

BGU ISE-CS-DT Cpu Cluster User Guide

10/04/2022

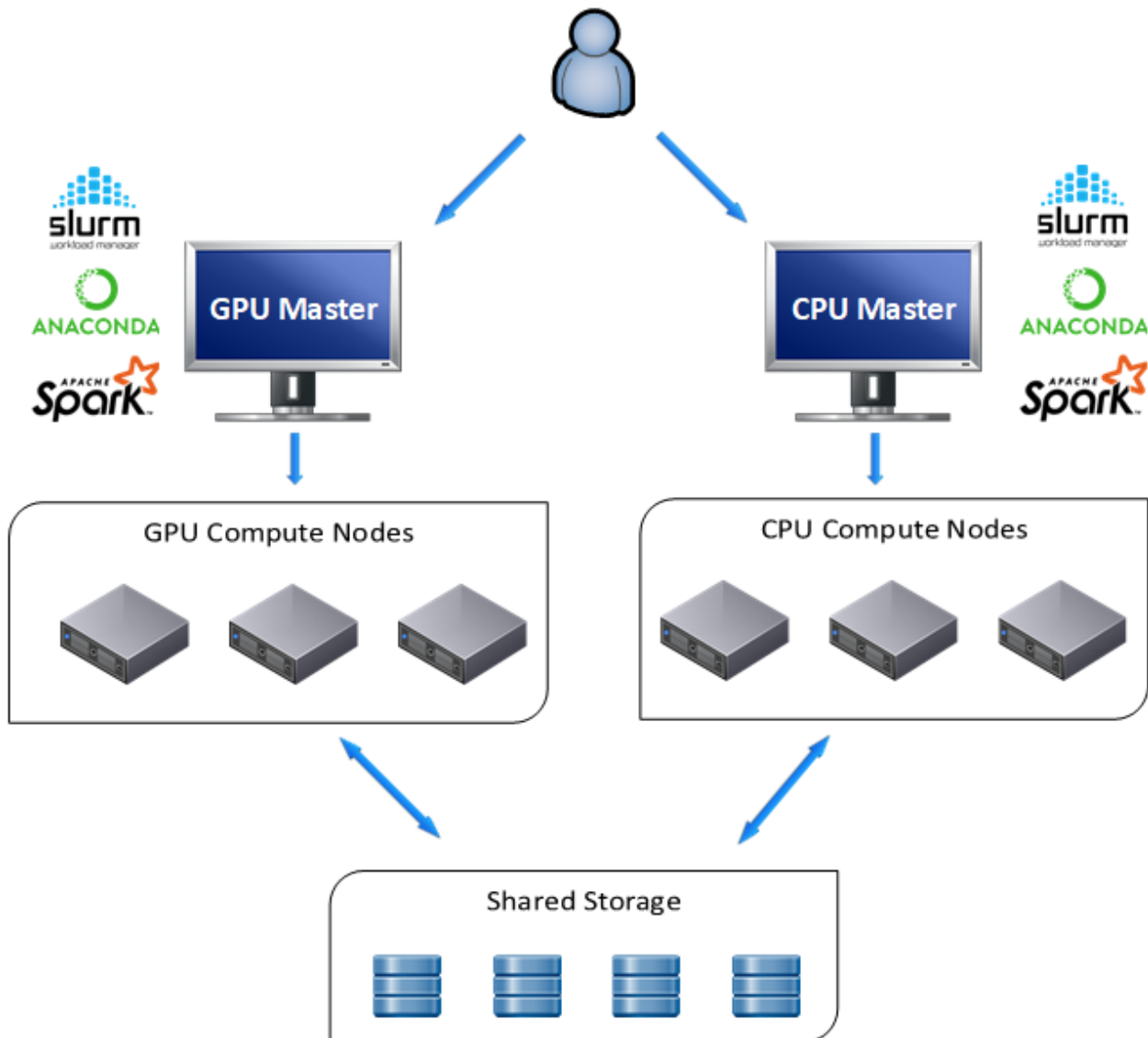
Contents

Abstract.....	4
Use	6
Submitting a Job.....	7
Batch File.....	7
Allocating Resources	8
Information about the compute nodes	9
List of My Currently Running Jobs	9
Cancel Jobs.....	9
Cancel All Pending jobs for a Specific User	9
Running Job Information	9
Complete Job Information	9
Advanced Topics	10
Jupyter Lab.....	10
Installation	10
Make the Conda Environment Available in Notebook’s Interface	10
Release Job Resources from Within Jupyter After Code Has Finished Running.....	10
How to add ipywidgets to Jupyter Lab.....	10
Tensorboard.....	11
Working with Notebooks	11
Allocate Extra RAM/CPUs	12
Working with the Compute Node SSD Drive	13
Job Arrays.....	14
Send Name of an Input File to Each Task.....	14
Read a Line from an Input File for Each Task.....	14
Email Notifications	14
Limiting the Number of Simultaneously Running Tasks from the Job Array	15
Job Dependencies	16
IDEs	17
pyCharm.....	17
Visual Studio Code	20
Docker	24
Installation	24

Test.....	24
Matlab.....	26
R	27
Command Line	27
C#	28
Install In Conda Environment.....	28
Use	28
Appendix	29
Step by Step Guide for First Use of Python and Conda	29
Conda	30
Viewing a list of your environments	30
list of all packages installed in a specific environment	30
Activating / deactivating environment	30
Create Environment	30
Update Conda	31
Compare Conda Environments	31
Transfer Files.....	32
To / From Your PC.....	32
Get a Public File.....	32
Deap.....	33
Create Environment.....	33
FAQ.....	34
Usage.....	34
Errors.....	34

Abstract

This document is located on the cluster in the '/storage' directory and being updated from time to time. Please make sure you have the most recent version.



