



INSTITUT DU
DÉVELOPPEMENT ET DES
RESSOURCES EN
INFORMATIQUE
SCIENTIFIQUE

www.idris.fr

JupyterHub sur Jean Zay

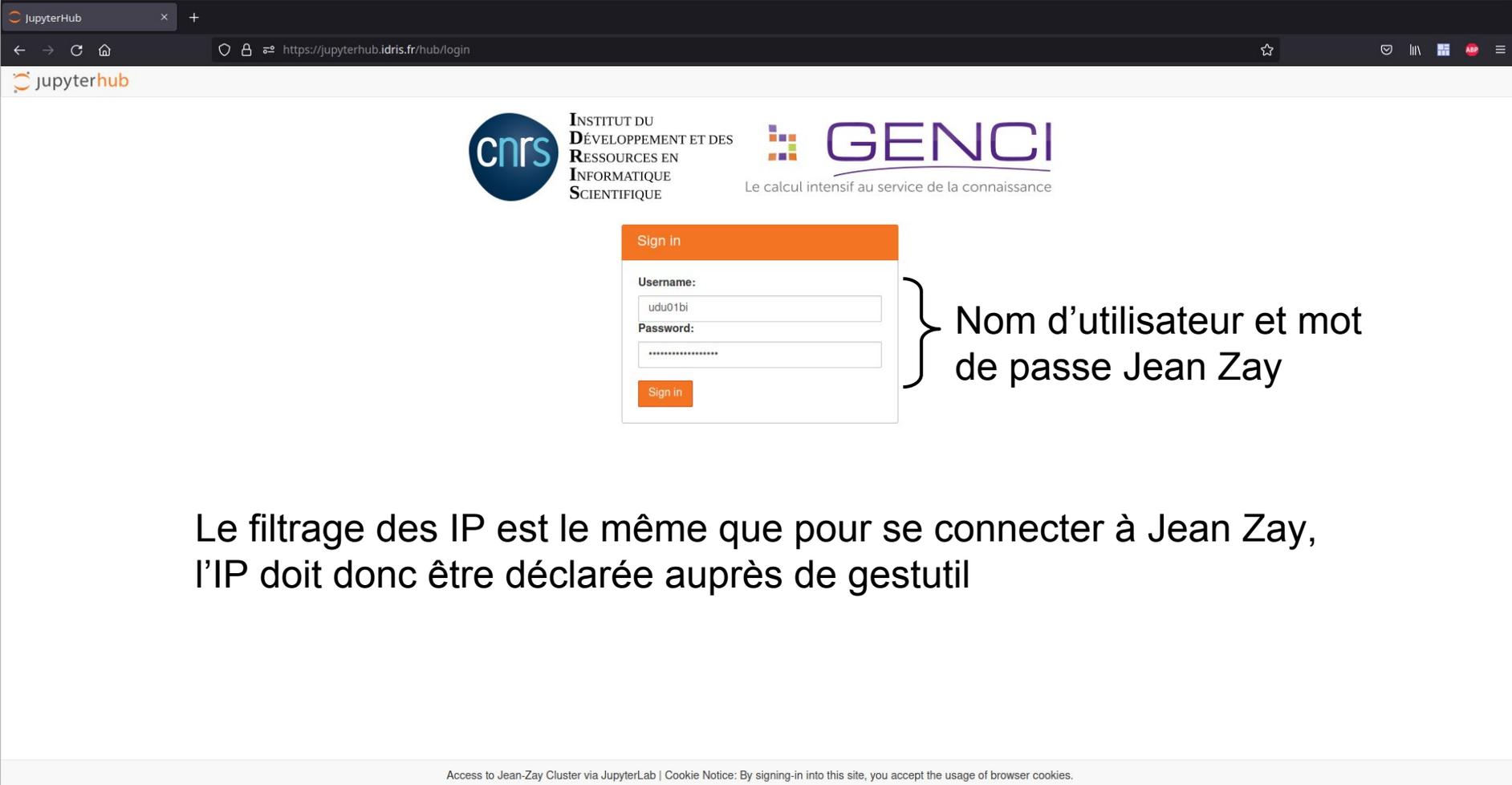


IDRIS – JupyterHub – CU du 16/09/2022

Qu'est-ce que JupyterHub ?

- Portail web de connexion au calculateur
- Permet de faire des allocations sur les différentes partitions et d'exécuter des notebooks sur les noeuds alloués
- Différents outils (SLURM manager, Tensorboard, Mlflow, etc)
- Accès : <https://jupyterhub.idris.fr>
- Documentation complète :
<https://jupyterhub.idris.fr/services/documentation/index.html>
- Documentation JupyterLab :
<https://jupyterlab.readthedocs.io/en/stable/>

Portail de connexion



Sign in

Username:
udu01bi

Password:

Sign in

} Nom d'utilisateur et mot de passe Jean Zay

Access to Jean-Zay Cluster via JupyterLab | Cookie Notice: By signing-in into this site, you accept the usage of browser cookies.

