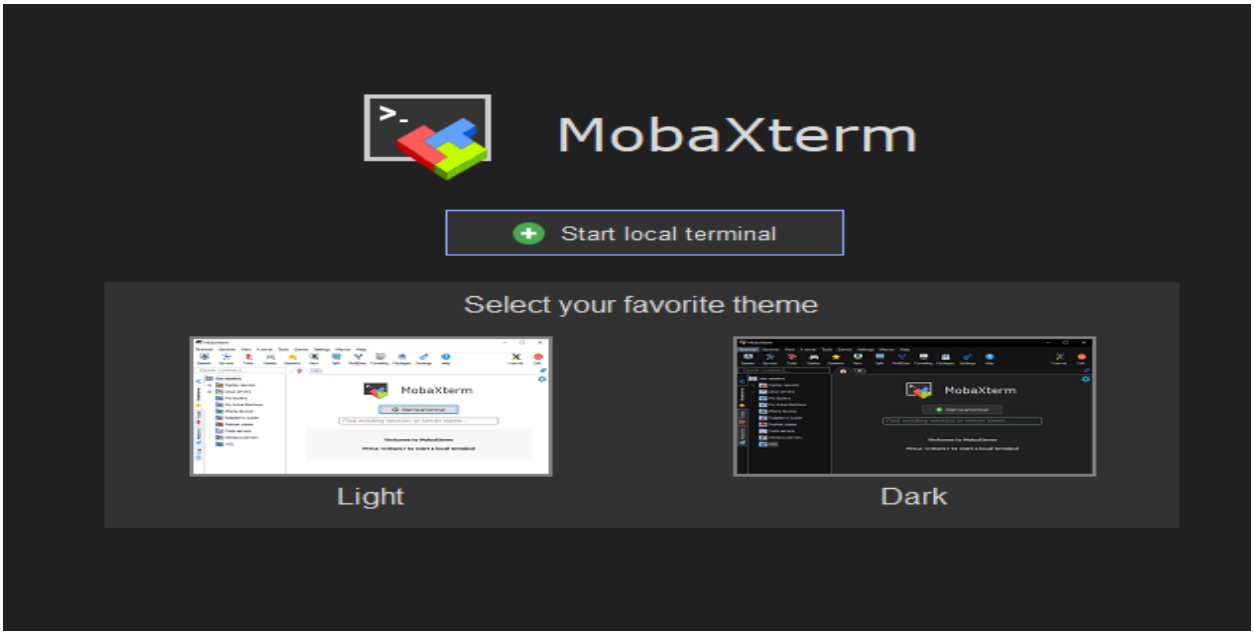
Compute Canada With Jupyter Lab

1. Download MobaXtrem at first.

2. After installing it, click on the Start the local terminal



3. Now in the terminal, login to the Compute Canada following the below steps:
   a. Login: **ssh -Y <your-username>@graham.computecanada.ca**
      Example: ssh -Y rumman@graham.computecanada.ca
   b. Enter your password at the prompt.
   c. After entering the correct credentials you will be able to see the following page.

```
(rumman@graham.computecanada.ca) Password:
(rumman@graham.computecanada.ca) Duo two-factor login for rumman

Enter a passcode or select one of the following options:

 1. Duo Push to Rumman's Phone (iOS)

Passcode or option (1-1): 897323
Success. Logging you in...
Last failed login: Sat May  4 17:40:00 EDT 2024 from 137.207.232.176 on ssh:notty
There were 3 failed login attempts since the last successful login.
Last login: Sat May  4 13:39:55 2024 from 137.207.232.176
*******************************************************************

Welcome to The Digital Research Alliance of Canada/SHARCNET cluster Graham.

 Documentation: https://docs.alliancecan.ca/wiki/Graham
Current issues: https://status.alliancecan.ca/
       Support: support@tech.alliancecan.ca

*******************************************************************

Graham has several types of GPUs, some of which are available with less wait:
 320 p100 2/node, 12GB, original
  70 v100 8/node, 16GB, newer, about 50% faster than P100 and with tensor cores
 144 t4   4/node, 16GB, newer, about half a V100, for compute & AI except much slower
FP64
More details: https://docs.alliancecan.ca/wiki/Graham#GPUs_on_Graham

************* NOTICES *************

Dec 20: /project issue: https://status.alliancecan.ca/view_incident?incident=1064

Jan 8: The data restore from the backup system is proceeding well. So
far over 5 million files have been successfully restored from tape. At
the current rate all files will be restored by early February. Files
will start appearing back in their original locations within the
project space this week.We are restoring the files in the most
efficient way possible. Files within a specific project may be
restored in several batches rather than all at once because of how
they are distributed across the backup tapes. Please watch for an
email with more details.
```

d. If “ls” is a common being type then it will show all the folders in that directory.

```
[rumman@gra-login3 ~]$ ls
jupyter1  nearline  nltk_data  projects  scratch
```

4. Now write the below commands one by one which will lead you to your folder. As my name is rumman that is why I went inside to that folder

```
[rumman@gra-login3 ~]$ ls
jupyter1  nearline  nltk_data  projects  scratc
[rumman@gra-login3 ~]$ cd projects
[rumman@gra-login3 projects]$ ls
def-masaduzz-ab
[rumman@gra-login3 projects]$ cd def-masaduzz-a
[rumman@gra-login3 def-masaduzz-ab]$ ls
masaduzz  rumman
[rumman@gra-login3 def-masaduzz-ab]$ cd rumman
```

5. Now here, **git clone https://github.com/tvhahn/compute-canada-hpc.git** write this command which will help cloning the repository whatever you want.

6. Now for creating the virtual environment you need to follow the below steps:
    a. Go to your home directory. The cd command takes you to your home directory.
    b. Load Python/3.10.13 .: module load python/3.10.13 (whichever is latest for you).
    c. Create the virtual environment in your home directory: virtualenv ~/jupyter1
    d. Activate the virtual environment you just created: source ~/jupyter1/bin/activate

7. One can install python packages here following the below steps:
    a. Install the packages you need to open up a Jupyter notebook and do data analysis.
    b. While the jupyter1 environment is active, upgrade the package manager, pip: pip install --no-index --upgrade pip You should always do this when setting up a new environment.
    c. Install basic data-science packages, scikit-learn, Pandas, Matplotlib: pip install --no-index pandas scikit_learn matplotlib seaborn

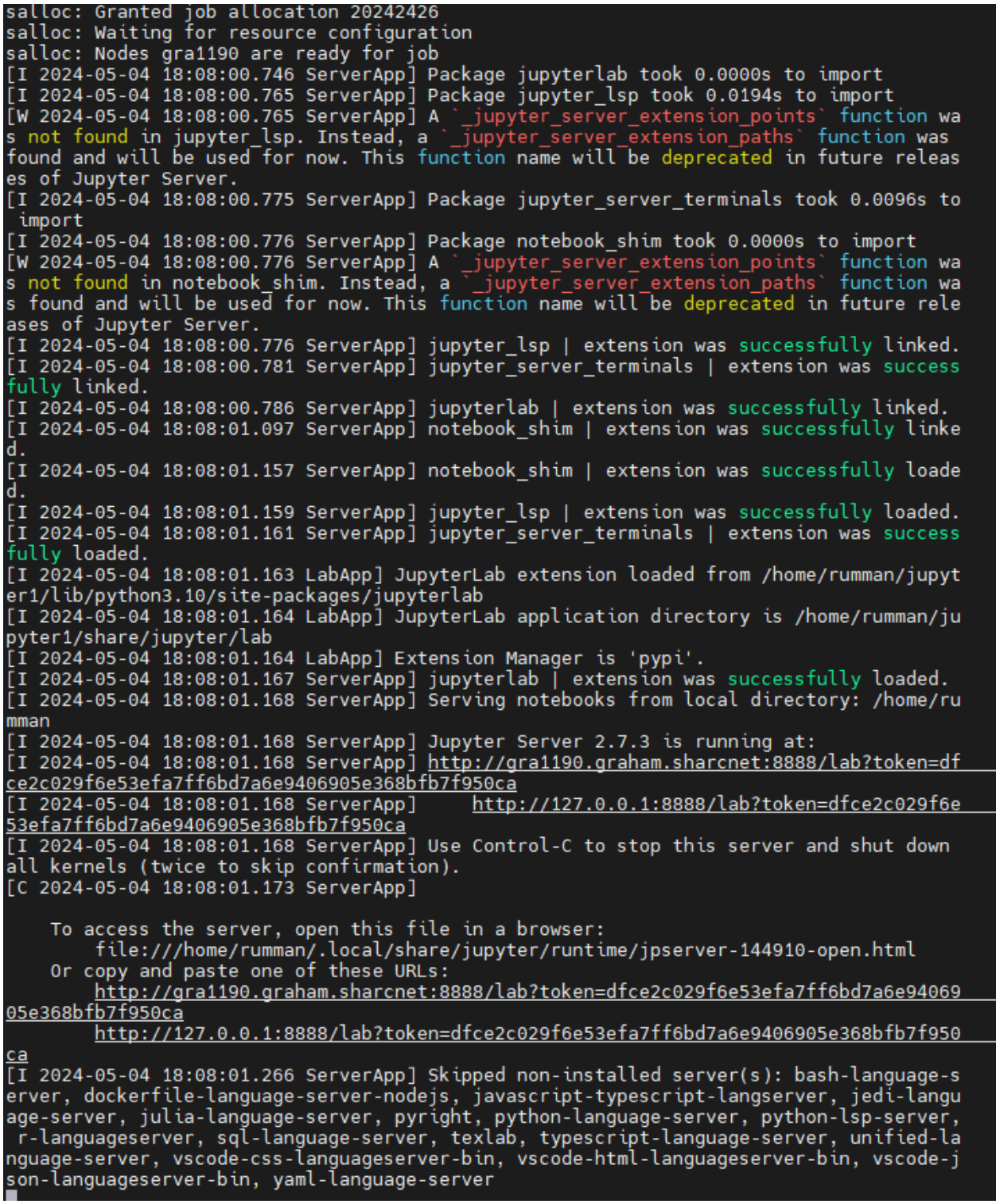
8. To launch jupyter lab you need to follow the below steps:
    a. Use nano (text editor in linux) to create a bash script that we'll call upon to open up a Jupyter Lab session.
    b. Create a script in your virtual environment (make sure jupyter1 is active), in the bin folder: nano $VIRTUAL_ENV/bin/notebook.sh
    c. This opens up the nano text editor, so that we can create the bash script
    d. Copy the following code in that file

```
#!/bin/bash
unset XDG_RUNTIME_DIR
jupyter-lab --ip $(hostname -f) --no-browser
```