BGU ISE, DT and CS departments have two Slurm clusters – a GPU cluster and a CPU cluster. The cluster is a job scheduler and resource manager. It consists of a manager node and several compute nodes.

The manager node is a shared resource used for launching, monitoring, and controlling jobs and should **NEVER** be used for computational purposes.

The compute nodes are powerful Linux machines.

The user connects to the manager node and launches jobs that are executed by compute nodes.

A job is allocation of compute resources such as RAM memory, cpu cores, etc. for a limited time. A job may consist of job steps which are tasks within a job.

In the following pages, *Italic* writing is saved for Slurm command line commands.

You may find abundance of information regarding Slurm, on the web.

Use

- Make sure you got admission to the cluster by your IT team.
- Ssh to the Manager Node: 132.72.65.199
- Use your BGU user name and password to login to the manager node. The default path is to your home directory on the storage.
- Python users: create your virtual environment on the manager node.
- If you copy files to your home directory, don't forget about file permissions. E.g. files that need execution permissions, do: `chmod +x <path to file>`
- Remember that the cluster is a shared resource. Currently, users are trusted to act with responsibility in regards to the cluster usage – i.e. **release unused allocated resources (with *scancel*), not allocate more than needed resources, erase unused files and datasets, etc.** Please release the resources even if you are taking a few hours break from interactively using them.
- Anaconda3 is already installed on the cluster.
- Please read thoroughly, the following page or two. If you are clueless about Linux, Conda and the rest of the environment then use the [Step by Step Guide for First Use](#) page.

Submitting a Job

`sbatch <batch file name>`

- ❖ **Conda users: Make sure you submit the job while virtual environment deactivated on the manager node ('conda deactivate')!**

Batch File

The batch file should look like the following:

```
#!/bin/bash

### sbatch config parameters must start with #SBATCH and must precede any other command. to ignore just add another # - like so ##SBATCH

#SBATCH --partition main          ### specify partition name where to run a job. main - 7 days time limit

#SBATCH --time 0-01:30:00        ### limit the time of job running. Make sure it is not greater than the partition time limit!! Format: D-H:MM:SS

#SBATCH --job-name my_job        ### name of the job. replace my_job with your desired job name

#SBATCH --output my_job-id-%J.out  ### output log for running job - %J is the job number variable

#SBATCH --mail-user=user@post.bgu.ac.il  ### users email for sending job status notifications

#SBATCH --mail-type=BEGIN,END,FAIL      ### conditions when to send the email. ALL,BEGIN,END,FAIL, REQUEU, NONE

##SBATCH --cpus-per-task=6        # 6 cpus per task – use for multithreading, usually with --tasks=1

##SBATCH --tasks=2                # 2 processes – use for processing of few programs concurrently in a job (with srun). Use just 1 otherwise

### Print some data to output file ###

echo "SLURM_JOBID"=$SLURM_JOBID

echo "SLURM_JOB_NODELIST"=$SLURM_JOB_NODELIST

### Start you code below        #####

module load anaconda             ### load anaconda module

source activate my_env           ### activating Conda environment, environment must be configured before running the job

python my.py my_arg              ### execute python script – replace with your own command
```

Example sbatch file location on cluster: `/storage/sbatch_cpu.example`

Should you need the IT team's support, in your request remember to state the job id and include the sbatch file and the output file.

Allocating Resources

Since the resources are expensive and in high demand, you should make use of the **minimum possible RAM**. If your code makes use of 30G then by all means, do NOT ask for 50G! (to tell how much RAM was used, when the job completes, use: `sacct -j <jobid> --format=JobName,MaxRSS`).

Same goes for the number of CPUs. There is no need to allocate more cores than threads.

Information about the compute nodes

sinfo shows cluster information.

sinfo -Nel

NODELIST – name of the node

S:C:T - sockets:cores:threads

List of My Currently Running Jobs

squeue --me

Cancel Jobs

scancel <job id>

scancel --name <job name>

Cancel All Pending jobs for a Specific User

scancel -t PENDING -u <user name>

Running Job Information

Use *sstat*. Information about consumed memory:

sstat -j <job_id> --format=MaxRSS,MaxVMSize

scontrol show job <job_id>

Complete Job Information

sacct -j <jobid>

sacct -j <jobid> --

format=JobName,MaxRSS,State,Elapsed,Start,ExitCode,DerivedExitcode,Comment

MaxRSS is the maximum memory the job needed.

Advanced Topics

Jupyter Lab

Installation

```
conda install jupyterlab
```

Make the Conda Environment Available in Notebook's Interface

```
python -m ipykernel install --user --name <conda environment> --display-name "<env name to show in web browser>"
```

e.g.:

```
python -m ipykernel install --user --name my_env --display-name "my best env"
```

Don't forget to choose the right kernel while in the notebook.

Release Job Resources from Within Jupyter After Code Has Finished Running

Add the following 3 lines at the end of your code to make the code release the job resources when done:

```
Import os
```

```
job_cancel_str="scancel " + os.environ['SLURM_JOBID']
```

```
os.system(job_cancel_str)
```

How to add ipywidgets to Jupyter Lab

Create a Conda environment with ipywidgets and install as lab extension:

```
conda create -n tqdm -c conda-forge jupyterlab nodejs widgetsnbextension ipywidgets -y
```

```
conda activate tqdm
```

```
pip install tqdm==4.32.1 ipykernel
```

```
python -m ipykernel install --user --name tqdm --display-name "Python (tqdm)"
```

```
jupyter labextension install @jupyter-widgets/jupyterlab-manager
```

```
conda deactivate
```

Tensorboard

Run:

```
tensorboard --port=9989 --logdir logs/fit
```

If port 9989 occupied, choose another random port of the range 9980-9999.

