Datarmor documentation

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What is Datarmor?

Figure 1: Datarmor

Applications

- Parallel computing (MPI, Fortran, C/C++)

- Data Analysis (Python, R, Matlab, Julia)
- JupyterHub (Notebooks, Jupyterlab)
- Machine Learning (TensorFlow)
- Data visualisation (VisIt, VMD)

Creating an account

To create an account, send me an email (nicolas.barrier@ird.fr) with:

- An **institutional** email address
- A phone number
- The names of your supervisors (if any)
- A short description of why you want to use Datarmor (projects, tools, etc.)

Support questions about Datarmor should be sent to assistance@ifremer.fr

Connection: Pulse Secure

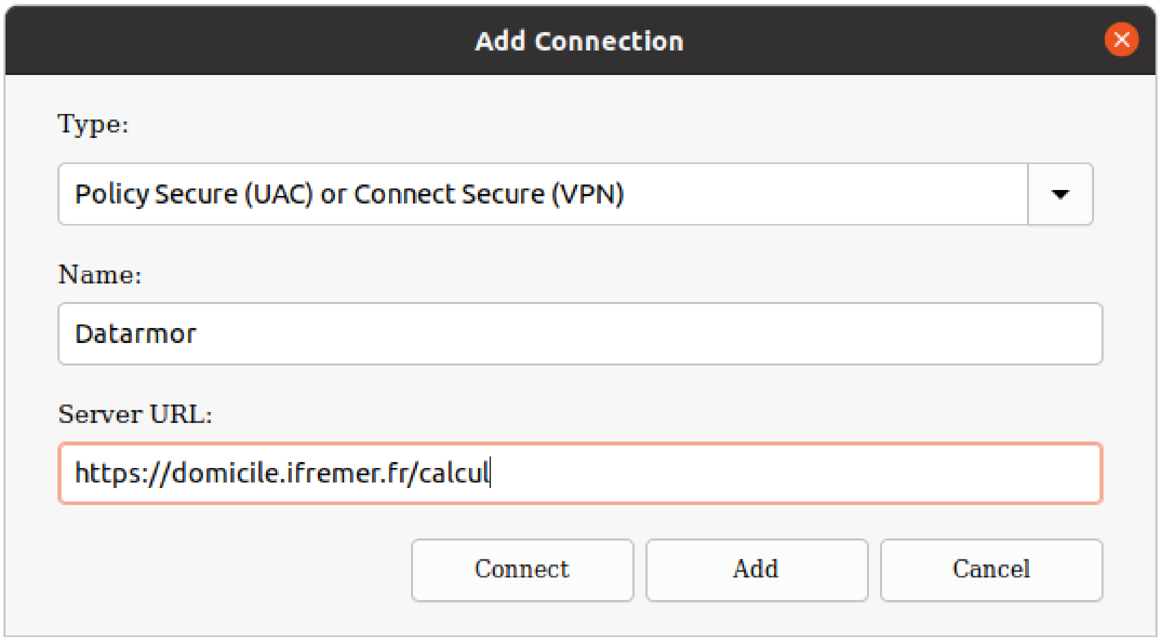
Outside the Ifremer Network, PulseSecure is required. It can be downloaded here.

Install the right version depending on your OS:

- Windows 64: `PulseSecure.x86.msi`
- Mac Os X 64: `PulseSecure.dmg`
- Ubuntu 20.04: `pulsesecure_9.1.R12_amd64.deb`
- Ubuntu 18.04: `pulse-9.1R8.x86_64.deb`

Connection: Pulse Secure

Now set-up a new connection as follows:



Type:

Policy Secure (UAC) or Connect Secure (VPN)

Name:

Datarmor

Server URL:

https://domicile.ifremer.fr/calcul

Connect to the Datarmor VPN using your **extranet** logins and leave it open until you have finished.

Connection: Terminal (Linux / Mac Os X)

For Linux/Mac Os X users, open a Terminal and types:

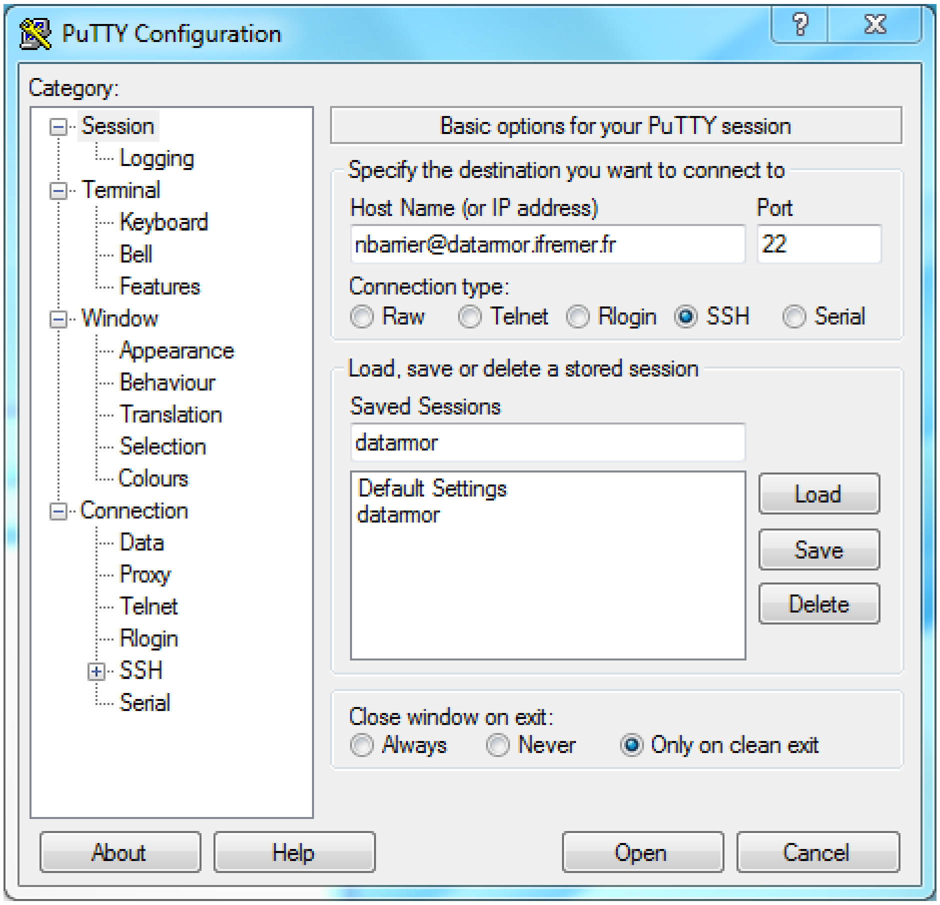
```
ssh -X nbarrier@datarmor.ifremer.fr
```

replacing `nbarrier` by your **intranet** login. The `-X` option allows display (for use of text editors for instance). If the `-X` option does not work, use `-Y`.

For Mac Os X users, I recommend to install and use iTerm2 Terminal application, which is more user friendly than the default one.

Connection: Putty or MobaXTerm (Windows)