Le filtrage des IP est le même que pour se connecter à Jean Zay, l'IP doit donc être déclarée auprès de gestutil

Menu d'accueil

The screenshot shows the JupyterHub interface. At the top, there is a navigation bar with the JupyterHub logo and links for Home, Token, Announcement, Documentation, and Support. The user is logged in as 'udu01bi' and has a 'Logout' button. The main content area is titled 'List of JupyterLab instances' and includes a sub-header: 'Every user may have 10 JupyterLab server(s) with names. This allows the user to have more than one JupyterLab server running at the same time.' Below this is a form with a text input field labeled 'Name your JupyterLab' and a link 'Add New JupyterLab Instance'. A table with the following columns is displayed: Instance name, URL, Node type, Project, Node list, Job ID, Last activity, and Actions.

Instance name	URL	Node type	Project	Node list	Job ID	Last activity	Actions
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Créer une nouvelle instance (1)

The screenshot shows the JupyterHub interface. At the top, there is a navigation bar with 'Home', 'Token', 'Announcement', 'Documentation', and 'Support'. Below this, the main heading is 'List of JupyterLab instances'. A sub-heading reads: 'Every user may have 10 JupyterLab server(s) with names. This allows the user to have more than one JupyterLab server running at the same time.' Below this text is a form with a text input field containing 'my-new-kernel' and a button labeled 'Add New JupyterLab Instance'. A table with columns 'Instance name', 'URL', 'Node type', 'Project', 'Node list', 'Job ID', 'Last activity', and 'Actions' is visible below the form. A large, semi-transparent box highlights the input field and the button, with a hand cursor pointing to the button. A blue arrow points from the input field in the highlighted box to the input field in the actual interface.

Le nom de la nouvelle instance est optionnel

Créer une nouvelle instance (2)

SLURM Job Configuration Options

The following fields are used in SLURM batch script submission. Only Account field is required and rest of them, if not provided, will use Jean Zay platform default settings.

Profile
Current SLURM job configuration parameters will be saved under this profile name which can be loaded using Load profile for subsequent spawns

Load profile
Load the existing SLURM job configuration from previously saved profiles

Account (--account)
bid@v100

Time (--time) (in hours)
2

Partition (--partition)
gpu_p13

QoS (--qos)
qos_gpu-dev

Number of nodes (--nodes)
1

Number of GPUs per node (--gres)
gpu:1

Number of tasks (--tasks)
1

Number of CPUs (--cpus-per-task)
10

Application hint (--hint)
nomultithread

Notebook directory (--NotebookApp.notebook_dir)
/gpfwork/rech/bid/udu01bi
Root directory of the JupyterLab file explorer is also set to this path

Extra #SBATCH directives (one per line)
#SBATCH --exclusive

Environment variables (one per line)
WHOAMI=JUPYTERHUB

Update notebook kernels
Check this option for newly added notebook kernels on Jean Zay platform to appear in the JupyterLab launcher

Submit

Rafraîchir la liste des environnements disponibles pour disposer des modules les plus récents du calculateur

Définition du Job Slurm (noeuds, QOS, comptabilité, etc)

Comptabilité de la nouvelle instance

SLURM Job Configuration Options

The following fields are used in SLURM batch script submission. Only Account field is required and rest of them, if not provided, will use Jean Zay platform default settings.

Account (--account)

- bid@cpu
- dum@cpu
- bid@v100
- dum@v100

Load profile

Current SLURM job configuration parameters will be saved under this profile name which can be loaded using Load profile for subsequent spawns

Load the existing SLURM job configuration from previously saved profiles

Time (--time) (in hours)

2

QoS (--qos)

Number of GPUs per node (--gres)

Number of tasks (--ntasks)

1

Application hint (--hint)

nomultithread

Notebook directory (--NotebookApp.notebook_dir)

/gpfswork/rech/bid/udu01bi

Root directory of the JupyterLab file explorer is also set to this path

Extra #SBATCH directives (one per line)

#SBATCH --exclusive

The user may use this field to add any additional #SBATCH directives that are not provided in the form

Environment variables (one per line)