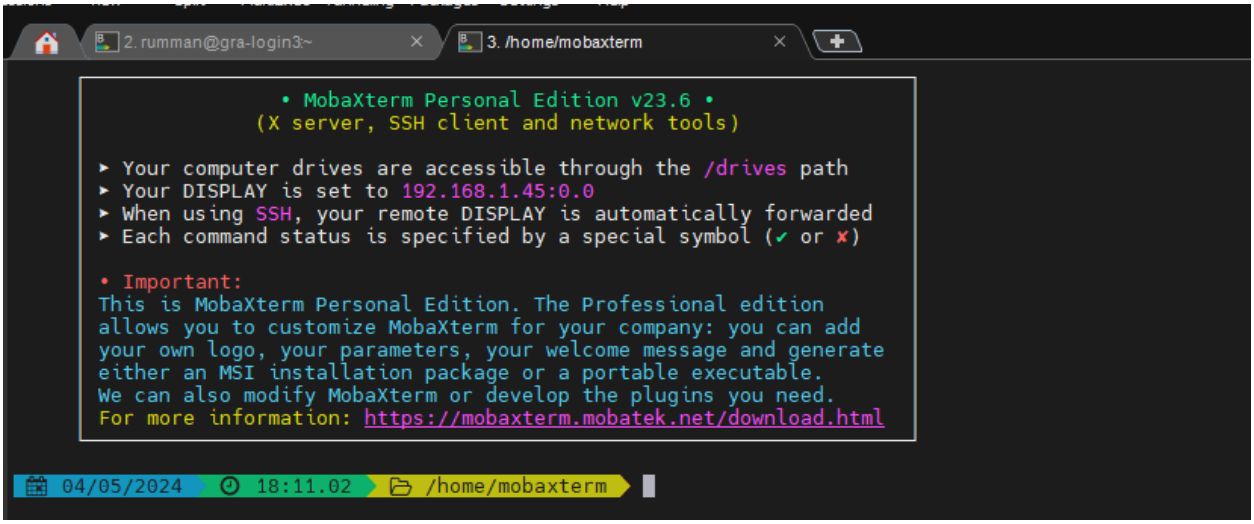
e. Press ctrl-O to save, and after that press enter and ctrl-X to exit.
f. Back in your home directory, change the user privileges of the notebook.sh that you just created (we'll allow the user, *u*, to execute, *x*, the file). This is needed so that we can run the script in the bin folder: chmod u+x $VIRTUAL_ENV/bin/notebook.sh

9. To run jupyter lab create an allocation by following the below steps:
    a. While in your virtual environment, run the following:
    salloc --time=1:0:0 --ntasks=1 --cpus-per-task=4 --mem-per-cpu=2048M --account=<your-account> srun $VIRTUAL_ENV/bin/notebook.sh
    b. Rename account name with your Compute Canada account name
    c. In the above command, 1 hour allocated for 1 task, using 4 cpus and 2048 MB of RAM/CPU. Allocated on the
    Warning: Try not to allocate more than you need so that the resources can be efficiently used between users.
    d. After running that command you will be able to see the following thing

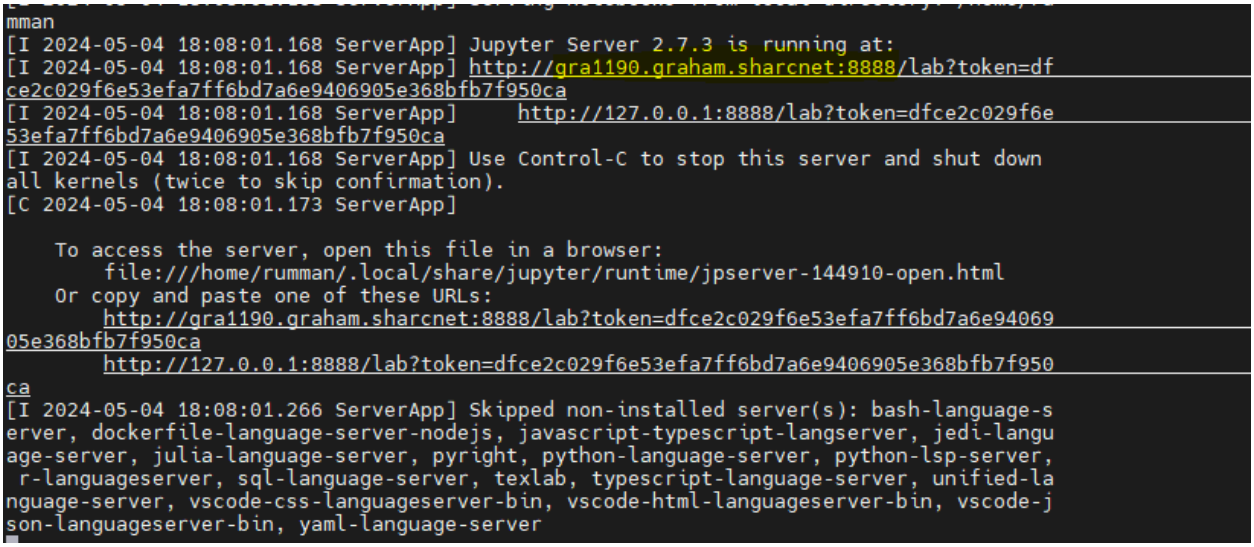
e.



10. Now open another new terminal side by side



11. In the new terminal, ssh into the graham server. Type something like this, based on what is shown the other terminal you have open showing the notebook access token: ssh -L 8888:[gra800.graham.sharcnet:8888(change this with new value)] rumman@graham.computecanada.ca
12. Replace the red one with the value marked as yellow which you got from the previous terminal



13. Now if you see the following picture in your new terminal, then your task is almost done:

```
Enter a passcode or select one of the following options:

 1. Duo Push to Rumman's Phone (iOS)

Passcode or option (1-1): 584134
Success. Logging you in...
Last failed login: Sat May  4 18:15:59 EDT 2024 from 137.207.232.176 on ssh:notty
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Last login: Sat May  4 12:49:37 2024 from 137.207.232.176
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efficient way possible. Files within a specific project may be
restored in several batches rather than all at once because of how
they are distributed across the backup tapes. Please watch for an
email with more details.

*******************************************************************************
```
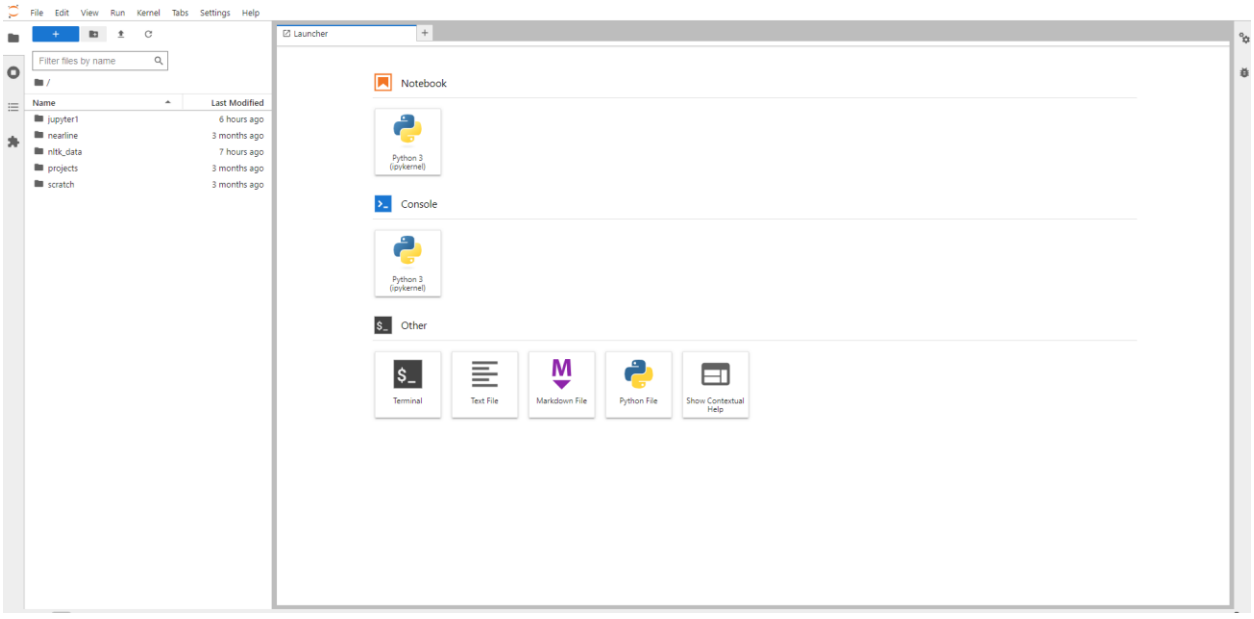