Open your web browser here: <http://132.72.X.Y:9989/> (change X, Y to form your compute node address).

If you cannot access Tensorboard then add, as another parameter: `--bind-all`

Working with Notebooks

Working with notebooks is interactive. If you closed your browser tab while a notebook's cell is running, it keeps running on the cluster, but you will lose the output. On the other hand, it is not always possible to leave your browser open. The simple solutions to that are either to write variable values and results into a file or to run the code as a python script instead of using a notebook.

In Ipython 6.0 and higher you can use `%capture cell` magic to save all output to file. Use the following line as the very first line of the cell: `%%capture cap_out`

Then, in order to save to variable, on the cell's last line: `var = cap_out.stdout`

If you rather print to file then: `with open('cap_output.txt', 'w') as f:`

```
    f.write(cap_out.stdout)
```

When you come back to the notebook you can print the content of `var` or `cap_out.show()` in another cell.

Allocate Extra RAM/CPU

In your sbatch file:

To override default ram:

```
#SBATCH --mem=58G
```

To override default cpu number

```
#SBATCH --cpus-per-task=16
```

Working with the Compute Node SSD Drive

You may want to use the compute node local drive for fast access to data. /scratch directory on the compute node is intended for that.

Add to the sbatch script file:

```
#SBATCH --tmp=100G      ### Asks to allocate enough space on /scratch
```

Then in users code section:

```
export SLURM_SCRATCH_DIR=/scratch/${SLURM_JOB_USER}/${SLURM_JOB_ID}  
cp /storage/*.img $SLURM_SCRATCH_DIR          ### copy data TO node's local storage  
mkdir $SLURM_SCRATCH_DIR/testtttt  
  
...  
some user code  
  
...  
cp -r $SLURM_SCRATCH_DIR $SLURM_SUBMIT_DIR    ### copy back final results to user home  
or other accessible location
```

When job has finished, canceled or failed, ALL data in \$SLURM_SCRATCH_DIR is erased! This temp folder lives with running jobs only!

Job Arrays

Job array feature allows you to run identical version of your script with different environment variables. This is useful for parameter tuning or averaging results over seeds.

To use job array, add the following line to your Slurm batch file:

```
#SBATCH --array=1-10 ### run parallel 10 times
```

Adding this will run your script 10 times in parallel, actually creating 10 jobs where each job gets the requested resources, e.g., if you requested 6 CPUs then each job shall get 6 CPUs. The environment variable `SLURM_ARRAY_TASK_ID` for each run will have different values (from 1 to 10 in this case). You can then set different parameter setting for each parallel run based on this environment variable.

Remember to change `#SBATCH --output=your_output.out` to `#SBATCH --output=output_file_name_%A_%a.out`, so the output of each parallel run be directed to a different file. `%a` will be replaced by the corresponding `SLURM_ARRAY_TASK_ID` for each run. `%A` will be replaced by the master job id.

To get the above `SLURM_ARRAY_TASK_ID` variable in python:

```
import sys  
jobid = sys.getenv('SLURM_ARRAY_TASK_ID')
```

In R:

```
task_id <- Sys.getenv("SLURM_ARRAY_TASK_ID")
```

Send Name of an Input File to Each Task

For example, if the input files end in `.txt`

```
file=$(ls *.txt | sed -n ${SLURM_ARRAY_TASK_ID}p)  
myscript -in $file
```

Read a Line from an Input File for Each Task

```
SAMPLE_LIST=$(cat input.list)  
SAMPLE=${SAMPLE_LIST[${SLURM_ARRAY_TASK_ID}]}
```

Email Notifications

If you would like to receive an email for each task in the array, rather than just for the whole job:

```
#SBATCH --mail-type=BEGIN,END,FAIL,ARRAY_TASKS
```

Limiting the Number of Simultaneously Running Tasks from the Job Array

For example, to limit the number of simultaneously running tasks from a 15 jobs job array to 4:

```
#SBATCH --array=0-15%4
```

Job Dependencies

Job dependencies are used to defer the start of a job based on other job's condition.

SBATCH --dependency=after:<other_job_id> <SBATCH_script> ### start job after other_job started

SBATCH --dependency=afterok:<other_job_id> <SBATCH_script> ### start job after other_job ends with ok status. E.g. sbatch --dependency=afterok:77:79 my_sbatch_script.sh -> start after both job 77 and 79 have finished

SBATCH --dependency=singleton ### This job can begin execution after any previously launched jobs, sharing the same job name and user, have terminated

IDEs

pyCharm

Make sure you have pyCharm Professional installed (free for students/academy people).

Create an interactive session:

Ssh to Slurm and copy the script file /storage/pycharm.sh to your working Slurm directory.

You can modify the following lines at the beginning of the file (just make sure GPU=0):

```
#####  
  
# USER MODIFIABLE PARAMETERS:  
  
PART=main # partition name  
  
TASKS=6 # 6 cores  
  
TIME="2:00:00" # 2 hours  
  
GPU=0 # Make sure this is 0  
  
QOS=normal # QOS Name  
  
#####
```