WHOAMI=JUPYTERHUB

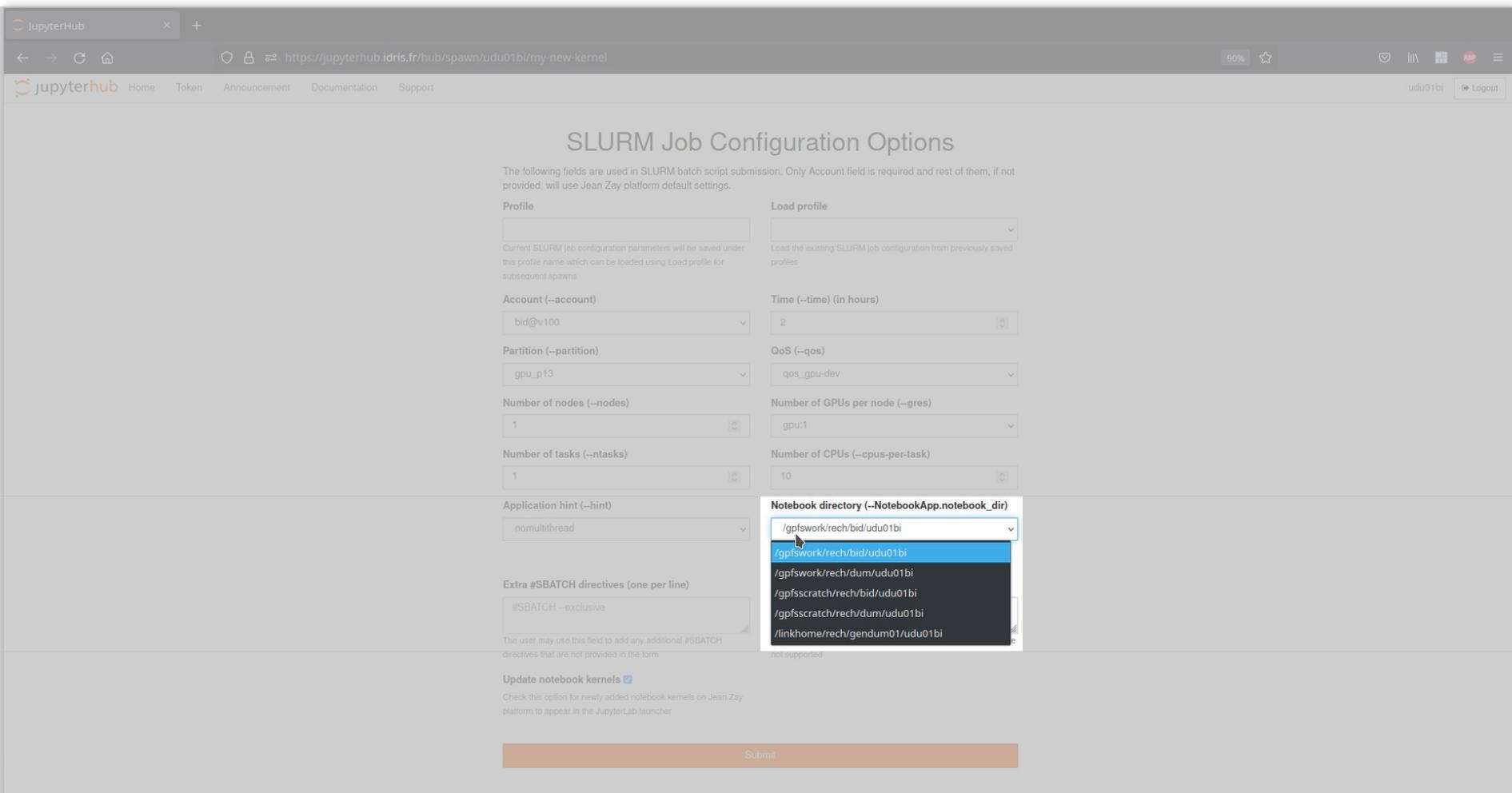
Custom environment variables can be defined here. Subshells are not supported

Update notebook kernels

Check this option for newly added notebook kernels on Jean Zay

Pour utiliser des noeuds A100, il faut sélectionner la comptabilité A100, la partition gpu_p5 et ajouter la directive #SBATCH -C a100

Workdir de la nouvelle instance



JupyterHub

https://jupyterhub.idris.fr/hub/spawn/udu01bi/my-new-kernel

Home Token Announcement Documentation Support

SLURM Job Configuration Options

The following fields are used in SLURM batch script submission. Only Account field is required and rest of them, if not provided, will use Jean Zay platform default settings.

Profile
Current SLURM job configuration parameters will be saved under this profile name which can be loaded using Load profile for subsequent spawns

Load profile
Load the existing SLURM job configuration from previously saved profiles

Account (--account)
bid@v100

Time (--time) (in hours)
2

Partition (--partition)
gpu_p13

QoS (--qos)
qos_gpu-dev

Number of nodes (--nodes)
1

Number of GPUs per node (--gres)
gpu:1

Number of tasks (--ntasks)
1

Number of CPUs (--cpus-per-task)
10

Application hint (--hint)
nomultithread

Extra #SBATCH directives (one per line)
#SBATCH --exclusive

The user may use this field to add any additional #SBATCH directives that are not provided in the form

Notebook directory (--NotebookApp.notebook_dir)

- /gpfswork/rech/bid/udu01bi
- /gpfswork/rech/bid/udu01bi
- /gpfswork/rech/dum/udu01bi
- /gpfsscratch/rech/bid/udu01bi
- /gpfsscratch/rech/dum/udu01bi
- /linkhome/rech/gendum01/udu01bi

not supported

Update notebook kernels

Check this option for newly added notebook kernels on Jean Zay platform to appear in the JupyterLab launcher

Submit

Sauvegarder une configuration

SLURM Job Configuration Options

The following fields are used in SLURM batch script submission. Only Account field is required and rest of them, if not provided, will use Jean Zay platform default settings.