For Windows Users, it is recommended to use Putty or MobaXTerm



Specify the destination you want to connect to

Host Name (or IP address): nbarrier@datarmor.ifremer.fr

Port: 22

Connection type: ○ Raw ○ Telnet ○ Rlogin ● SSH ○ Serial

Load, save or delete a stored session

Saved Sessions: datarmor

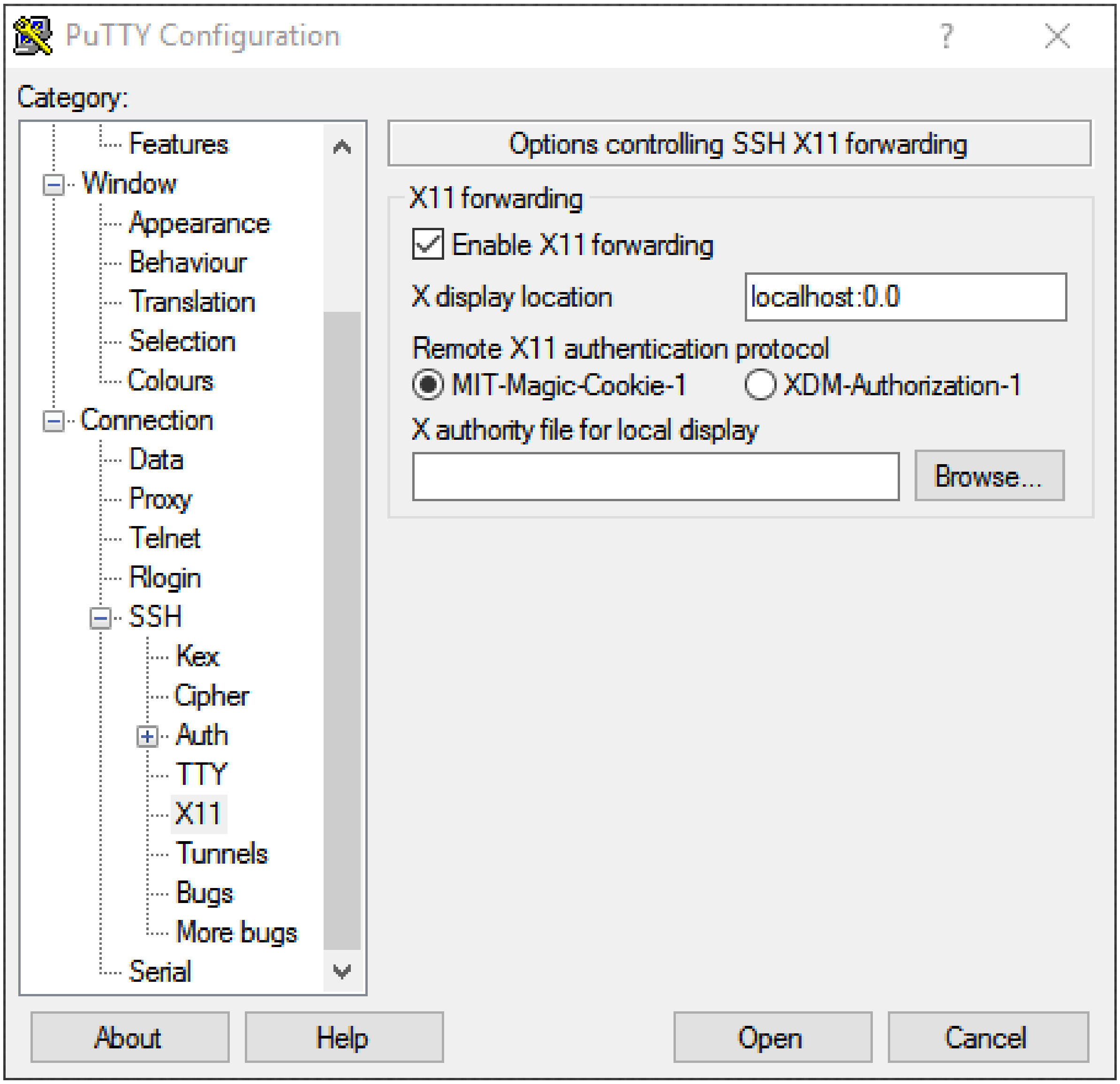
Default Settings
datarmor

Close window on exit: ○ Always ○ Never ● Only on clean exit

Figure 2: Putty connection window

Connection: Putty (Windows)

To allow display, you need to enable X11 forwarding on the `Connection > SSH` menu:



Options controlling SSH X11 forwarding

X11 forwarding

☑ Enable X11 forwarding

X display location: localhost:0.0

Remote X11 authentication protocol

● MIT-Magic-Cookie-1 ○ XDM-Authorization-1

X authority file for local display

Figure 3: Putty configuration window

RSA keys (Linux / Mac Os X)

To connect on Datarmor without typing the password, you need to use an ED25519 key. First, check if one already exists on your local computer:

```
ls $HOME/.ssh/id_ed25519.pub
```

If no such file, generate a key using

```
ssh-keygen -t ed25519
```

and follows instructions. Then, send it to Datarmor (the intranet password is needed):

```
ssh-copy-id nbarrier@datarmor.ifremer.fr
```

Use your login instead of `nbarrier`. Now you should be able to connect to Datarmor without typing your password.

Navigating on Datarmor

Datarmor is a Unix computer. You need some Linux background.

- Change directory: `cd my/new/directory`
- Find current directory: `pwd`
- List directory content: `ls`
- Go to parent directory: `cd ..`

- Create new folder: `mkdir -p folder_name`
- Create an empty file: `touch file.txt`
- Copy a file: `cp file.txt save_file.txt`
- Remove a file/folder: `rm -r file.txt`
- Rename/Move a file: `mv file.text my/dest/renamed.txt`

Visit linux-commands-cheat-sheet for a summary of essentials Linux commands.

Datarmor: important folders

Important folders are:

- `$HOME`: main folder (50 Go, backed-up). For codes and important things
- `$DATAWORK`: data folder (1 To, **no back-up**). For data.
- `$SCRATCH`: temporary folder (10 To, files older than 10 days are automatically removed). For running computation.
- `/dataref`: folder containing some reference data (Copernicus data, atmospheric forcings, etc.)
- `/home/datawork-marbec-pmod`: Marbec DEN folder (limited access)

  To recover deleted files from `$HOME`, send an email to assistance@ifremer.fr

Modules (1/2)

To work with external tools, you need to load them into Datarmor's memory. This is done as follows:

```
module load R   ## load one module
module load java NETCDF  ##  load 2 modules
module load vacumm/3.4.0-intel  ## load a specific version
```

To list all the available modules:

```
module avail
```

Modules (2/2)

To list the modules that are loaded:

```
module list
```

To unload a module:

```
module unload R
```

To unload all the modules at once:

```
module purge
```

Default settings (1/2)

By default, the `rm` command does not ask you whether you are sure or not. Might be error prone. We might want to correct it.

