JUPYTERLAB -SUPERCOMPUTING IN YOUR BROWSER

Training course "Introduction to the usage and programming of supercomputer resources in Jülich"

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Member of the Helmholtz Association

JÜLICH
Forschungszentrum

MOTIVATION

your thinking, your reasoning, your insides, your ideas

“It is all about using and building a machinery **interface** **between** computational researchers and data, supercomputers, laptops, cloud **and** your thinking, your reasoning, your insides, your ideas about a problem.”

Fernando Perez, Berkely Institute for Data Science
Founder of Project Jupyter

https://jupyter.org

MOTIVATION

Rise of Jupyter´s popularity

If popularity can be counted by

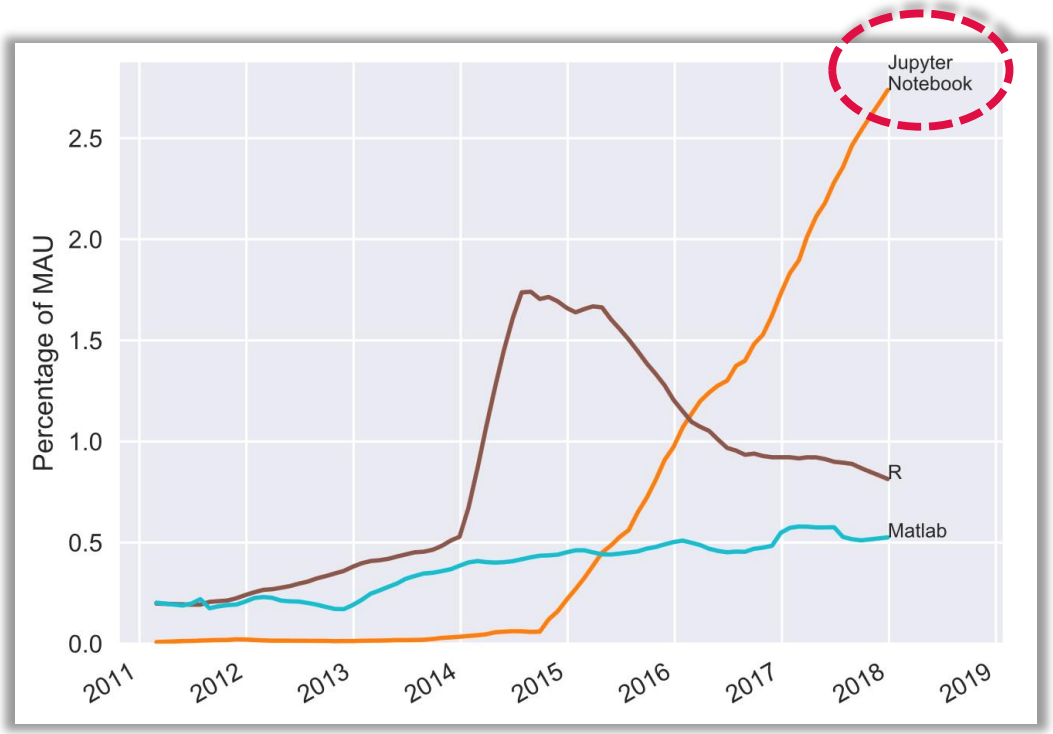
- Monthly aggregated number of user interactions with GitHub repos (= Monthly Active Users (MAU))

and

- Each repository is assigned to a single language
  (by looking at which language has the most bytes in the repo)

Jupyter Notebooks have seen significant and steady growth over the last years (still rising).

- Of course the popularity of Python in general is pushing this trend.



https://www.benfrederickson.com/ranking-programming-languages-by-github-users/
https://github.com/benfred/github-analysis