14. Then on local browser, copy the link to Jupyter lab with the access token, like: http://localhost:8888/?token=<token>
15. Now, Replace the token value with previous terminal's token value which has been marked yellow in the below picture:
16. Now you will be able to have the access to your server

```
[I 2024-05-04 18:08:00.776 ServerApp] Package notebook_shim took 0.0000s to import
[W 2024-05-04 18:08:00.776 ServerApp] A `_jupyter_server_extension_points` function wa
s not found in notebook_shim. Instead, a `_jupyter_server_extension_paths` function wa
s found and will be used for now. This function name will be deprecated in future rele
ases of Jupyter Server.
[I 2024-05-04 18:08:00.776 ServerApp] jupyter_lsp | extension was successfully linked.
[I 2024-05-04 18:08:00.781 ServerApp] jupyter_server_terminals | extension was success
fully linked.
[I 2024-05-04 18:08:00.786 ServerApp] jupyterlab | extension was successfully linked.
[I 2024-05-04 18:08:01.097 ServerApp] notebook_shim | extension was successfully linke
d.
[I 2024-05-04 18:08:01.157 ServerApp] notebook_shim | extension was successfully loade
d.
[I 2024-05-04 18:08:01.159 ServerApp] jupyter_lsp | extension was successfully loaded.
[I 2024-05-04 18:08:01.161 ServerApp] jupyter_server_terminals | extension was success
fully loaded.
[I 2024-05-04 18:08:01.163 LabApp] JupyterLab extension loaded from /home/rumman/jupyt
er1/lib/python3.10/site-packages/jupyterlab
[I 2024-05-04 18:08:01.164 LabApp] JupyterLab application directory is /home/rumman/ju
pyter1/share/jupyter/lab
[I 2024-05-04 18:08:01.164 LabApp] Extension Manager is 'pypi'.
[I 2024-05-04 18:08:01.167 ServerApp] jupyterlab | extension was successfully loaded.
[I 2024-05-04 18:08:01.168 ServerApp] Serving notebooks from local directory: /home/ru
mman
[I 2024-05-04 18:08:01.168 ServerApp] Jupyter Server 2.7.3 is running at:
[I 2024-05-04 18:08:01.168 ServerApp] http://gra1190.graham.sharcnet:8888/lab?token=df
ce2c029f6e53efa7ff6bd7a6e9406905e368bfb7f950ca
[I 2024-05-04 18:08:01.168 ServerApp]     http://127.0.0.1:8888/lab?token=dfce2c029f6e
53efa7ff6bd7a6e9406905e368bfb7f950ca
[I 2024-05-04 18:08:01.168 ServerApp] Use Control-C to stop this server and shut down
all kernels (twice to skip confirmation).
[C 2024-05-04 18:08:01.173 ServerApp]

    To access the server, open this file in a browser:
        file:///home/rumman/.local/share/jupyter/runtime/jpserver-144910-open.html
    Or copy and paste one of these URLs:
        http://gra1190.graham.sharcnet:8888/lab?token=dfce2c029f6e53efa7ff6bd7a6e94069
05e368bfb7f950ca
        http://127.0.0.1:8888/lab?token=dfce2c029f6e53efa7ff6bd7a6e9406905e368bfb7f950
ca
[I 2024-05-04 18:08:01.266 ServerApp] Skipped non-installed server(s): bash-language-s
erver, dockerfile-language-server-nodejs, javascript-typescript-langserver, jedi-langu
age-server, julia-language-server, pyright, python-language-server, python-lsp-server,
 r-languageserver, sql-language-server, texlab, typescript-language-server, unified-la
nguage-server, vscode-css-languageserver-bin, vscode-html-languageserver-bin, vscode-j
son-languageserver-bin, yaml-language-server
srun: interrupt (one more within 1 sec to abort)
srun: StepId=20242426.0 task 0: running
```

17. Now you will have the access to your server



18. Now for the scheduling jobs follow the following steps:
    a. Now create a file (ex: random_search_cpu.sh)
    b. Inside this file add the following bash script

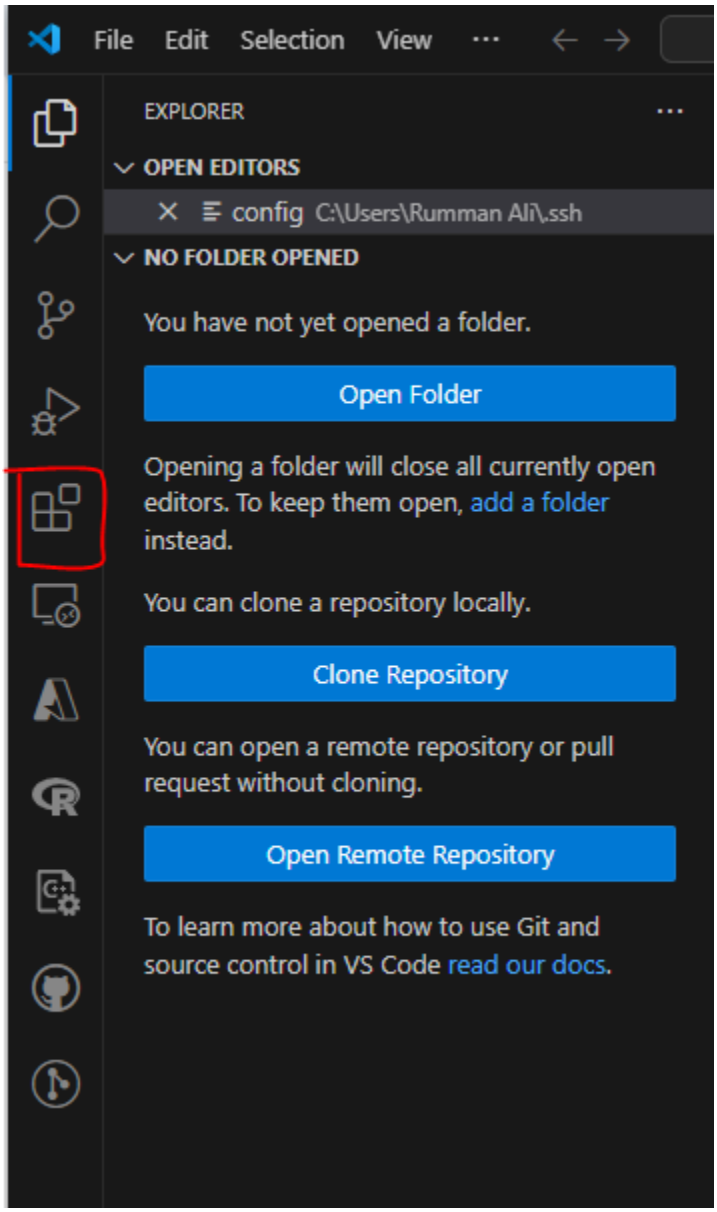
```
#!/bin/bash
#SBATCH --account=<your-account>
#SBATCH --cpus-per-task=4   # number of cores
#SBATCH --mem=4G          # memory for the entire job across all cores (4GB)
#SBATCH --time=0-00:10     # time (DD-HH:MM)
#SBATCH --output=%N-%j.out  # %N for node name, %j for jobID
#SBATCH --mail-type=ALL            # Type of email notification-
BEGIN,END,F$
#SBATCH --mail-user=<your-email> # Email to which notifications will be $


module load python/3.10.13
source ~/jupyter1/bin/activate

python train_model_tcn.py
```

    c. The email id is provided so that when this will start and finish it will be sent to the provided mail id.
    d. Account name will be replaced by your own account name, time can be updated with requirement and email id.
    e. For submitting the bash job do the following command:
       sbatch random_search_cpu.sh
    f. To see the progress of the bash job type the following command:
       squeue -u rumman