To change some default behaviours, you need to create/edit a Linux configuration file.

```
gedit ${HOME}/.cshrc &
```

> The `&` character implies that you will keep access to your terminal. Else, the terminal will be back once the text editor is closed.

Default settings (2/2)

In the `.cshrc` file, you can overwrite existing commands and create new ones:

```
alias x 'exit'
alias rm 'rm -i -v'
alias cp 'cp -i -v'
alias mv 'mv -i -v'
```

You can also create environment variables (accessible via `$`):

```
setenv R_LIBS_USER $HOME/libs/R/lib
```

You can also load your favorite modules automatically by adding the `module load` command in your `.cshrc` file:

```
module load R
```

Running a calculation: warning!

When you connect on Datarmor, you end-up on the **login node**. It is used for navigation, small file manipulation, text edition, code compilation **but nothing more!**

Absolutely no computation or heavy file manipulation should be done from here!!!

Heavy stuff should be done on a compute node, which are accessible by submitting a PBS job using the `qsub` command.

Running a job: interactive mode.

To run an interactive job, type the following command line

```
qsub -I -l walltime=01:00:00 -l mem=50M
```

The `-l mem` specifies the requested memory, `-l walltime` specifies the requested calculation time.

Job is ended by typing `exit` on the terminal.

> **Running interactive jobs imply that you leave your connection open until the job is finished.**

Running a job: PBS script

To run a job in a non-interactive way, you need to create a `.pbs` file, which contains the instructions for running your job.

When done, run the calculation as follows:

```
qsub run_script.pbs
```

Job output files will be provided in a `run_script.pbs.oXXXX` file, with `XXXX` the job ID.

Some examples are provided in Datarmor's `/appli/services/exemples/` folder (see the `R` and `pbs` sub-folders).

Running a job: PBS script (sequential)

```
#!/bin/csh
#PBS -l mem=100M
#PBS -l walltime=01:00:00

## Load the modules that will be used to do the job
source /usr/share/Modules/3.2.10/init/csh
module load R

## go to the directory where the job has been launched
```

```
cd $PBS_O_WORKDIR


## Run R
Rscript script.R >& output.log  ## redirects outputs into log
```

Running a job: PBS script (parallel)

Parallel jobs are run in the same way, except that a queue (`-q`) parameter is added. It specifies the resources that you will use.

```
#!/bin/csh
#PBS -l mem=100M
#PBS -q mpi_2
#PBS -l walltime=01:00:00
cd $PBS_O_WORKDIR


source /usr/share/Modules/3.2.10/init/csh
module load NETCDF/4.3.3.1-mpt-intel2016


$MPI_LAUNCH program.exe >& out
```

In the above, 2 nodes, each containing 28 cores are requested, so 56 cores in total

Running a job: queues

The full description of Datarmor queues is provided here. Most important ones are:

- `sequentiel`: the default one (single core)
- `omp`: shared-memory queue (several nodes with access to the same memory).
- `mpi_N`: distributed memory queue (several nodes with independent memories), with `N` ranging from 1 (28 cores) to 18 (504 cores)
- `big`: distributed memory with 1008 cores.
- `ftp`: queue used to upload/download data to/from remote FTP servers
- `gpuq`: GPU queue.

Running a job: good practice

A good practice is to copy everything you need (code + data) to `$SCRATCH` and run your calculation from here:

```
#!/bin/csh
#PBS -l mem=100M
#PBS -q mpi_2
#PBS -l walltime=01:00:00

source /usr/share/Modules/3.2.10/init/csh
module load NETCDF/4.3.3.1-mpt-intel2016
```

```
cp -r $HOME/code.exe $SCRATCH
cp -r $DATAWORK/data $SCRATCH
cd $SCRATCH
$MPI_LAUNCH code.exe >& out
cp -r output $DATAWORK
```

Running a job: array

To repeat a job a certain number of times (if your model has stochasticity for instance), you can use job arrays:

```
#!/bin/csh
#PBS -l mem=10M
#PBS -l walltime=00:01:00

cd $PBS_O_WORKDIR

mkdir -p output_${PBS_ARRAY_INDEX}
touch output_${PBS_ARRAY_INDEX}/toto.txt
```

To run the job:

```
qsub -J 0-10 seq.array
```

It will run the job 11 times, with `PBS_ARRAY_INDEX` ranging from `0` to `10`.