TERMINOLOGY

What is JupyterLab

JupyterLab

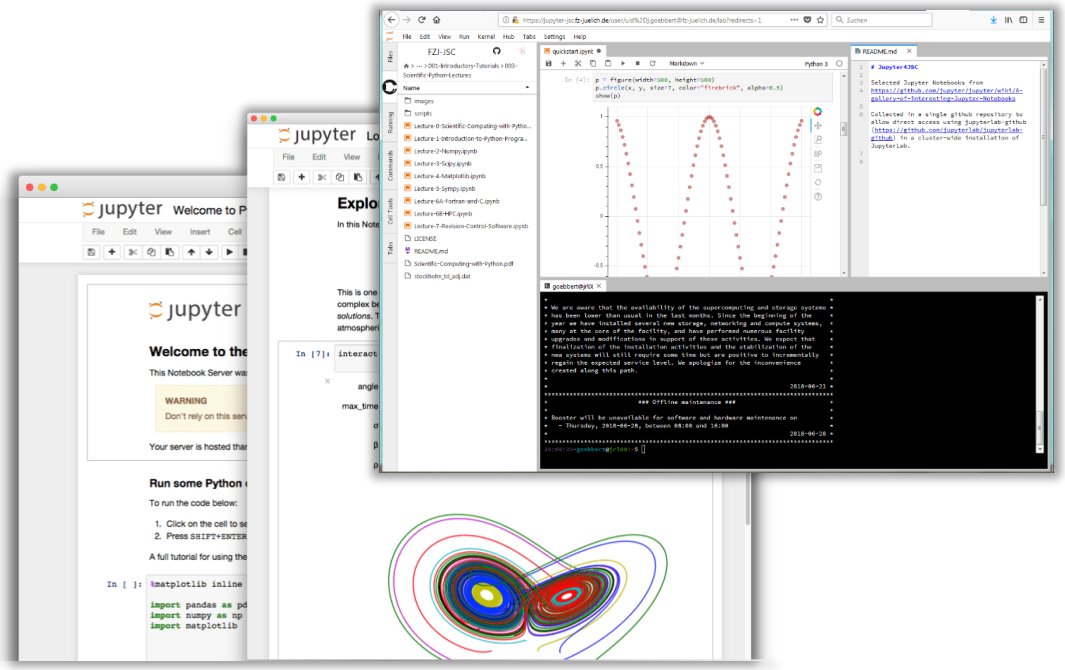
- **Interactive** working environment in the web browser
- For the creation of **reproducible** computer-aided narratives
- Very **popular** with researchers from all fields
- Jupyter = Julia + Python + R

Multi-purpose working environment

- Language agnostic
- Supports execution environments (“*kernels*”)
  - For dozens of languages: Python, R, Julia, C++, ...
- Extensible software design („*extensions*“)
  - many server/client plug-ins available
  - Eg. in-browser-terminal and file-browsing

Document-Centered Computing (“*notebooks*”)

- Combines code execution,
  rich text, math, plots and rich media.
- All-in-one document called Jupyter Notebook



https://jupyterlab.readthedocs.io

TERMINOLOGY

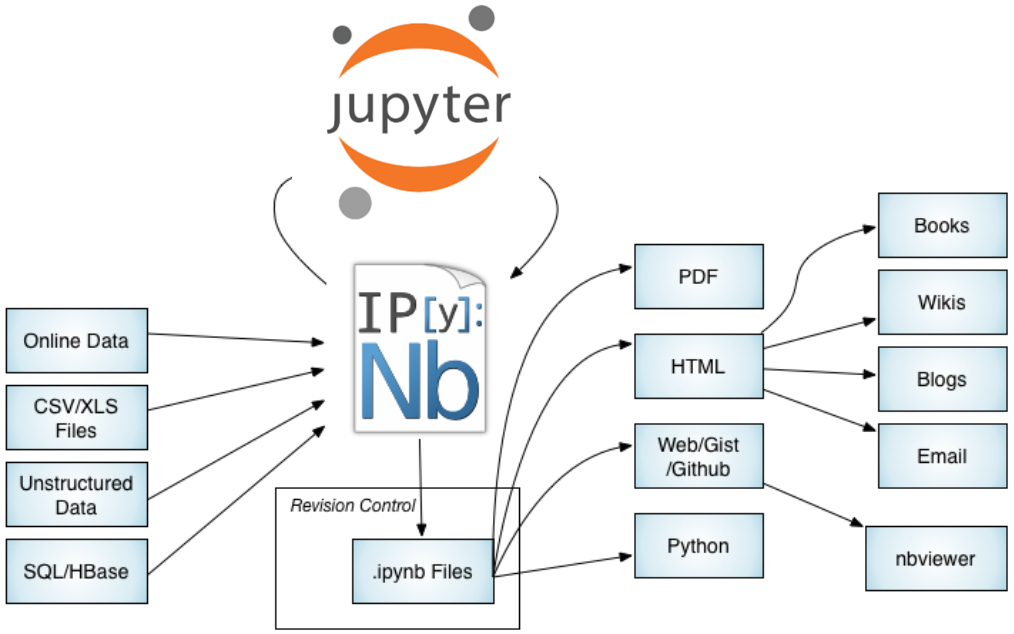
What is a Jupyter Notebook?

Jupyter Notebook
A notebook document (file extension .ipynb)
is a document that can be rendered in a web browser

- It is a file, which stores your work in JSON format
- Based on a set of open standards for interactive computing

- Allows development of custom applications with embedded interactive computing.
- Can be extended by third parties

- Directly convertible to PDF, HTML, LateX ...
- Supported by many applications
  such as GitHub, GitLab, etc..



https://jupyter-notebook.readthedocs.io/
https://github.com/jupyter/jupyter/wiki/A-gallery-of-interesting-Jupyter-Notebooks

TERMINOLOGY

What is a Jupyter Kernel?

Jupyter Kernel
A “kernel” refers to the separate process
which executes code cells within a Jupyter notebook.

Jupyter Kernel

- **run code** in different programming languages and environments.
- can be **connected to** a notebook (one at a time).
- **communicates** via ZeroMQ with the JupyterLab.