Profile
ma_config
Current SLURM job configuration parameters will be saved under this profile name which can be loaded using Load profile for subsequent spawns

Load profile
Load the existing SLURM profiles

Account (--account)
bid@v100

Partition (--partition)
gpu_p13

Number of nodes (--nodes)
1

Number of tasks (--tasks)
1

Application hint (--hint)
nomultithread

Extra #SBATCH directives (one per line)
#SBATCH --exclusive

Update notebook kernels
Check this option for newly added notebook kernels on Jean Zay platform to appear in the JupyterLab launcher

Time (--time) (in hours)
2

QoS (--qos)
qos_gpu-dev

Number of GPUs per node (--gres)
gpu:1

Number of CPUs (--cpus-per-task)
10

Notebook directory (--NotebookApp.notebook_dir)
/gpfswork/rech/bid/udu01bi
Root directory of the JupyterLab file explorer is also set to this path

Environment variables (one per line)
TESTVARIABLE=123456789
Custom environment variables can be defined here. Subshells are not supported

Submit

Lors de la soumission du job, si un nom de profil est renseigné, la configuration sera enregistrée sous ce nom

Restaurer une configuration

Lors des soumissions suivantes, il est alors possible de basculer d'une configuration à l'autre à volonté

SLURM Job Configuration Options

The following fields are used in SLURM batch script submission. Only Account field is required and rest of them, if not provided, will use Jean Zay platform default settings.

Profile

This profile name which can be loaded using Load profile for

Account (--account)

Load profile

cpu

ma_config

autre_config

cpu

Partition (--partition)

cpu_p1

Number of nodes (--nodes)

1

Number of tasks (--ntasks)

1

Application hint (--hint)

nomultithread

Extra #SBATCH directives (one per line)

#SBATCH --exclusive

The user may use this field to add any additional #SBATCH directives that are not provided in the form

Update notebook kernels

Check this option for newly added notebook kernels on Jean Zay platform to appear in the JupyterLab launcher

QoS (--qos)

qos_cpu-dev

Number of GPUs per node (--gres)

Number of CPUs (--cpus-per-task)

10

Notebook directory (--NotebookApp.notebook_dir)

/gpfsscratch/rech/dum/udu01bi

Root directory of the JupyterLab file explorer is also set to this path

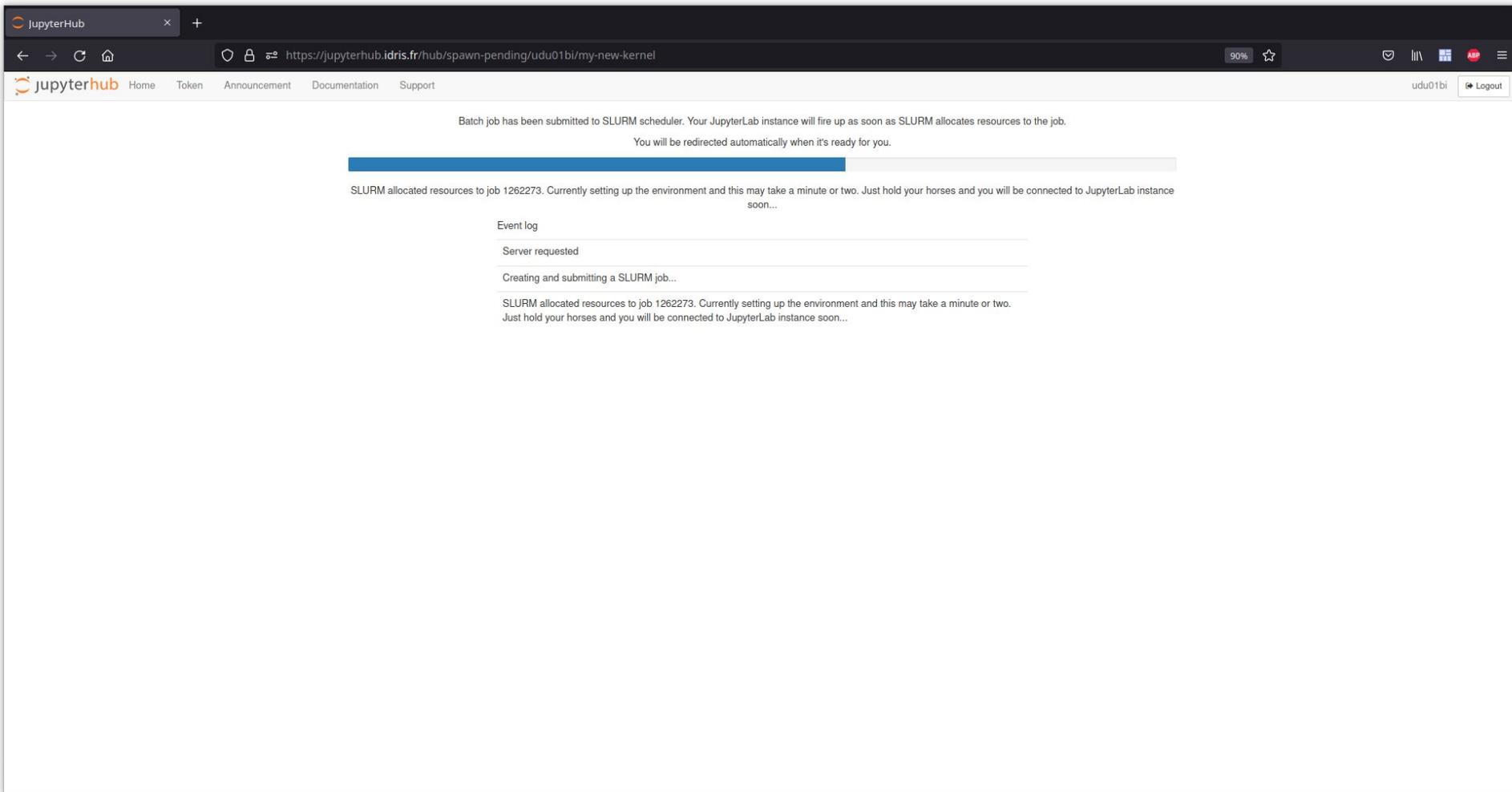
Environment variables (one per line)