Running a job: chained jobs (Advanced users)

To run a job in a chained mode (i.e.`job2` depends on `job1`), first run a job using the `-h` option (freeze the job):

```
qsub -h -N Job1 script1.pbs
```

Now, run a second job depending on the result of the first job:

```
qsub -N Job2 -W depend=afterany:'qselect -N Job1 -u $USER' script2.pbs
```

Finally, release the first job:

```
qrls 'qselect -N Job1 -u $USER'
```

Note: replace `afterany` by `afterok` (no error) or `afternotok` (error)

Running a job: follow-up

To follow the status of your job:

```
qstat -u nbarrier
```

Table 1: Job status provided by `qstat`

Status	Description
C	Job is completed after having run
E	Job is exiting after having run
H	Job is held
Q	Job is queued, eligible to run or routed
R	Job is running

Running a job: follow-up

To suppress a job:

```
qdel 9255575.datarmor0  ## replace by the ID of the job to kill
```

At the end of the job, check the email you receive and look for the following lines:

```
resources_used.mem=12336kb
resources_used.walltime=00:00:24
```

If you requested more memory/walltime than you used, adapt your needs for the next time (cf. here for more details)

Exchange between Datarmor and local computer

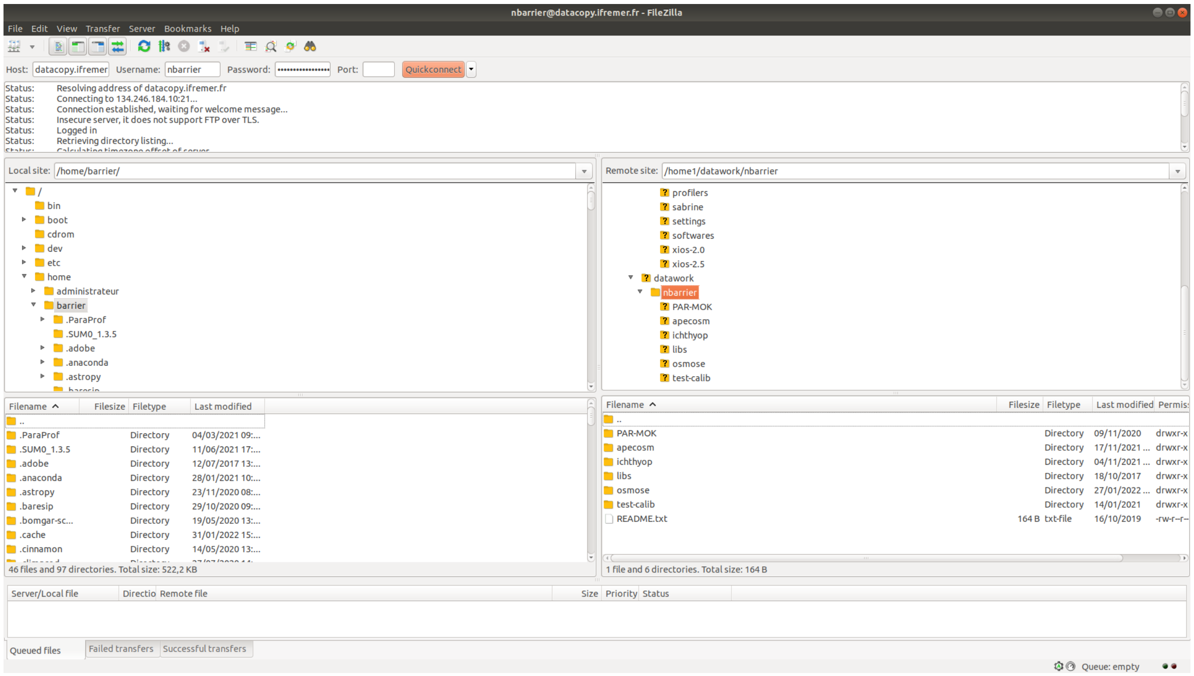
Data exchange between local computer and Datarmor should not be done on the compute node, especially so for heavy files (**no use of `scp`**).

To exchange data, use the `datacopy.ifremer.fr` server, to which you can connect using FTP. Your **intranet** logins are required.

> **Note:** you need to be on the Ifremer network. If not, the VPN should be on.

