

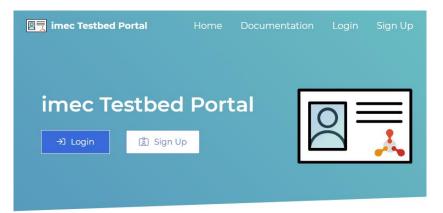
GPULAB AND JUPYTERHUB INTRODUCTION

PREREQUISITES

REQUEST OR JOIN A PROJECT

For IDLab members/students:

https://account.ilabt.imec.be



For External Users:

https://portal.slices-sc.eu

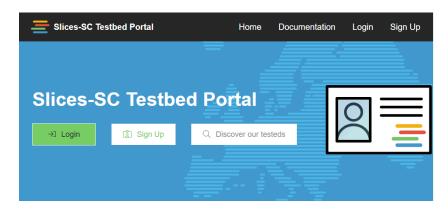










TABLE OF CONTENTS

- Features of GPULab
- Architecture of GPULab
- JupyterHub on GPULab
- Using GPULab directly
 - jobDefinition
 - Storage
 - Opening network ports
 - Accessing logs
 - SSH access







FEATURES OF GPULAB



Access to a lot of GPUs:

12x A40 – 48 GB, 40x Tesla V100 – 32 GB, 11x RTX 4090 – 24GB, 33x GTX 1080 Ti – 12 GB, ...



Your pip/conda packages are installed and ready to use!

Choose any Docker image with your packages pre-installed



Isolated Storage

Separate storage per project



Automatic Job Scheduling

Jobs are started in FIFO order





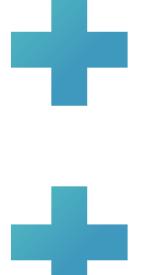


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ARCHITECTURE OF GPULAB

Thin wrapper around GPU-enabled Docker containers:

- Hides complexities of mounting storage, CPU/GPU isolation, etc.
- No need to install CUDA, Tensorflow,
 PyTorch, etc. on the machine yourself



Job Scheduler:

- Over multiple machines
- With I or more GPUs
- Reservations possible

Authentication:

- Via imec iLab.t or Slices portal
- Concept of 'projects' for sharing of resources









TOPOLOGY OF GPULAB

The GPULab slaves (=servers) are:

- Spread over 2 locations: iGent DC and UAntwerp DC:
 - Different storage options
 - Different network
- Divided into clusters: servers with the similar properties:
 - Same location,
 - Same GPU type







Available on https://jupyterhub.ilabt.imec.be

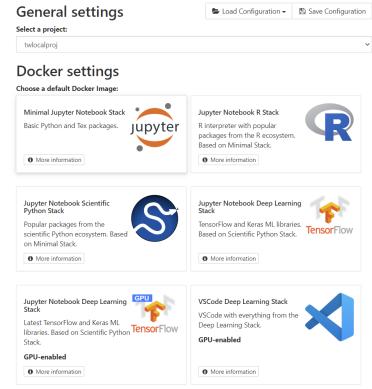


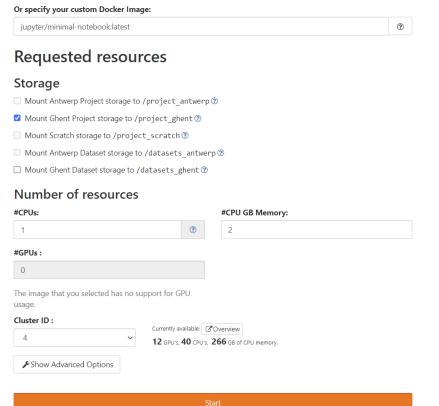
- Hosted Jupyter Notebook service which provides easy access to GPULab resources
 - Similar to Google CoLab
 - No setup required!
- <u>Ideal for</u>: interactive development of your code and short training runs
- Use GPULab directly for long running jobs





Available on https://jupyterhub.ilabt.imec.be













HOW DOES IT WORK?