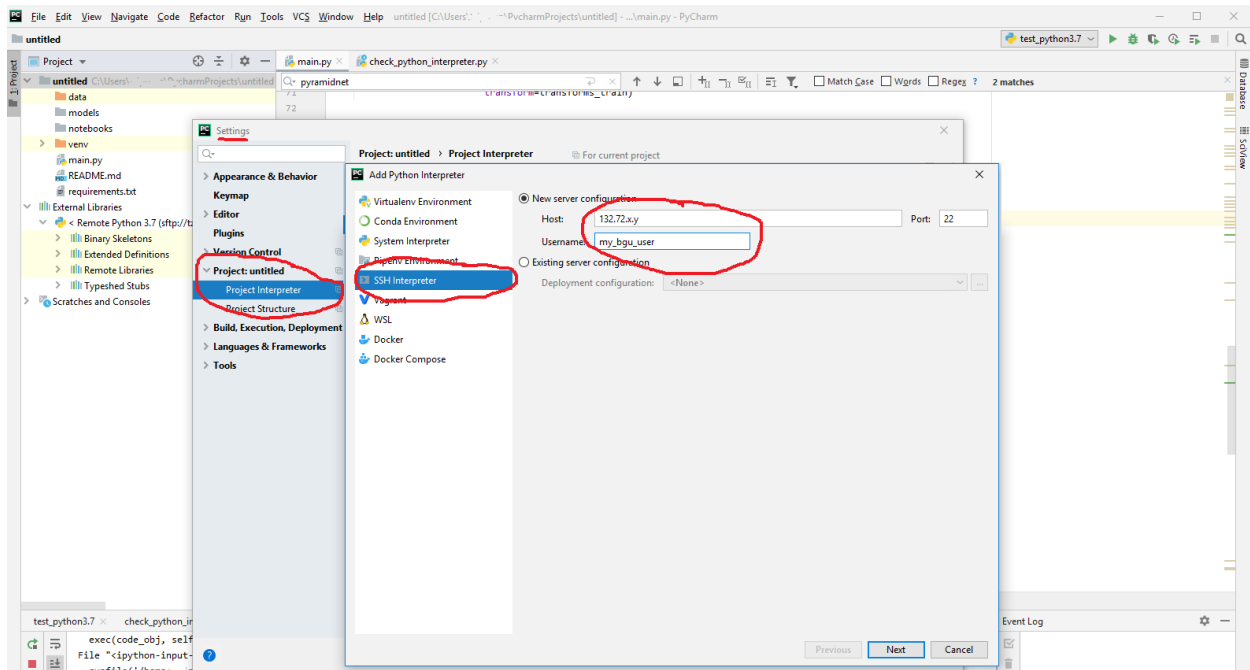
Run the script by typing: `./pycharm.sh`

The output lists the node's ip address and the job id.

Open pyCharm.

Go to settings->Project->Project Interpreter

On the upper right hand corner next to Project Interpreter: press the settings icon, choose 'add'

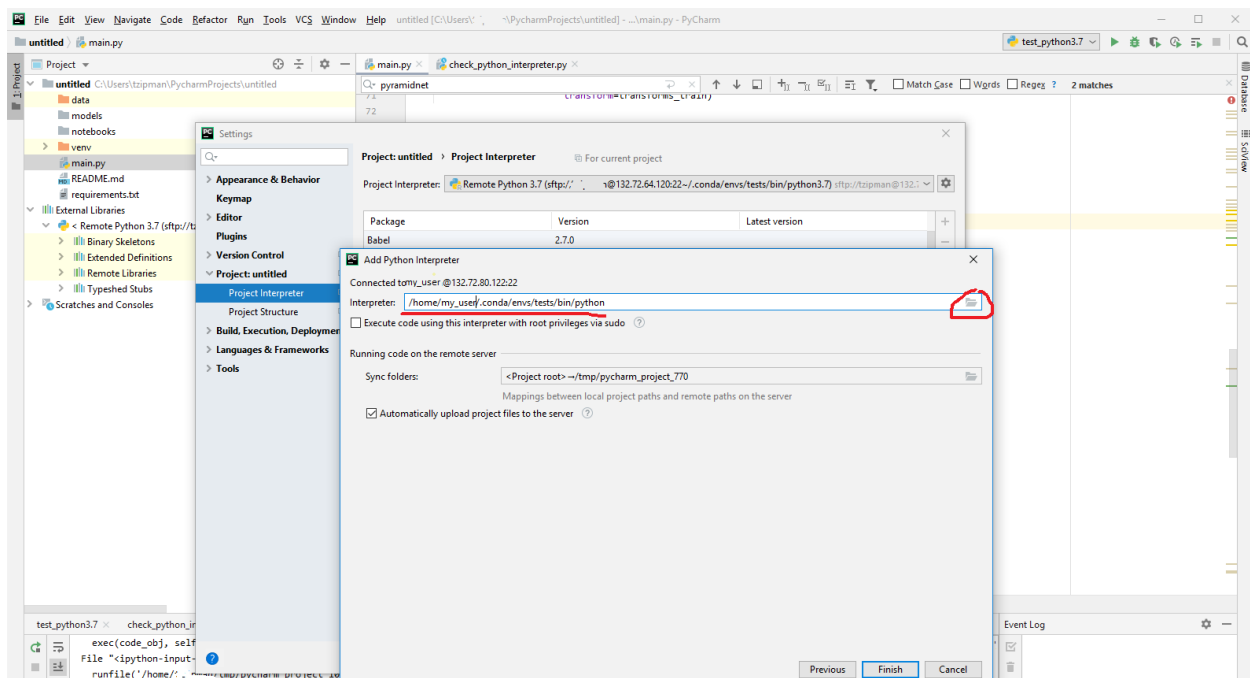


On the left hand side choose SSH Interpreter. Under 'New server configuration' fill in the compute node's ip address and your BGU user name. Click Next.

You might get a message about the authenticity of the remote host, asking if you want to continue connecting. Click 'yes'.

Enter your BGU password. Click Next.

In the 'Interpreter:' line, enter the path to the desired interpreter. You can find your environments interpreters under `/home/<your_user>/<your_environment>/bin/python`.



Click Finish.

Give pyCharm some time to upload files to the cluster (upload status is shown on the status bar).

Make pyCharm Continue Running Script When Sessions is Disconnected

The `offline_training.py` script in the frame below, launches another script with arguments:

```
train.py -- size 192
```

The output be redirected into `result.txt` file.