Is is advised to use FileZilla to do that

Exchange between Datarmor and local computer



Host: datacopy.ifremer Username: nbarrier Password: ••••••••••••••••• Port:

```
Status:     Resolving address of datacopy.ifremer.fr
Status:     Connecting to 134.246.184.10:21...
Status:     Connection established, waiting for welcome message...
Status:     Insecure server, it does not support FTP over TLS.
Status:     Logged in
Status:     Retrieving directory listing...
```

Local site: /home/barrier/

```
▾ /
    bin
  ▸ boot
    cdrom
  ▸ dev
  ▸ etc
  ▾ home
    ▸ administrateur
    ▾ barrier
      ▸ .ParaProf
        .SUM0_1.3.5
      ▸ .adobe
      ▸ .anaconda
      ▸ .astropy
```

Remote site: /home1/datawork/nbarrier

```
      profilers
      sabrine
      settings
      softwares
      xios-2.0
      xios-2.5
  ▾ datawork
    ▾ nbarrier
        PAR-MOK
        apecosm
        ichthyop
        libs
        osmose
        test-calib
```

Filename	Filesize	Filetype	Last modified
..			
.ParaProf		Directory	04/03/2021 09:...
.SUM0_1.3.5		Directory	11/06/2021 17:...
.adobe		Directory	12/07/2017 13:...
.anaconda		Directory	28/01/2021 10:...
.astropy		Directory	23/11/2020 08:...
.baresip		Directory	29/10/2020 09:...
.bomgar-sc...		Directory	19/05/2020 13:...
.cache		Directory	31/01/2022 15:...
.cinnamon		Directory	14/05/2020 13:...

46 files and 97 directories. Total size: 522,2 KB

Filename	Filesize	Filetype	Last modified	Permis:
..				
PAR-MOK		Directory	09/11/2020	drwxr-x
apecosm		Directory	17/11/2021 ...	drwxr-x
ichthyop		Directory	04/11/2021 ...	drwxr-x
libs		Directory	18/10/2017	drwxr-x
osmose		Directory	27/01/2022 ...	drwxr-x
test-calib		Directory	14/01/2021	drwxr-x
README.txt	164 B	txt-file	16/10/2019	-rw-r--r--

1 file and 6 directories. Total size: 164 B

Server/Local file	Directio	Remote file	Size	Priority	Status

Figure 4: Filezilla windows

Exchange between Datarmor and remote server

To recover data from a remote FTP server, submit a job on the `ftp` queue. An exemple is provided below (inspired from `/appli/services/exemples/pbs/ftp.pbs`)

```
#!/bin/csh

#PBS -q ftp

#PBS -l walltime=02:15:00
```

```
cd $DATAWORK
```

```
time rsync -av login@server:/source/folder /destination/folder/ >& output
```

This will need some adaptation depending on the remote server.

Conda

Sometimes, you might need external tools that are not available on modules. One way to use these tools is to create your own Conda environments, which is possible on Datarmor (cf. Conda sur Datarmor).

First, edit your `.cshrc` file (using `gedit $HOME/.cshrc &`) and add:

```
source /appli/anaconda/latest/etc/profile.d/conda.csh
```

Then, close and reopen the datarmor connection and type

```
which conda
```

to see if `conda` commands are accessible.

Conda: settings

Now, create a `.condarc` using `gedit $HOME/.condarc &` and write:

```
envs_dirs:
- /my/env/folder
- /home1/datahome/nbarrier/softwares/anaconda3-envs
- /appli/conda-env
- /appli/conda-env/2.7
- /appli/conda-env/3.6
channels:
  - conda-forge
  - defaults
```

Replace the first line by a folder of your choice. It will contain your own environments.

Conda: using existing environments

To list the environments:

```
conda env list
```

To activate an environment:

```
conda activate pyngl
```

To deactivate an environment:

```
conda deactivate pyngl
```

Conda: creating environments

To create a new environment:

```
conda create --name new-env
```

To install packages in the activated environment:

```
conda install package_name
```

For a R environment:

```
conda create --name r-env
conda activate r-env
conda install r r-base
```