- Multiple **preinstalled** Jupyter Kernels can be found on our clusters
  - Python, R, Julia, Bash, C++, Ruby, JavaScript
  - Specialized kernels for visualization, quantumcomputing

- You can easily **create your own kernel** which for example runs your specialized virtual Python environment.

https://jupyter-notebook.readthedocs.io/
https://github.com/jupyter/jupyter/wiki/Jupyter-kernels
https://zeromq.org

TERMINOLOGY

What is a JupyterLab Extension?

JupyterLab Extension

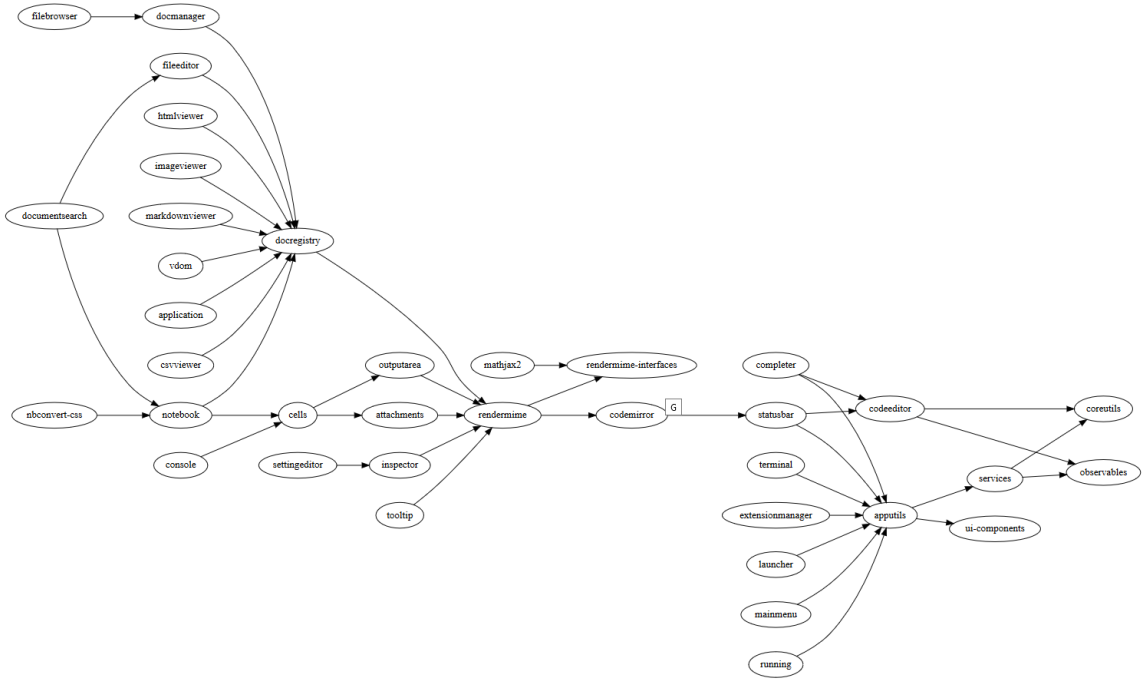
JupyterLab extensions can customize or enhance any part of JupyterLab.

JupyterLab Extensions

- provide new file viewers, editors, themes
- provide renderers for rich outputs in notebooks
- add items to the menu or command palette
- add keyboard shortcuts
- add settings in the settings system.

- Extensions can even provide an API for other extensions to use and can depend on other extensions.