Jupyterhub

- Generates and starts a GPULab job for you
- Redirects you to your Jupyter notebook server once started

Gotchas:

- Server start will timeout after 5 minutes (ex. no GPUs available in chosen cluster)
- Job will be cancelled after I hour of inactivity in the browser, even if a computation is running!
- Job will always stop after 24 hours
- Custom docker images must descend from jupyter/base-notebook







FAIR USAGE POLICY

- Use JupyterHub only for interactive development and short training runs.
- Request I GPU, maximum 2 if you need to validate concurrency
- Request a reasonable amount of CPU's and CPU memory
- Does your code need multiple hours to run? Do you need to scale up the number of GPU's? → Use GPULab directly instead.







HANDS ON

- Go to https://jupyterhub.ilabt.imec.be
- Choose a default Docker image of your liking
- Select the storage you want to use
 - Note: illegal combinations are automatically prevented
- Define number of CPU's/GPU's memory
- Optional: define a cluster ID
- Click 'Start'

Create or Upload a Python script / Jupyter notebook that you want to execute



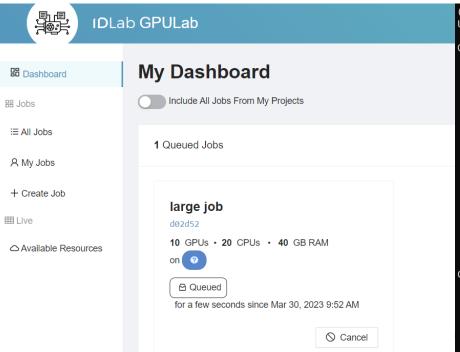




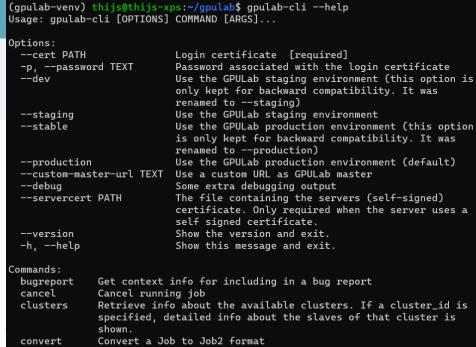


USING GPULAB DIRECTLY

Website https://gpulab.ilabt.imec.be for monitoring/submitting simple jobs



 gpulab-cli for submitting jobs from the command line



DEFINING A GPULAB JOB

GPULab-specific bookkeeping

```
"jobDefinition": {
  "name": "helloworld",
  "description": "Hello world!",
  "request": {
    "resources": {"gpuModel": "1080",
                  "gpus": 1, "cpus": 2, "cpuMemoryGb": 2000, },
    "docker": { "image": "nvidia/cuda:12.1.0-runtime-ubuntu22.04",
                "command": "echo 'Hello World'",
                "environment": { },
                "storage": [ { "containerPath": "/project ghent"} ],
                "portMappings": [ { "containerPort": 80 } ],
```





Passed to Docker for starting the container

innec

USING GPULAB

SUBMITTING A JOB VIA THE CLI

```
thijs@ibcn055:~$ gpulab-cli submit --project twalcari-test < jupyter-scipy.json
87914bc6-10ec-11ea-93a1-d7177117bc9b
thijs@ibcn055:~$ gpulab-cli jobs 87914bc6-10ec-11ea-93a1-d7177117bc9b
        Job ID: 87914bc6-10ec-11ea-93a1-d7177117bc9b
          Name: Jupyter SciPy
   Description: Scipy jupyter notebook server
       Project: twalcari-test
      Username: twalcari
  Docker image: jupyter/scipy-notebook:latest
       Command:
        Status: RUNNING
       Created: 2019-11-27T09:04:26+01:00
 State Updated: 2019-11-27T09:04:35+01:00
        Oueued: 2019-11-27T09:04:26+01:00
    Cluster ID: 4
     Worker ID: 3
   Worker Name: n051-02
 Port Mappings: 8888/tcp -> 32814
   Worker Host: n051-02.wall2.ilabt.iminds.be
    SSH login:: ssh FCXDN232@n051-02.wall2.ilabt.iminds.be
       Started: 2019-11-27T09:04:34+01:00
      Duration: 11 seconds
      Finished: -
      Deadline: 2019-11-27T19:04:34+01:00
```