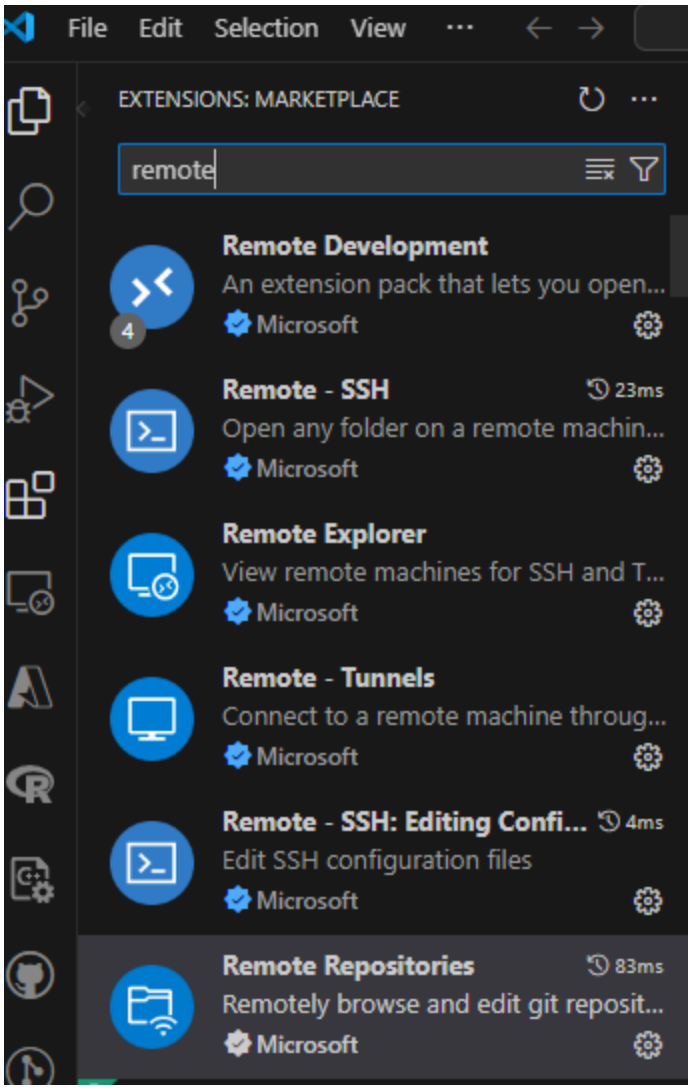
Referenced Video: https://www.youtube.com/watch?v=K8wuaIKW6aU

Compute Canada With Visual Studio

1. Download Visual Studio Code Community edition
2. Now go to visual studio code. Need to add the following extensions:
    a. Click on this extension tab



    b. Now search remote and download the following extensions



3. Next step is to generate a public key and add that key in Compute Canada as well.
    a. Enter the following command which will result in creating the public key. At the end, add your own email address
    ssh-keygen -t rsa -b 4096 -C <your-email>

```
C:\Users\Rumman Ali>ssh-keygen -t rsa -b 4096 -C ali5i@uwindsor.ca
Generating public/private rsa key pair.
Enter file in which to save the key (C:\Users\Rumman Ali/.ssh/id_rsa):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in C:\Users\Rumman Ali/.ssh/id_rsa.
Your public key has been saved in C:\Users\Rumman Ali/.ssh/id_rsa.pub.
The key fingerprint is:
SHA256:Z2+eLl7roHPFxkIdYTSqjSjhiX7CtcVmjPdUROmvO1c ali5i@uwindsor.ca
The key's randomart image is:
+---[RSA 4096]----+
|          .oo=.  |
|          ..o..  |
|     .    .o. .  |
|   o * . =o .    |
|  . * O S.++     |
| o . B o o..* E  |
|  + o   . .=+.   |
|   o    ..==.o   |
|        .+oB*    |
+----[SHA256]-----+
```

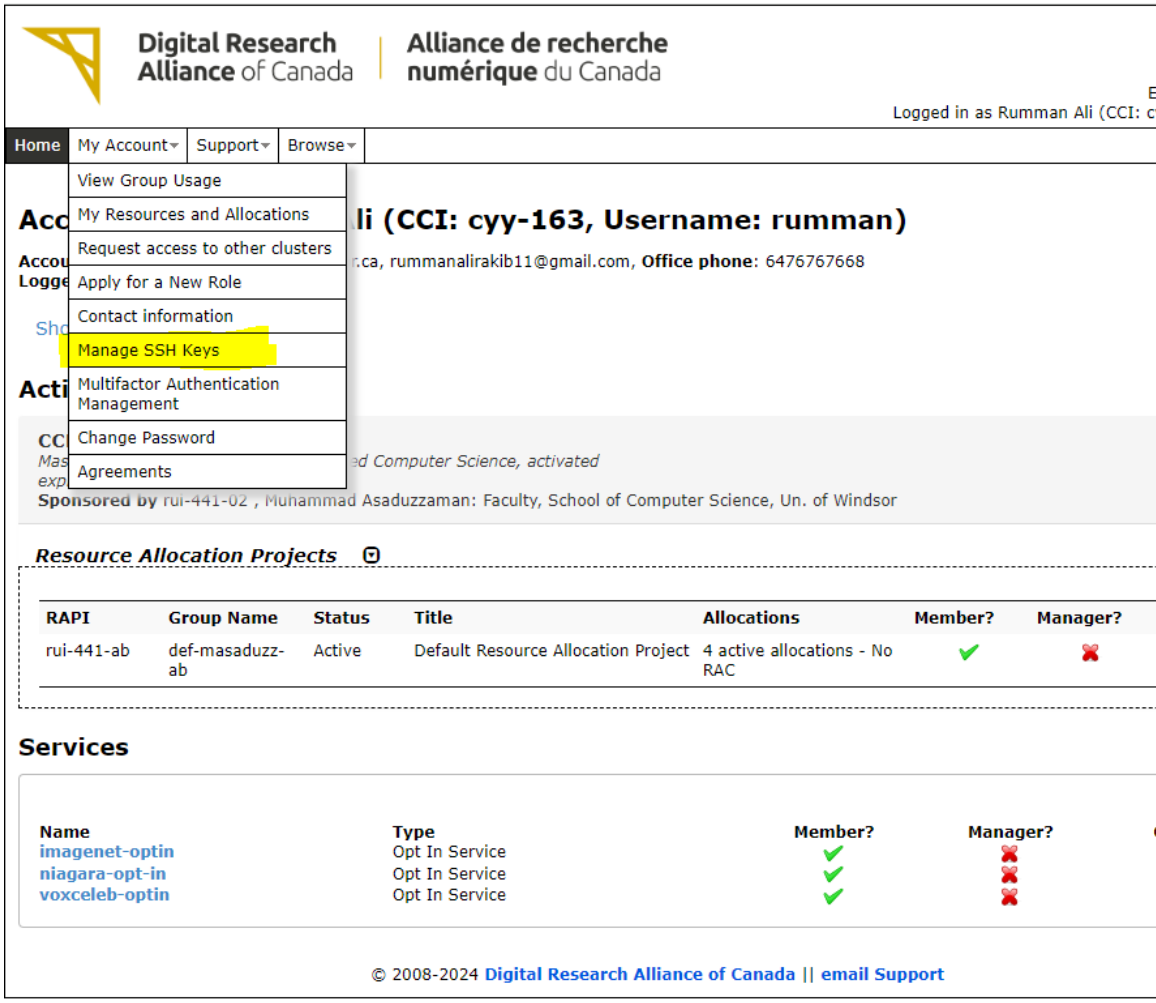
b. It will ask for the location where you want to save the key pair. If you press enter then C:\Users\Rumman Ali/.ssh/id_rsa this will be its default location.

c. And be careful about the passphrase, if you are providing one then do remember it.