`offline_training.py`

```
import os
import sys

os.system("nohup bash -c '" +
          sys.executable + " train.py --size 192 >result.txt" +
          "' &")
```

The `result.txt` file may be found on the compute node. Once you run `offline_training.py` In Pycharm, on the 'Python Console' pane, the next line should show up:

```
runfile('/tmp/pycharm_project_<some_number>/<your_offline_running_file>.py',
wdir='/tmp/pycharm_project_<some_number>')
```

The path is the path to the folder in the compute node where your local files are synced. Ssh to the compute node and you may find `result.txt` at that path.

Remember that once the job ends, that folder is erased!

Visual Studio Code

Create an interactive session:

Ssh to Slurm and copy the script file /storage/pycharm.sh to your working Slurm directory.

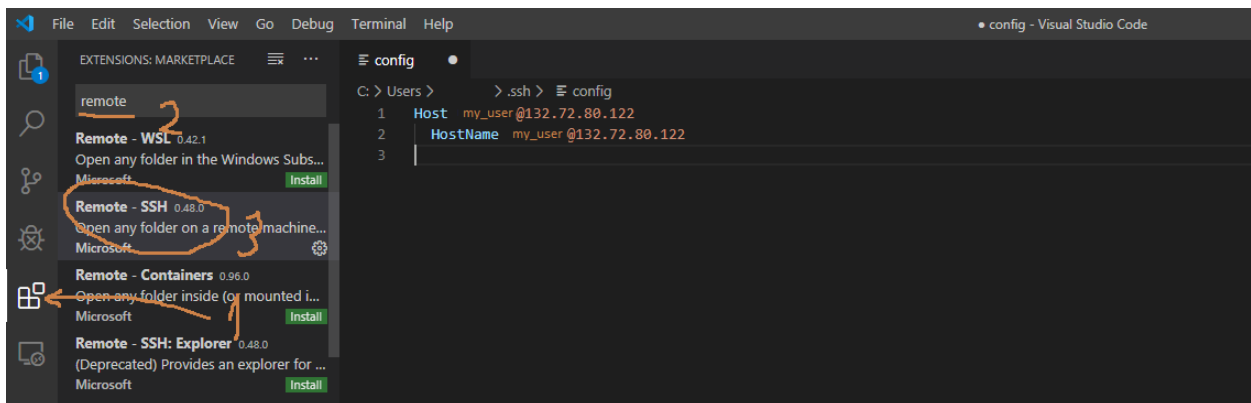
You can modify the following lines at the beginning of the file (just make sure GPU=0):

```
#####  
  
# USER MODIFIABLE PARAMETERS:  
  
PART=main # partition name  
  
TASKS=6 # 6 cores  
  
TIME="2:00:00" # 2 hours  
  
GPU=0 # Make sure this is 0  
  
QOS=normal # QOS Name  
  
#####
```

Run the script by typing: ./pycharm.sh

The output lists the newly allocated compute node's ip address and the job id.

Assuming you have VS Code installed and a supported OpenSSH client installed, install the 'Remote – SSH' pack.

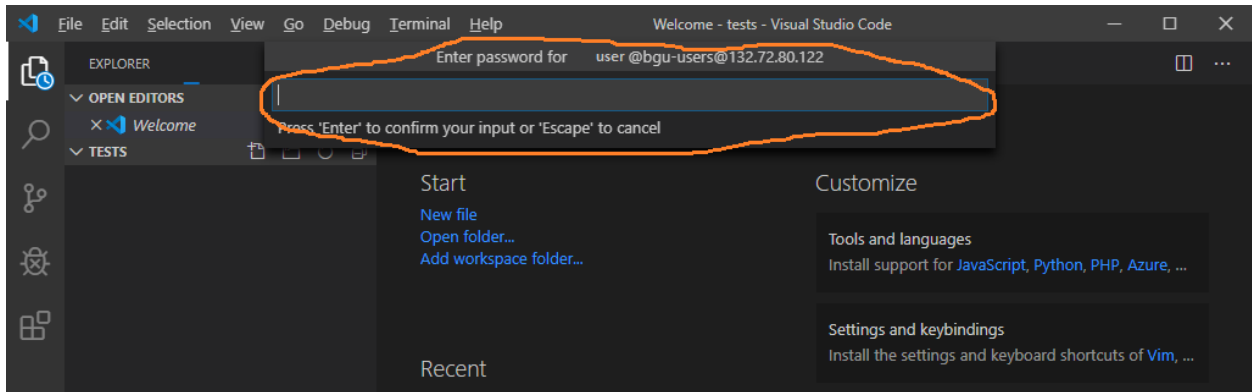


Install the Python package, if needed.