To remove an environment:

```
conda env remove --name r-env
```

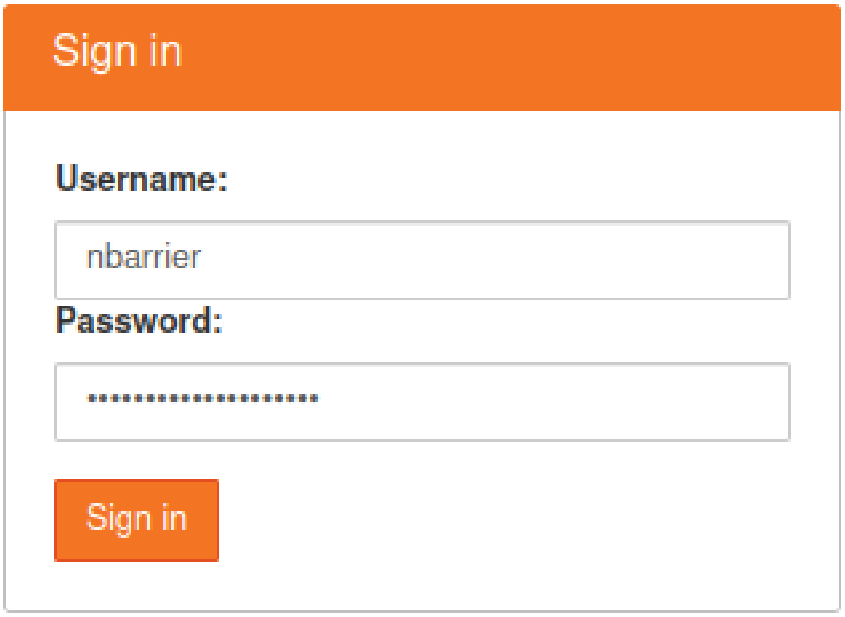
Conda: running jobs

Conda can be used to run PBS jobs as follows:

```
#!/bin/csh
#PBS -l mem=4g
#PBS -l walltime=00:10:00

## for CSH
source /appli/anaconda/latest/etc/profile.d/conda.csh

## for BASH
#. /appli/anaconda/latest/etc/profile.d/conda.csh

conda activate myconda

python toto.py >& output
```

Jupyterhub

In order to process data in a fancy way, you can use Jupyter. To do so, connect on https://datarmor-jupyterhub.ifremer.fr/ with your Intranet login.



Username: nbarrier

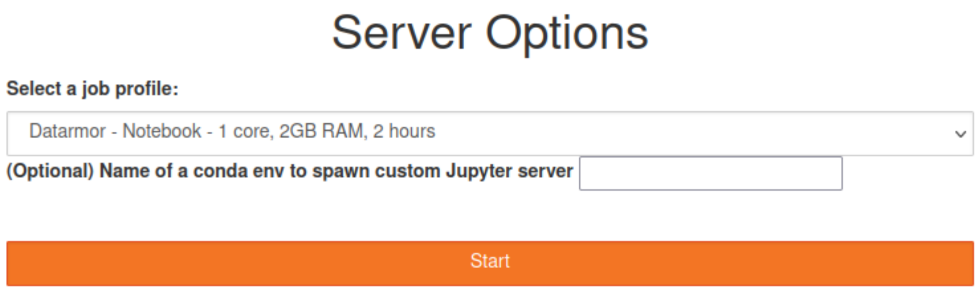
Password: ••••••••••••••••••••

Figure 5: Jupyter connection window

Note: you also need to be on Ifremer Network or with the Datarmor VPN activated

Jupyterhub

Now, select the resources that you want (core + memory)



Server Options

Select a job profile:

Datarmor - Notebook - 1 core, 2GB RAM, 2 hours

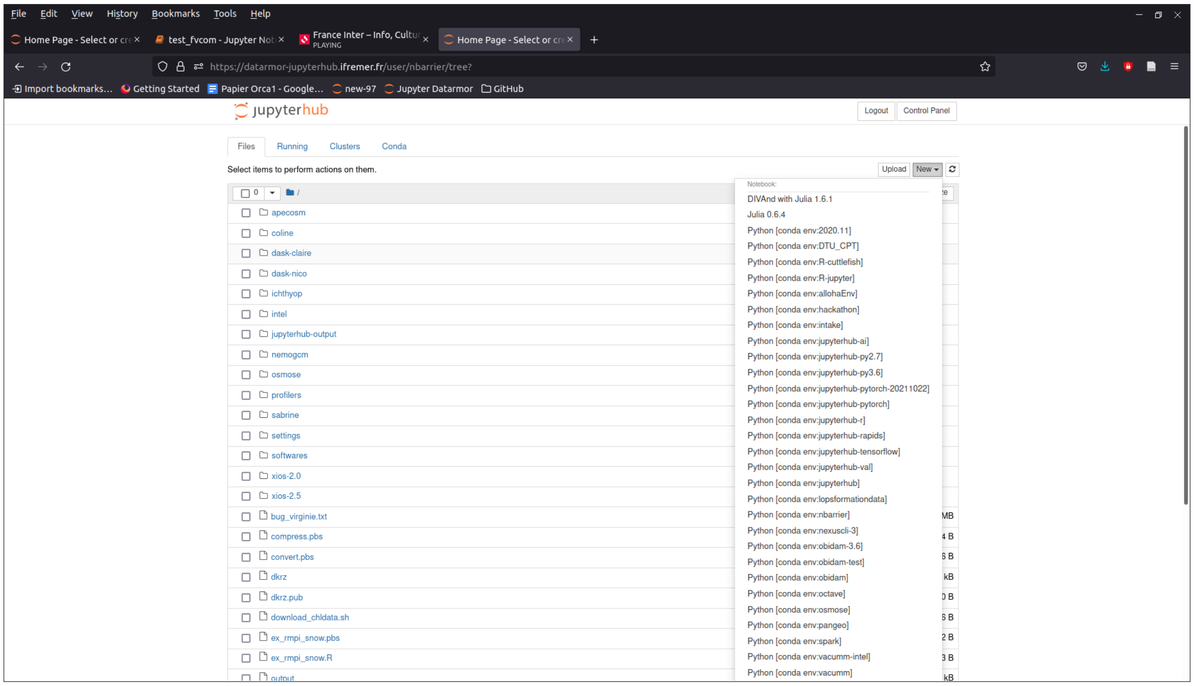
(Optional) Name of a conda env to spawn custom Jupyter server