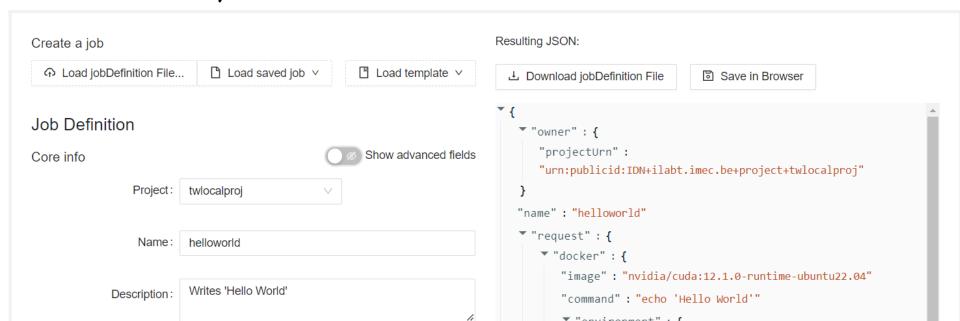






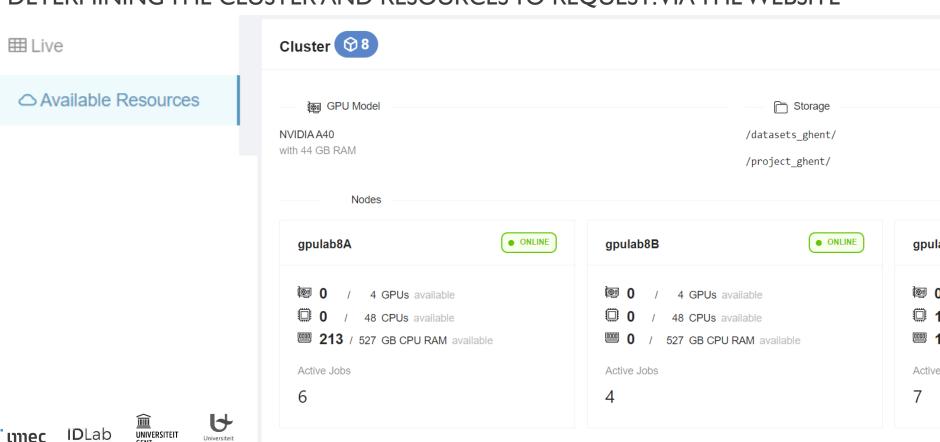
DEFINING A GPULAB JOB

- Modify an example
 - Consult documentation on https://doc.ilabt.imec.be/ilabt/gpulab/jobdefinition.html
- Use the 'Create job' function on the website



DEFINING A GPULAB JOB

DETERMINING THE CLUSTER AND RESOURCES TO REQUEST: VIA THE WEBSITE



DEFINING A GPULAB JOB DETERMINING THE CLUSTER AND RESOURCES TO REQUEST: VIA THE CLI

(gpulab-venv) thijs@thijs-xps:~/gpulab\$ gpulab-cli clusters					
ID	GPU Model	Comment	Slaves	GPUs	CPUs
1 stable		1x 2x GF GTX 1080 Ti	0	0/0	0/0
2 stable		temporary cluster	0	0/0	0/0
3 stable	NVIDIA GeForce RTX 2080 Ti	1x RTX2080	1	1/1	10/12
4 stable	NVIDIA GeForce GTX 1080 Ti	4x 11x GF GTX 1080 Ti	4	19/44	55/128
5 stable	Quadro RTX 4000	UAntwerp: 2x 4x RTX4000	3	0/8	21/80
6 stable	Tesla V100-SXM3-32GB	1x HGX-2 - 16xTesla V100	1	1/16	46/96
7 stable	Tesla V100-SXM2-32GB,Tesla V100-SXM3-32GB	UAntwerp: DGX-1 + DGX-2 - (8+16)x Tesla V100	4	0/24	17/176