WHOAMI=JUPYTERHUB

Custom environment variables can be defined here. Subshells are not supported

Submit

Allocation du job (écran de chargement)



The screenshot shows a web browser window with the JupyterHub interface. The address bar displays the URL `https://jupyterhub.idris.fr/hub/spawn-pending/udu01bi/my-new-kernel`. The page content includes a progress bar at 90% and an event log with the following entries:

- Batch job has been submitted to SLURM scheduler. Your JupyterLab instance will fire up as soon as SLURM allocates resources to the job.
- You will be redirected automatically when it's ready for you.
- SLURM allocated resources to job 1262273. Currently setting up the environment and this may take a minute or two. Just hold your horses and you will be connected to JupyterLab instance soon...
- Event log
 - Server requested
 - Creating and submitting a SLURM job...
 - SLURM allocated resources to job 1262273. Currently setting up the environment and this may take a minute or two. Just hold your horses and you will be connected to JupyterLab instance soon...

Sur la liste des instances

The screenshot shows the JupyterHub interface with a table of instances. The table has columns for Instance name, URL, Node type, Project, Node list, Job ID, Last activity, and Actions. Two instances are listed: 'jupyterlab_0' and 'my-new-kernel'. The 'my-new-kernel' instance has a 'cancel' button in the Actions column. Annotations with arrows point to various parts of the interface: 'En cours d'exécution' points to the 'jupyterlab_0' instance; 'Accès à l'instance' points to the URL of 'my-new-kernel'; 'Libérer les ressources (tue le job)' points to the 'cancel' button; 'Redémarrage de l'instance (nouveau job)' points to the 'start' button; and 'Suppression de l'instance' points to the 'delete' button.

Instance name	URL	Node type	Project	Node list	Job ID	Last activity	Actions
jupyterlab_0		cpu	dum	r1i1n25	1262289	a minute ago	start delete
my-new-kernel	/user/udu01bi/my-new-kernel	v100	bid	r13i3n5	1262273	a few seconds ago	cancel

En cours d'exécution →

Accès à l'instance ↗

Libérer les ressources (tue le job) ↑

Redémarrage de l'instance (nouveau job) ↘

Suppression de l'instance ←

JupyterHub garde un historique des instances après la fin de l'exécution, conservant des informations sur le noeud, l'allocation, le job id, etc. On peut la supprimer ou la redémarrer (écrasant les informations enregistrées)

Lancer un notebook (1)

The screenshot displays the JupyterLab interface. The browser address bar shows the URL `https://jupyterhub.idris.fr/user/udu01bi/my-new-kernel/lab`. The interface includes a left sidebar with a file browser showing folders like 'jupyter_slurm_1...', 'POT', 'TV', and 'Untitled.ipynb'. The main area is titled 'Launcher' and contains a welcome message: 'Welcome to the JupyterLab instance on Jean Zay' and 'Your current working directory is'. Below this is a 'Notebook' section with a grid of 56 environment icons, each featuring the Python logo and a specific environment name. A tooltip is visible over the 'pytorch-gpu-1.11.0+py3.9.12' icon. At the bottom, there is an 'Applications' section with three icons. The system tray at the bottom left shows 'Simple' mode and 'Mem: 164.39 MB'. The bottom right corner of the interface says 'Launcher'.

Environment Name
Python3 (default)
alphafold2.1.2
atomistic_simulation
climate_science
colabfold
mxnet-gpu-1.8.0
parcels
parcels_seq
python-3.10.4
python-3.6.15
python-3.7.10
python-3.9.12
python3.8.8
pytorch-1.8.1+py3.8.8-its
pytorch-cpu-1.7.1
pytorch-gpu-1.1
pytorch-gpu-1.10.0+py3
pytorch-gpu-1.10.1+py3
pytorch-gpu-1.11.0+py3
pytorch-gpu-1.11.0+py3.9.12
pytorch-gpu-1.3
pytorch-gpu-1.3.1
pytorch-gpu-1.3.1+nccl
pytorch-gpu-1.4.0
pytorch-gpu-1.5.0
pytorch-gpu-1.5.1
pytorch-gpu-1.6.0
pytorch-gpu-1.7.0
pytorch-gpu-1.7.0+hvd
pytorch-gpu-1.7.1
pytorch-gpu-1.7.1
pytorch-gpu-1.7.1+nccl
pytorch-gpu-1.8.0
pytorch-gpu-1.9.0+py3.9
rapids-0.14
rapids-21.08
tensorflow-gpu-2.7.0+py3.9
tensorflow-gpu-2.9.1+py3.10
tensorflow-gpu-1.13.2
tensorflow-gpu-1.14
tensorflow-gpu-1.14-mpi
tensorflow-gpu-1.14
tensorflow-gpu-1.15.2
tensorflow-gpu-1.8
tensorflow-gpu-2.0.0
tensorflow-gpu-2.1.0
tensorflow-gpu-2.1.0+hvd-0
tensorflow-gpu-2.2.0
tensorflow-gpu-2.3.0
tensorflow-gpu-2.3.1
tensorflow-gpu-2.3.1+hvd
tensorflow-gpu-2.4.0
tensorflow-gpu-2.4.0
tensorflow-gpu-2.4.1
tensorflow-gpu-2.4.1+cuda
tensorflow-gpu-2.4.1+nccl
tensorflow-gpu-2.5.0
tensorflow-gpu-2.5.0
tensorflow-gpu-2.5.0+nccl
tensorflow-gpu-2.6.0
tensorflow-gpu-2.8.0+py3.9