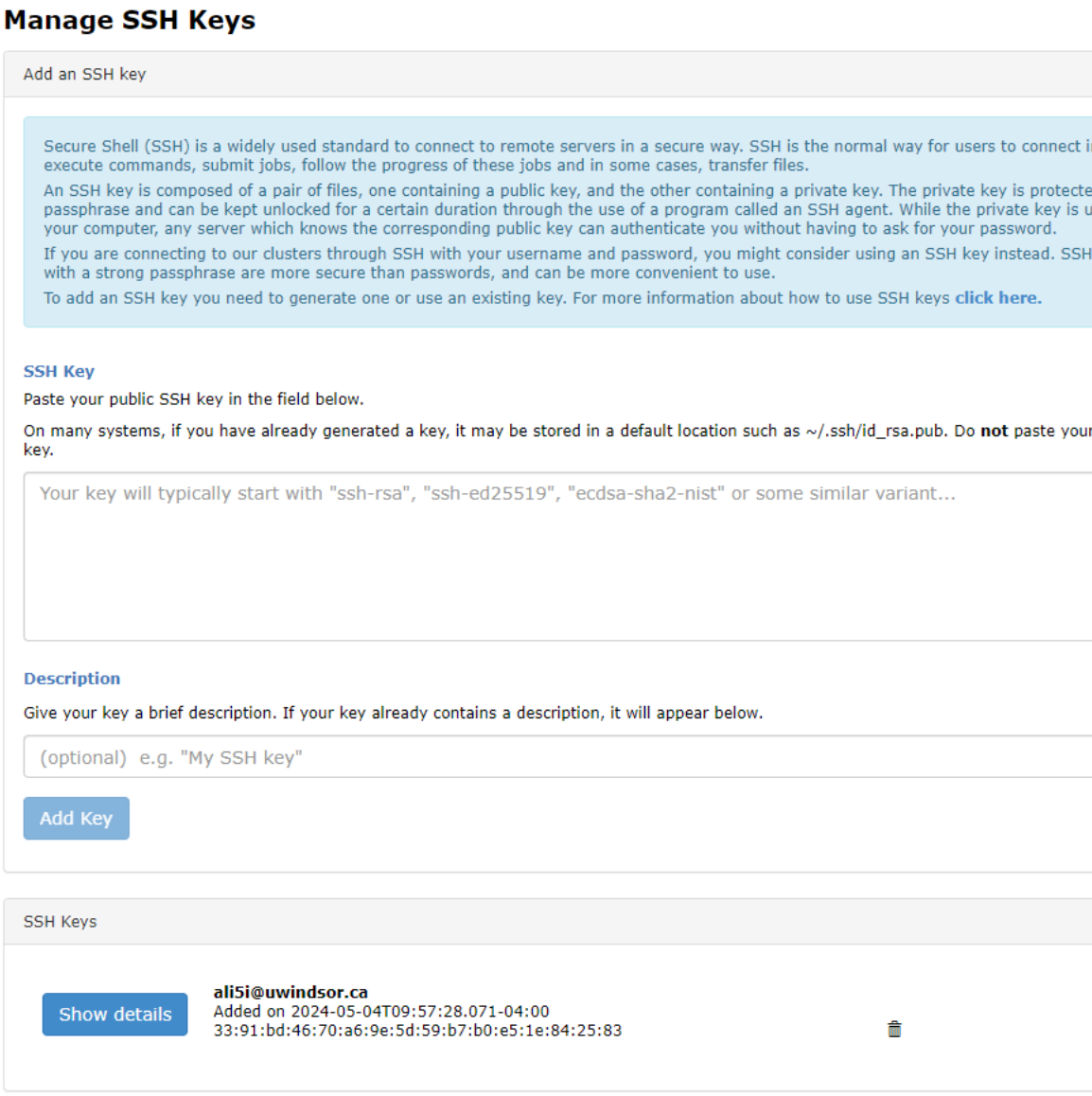
d. With the following command, you can see your public key in the command line or you open it from the folder as well.
Command is: cat ~/.ssh/id_rsa.pub

```
C:\Users\Rumman Ali>cat ~/.ssh/id_rsa.pub
ssh-rsa AAAAB3NzaC1yc2EAAAADAQABAAACAQCyP0kQ5MuOvq7QPHOq5atfKxow41u7z6XT8kO4wfIdN9ZdpvCNa/NtFaB6WLmEWL8YBu9LE3rxFOj3hhBw6GJqlGERw6dXK3tsLSnqYbgnvrH
m07ZHHgw9KeTjpyv9NnJxo4MGpHx+T7skAjdyIWY8b7BzDC26WMhz3mJke2CFd9pQWHDW8YpOGyTGa3fccANGuGI09GWhFPhAOWc+bkbInzDpjNX7G5gzv9fkjVNnodgZ65HcSn0dC4+QvCcng1
mfZlpyXlWvZ+Nyfobtxa7vySdOs2zJT4U/xMk612DeMmyY7je6zMNqjlmkjp27KMMon+VcK4aFrV081kRpQV24H4/X+/hQEUIvMMisSGqVbiUAl+oJ5ydNmidzOmDc9u5T6Q1pRA/Se6R9np14C
Na6NZG9STNuPvMqwh/yBmoEII7eLlAbRn22mRSQ4WCPAy2BPrBDRPc4hJxaaHJ3NMfcwxu0b6YpdUdcbruJVaeHYNK0+XVut9GHhgTfXzKuDJT2xCLHajIqtbuVhB9CSC2LXbviriwD2ru8LZOc
gAXR2Y1tASCgMQL6c+BPKk3u5A3+kwyW02y7xlQQ9X43soWrmrvw94OR8vMH4IrYYZ4NvUpgRJTrLtH6Qnef2UsBLQ== ali5i@uwindsor.ca
```

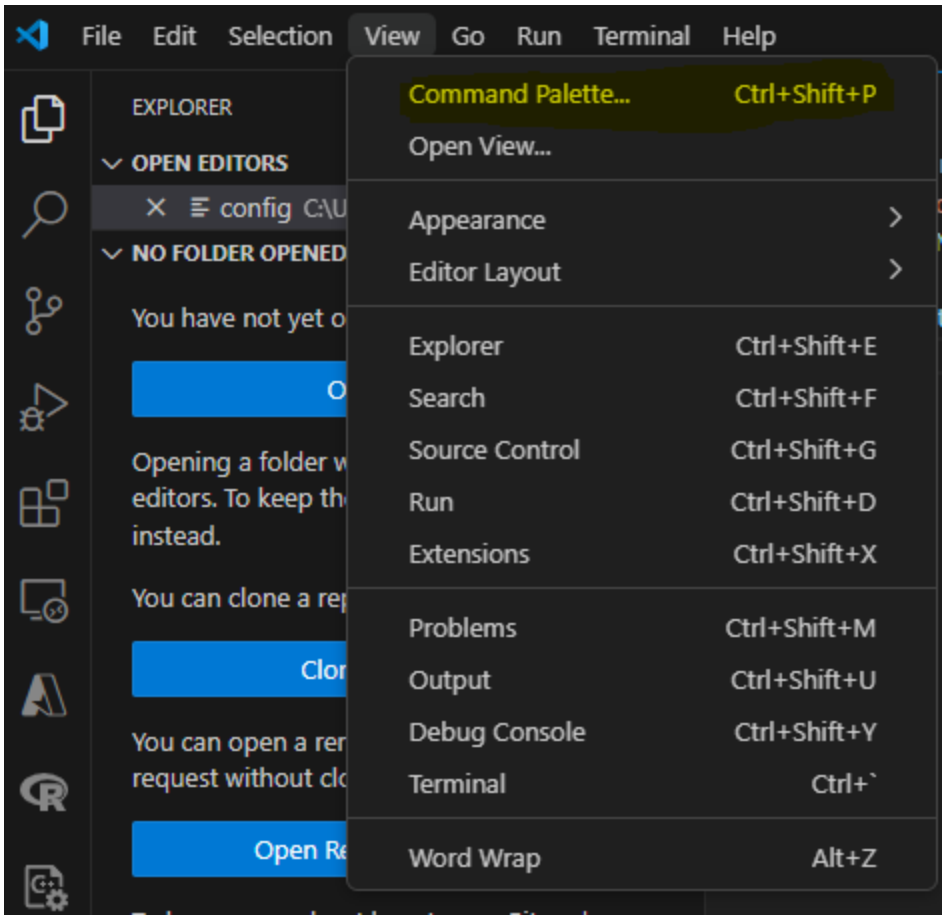
e. Log into Compute Canada. After logging in go to the Manage SSH Keys



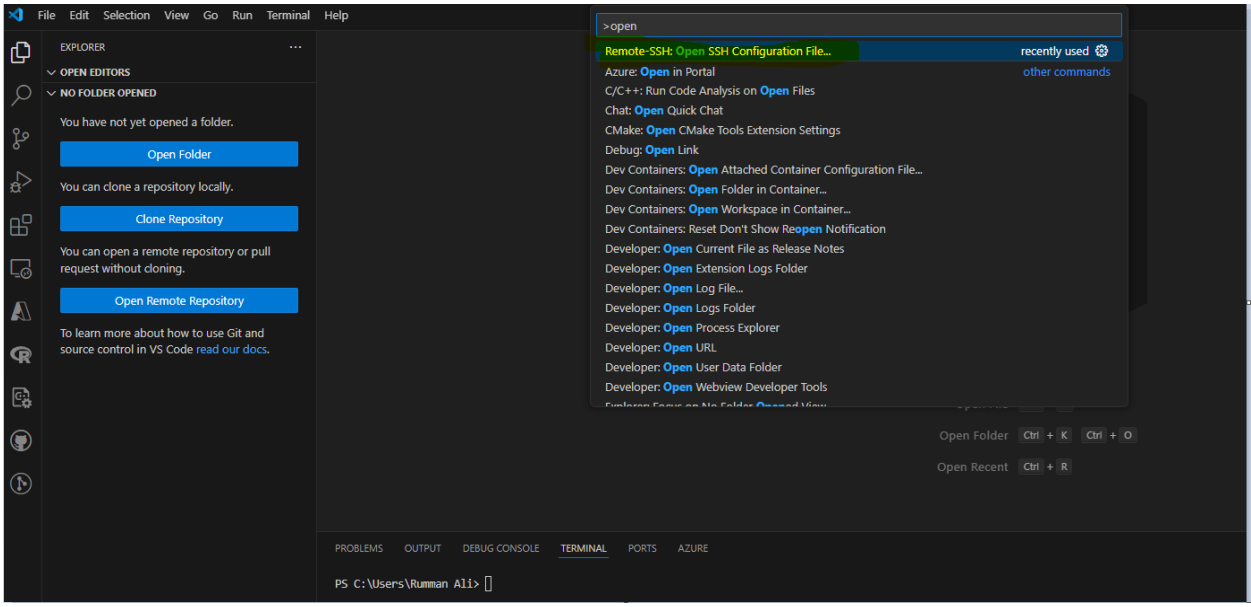
f. Paste the public key in the SSH Key section. After pasting the public key in that box. Now, click on the button Add Key which will result in adding the key.