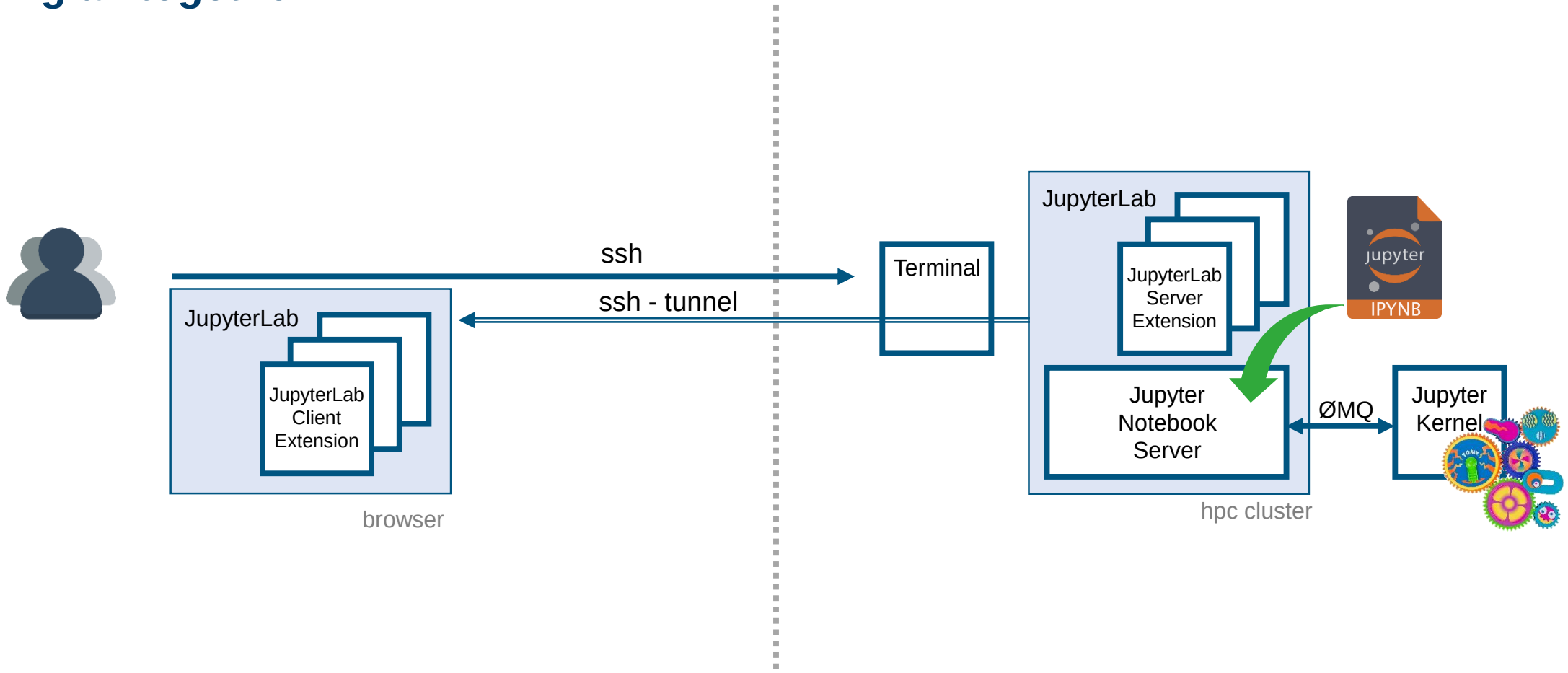
The whole JupyterLab itself is simply a **collection of extensions** that are no more powerful or privileged than any custom extension.



https://jupyterlab.readthedocs.io/en/stable/user/extensions.html
https://github.com/topics/jupyterlab-extension

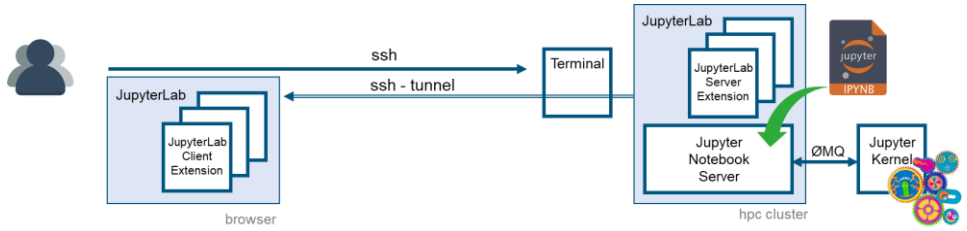
TERMINOLOGY

Bringing all together



JUPYTER – START & TUNNEL

Start your JupyterLab (the hard way)



Start Jupyter on the login node

```
Lnode:> module purge
Lnode:> module use $OTHERSTAGES
Lnode:> module load Stages/Devel-2019a
Lnode:> module load GCC/8.3.0
Lnode:> module load JupyterCollection/2019a.2.4

Lnode:> cd $PROJECT_<my_project>
Lnode:> jupyter lab
```

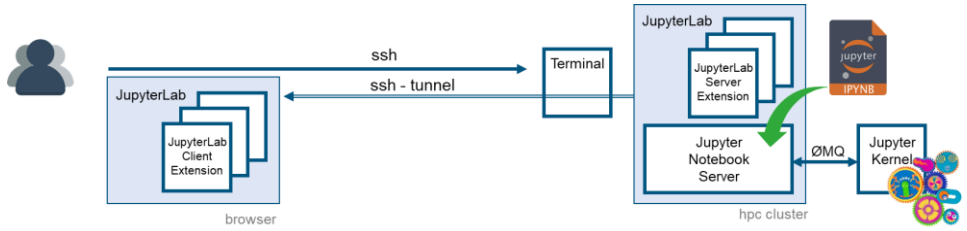
JupyterCollection is a meta-module, which loads the modules:

- JupyterKernel-Bash/0.7.1-2019a.2.4
- JupyterKernel-Cling/0.6-2019a.2.4
- JupyterKernel-JavaScript/5.2.0-2019a.2.4
- JupyterKernel-Julia/1.3.1-2019a.2.4
- JupyterKernel-Octave/5.1.0-2019a.2.4
- JupyterKernel-PyParaView/5.8.0-2019a.2.4
- JupyterKernel-PyQuantum/1.0-2019a.2.4
- JupyterKernel-R/3.5.3-2019a.2.4
- JupyterKernel-Ruby/2.6.3-2019a.2.4
- Jupyter/2019a.2.4-Python-3.6.8

```
[I 20:44:05.916 NotebookApp] Writing notebook server cookie secret to
/run/user/12885/jupyter/notebook_cookie_secret
[…]
Copy/paste this URL into your browser when you connect for the first time, to
login with a token:
http://localhost:8888/?token=7f1f8d7d9414a8b72j2e2cc2c2866c29fb557677e9a08042
```

JUPYTER – START & TUNNEL

Start your JupyterLab (the hard way)




```
[I 20:44:05.916 NotebookApp] Writing notebook server cookie secret to
/run/user/12885/jupyter/notebook_cookie_secret
[…]
Copy/paste this URL into your browser when you connect for the first
time, to login with a token:
http://localhost:8888/?token=7f1f8d7d9414a8b72j2e2cc2c2866c29fb557677e9a
08042
```

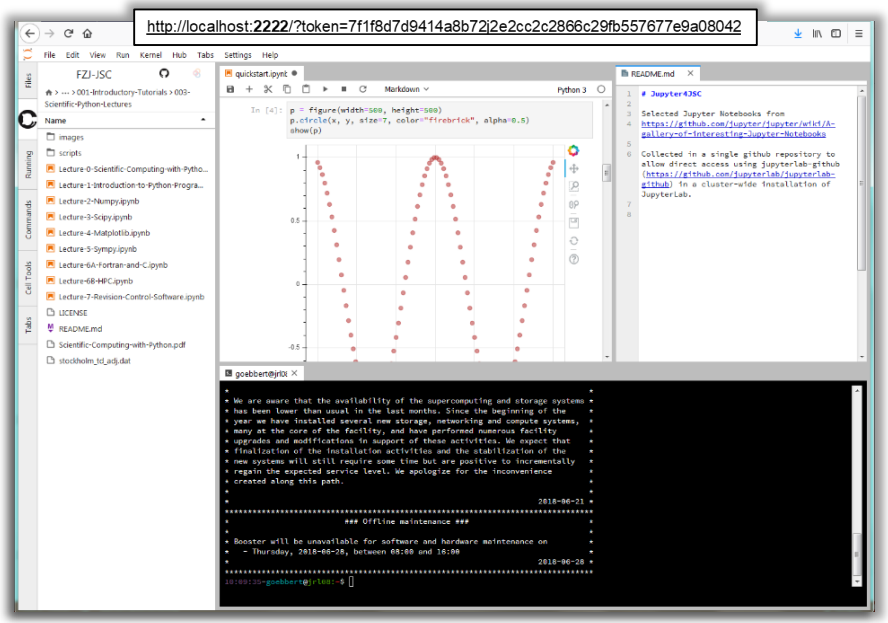
Tunnel Jupyter port to workstation

```
Wrkst:> ssh -4 -N -L 2222:localhost:<jupyter-port> \
                   <username>@juwels<no>.fz-juelich.de
```