Lancer un notebook (2)

The screenshot shows the JupyterLab interface. At the top, there is a navigation bar with the following items: Documentation, Hub Control Panel, Log Out, a theme selector (currently set to 'light'), and Mem:367 MB. Below this, the main area displays a grid of kernel options. A white box highlights the top navigation bar with the following text: Documentation | Hub Control Panel | Log Out | light | Mem:367 MB. A blue arrow points from the 'Hub Control Panel' link to the 'Mode sombre' label. Another blue arrow points from the 'Log Out' link to the 'Déconnexion' label. A third blue arrow points from the 'Mem:367 MB' text to the 'Mémoire CPU consommée' label. The kernel options include Python3 (default), Python 3.6.15, Python 3.7.10, and various TensorFlow and GPU configurations. A 'Menu principal (liste des instances)' label is placed over the grid of kernels. At the bottom left, there is a link to the online documentation: <https://jupyterhub.idris.fr/services/documentation/index.html>. The bottom status bar shows 'Simple' and 'Mem: 164.39 MB'.

Menu principal (liste des instances)

Mode sombre

Documentation | Hub Control Panel | Log Out | light | Mem:367 MB

Documentation en ligne <https://jupyterhub.idris.fr/services/documentation/index.html>

Déconnexion

Mémoire CPU consommée

Notebook



The screenshot displays a Jupyter Notebook interface. The left sidebar shows a file browser with a table of files:

Name	Last Modified
jupyter_sturm_1...	8 minutes ago
POT	19 hours ago
TV	2 months ago
Untitled.ipynb	18 hours ago
Untitled1.ipynb	a minute ago

The main notebook area shows the following code cells:

```
[1]: import torch
     torch.__version__

[1]: '1.11.0'

[2]: import os

[3]: os.environ["TESTVARIABLE"]

[3]: '123456789'
```

The output of the third cell is highlighted with a box containing the text: `pytorch-gpu-1.11.0+py3.9.12`. A blue arrow points from this box to the environment name `pytorch-gpu-1.11.0+py3.9.12` in the top right corner of the notebook interface.

On retrouve l'environnement qu'on a chargé ainsi que les variables d'environnement demandées à la création du job.

