## Conda

| conda info   | Verify Conda is installed, check version number.   |  |
|--|--|--|
| conda update conda                                     | Update conda package and environment manager to current version.                               |  |
| conda list   | List linked packages in a conda environment.   |  |
| conda createname ENVNAME python=3.6<br>"PKG1>7.6" PKG2 | Create a new environment named ENVNAME with specific version of Python and packages installed. |  |
| conda activate ENVNAME                                 | Activate the conda environment named ENVNAME.  |  |
| conda listname ENVNAME                                 | List all packages and versions in the environment named ENVNAME.                               |  |
| conda install PKGNAME==3.1.4                           | Install a package by exact version number (3.1.4).   |  |
| conda uninstall PKGNAMEname ENVNAME                    | Remove a package from an environment named ENVNAME.  |  |
| conda env exportname ENVNAME ><br>envname.yml          | Export an environment named ENVNAME to a YAML file.  |  |
| conda env createfile envname.yml                       | Create an environment from a YAML file.  |  |
| conda clean  | Remove unused packages and caches.   |  |
| conda deactivate                                       | Deactivate the current active conda environment.   |  |

### **DOCKER**

| docker search <myapp></myapp>   | Search for an image of <myapp> in dockerhub</myapp>                     |
|---|---|
| docker pull <imagedocker:1.0></imagedocker:1.0>   | Install the image "imageDocker" with version "1.0"                      |
| docker images   | List all images available   |
| docker inspect <imagedocker:1.0></imagedocker:1.0>  | Obtain a description of the image in JSON format                        |
| docker run <imagedocker:1.0> <mycommand></mycommand></imagedocker:1.0>  | Run the command of the application                                      |
| docker run -v <localpath:imagepath> <imagedocker:1.0> <mycommand></mycommand></imagedocker:1.0></localpath:imagepath> | Map a local volume to a volume in the image while running a command     |
| docker build -t <mydockerfile:1.0> <path dockerfile="" to=""></path></mydockerfile:1.0>                               | Create an image named "myDockerfile:1.0" from a file named "dockerfile" |
| docker ps -l  | List the containers (-I for the last container)                         |
| docker start <mycontainer></mycontainer>  | Restart a stopped container (it will be detached)                       |
|   |   |

## **DOCKER**

| docker stop myContainer                       | Stop the container "myContainer"                 |
|---|--|
| docker exec myContainer myCommand             | Run command in a running container               |
| docker commit myContainer myImage:1.0         | Create an image from a container                 |
| docker save mylmage:1.0 > path/savedImage.tar | Save an image into a file                        |
| docker load < path/savedImage.tar             | Load an image from a saved image file            |
| docker rm containerid                         | Removing one local container                     |
| docker rmi mylmage:1.0                        | Removing one local image                         |
| docker system prune                           | Clean stopped containers, residual images, cache |
|   |  |

#### **Snakemake**

| <pre>docker pull snakemake/snakemake conda create -n smk-env -c bioconda snakemake</pre>                         | Downloads and installs snakemake respectively within docker or conda (using bioconda)                                 |
|--|---|
| <pre>docker run -v \${PWD}:/data -w /data snakemake/snakemake conda activate smk-env module load snakemake</pre> | Activates snakemake environment within docker/conda/an HPC cluster respectively                                       |
| <pre>snakemakecores 1snakefile ex1_o1.smkuse-conda/envmodule/singularity</pre>                                   | Runs the pipeline described in ex1_o1.smk on 1 core within a conda/SLURM module/singularity environment               |
| <pre>snakemake -c1 -s ex1_o1.smkconfigfile myConfig.yml</pre>  | Runs the pipeline described in ex1_o1.smk on 1 core using a YAML config file containing parameters and paths to files |
| <pre>snakemakecores allsnakefile ex1_o1.smk</pre>  | Runs the pipeline described in ex1_o1.smk on all cores available  |
| <pre>snakemakecores 8snakefile ex1_o1.smk -R fastqc</pre>  | Redoes rule/step fastqc within the pipeline described in ex1_o1.smk on 8 cores  |
|  |   |

.smk files describe the pipeline with "rules": named descriptions of each step, including names of input and output files, and command lines to be launched. The first rule must describe the end files as input and the others can be written in any order provided the output files are exactly the same as the input files of the next rule/step in the pipeline. Rules will be recursively examined until the latest files are found, and the pipeline will be redone from there.

output:

input:

"FastQC/SRR3099585\_chr18\_fastqc.zip",
"FastQC/SRR3099585\_chr18\_fastqc.html"

"Data/SRR3099585\_chr18.fastq.gz"
shell: "fastqc --outdir FastQC/ {input}"



## Rmarkdown Notebook

| Rmarkdown documentation File: my_Rmarkdown_Notebook.Rmd   |                           |
|---|---------------------------|
| Header: yml format  | <br>key:value<br>         |
| Text: explanation (markdown formatted)  | # title<br>## subtitle    |
| Chunk: place for code (specify the language between {}) Add {r, eval=FALSE} to present code and not the result of its execution | ```{r}<br>i <- i+1<br>``` |

# Jupyter Notebook



| Jupyter documentation File: my_Jupyter_Notebook.ipynb | Nbviewer : static renderer for notebooks Binder : Jupyter + Docker |
|---|--|
| Header: ??  |  |
| Text:   |  |
| Cells: place for code                                 |  |

- Choose/create a folder for the content of the website (can be the root of the repository)

- Go to GitHub Settings ->
   Options -> paragraph GitHub

   Pages
- Choose the source (branch / folder) and save
- Choose the theme and select
- Create HTML/MD files for the content in the repository

- Fork the repository

- Create a branch in the forked repository
- Clone/edit the forked repository
- Push changes to the forked repository
- Pull request to the initial repository



- "Create a new release"

- Choose a tag, i.e.
   vMAJOR.MINOR.PATCH
- Choose a branch
- Provide a title and description
- (optional) attach binaries
- Click on Publish the release

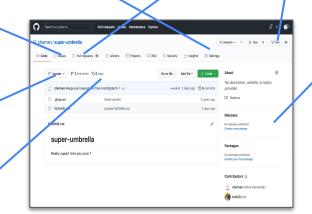
- Choose a Licence on GitHub

- Create a Zenodo account with GitHub identifiers
- Zenodo Settings -> GitHub tab
- Flip the switch for the repository to connect (adds a webhook on GitHub)
- Integrate the badge on GitHub (README)
- Any new release on GitHub will generate a DOI on Zenodo

To keep track of problems/bugs

- Created by users
- Created by yourself to communicate with users
- New branch : provide a new name
- Switch branch : select an existing branch

Add a label to the repository in a specific status at a given time



request

Fork

cenodo

Se

elea