- File system within your GPULab job is ephemeral:
 - Jobs start with file system defined within the Docker image that you start
 - when the job ends, all changes to the file system are lost
- Exception: any permanent storage that you attach to the GPULab job: use this for storing all your datasets, code, logs, results









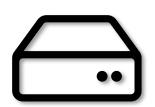
- GPULab slaves are spread over 2 datacenters, each with their own storage:
 - /project_antwerp : cluster 5 & 7
 - /project_ghent : all other clusters
- Some slaves have very fast local scratch storage: /project_scratch
- Use CPU memory as storage by mounting it as tmpfs

 Use request → docker → storage to set storage mount points









/project_ghent

/project_antwerp

I I 5 TB backed by NVMe disks
Connected by Infiniband to Cluster 6

I 05TB backed by DDN A³I storage Connected by Infiniband to Cluster 5 & 7

"Fair use policy", but no hard limits

"Fair use policy", but no hard file size limits Quota of 500.000 inodes







Documentation:

https://doc.ilabt.imec.be/ilabt/gpulab/storage.html



/project_scratch

- Slave-specific:
 - **6A**: 94TB
 - **7A**: 28TB
 - **7B**: 7TB
- Use request → resources → slaveName to request specific slave

 RAID0 storage over multiple local NVMe disks

Example: 6A uses 16 enterprise-grade NVMe disks with each a MTBF of 2.000.000 hours



WARNING

Do NOT store anything here that you cannot afford to lose!









TMPFS



Due to limited local storage on each slave, you can use a **maximum of IOGB** of disk space outside of the mounted storage paths.

Using more will kill your job.

Solution 1: make sure that all necessary dependencies are already installed in the Docker image that you are using

Solution 2: mount a part of the available CPU memory as an ephemeral tmpfs

```
"storage": [
    {
        "hostPath": "tmpfs",
        "containerPath": "/my_tmp_dir",
        "sizeGb": 4
    }
]
```

Documentation:

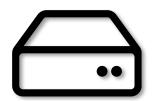
https://doc.ilabt.imec.be/ilabt/gpulab/storage.html#tmpfs





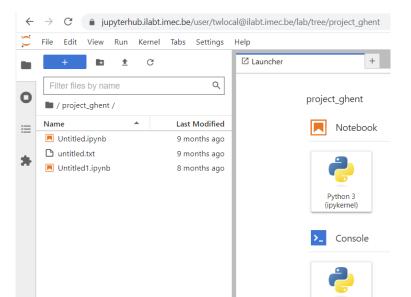


IMPORTING YOUR DATA INTO GPULAB



Small uploads?

Start a JupyterHub session and upload via the browser



Large uploads?

Connect via SFTP to your job

- Use the SSH credentials supplied by your job to connect
- Use login certificate as credentials



.

EXPOSING PORTS OF YOUR CONTAINER



- You can define ports to be exposed in request → docker → portMappings
- Use containerPort to specify which port of your container you want to access
- Host address/port is determined during job scheduling
- Ghent-based nodes:
 - only have public IPv6 address
 - use iGent VPN for IPv4 access
- Antwerp-based nodes:
 - use IDLab Antwerp VPN for access

```
"portMappings": [
    {
       "containerPort": 5000
    },
      {
       "containerPort": 5001,
       "hostPort": 5001
    }
]
```

WARNING: Job will fail if another container is already mapped to that port!