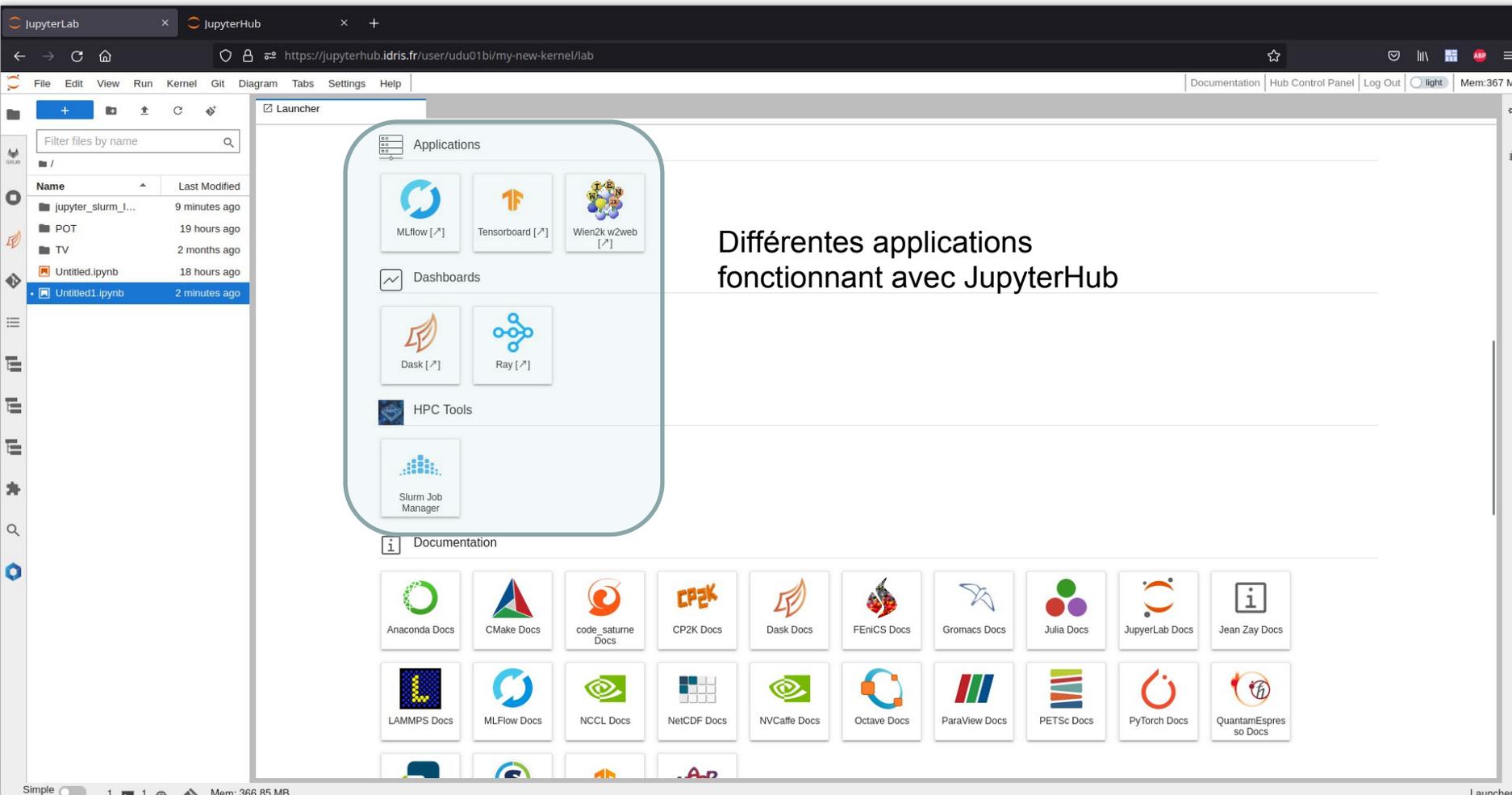
Documentations

The screenshot shows a JupyterLab interface with a 'Launcher' view. The interface includes a file browser on the left, a top menu bar, and a main workspace. The 'Launcher' view displays several categories of tools and documentation:

- Applications:** MLflow, Tensorboard, Wien2k w2web.
- Dashboards:** Dask, Ray.
- HPC Tools:** Slurm Job Manager.
- Documentation:** A grid of 18 documentation links, including Anaconda Docs, CMake Docs, code_saturne Docs, CP2K Docs, Dask Docs, FEniCS Docs, Gromacs Docs, Julia Docs, JupyterLab Docs, Jean Zay Docs, LAMMPS Docs, MLFlow Docs, NCCL Docs, NetCDF Docs, NVcaffe Docs, Octave Docs, ParaView Docs, PETSc Docs, PyTorch Docs, and QuantamEspres so Docs.

A red box highlights the 'Documentation' section, and the text 'Accès rapide aux docs en ligne des outils' is overlaid on the right side of the image.

Outils divers



The image shows a screenshot of the JupyterLab Launcher interface. The browser address bar displays `https://jupyterhub.idris.fr/user/udu01bi/my-new-kernel/lab`. The interface includes a file browser on the left, a central launcher area, and a documentation grid at the bottom. A blue rounded rectangle highlights the 'Applications' section, which contains icons for MLflow, Tensorboard, Wien2k w2web, Dask, and Ray. Below this, the 'HPC Tools' section features the Slurm Job Manager icon. The 'Documentation' section at the bottom contains a grid of 24 icons representing various software documentation pages, including Anaconda Docs, CMake Docs, code_saturne Docs, CP2K Docs, Dask Docs, FEniCS Docs, Gromacs Docs, Julia Docs, JupyterLab Docs, Jean Zay Docs, LAMMPS Docs, MLFlow Docs, NCCL Docs, NetCDF Docs, NVcaffe Docs, Octave Docs, ParaView Docs, PETSc Docs, PyTorch Docs, and QuantamEspres so Docs. The top right of the interface shows 'Mem:367 MB' and 'light' theme. The bottom left shows 'Simple' mode and 'Mem: 366.85 MB'.

Différentes applications fonctionnant avec JupyterHub

SLURM Queue Manager

Permet de contrôler ses jobs, ou en lancer de nouveaux

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
1262273	gpu_p13	my-new-k	udu01bi	R	13:43	1	r133n5

Tensorboard (1)

The screenshot shows the JupyterLab interface with a grid of available kernels. A search bar at the top left contains the text "tensorflow-gpu/py3/2.". A large blue arrow points from the search bar to the "Load" button next to the "tensorflow-gpu/py3/2.6.0" kernel in the available modules list. A second, smaller search bar is overlaid on the right side of the interface, showing the loaded modules for the selected kernel, including "tensorflow-gpu/py3/2.6.0".

Charger un module où tensorboard est installé

Le module tensorboard ainsi que ses dépendances sont maintenant chargés

Tensorboard (2)

The screenshot shows the JupyterLab Launcher interface. On the left, there is a file browser showing a directory structure with folders like 'miruns', 'POT', 'runs', and 'TV'. The main area displays a grid of application icons for various TensorFlow GPU environments, such as 'tensorflow-gpu-2.0.0', 'tensorflow-gpu-2.1.0+hvd-0', and 'tensorflow-gpu-2.5.0+nccl-2'. Below the grid, there are sections for 'Applications', 'Dashboards', 'HPC Tools', and 'Documentation'. The 'Applications' section has 'Tensorboard' selected. A modal dialog titled 'Set up Tensorboard' is open, showing CLI arguments and environment variables.

