Let's go!!
Cancel
Select a receptor File(pdb)
OK
Recent
Home
Desktop
Documents
Downloads
Music
Pictures
Videos
Final_touch_gmx_qk
Other Locations
Documents
harry_maan
Final_touch_gmx_qk
file_simul
Name
Size
Type
Modified
16_ligand.pdb
4.5 kB
Document
Yesterday
lig16_ligand.itp
30.2 kB
Text
Yesterday
step1_pdbreader_protein.pdb
177.2 kB
Document
Yesterday


ajay@ajay-MS-7B93: /...
ajay@ajay-MS-7B93:/media/ajay/e64e5c93-92d9-4629-a905-5f74efd31865/ajay/Documents/harry_maan/Final_touch_gmx_qk$ bash gmx_qk.sh
Let's go!!
Cancel
Select a ligand File(pdb)
OK
Recent
Home
Desktop
Documents
Downloads
Music
Pictures
Videos
Final_touch_gmx_qk
Other Locations
Documents
harry_maan
Final_touch_gmx_qk
file_simul
Name
Size
Type
Modified
16_ligand.pdb
4.5 kB
Document
Yesterday
lig16_ligand.itp
30.2 kB
Text
Yesterday
step1_pdbreader_protein.pdb
177.2 kB
Document
Yesterday


ajay@ajay-MS-7B93: /...
ajay@ajay-MS-7B93:/media/ajay/e64e5c93-92d9-4629-a905-5f74efd31865/ajay/Documents/harry_maan/Final_touch_gmx_qk$ bash gmx_qk.sh
Let's go!!
Cancel
Select a ligand ITP File(itp)
OK
Recent
Home
Desktop
Documents
Downloads
Music
Pictures
Videos
Final_touch_gmx_qk
Other Locations
Documents
harry_maan
Final_touch_gmx_qk
file_simul
Name
Size
Type
Modified
16_ligand.pdb
4.5 kB
Document
Yesterday
lig16_ligand.itp
30.2 kB
Text
Yesterday
step1_pdbreader_protein.pdb
177.2 kB
Document
Yesterday


ajay@ajay-MS-7B93: /...
ajay@ajay-MS-7B93:/media/ajay/e64e5c93-92d9-4629-a905-5f74efd31865/ajay/Documents/harry_maan/Final_touch_gmx_qk$ bash gmx_qk.sh
Let's go!!
topology or Simulation
Combo name
Select what you want to do
Simulate the P-L complex
Cancel
OK


ajay@ajay-MS-7B93: /...
ic box
See the GROMACS manual for a description of the re
quirements that
must be satisfied by descriptions of simulation ce
lls.
GROMACS reminds you: "May the Force Be With You" (
Star Wars)
('Total Matched lines : ', 1)
('Total Matched lines : ', 1)
MD Parameters
1. Please enter digits only in picoseconds.
2. Please eneter digits only in picoseconds
3. String for output file name
Simulation Course (picoseconds)
10
Energy minimization
100
Name of output
first_simulation
Cancel
OK


ajay@ajay-MS-7B93: /...
starting mdrun 'Protein in water'
5000 steps, 10.0 ps.
Writing final coordinates.
Core t (s) Wall t (s) (%)
Time: 49.459 4.122 1200.0
(ns/day) (hour/ns)
Performance: 209.667 0.114
GROMACS reminds you: "Before we work on artificial intelligence why don't we do something about natural stupidity?" (Steve Polyak)
ajay@ajay-MS-7B93:/media/ajay/e64e5c93-92d9-4629-a905-5f74efd31865/ajay/Documents/harry_maan/Final_touch_gmx_qk$
ajay
Documents
harry_maan
Final_touch_gmx_qk
Recent
Starred
Home
Desktop
Documents
Downloads
Music
Pictures
Videos
Trash
STRONTI...
Other Locations
Final_touch_gmx_qk
Pictures
bin
Name
Size
Modified
file_simul 3 items 10:15
output 7 items Yesterday
RPubs - Document_files 18 items Yesterday
first_simulation.tar.gz 437.5 MB 11:00
gmx_qk.sh 18.5 kB 10:27
mera.tar.gz 437.4 MB 10:29
my.html 476 bytes 10:49
RPubs - Document.html 10.0 kB Yesterday
#topol.top.1# 638.9 kB 10:27
#topol.top.2# 639.0 kB 10:28
#topol.top.3# 638.9 kB 10:58
#topol.top.4# 639.0 kB 10:58

Addition Notes

1. **Install gromacs in the two different location for example**
   a) /opt/ gromacs version 5.0 (https://gromacs-www-legacy.biophysics.kth.se/Downloads_of_outdated_releases)
   b) /usr/local/ gromacs 2021.4 (https://ftp.gromacs.org/gromacs/gromacs-2021.4.tar.gz)
2. **Install Zenity from "sudo apt-get install -y zenity"**
3. **Install python**
4. **Clean your receptor.pdb file**
5. **Generate itp file for your ligand from https://www.swissparam.ch or http://zarbi.chem.yale.edu/ligpargen**
6. **This program only uses charmm27.ff and TIP3P water model (More options will be added in upcoming versions)**
7. **MD simulation performance will be as per your gromacs installation and machine configuration i.e. RAM and GPU (CUDA toolkit)**

A big Thankyou for using gmx_qk