Open Jupyter in the local browser

```
Wrkst-Browser:>
```

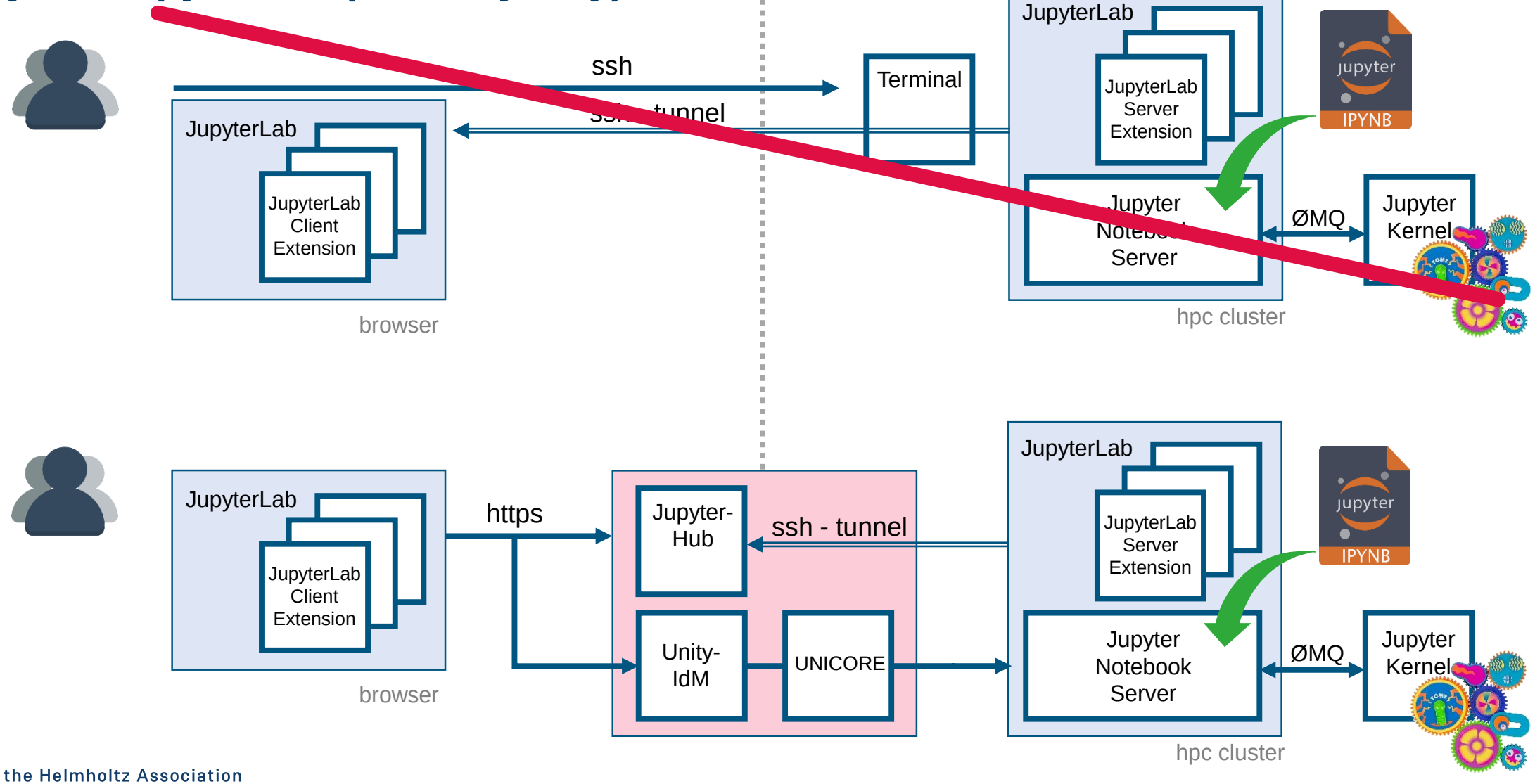
http://localhost:**2222**/?token=7f1f8d7d9414a8b72j2e2cc2c2866c29fb557677e9a08042



- You will see the view on the filesystem **from working directory** of the jupyter command.
- You can only enter sub-directories – you **CANNOT** enter any directory above.
  Please add **softlinks** to directories like $PROJECT, $SCRATCH, etc.

JUPYTER-JSC WEBSERVICE

Start your JupyterLab (the easy way)



JUPYTER-JSC WEBSERVICE

Start your JupyterLab (the easy way)

JupyterHub
is used to make Jupyter available to a group of HPC users.

- Creates/manages JupyterLabs for single users.
- Connects JupyterLabs to users via a configurable HTTP proxy.

- Supports custom spawners
  - UNICORE at JSC
- Supports custom authenticators
  - Unity-IdM at JSC

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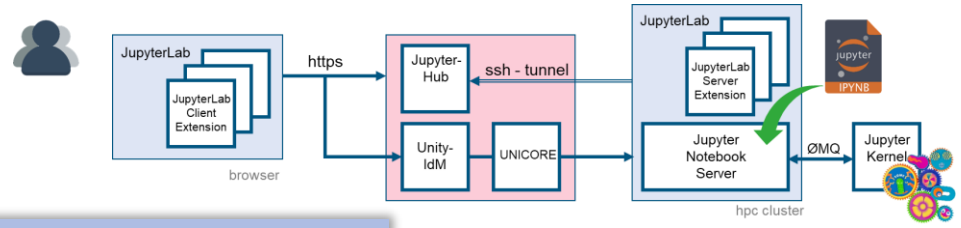
JUPYTER-JSC WEBSERVICE