EXPOSING PORTS OF YOUR CONTAINER FINDING THE HOST/PORT VIA THE WEBSITE OR CLI

\$ gpulab-cli jobs <job_id>

```
(gpulab-venv) thijs@thijs-xps:~/gpulab$ gpulab-cli jobs ae9e8923
        Job ID: ae9e8923-f2a9-4f1a-ad76-ae1680a9efd9
          Name: JupyterHub-singleuser
   Description: Single Jupyter notebook instance for JupyterHub
       Project: twlocalproj
      User URN: urn:publicid:IDN+ilabt.imec.be+user+twlocal
       User ID: twlocal@ilabt
  Docker image: jupyter/minimal-notebook:latest
       Command: start-notebook.sh --notebook-dir=/ --SingleUserNotebookApp.default_url='/lab/tr
        Status: RUNNING
    Cluster ID: 4
     Worker ID: 8
   Worker Name: gpulab4C
  Port Mappings: 8888 -> 33400, 8888 -> 33400
   Worker Host: 4c.gpulab.ilabt.imec.be
    SSH login:: ssh -i '/home/thijs/.ssh/twlocal_unlocked.pem' ELWHKEIY@4c.gpulab.ilabt.imec.be
em' ffftwlocal@bastion.ilabt.imec.be -W %h:%p"
        Timing:
             Created: 2023-03-30T11:25:35+02:00 (5 minutes, 48 seconds ago)
             Queued: 2023-03-30T11:25:35+02:00 (less than 1 second after job creation)
           Assigned: 2023-03-30T11:25:38+02:00 (3 seconds after QUEUED)
           Starting: 2023-03-30T11:25:41+02:00 (3 seconds after ASSIGNED)
            Running: 2023-03-30T11:25:43+02:00 (2 seconds after STARTING)
               Ended: -
           Duration: 5 minutes, 40 seconds
      State Updated: 2023-03-30T11:25:43+02:00 (5 minutes, 40 seconds ago)
```



Host Summary: 4C

Cluster:

Slave: gpulab4C

SSH: ELWHKEIY @ 4c.gpulab.ilabt.imec.be

Port mappings

Port 8888 → 4c.gpulab.ilabt.imec.be:33400

Port 8888 → 4c.gpulab.ilabt.imec.be:33400







CHECKING THE LOGS OF YOUR CONTAINER ON THE CLI



\$ gpulab-cli log <job_id>

```
(gpulab-venv) thijs@thijs-xps:~/gpulab$ gpulab-cli log ae9e8923
2023-03-30T11:25:42.854890278+02:00 WARNING: using start-singleuser.sh instead of start-notebook.sh to start a server a 2023-03-30T11:25:42.859173254+02:00 Entered start.sh with args: jupyterhub-singleuser --ip=0.0.0.0 --notebook-dir=/ --S b/tree/project_ghent'
2023-03-30T11:25:42.923211639+02:00 Updated the jovyan user:
2023-03-30T11:25:42.923275604+02:00 - username: jovyan -> twlocal
2023-03-30T11:25:42.923370399+02:00 - home dir: /home/jovyan -> /home/twlocal
2023-03-30T11:25:42.930787366+02:00 Update twlocal's UID:GID to 1000:7123
2023-03-30T11:25:42.971664391+02:00 userdel: group twlocal not removed because it is not the primary group of user twlo 2023-03-30T11:25:43.051739125+02:00 Attempting to copy /home/jovyan to /home/twlocal...
2023-03-30T11:25:43.059861132+02:00 Success!
2023-03-30T11:25:43.059889846+02:00 Changing working directory to /home/twlocal/
2023-03-30T11:25:43.067453762+02:00 Granting twlocal passwordless sudo rights!
2023-03-30T11:25:43.067769575+02:00 Running as twlocal: jupyterhub-singleuser --ip=0.0.0.0 --notebook-dir=/ --SingleUse
```



roject_ghent'

3.6.2





2023-03-30T11:25:46.163553566+02:00 [I 2023-03-30 09:25:46.163 SingleUserLabApp mixins:609] Starting jupyterhub single-2023-03-30T11:25:46.163744884+02:00 [I 2023-03-30 09:25:46.163 SingleUserLabApp mixins:623] Extending jupyterlab.labhub

CHECKING THE LOGS OF YOUR CONTAINER

ON THE WEBSITE

Job ae9e8923-f2a9-4f1a-ad76-ae1680a9efd9 RUNNING



Creator: twlocal Project: twlocalproj

Name: JupyterHub-singleuser Description: Single Jupyter notebook instance for JupyterHub

General Info Debugging Logs Usage Graphs

2023-03-30T11:25:42.854890278+02:00 WARNING: using start-singleuser.sh instead of start-notebook.sh to start a server associated with JupyterHub. 2023-03-30T11:25:42.859173254+02:00 Entered start.sh with args: jupyterhub-singleuser --ip=0.0.0.0 --notebook-dir=/ --SingleUserNotebookApp.default url='