Set up Tensorboard

CLI arguments:

```
--logdir /gpfswork/rech/bid/udu01bi/runs
```

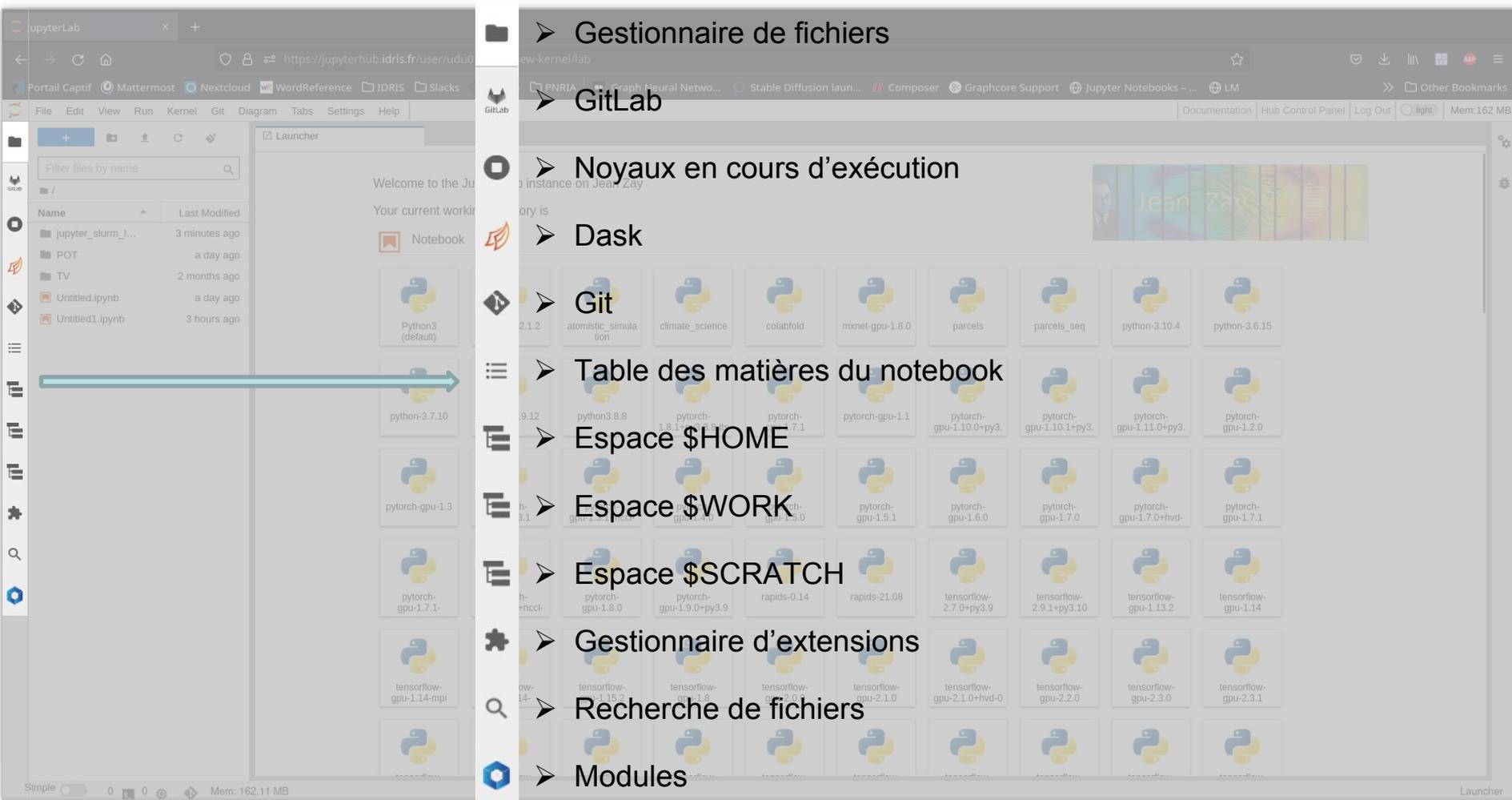
Environment variables:

```
TOM=CAT JERRY=MOUSE
```

Buttons: Cancel, Launch

Lancez tensorboard depuis le launcher, une nouvelle fenêtre s'ouvrira alors avec ledit tensorboard

Autres fonctionnalités



The image shows a screenshot of the JupyterLab interface. On the left, the Launcher sidebar is visible, showing a list of files and folders. A blue arrow points from the sidebar to the main area. The main area displays a grid of kernels, each with a Python logo and a name. The kernels are arranged in a grid, with some having a 'Python3 (default)' label and others having specific versions and configurations like 'python-3.7.10', 'pytorch-gpu-1.3', 'tensorflow-gpu-1.14-mpi', etc. The interface includes a top navigation bar with various icons and a bottom status bar showing memory usage.

- Gestionnaire de fichiers
- GitLab
- Noyaux en cours d'exécution
- Dask
- Git
- Table des matières du notebook
- Espace \$HOME
- Espace \$WORK
- Espace \$SCRATCH
- Gestionnaire d'extensions
- Recherche de fichiers
- Modules