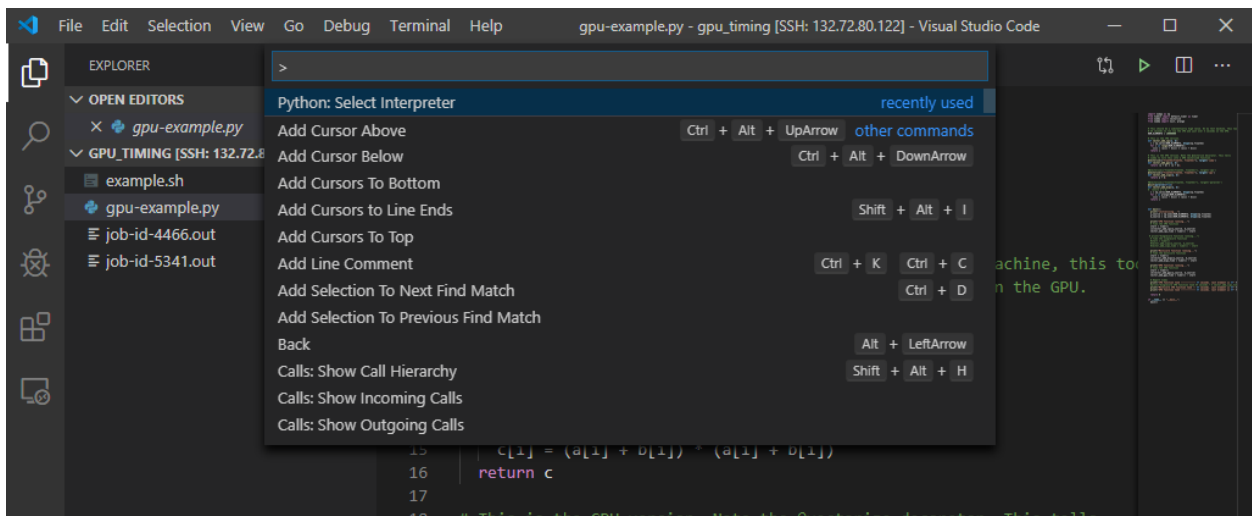
Press the green button (>) on the most lower left side of the window (under the 'settings' button).

On the middle upper side of the window, choose "Remote – SSH: Connect to host..." and enter <your_BGU_user>@<compute_node_ip_address>

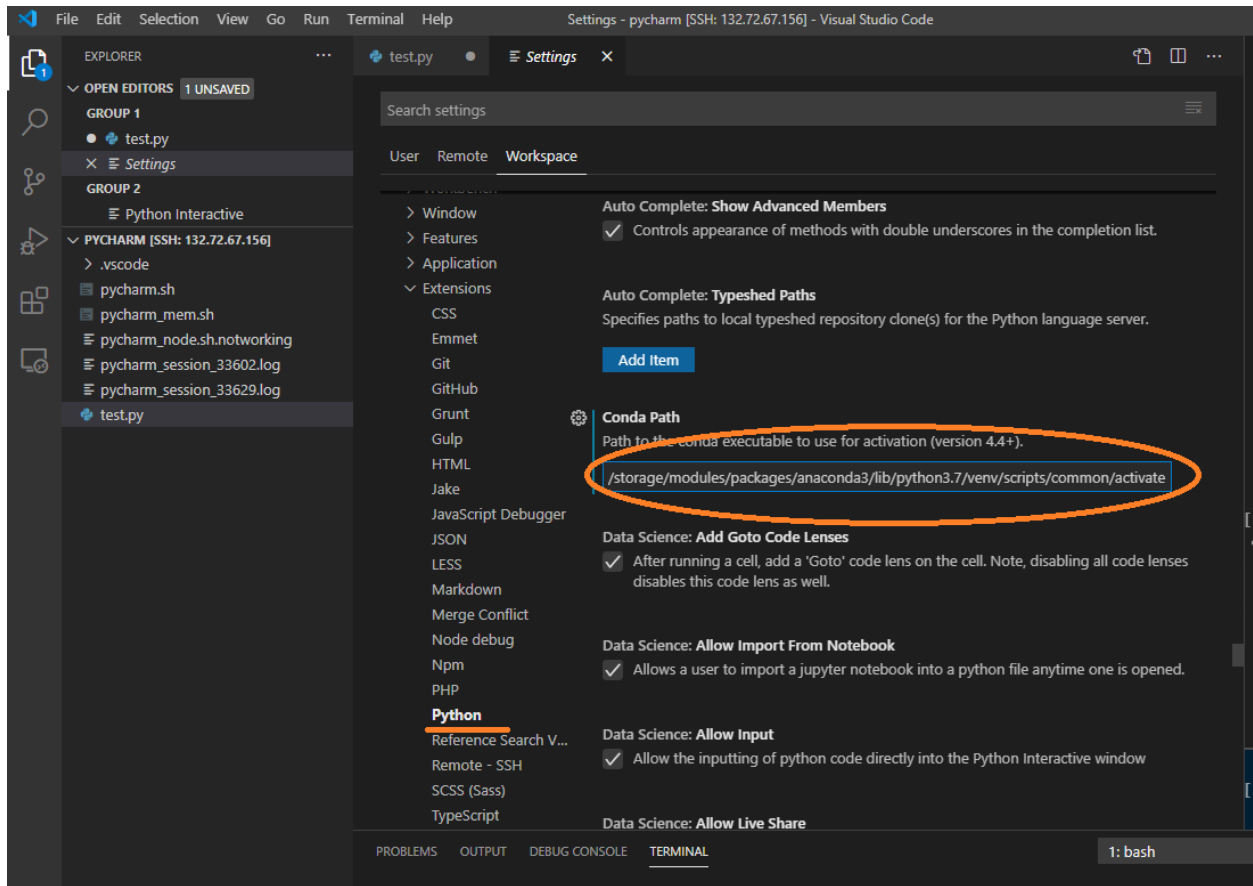
A new window opens. Enter your BGU password, when prompted.



Ctrl+Shift+P for the Command Palette then choose 'Python: Select Interpreter' (start typing – it will show up) and choose the interpreter from your desired environment (~/.conda/envs/<environment>/bin/python).



To enable interactive work with notebook like cells, Ctrl+Shift+P for the Command Palette then choose 'Preferences: Open Workspace Settings' (start typing – it will show up) and click 'Python'. Scroll down until you find 'Conda Path' and fill in '/storage/modules/packages/anaconda3/lib/python3.7/venv/scripts/common/activate'.



To solve an errata with finding the actual path of the python script add the following line to launch.json file:

```
"cwd": "${fileDirname}"
```

Refer to the following paragraph for instructions as to how to place it in the file and where.