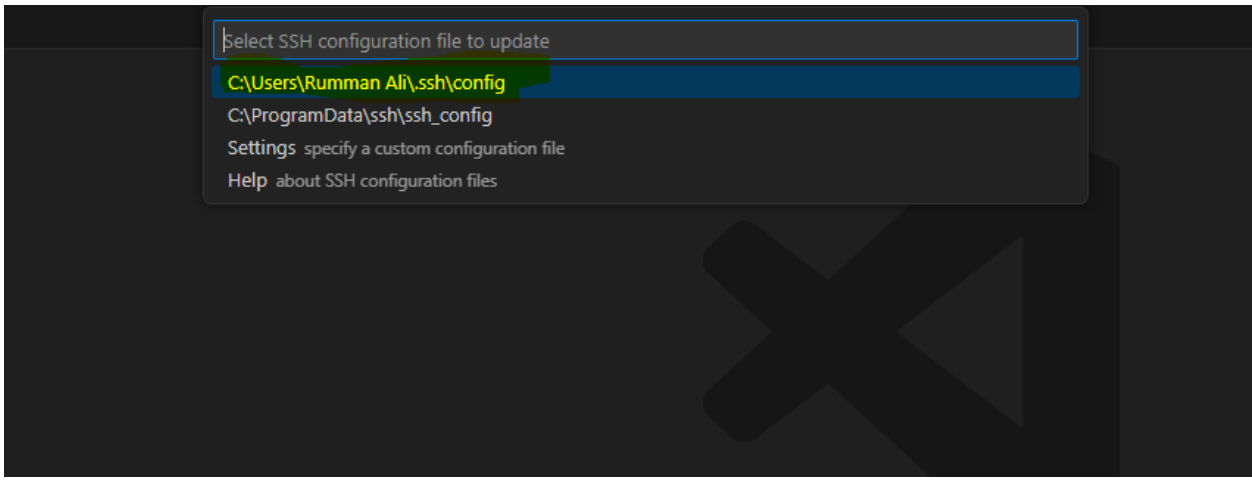
4. Now go to Visual Studio Code and open Command Palette from view or by using shower key Ctrl+Shift+P



5. Now after that go to Remote SSH: Open SSH Configuration file



6. Now just go with the default one:

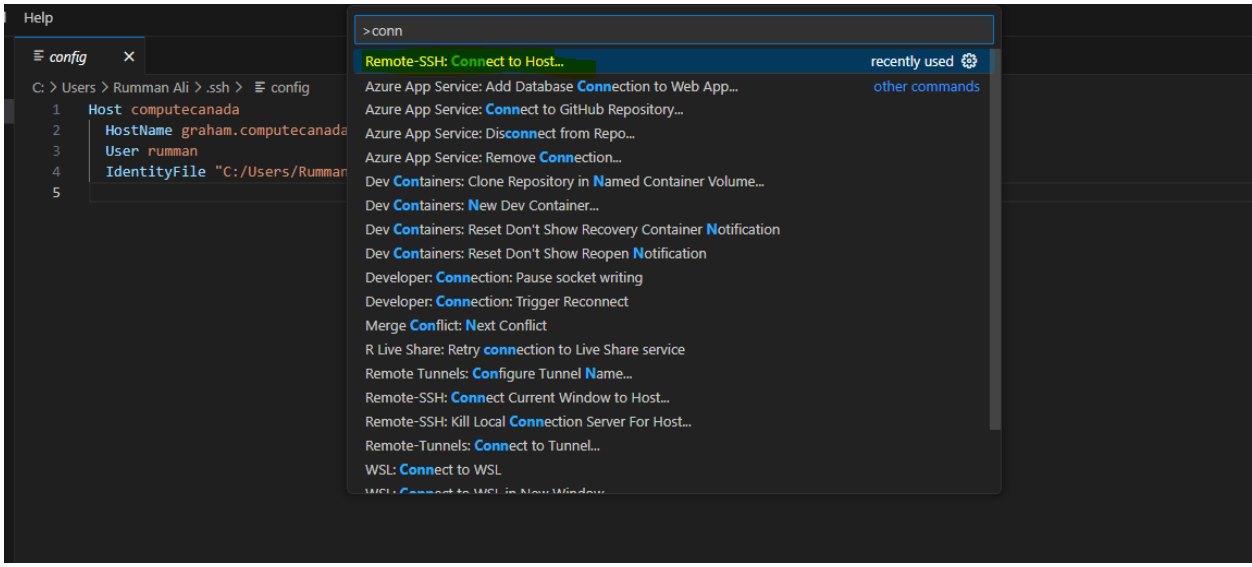


7. Now in that file add the following things:

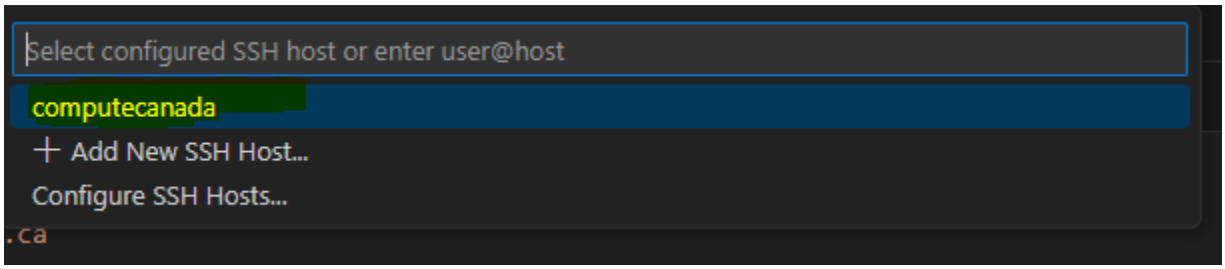
```
Host computecanada
  HostName graham.computecanada.ca
  User rumman
  IdentityFile "C:/Users/Rumman Ali/.ssh/id_ed25519"
```

Add the value with your own values. After that in the IdentifyFile just add the location of your public key in the quotation mark.

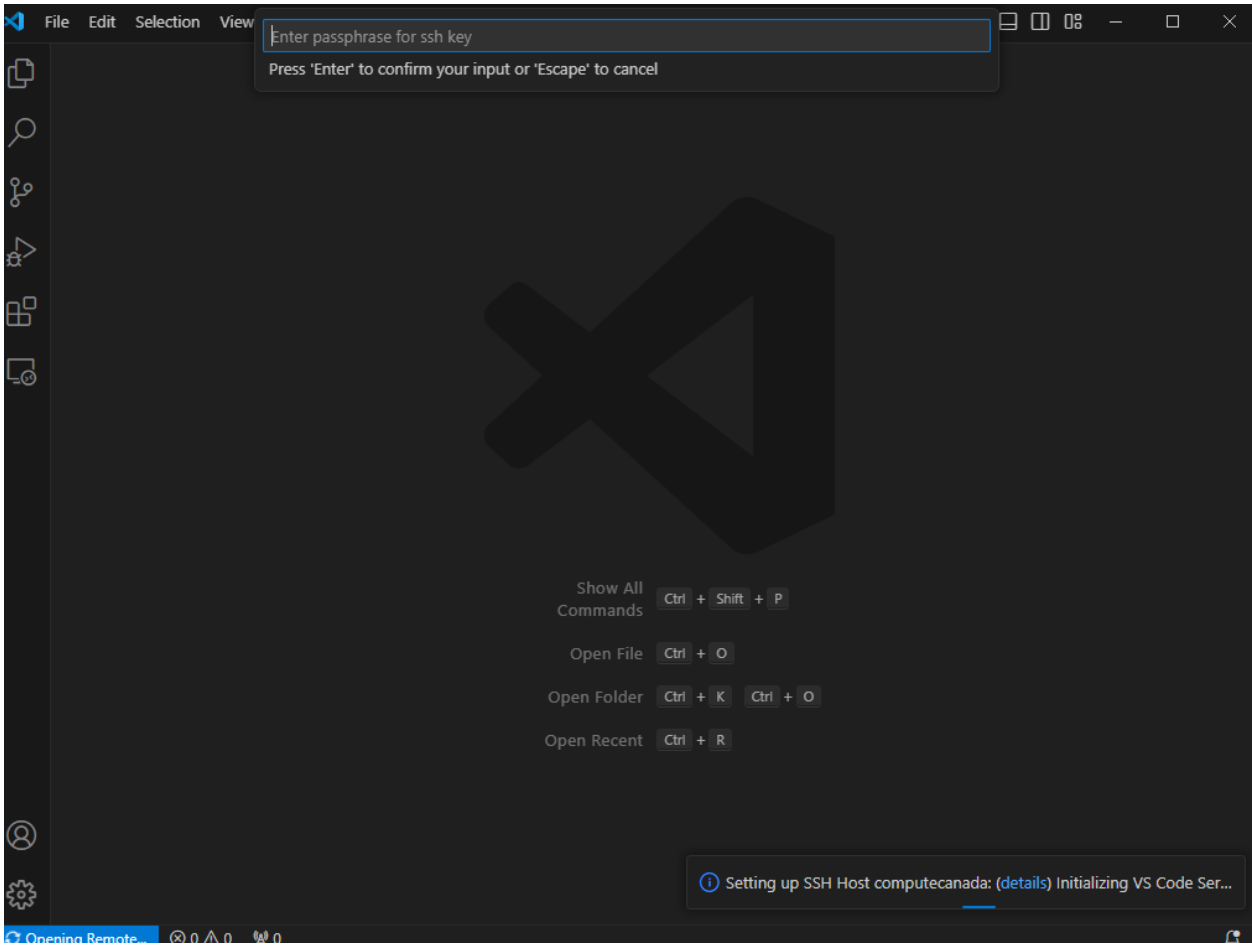
8. Now, again open Command Palette select the Remote-SSH: Connect to Host