Raw Job JSON

2023-03-30T11:25:42.923211639+02:00 Updated the jovyan user:

2023-03-30T11:25:42.923275604+02:00 - username: jovyan -> twlocal

2023-03-30T11:25:42.923370399+02:00 - home dir: /home/jovyan -> /home/twlocal

2023-03-30T11:25:42.930787366+02:00 Update twlocal's UID:GID to 1000:7123

2023-03-30T11:25:42.971664391+02:00 userdel: group twlocal not removed because it is not the primary group of user twlocal.

2023-03-30T11:25:43.051739125+02:00 Attempting to copy /home/jovyan to /home/twlocal...

2023-03-30T11:25:43.059861132+02:00 Success!

2023-03-30T11:25:43.059889846+02:00 Changing working directory to /home/twlocal/

2023-03-30T11:25:43.067453762+02:00 Granting twlocal passwordless sudo rights!

2023-03-30T11:25:43.067769575+02:00 Running as twlocal: jupyterhub-singleuser --ip=0.0.0.0 --notebook-dir=/ --SingleUserNotebookApp.default url='/lab/tre

2023-03-30T11:25:46.163553566+02:00 [I 2023-03-30 09:25:46.163 SingleUserLabApp mixins:609] Starting jupyterhub single-user server version 3.1.1

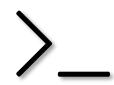
2023-03-30T11:25:46.163744884+02:00 [I 2023-03-30 09:25:46.163 SingleUserLabApp mixins:623] Extending jupyterlab.labhubapp.SingleUserLabApp from jupyterl

2023-03-30T11:25:46.163979141+02:00 [I 2023-03-30 09:25:46.163 SingleUserLabApp mixins:623] Extending jupyter server.serverapp.ServerApp from jupyter ser

2023-03-30T11:25:46.188658587+02:00 /opt/conda/lib/python3.10/site-packages/traitlets/traitlets.py:2548: FutureWarning: Supporting extra quotes around st

2023-03-30T11:25:46.188700697+02:00 2022-02-20T11:25:46 100510200+02:00 [N 2022-02-20 00:25:46 100 Single North Configurable:2001 Configur

GETTING SSH-ACCESS TO YOUR CONTAINER



\$ gpulab-cli ssh <job-id>

```
(gpulab-venv) thijs@thijs-xps:~/gpulab$ gpulab-cli ssh ae9e8923
Warning: Permanently added the ECDSA host key for IP address '10.2.47.43' to the list of known host
Welcome to Ubuntu 22.04.2 LTS (GNU/Linux 5.15.0-58-generic x86_64)
```

- * Documentation: https://help.ubuntu.com
- * Management: https://landscape.canonical.com * Support: https://ubuntu.com/advantage
- This system has been minimized by removing packages and content that are not required on a system that users do not log into.
- To restore this content, you can run the 'unminimize' command.
- The programs included with the Ubuntu system are free software; the exact distribution terms for each program are described in the individual files in /usr/share/doc/*/copyright.
- Ubuntu comes with ABSOLUTELY NO WARRANTY, to the extent permitted by applicable law.

GETTING SSH-ACCESS TO YOUR CONTAINER



- SSH access to GPULab jobs is a hack on top of `docker exec -ti /bin/bash` into the container.
- Can only be used for shell access and SFTP access
- No support for additional SSH channels:
 - No port forwarding
 - No SCP
 - No support for VSCode Remote Development