Run/Debug with Arguments

Press the Debug symbol on the left vertical ribbon. Click 'create a launch.json file' on the left pane.

Open file launch.json and add another line within 'configurations like so (example for 4 arguments):

```
"args": ["-arg_name1", "value_1", "-arg_name2", "value_2"]
```

Here is an example:

```
"configurations": [
  {
    "name": "Python: Current File",
```

```
    "type": "python",
    "request": "launch",
    "program": "${file}",
    "console": "integratedTerminal",
    "cwd": "${fileDirname}",
    "args": ["cuda", "100", "exit"]
  }
]
```

Docker

Running Docker containers on the cluster may be done using UDOCKER. UDOCKER shall be installed in a Conda environment.

Installation

- Installation for Python3 udocker. For Python2: remove the “python=3.8” string in the next line.

```
conda create -n udocker_env python=3.8
```

```
conda activate udocker_env
```

```
conda install configparser
```

```
pip install udocker
```

Test

Test a tensorflow-gpu container. Copy paste the following at the end of an sbatch file:

```
module load anaconda
source activate udocker_env
# pull image, create container and '--rm' remove 'hello-world' container after run
udocker run --rm hello-world
```

Once udocker environment is activated you can use:

```
udocker --help – info about commands and way of use
```

```
udocker run --help – help for the ‘run’ command. This can be done also with other commands
```

```
udocker ps – list your containers
```

```
udocker images – list your images
```

```
udocker rm <container name/id> - remove container
```

```
udocker rmi <image id> - remove image
```


There is no need to pull the image every time.

There is no need to create the container if it already exists.

Matlab

Run Matlab GUI straight from terminal (no need for sbatch):

```
module load matlab
```

```
srun --x11 --nodes=1 --mem=24G --cpus-per-task=4 --partition=main matlab -desktop -sd ~
```

Make sure your ssh terminal supports x11 forwarding!

Send Matlab script to run as batch by headless Matlab:

```
srun --nodes=1 --mem=24G --cpus-per-task=4 --partition=main matlab -nosplash -nodisplay -nodesktop -sd ~ -batch "my_matlab_script"
```

Headless Matlab may be run by sbatch as well.

- Cluster params:
 - --nodes – number of allocated cluster nodes (must be 1)
 - --mem=24G – memory allocation
 - --cpus-per-task – number of CPUs
 - --gpus – number of GPUs
 - --partition – partition name
- Matlab params:
 - -desktop – run matlab in GUI mode
 - -sd – matlab working directory

R

Command Line

- Create an R conda environment. E.g.: `conda create -n r_env r-essentials r-base`
- Copy the following file: `/storage/pycharm_mem.sh`
- Edit the first section of the above file to suit your demands.
- Execute the file: `./pycharm_mem.sh`
- Wait for the resources to be allocated.
- Copy the compute node's ip address from the script output.
- SSH to the compute node.
- Type: `conda activate r_env`
- Type: `R`

C#

Install In Conda Environment

```
conda install -c conda-forge dotnet-sdk
```

Use

- Use `./pycharm.sh` script (see [pyCharm](#)) to allocate a compute node.
- ssh to the compute node
- Activate environment: `conda activate <your dotnet environment name>`
- Create a new dotnet project: `dotnet new console -o myApp`
- `cd myApp`
- Run: `dotnet run`

Appendix

Step by Step Guide for First Use of Python and Conda

1. Make sure you are connected through VPN or from within BGU campus.
2. Download a SSH terminal (<https://mobaxterm.mobatek.net/download.html>).
3. Open the SSH terminal and start a SSH session (port 22). The remote host is 132.72.65.199 , the username is your BGU username and the password is your BGU password.
4. Once logged into the cluster's manager node, create your Conda environment. E.g.:

```
conda create -n my_env python=3.7
```

5. `conda activate my_env`
6. `pip install <whatever package you need>` or `conda install <whatever package you need>`

In most cases it is advisable to use 'conda install' rather than 'pip install'

7. `conda deactivate`
8. Copy the sbatch file (job launching file) by typing (do not forget the dot at the end!):

```
cp /storage/sbatch_cpu.example .
```

9. Edit the file using nano editor: `nano sbatch_cpu.example`
10. You may change the job name by replacing my_job with your own string.
11. Go to the last lines of the file. 'source activate my_env': if needed, replace 'my_env' with your environment name that you have created on paragraph 4.
12. 'python my.py my_arg' is the program to run on the compute node. You may use another command instead.
13. Press '<ctrl>+x', then 'y' and '<Enter>' to save and leave the file.
14. Launch a new job: `sbatch sbatch_cpu.example`
15. You should, instantly, get the job id.
16. To see the status of your job(s) type `squeue --me`
17. Under 'ST' (state) column if the state is 'PD' then the job is pending. If the the state is 'R' then the job is running and you can look at the output file for initial results (jupyter results will take up to a minute to show): `less job-<job id>.out`
18. If you asked for jupyter, then copy the 2nd link (which starts with 'https://132.72.'). Copy the whole link, including the token, and paste it in the address bar of your web browser. Make the browser advance (twice) in spite of its warnings.

Conda

Viewing a list of your environments

```
conda env list
```

list of all packages installed in a specific environment

```
conda list
```

to see a not activated environment

```
conda list -n <my_env>
```

Activating / deactivating environment

```
source activate <my_env>
```

or (depends on conda version)

```
conda activate <my_env>
```

```
conda deactivate
```

Create Environment

```
conda create -n <my_env>
```

with specific python version

```
conda create -n <my_env> python=3.4
```

with specific package (e.g. scipy)

```
conda create -n <my_env> scipy
```

Or

```
conda create -n <my_env> python
```

```
conda install -n <my_env> scipy
```

with specific package version

```
conda create -n <my_env> scipy=0.15.0
```

with multiple packages

```
conda create -n <my_env> python=3.4 scipy=0.15.0 astroid babel
```

Update Conda

```
conda update conda
```

Compare Conda Environments

The following python (2) script compares 2 conda environments and can be found in '/storage' directory.

```
python conda_compare.py <environment1> <environment2>
```

Transfer Files

To / From Your PC

You can use WinSCP to transfer files, or if you use MobaXTerm then it has its own file browser.