First time login

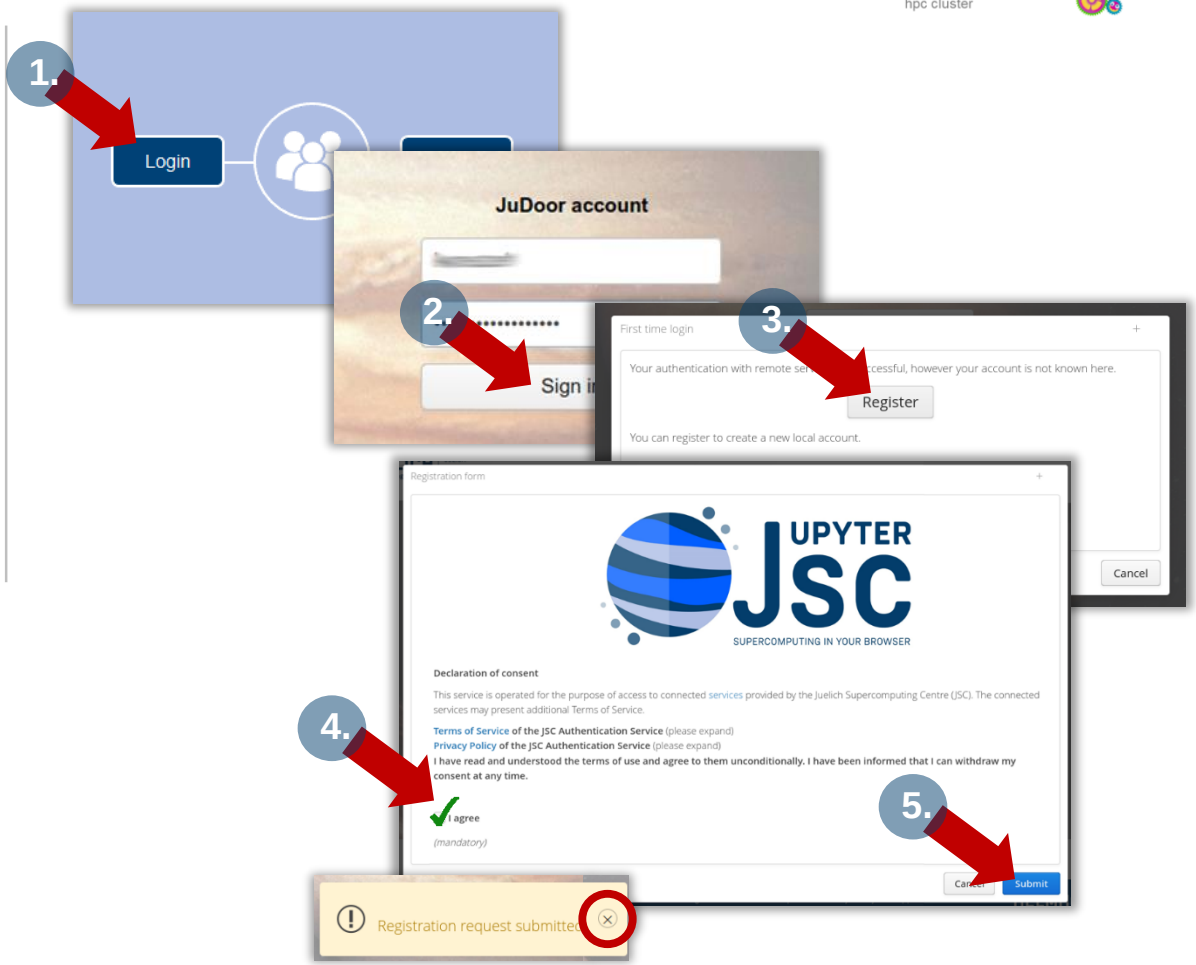


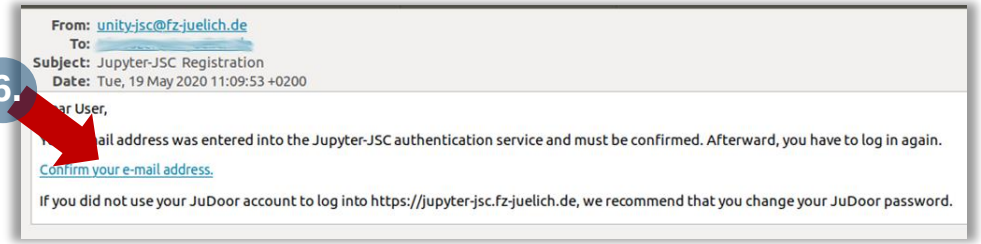
=> https://jupyter-jsc.fz-juelich.de

Jupyter-JSC first time login

- Requirements:
  - Registered at **judoor.fz-juelich.de**
    - **(with "Connected Services" = jupyter-jsc)**

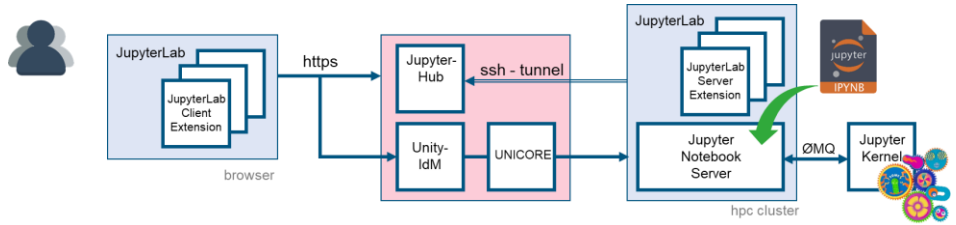
1. Login at jupyter-jsc.fz-juelich.de
2. Sign in with your JSC account
3. Register to Jupyter-JSC
4. **Accept usage agreement**
5. Submit the registration
6. Wait for email and confirm your email address