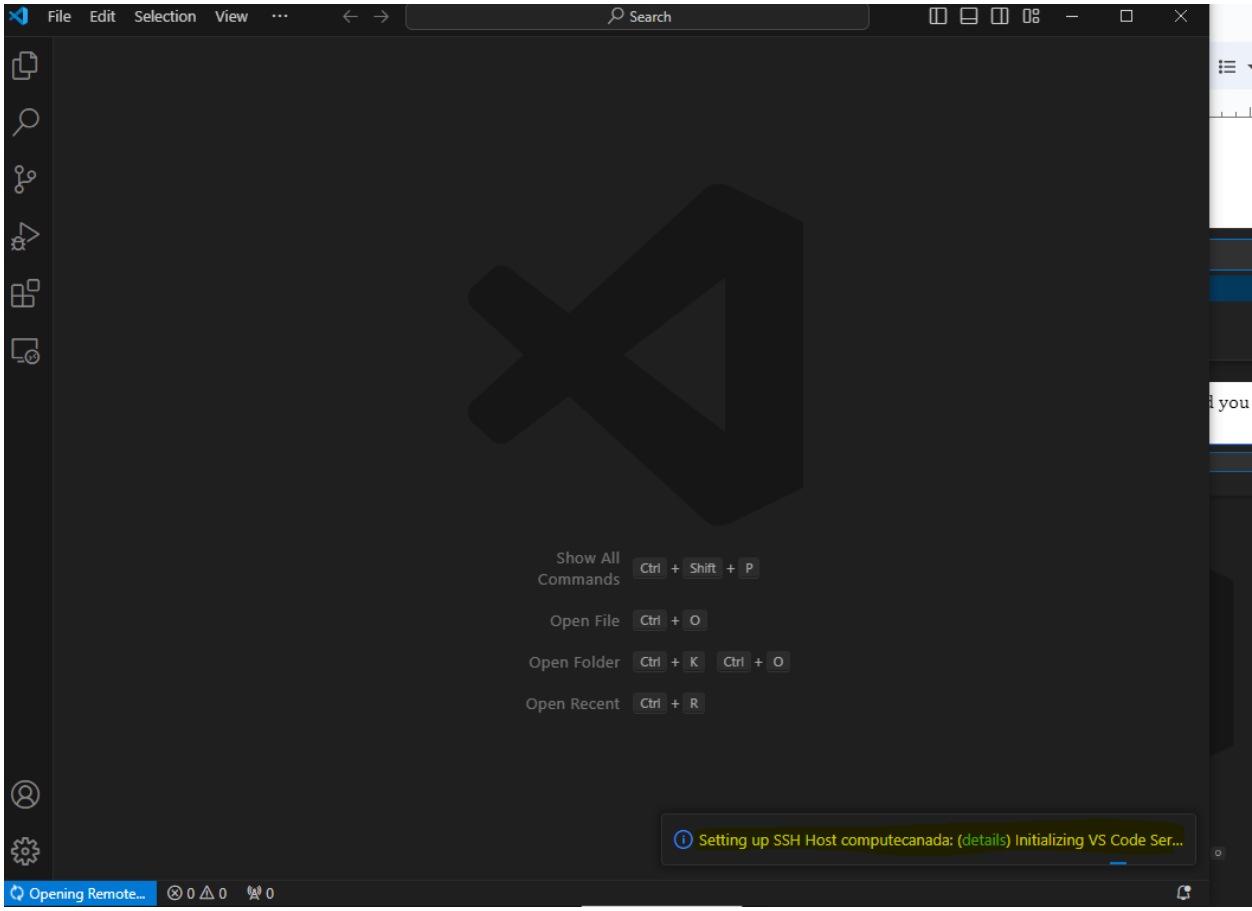
9. Now, Select the Host you provided



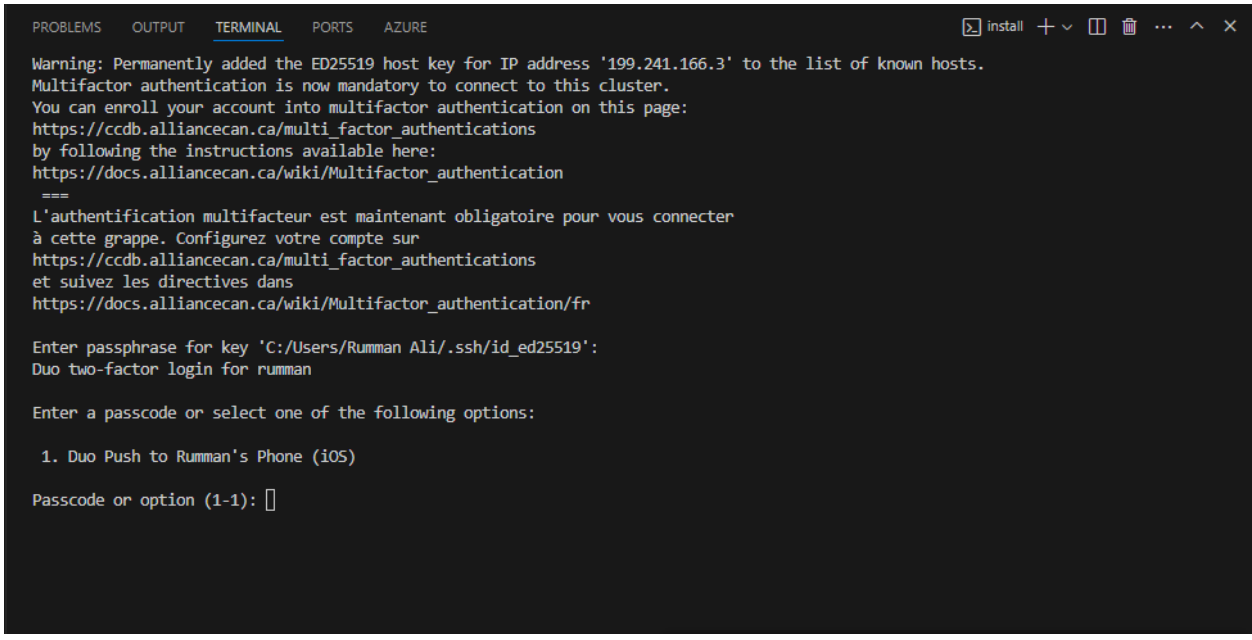
10. Now it will redirect you to the new visual studio code. And you will have to provide your passphrase



11. Now click on the details. Otherwise it will keep on running.



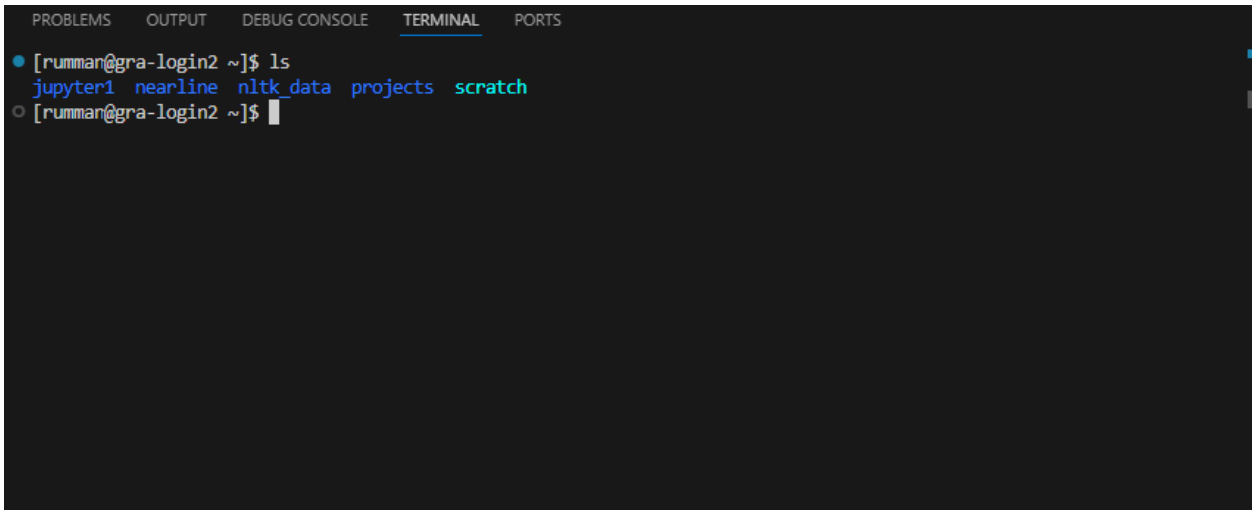
12. Now provide the passcode for your two step verification