In Windows, SISE department students can also map their cluster home directory like so:

1. connect to BGU vpn
2. open file explorer.
3. on the left pane right click "This PC".
4. on the menu that will open, click on "map network drive".
5. choose a drive letter or leave the default letter in place.
6. in the "Folder" field write down: \\132.72.65.201\usr_home\- 7. you can choose to check or uncheck "Reconnect at sign-in".
- 8. you must check "Connect using different credentials".
- 9. click on "Finish" button.
- 10. a new authentication window will open, in the Username field write down: bgu-users\- 11. in the Password field write down your BGU password.

Get a Public File

from AWS s3

Use wget:

```
wget --no-check-certificate --no-proxy 'https://<your bucket name>.s3.amazonaws.com/<path and name of file>'
```

from Google Drive

Use wget:

```
wget --no-check-certificate 'https://drive.google.com/uc?id=<file id> -O <file name to save>
```

where file-id is the alphanumeric long string that shows when you right click the file in Chrome and view the file's link. for example:

```
wget --no-check-certificate 'https://drive.google.com/uc?id=1A3Ef4gHdhsdjkln6o' -O my_file.txt
```


Deap

Create Environment

1. `conda create -n DEAP -y python=3`
2. `conda activate DEAP`
3. `conda install -c cyclus java-jdk`
4. `pip install deap`
5. `conda deactivate`

FAQ

Usage

- ❖ [Can I ssh the cluster when I am away from university?](#)

This can be done by using VPN.

- ❖ [I uploaded files to the cluster, while logged in to the manager node, can a compute node find these files?](#)

The files were uploaded to the storage. **All** cluster nodes have access to your files on the storage.

- ❖ [I need sudo to install library X / tool Y](#)

Install it in your conda environment, using 'conda install' or 'pip install'

- ❖ [Is Git installed on the cluster?](#)

Git is installed on the manager node.

- ❖ [Why is my job pending? What's the meaning of REASON?](#)

PartitionTimeLimit – the 'time' variable in your sbatch file is set to time limit greater than the partition's maximum possible time limit (usually 7 days).

Resources – currently, the cluster has insufficient resources to fulfill your job.

Priority – job is queued behind higher priority jobs. You may have exceeded your group QoS priority resources – You can launch a job with no QoS priority or wait for QoS priority resource to be available.

QOSMaxJobsPerUserLimit – you have reached the maximum allowed concurrent jobs for the requested partition.

- ❖ [In python app I print some run time info but they are buffered and being printed all at once.](#)

To use unbuffered print to output: `python -u my_py_app.py`

u – unbuffered.

Another option is to add the following line to your sbatch scripy:

```
export PYTHONUNBUFFERED=TRUE
```

Please note it has performance toll, so it is not advisable to use it when not debugging.

Errors

- ❖ [I installed wget python package like so: 'conda install wget', and I get 'ModuleNotFoundError: No module named wget' error.](#)

Use: pip install wget

- ❖ Output file shows: slurmstepd: error: _is_a_lwp: open() /proc/60830/status failed: No such file or directory

It's a rare Slurm accounting error message that should not affect the job. Just ignore it.

- ❖ In my conda environment I installed a package which is a python wrapper of binary code. Running a code that uses it, with Jupyter notebook was successful, but running the very same code from pycharm, failed with the message 'NotImplementedError: "... does not appear to be installed or on the path, so this method is disabled. Please install a more recent version of ... and re-import to use this method.'

This happens because with pycharm, the environment variable 'PATH' remains unchanged, unlike with Jupyter that when choosing conda environment, 'PATH' gets modified. The solution is to modify 'PATH' **prior** to **importing** the wrapper package in your python code, as follows (replace <your_user> and <your_env> with yours):

```
import os
os.environ['PATH'] =
'/home/<your_user>/.conda/envs/<your_env>/bin:/storage/modules/packages/anaconda3/bin:/storage/modules/bin:/storage/modules/packages/anaconda3/condabin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/storage/modules/packages/matlab/R2019B/bin:/home/<your_user>/.local/bin:/home/<your_user>/bin'
import <python wrapper package>
...
```

- ❖ Working with udocker I get these errors when pulling an image. TypeError: unicode argument expected, got 'str', Error: manifest not found or not authorized

Your udocker installation uses python2, instead of python3. Refer to [Docker Installation](#).

- ❖ VSCode error: windows remote host key has changed port forwarding is disabled

OR: Could not establish connection to "x.x.x.x": Remote host key has changed, port forwarding is disabled.

OR: visual studio code could not establish connection... the process tried to write to a nonexistent pipe

These errors mean that the remote host key does not match to the key saved locally, anymore. The keys mismatch may be a result of reinstalling the remote host. If that is the reason go to C:\Users\<your Windows user>\.ssh\ and change the names of the files. Windows will create new updated files instead.

- ❖ Got an error like this: libstdc++.so.6: version 'GLIBCXX_3.4.26' not found

If you already installed libgcc in your conda environment (like so: conda install libgcc), add the following line to your sbatch script right after the #SBATCH lines (replace 'username' and 'my_env' with yours):

```
export LD_LIBRARY_PATH=/home/username/.conda/envs/my_env/lib:$LD_LIBRARY_PATH
```