CHECKING CPU/GPU UTILIZATION

General Info

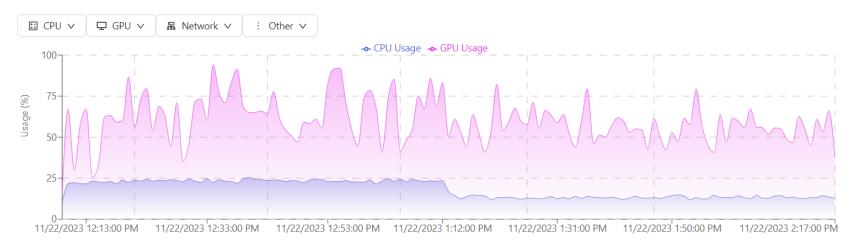
₽ Logs

Debugging Logs

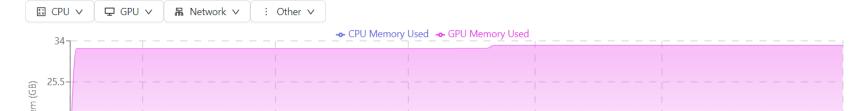
Usage Graphs

■ Raw Job JSON

CPU/GPU Utilization



Memory Utilization



FAIR USAGE POLICY

- Non-interactive GPULab jobs should:
 - Not require manual intervention to start their computations
 - Stop automatically when computations have ended
 - Be efficient:
 - Use all the GPU's they requested
 - Request enough CPU/memory to support your GPU ...
 - ... but not more than necessary







SUGGESTED WORKFLOW

- 1. Develop and test your code locally or in a Jupyter notebook
 - Create your own Docker image with custom software if necessary
- 2. Scale up to the full dataset once your code is ready:
 - Split your work into multiple jobs if possible (ex. Parameter sweep)
- 3. Add checkpointing for your intermediate results (e.g. if your job or server would crash)







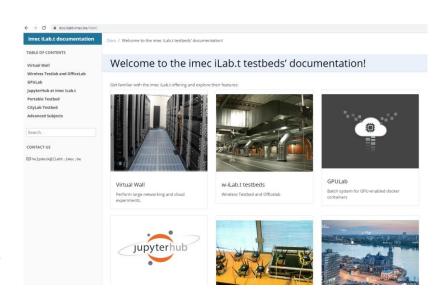
GET STARTED!

- Documentation: http://doc.ilabt.imec.be
- GPULab: https://gpulab.ilabt.imec.be
- JupyterHub: https://jupyterhub.ilabt.imec.be

SUPPORT



helpdesk@ilabt.imec.be









HANDS ON: YOUR FIRST GPULAB JOB

- Go to https://gpulab.ilabt.imec.be
- Click on + New Job
- Complete the form to execute the Python script / Jupyter notebook:
 - Image: you can reuse the Jupyter 'Docker stacks' images
 - Command:
 - python /project_ghent/path/to/my/script.py
 - bash -c '/project_ghent/my/script.py > /project_ghent/log.txt'
 - jupyter nbconvert --to notebook --execute /project_ghent/example.ipynb
 - Resources / input and output: complete as necessary
 - Scheduling: leave 'Interactive' unchecked.
- Click 'Start'

Interactive jobs will never queue, but fail instead. Useful for when you need to interact with the job (via SSH/SFTP/Jupyter server/ ...)



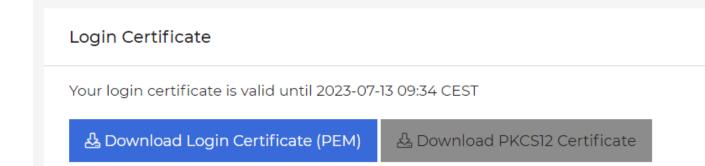




YOUR FIRST GPULAB JOB VIA THE CLI

SETTING UP THE CLI

- Only supported on Linux/Mac (On Windows: use WSL)
- Install the CLI: sudo pip install imecilabt-gpulab-cli
- Get your Login Certificate (PEM) from: https://account.ilabt.imec.be/profile or https://portal.slices-sc.eu/