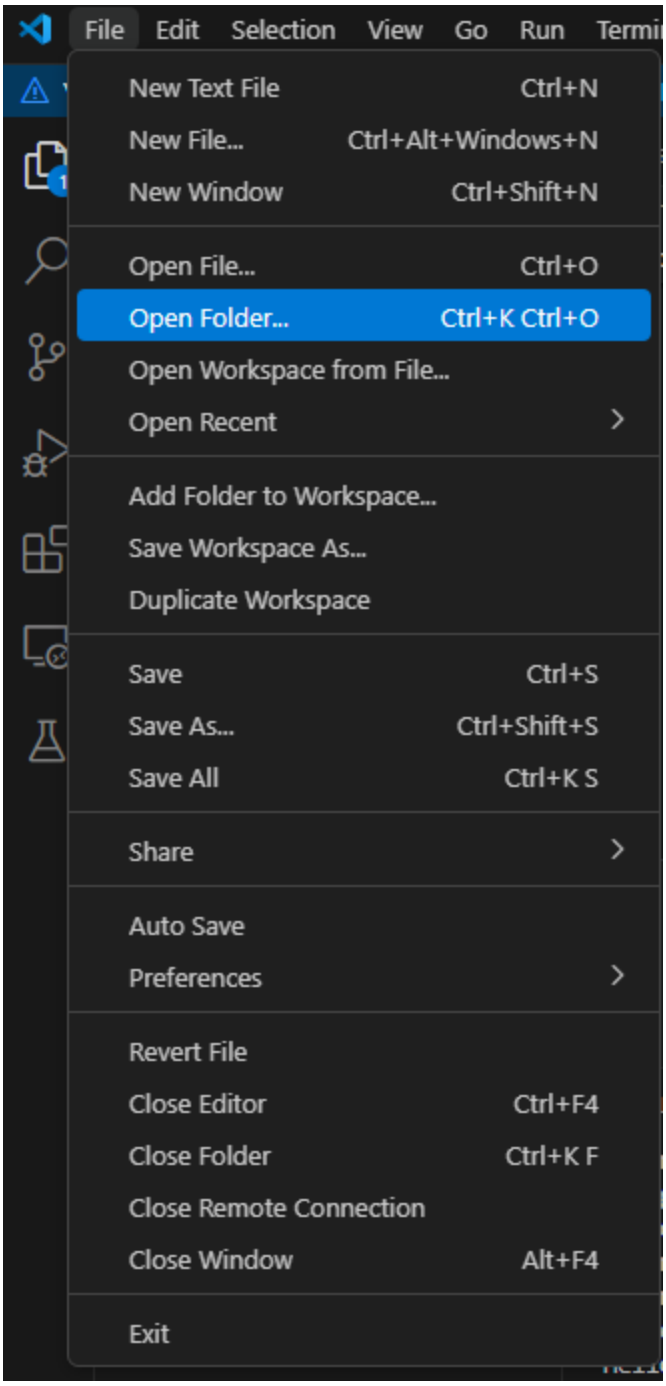
13. Now, after the successful connection, you will be able to see the following things

```
    __lmod_my_status=$?;
    if [ -n "${__lmod_sh_dbg:-}" ]; then
    echo "Shell debugging restarted" 1>&2;
    set -$__lmod_sh_dbg;
    fi;
    unset __lmod_sh_dbg;
    return $__lmod_my_status
   }
   _=/cvmfs/soft.computecanada.ca/gentoo/2023/x86-64-v3/usr/bin/printenv
Removing old logfile at /home/rumman/.vscode-server/.cli.b58957e67ee1e712cebf466b995adf4c5307b2bd.log
Spawned remote CLI: 22014
Waiting for server log...
76ee38927c63: start
SSH_AUTH_SOCK====
DISPLAY====
listeningOn==127.0.0.1:39304==
osReleaseId==centos==
arch==x86_64==
vscodeArch==x64==
bitness==64==
tmpDir==/tmp==
platform==linux==
unpackResult====
didLocalDownload==0==
downloadTime====
installTime====
serverStartTime==113==
execServerToken==371686a5-4d47-4273-af4d-3c0eb6120cb0==
76ee38927c63: end
```

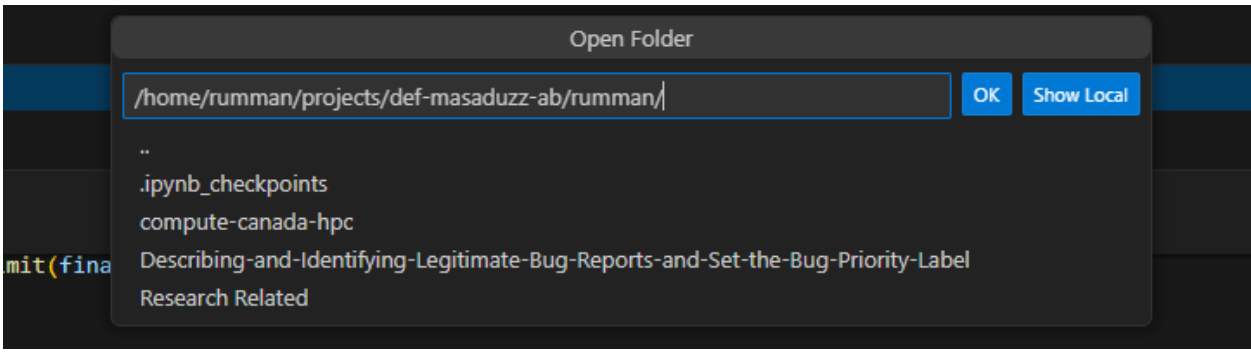
14. Now, if you open your new terminal in the VS code then you will be able to see that, you are now connected with your Compute Canada server



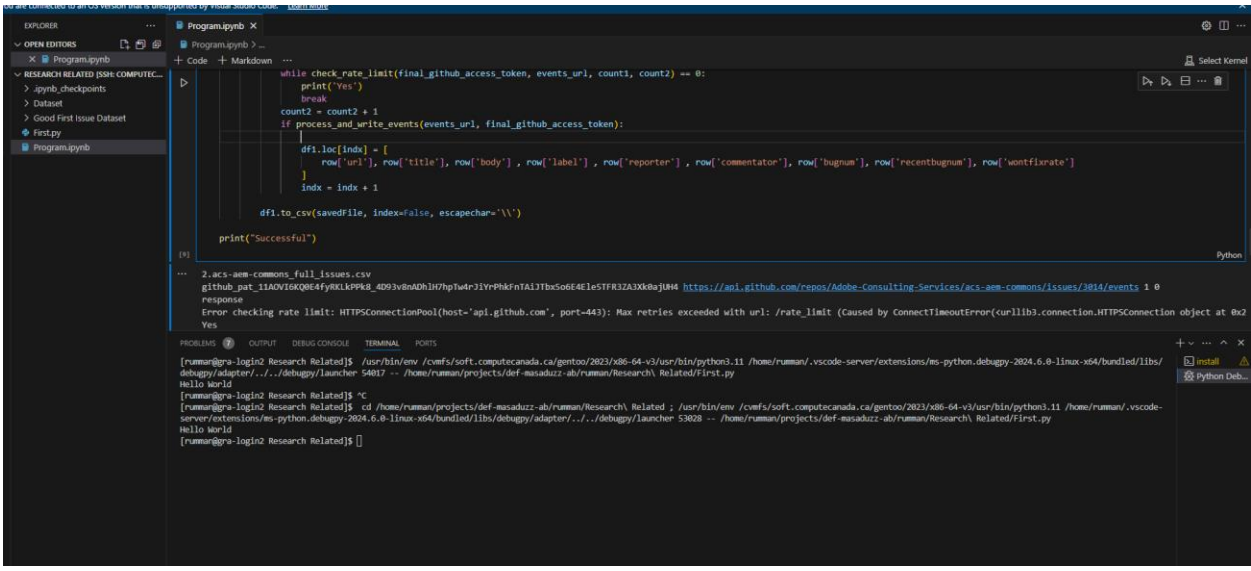
15. Now go to file and open folder



16. After that, it will ask you to redirect to the folder you want to work on.



17. And after selecting the folder, now you can write your code and run your file.



Referenced Video: https://www.youtube.com/watch?v=lKXMyln_5q4