Figure 6: Jupyter resource selection window

Warning: do not specify an optional environment

Jupyterhub

When the server is on, click on the `New` button and choose the Conda environment of your choice.



Select items to perform actions on them.

□ 0 /

□ apecosm
□ coline
□ dask-claire
□ dask-nico
□ ichthyop
□ intel
□ jupyterhub-output
□ nemogcm
□ osmose
□ profilers
□ sabrine
□ settings
□ softwares
□ xios-2.0
□ xios-2.5
□ bug_virginie.txt
□ compress.pbs
□ convert.pbs
□ dkrz
□ dkrz.pub
□ download_chldata.sh
□ ex_rmpi_snow.pbs
□ ex_rmpi_snow.R
□ output

Notebook:

DIVAnd with Julia 1.6.1
Julia 0.6.4
Python [conda env:2020.11]
Python [conda env:DTU_CPT]
Python [conda env:R-cuttlefish]
Python [conda env:R-jupyter]
Python [conda env:allohaEnv]
Python [conda env:hackathon]
Python [conda env:intake]
Python [conda env:jupyterhub-ai]
Python [conda env:jupyterhub-py2.7]
Python [conda env:jupyterhub-py3.6]
Python [conda env:jupyterhub-pytorch-20211022]
Python [conda env:jupyterhub-pytorch]
Python [conda env:jupyterhub-r]
Python [conda env:jupyterhub-rapids]
Python [conda env:jupyterhub-tensorflow]
Python [conda env:jupyterhub-val]
Python [conda env:jupyterhub]
Python [conda env:lopsformationdata]
Python [conda env:nbarrier]
Python [conda env:nexuscli-3]
Python [conda env:obidam-3.6]
Python [conda env:obidam-test]
Python [conda env:obidam]
Python [conda env:octave]
Python [conda env:osmose]
Python [conda env:pangeo]
Python [conda env:spark]
Python [conda env:vacumm-intel]
Python [conda env:vacumm]

Figure 7: Jupyter notebook window

Jupyterhub: personal Conda environments

To use Jupyter with your own R, Python or Matlab environments, you will need to install the following additional libraries to your Conda environments:

```
conda install r-irkernel  ## for R
conda install ipykernel  ## for Python
conda install matlab_kernel  ## for matlab
```

To use Jupyter with Julia, run Julia (installed with `conda`) from your environment and type:

```
using Pkg
Pkg.add("IJulia")
```

Jupyterhub: manual installation of kernel

If all your R libraries have been installed with a R version provided by Datarmor, you must manually install the R Kernel. To do so:

- Activate the JupyterHub environment of Datarmor: `conda activate jupyterhub`
- Load the R module of your choice, for instance `module load R/3.6.3-intel-cc-17.0.2.1`
- Open an R console by typing `R`. Then type:

  ```
  install.packages('IRkernel')
  IRkernel::installspec(name = 'my-r', displayname = 'My R')
  ```

- Leave the R console (`quit()`). You should have a new folder in `$HOME/.local/share/jupyter/kernels/my-r`.
- Type `echo $LD_LIBRARY_PATHS` and copy the output that is prompted in the Terminal.
- In the `my-r` folder, edit the `kernel.json` file and edit it by adding a `env` variable that contains the output of the `LD_LIBRARY_PATH`. It should look like this

```
{
  "argv": ["/appli/R/3.6.3-intel-cc-17.0.2.174/lib64/R/bin/R", "--slave", "
  "display_name": "R/3.6.3-intel-cc-17.0.2.174",
  "language": "R",
  "env": {"LD_LIBRARY_PATH": "..."}
}
```

- Restart your JupyterHub server. You should see your environment.

Datarmor acknowledgements

To acknowledge Datarmor on your publications, add the following lines to your paper:

The authors acknowledge the Pôle de Calcul et de Données Marines (PCDM, http://www.ifremer.fr/pcdm) for providing DATARMOR storage, data access, computational resources, visualization and support services.