YOUR FIRST GPULAB JOB VIA THE CLI **USING THE CLI**

\$ gpulab-cli --cert /path/to/cert.pem clusters

(gpulab-venv) thijs@thijs-xps:~/gpulab\$ gpulab-clicert /home/thijs/.ssh/login_ilabt_imec_be_twlocal.pem clusters Enter PEM pass phrase:							
ID	GPU Model	Comment	Slaves	GPUs	CPUs		
1 stable		1x 2x GF GTX 1080 Ti	0	0/0	0/0		
2 stable		temporary cluster	0	0/0	0/0		
3 stable	NVIDIA GeForce RTX 2080 Ti	1x RTX2080	1	0/1	8/12		
4 stable	NVIDIA GeForce GTX 1080 Ti	4x 11x GF GTX 1080 Ti	4	9/44	35/128		
5 stable	Quadro RTX 4000	UAntwerp: 2x 4x RTX4000	3	2/8	8/80		
6 stable	Tesla V100-SXM3-32GB	1x HGX-2 - 16xTesla V100	1	1/16	45/96		
7 stable	Tesla V100-SXM2-32GB,Tesla V100-SXM3-32GB	UAntwerp: DGX-1 + DGX-2 - (8+16)x Tesla V100	4	0/24	2/176		
8 stable	NVIDIA A40	12x A40 48GB	3	0/12	17/144		

imec





YOUR FIRST GPULAB JOB VIA THE CLI USING THE CLI

Tired of passing your certificate as a parameter?

Add the following line to your ~/.bashrc:

Tired of entering your password?

Decrypt your private key with OpenSSL

→ see CLI documentation

export GPULAB_CERT=/path/to/cert.pem

(gpulab-venv) thijs@thijs-xps:~/gpulab\$ gpulab-cli clusters Enter PEM pass phrase:			
ID	GPU Model	Comment	
1 stable	 	1x 2x GF GTX 1080 Ti	
2 stable	 	temporary cluster	
3 stable	NVIDIA GeForce RTX 2080 Ti	1x RTX2080	
4 stable	NVIDIA GeForce GTX 1080 Ti	4x 11x GF GTX 1080 Ti	
5 stable	Quadro RTX 4000	UAntwerp: 2x 4x RTX4000	
6 stable	Tesla V100-SXM3-32GB	1x HGX-2 - 16xTesla V100	







YOUR FIRST GPULAB JOB VIA THE CLI

STARTING AN INTERACTIVE JOB

(gpulab-venv) thijs@thijs-xps:~/gpulab\$ gpulab-cli interactivehelp Usage: gpulab-cli interactive [OPTIONS]			
Options:			
project TEXT	[required]		
duration-minutes TEXT	[required]		
docker-image TEXT	[required]		
-p,proxy	Use the jFed proxy to reach the container		
-P,no-proxy	Don't use the jFed proxy to reach the container		
	(requires IPv6 or VPN)		
auto-proxy	Automatically use the jFed proxy to reach the		
	container		
only-show	Do nothing except showing the job request		
cpus INTEGER	Number of CPU cores required (default 1)		
gpus INTEGER	Number of GPU's required (default 1)		
mem INTEGER	Memory required, in GB (default 2)		
cluster-id INTEGER	Wanted cluster ID (default any)		
ssh-pub-key TEXT	Add an SSH public key. This can be used to access		
	the running job's container. Uses the openssh		
	public key format. This option can be specified		
	more than once, to add multiple keys.		

YOUR FIRST GPULAB JOB VIA THE CLI

STARTING A JOB USING A JOBDEFINITION

Fill in the 'Create Job' form on the GPULab website, and click 'Download jobDefinition File':

"name": "exampleJob"

▼ "request" : {

▼ "owner" : {

Save in Browser

"projectUrn": "urn:publicid:IDN+ilabt.imec.be+project+twlocal

 Manually tweak your jobDefinition file if necessary

Start the job as follows:

\$ gpulab-cli submit --project my project < my jobdef file.json</pre>





ADVANCED TOPICS

PARAMETER SWEEP

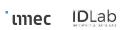
Want to do a parameter sweep?

Split it in multiple jobs!

I. Generate the correct jobDefinition JSON in the language of your choice

Pass it on the STDIN to `gpulab-cli submit --project my_project`

```
#!/bin/bash
sweep parameter=({100..1000..50})
for param in ${sweep_parameter[@]}
do
        gpulab-cli submit --project my project <<EOF</pre>
 "jobDefinition": {
     "name": "My Parameter sweep with param ${param}",
     "command": "/project_ghent/my/script.sh ${param}'",
     . . .
EOF
done
```







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