JUPYTER-JSC WEBSERVICE

Control Panel



A. Jupyter-JSC – Add new JupyterLab

- Name your new JupyterLab configuration
  - Unique Jupyter workspace in `~/.jupyter`
- => the **JupyterLab Options** page will open

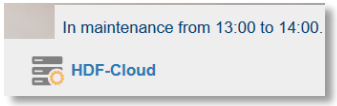
B. Jupyter-JSC – Actions

If a configuration has been added

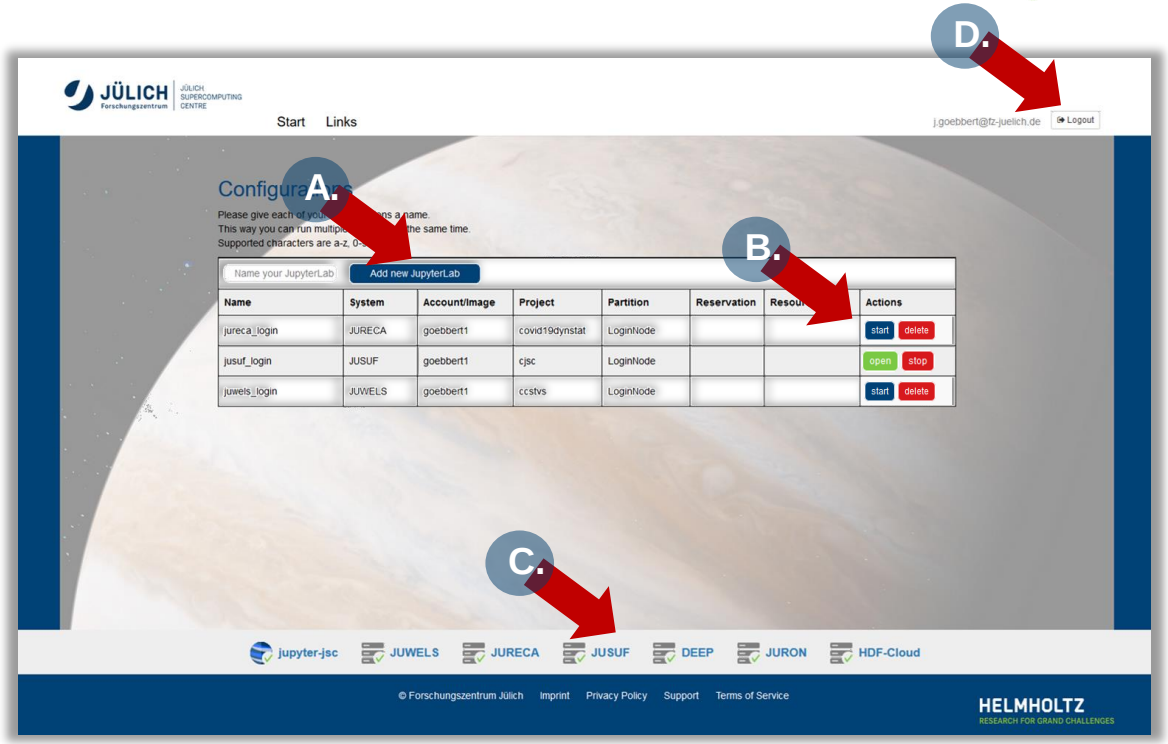
- Start/delete the named configuration (workspace will not be deleted)
- Open/stop a **running** JupyterLab

C. Jupyter-JSC -- Statusbar

- Upcoming maintenance (mouse hover for details)

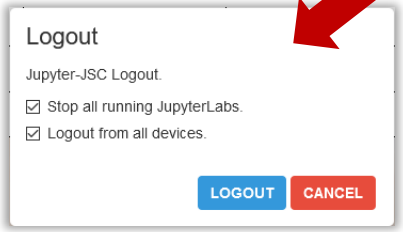


- System offline



B. Jupyter-JSC – Logout

Logout will ask what you want to do with the running JupyterLabs – be careful what you answer!



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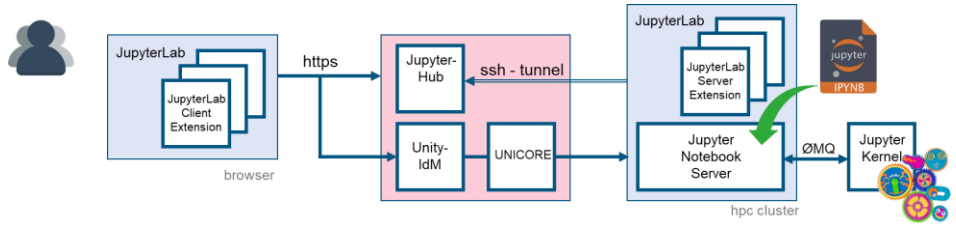
JUPYTER-JSC WEBSERVICE

JupyterLab Options



Jupyter-JSC – Options

Available options **depend on**

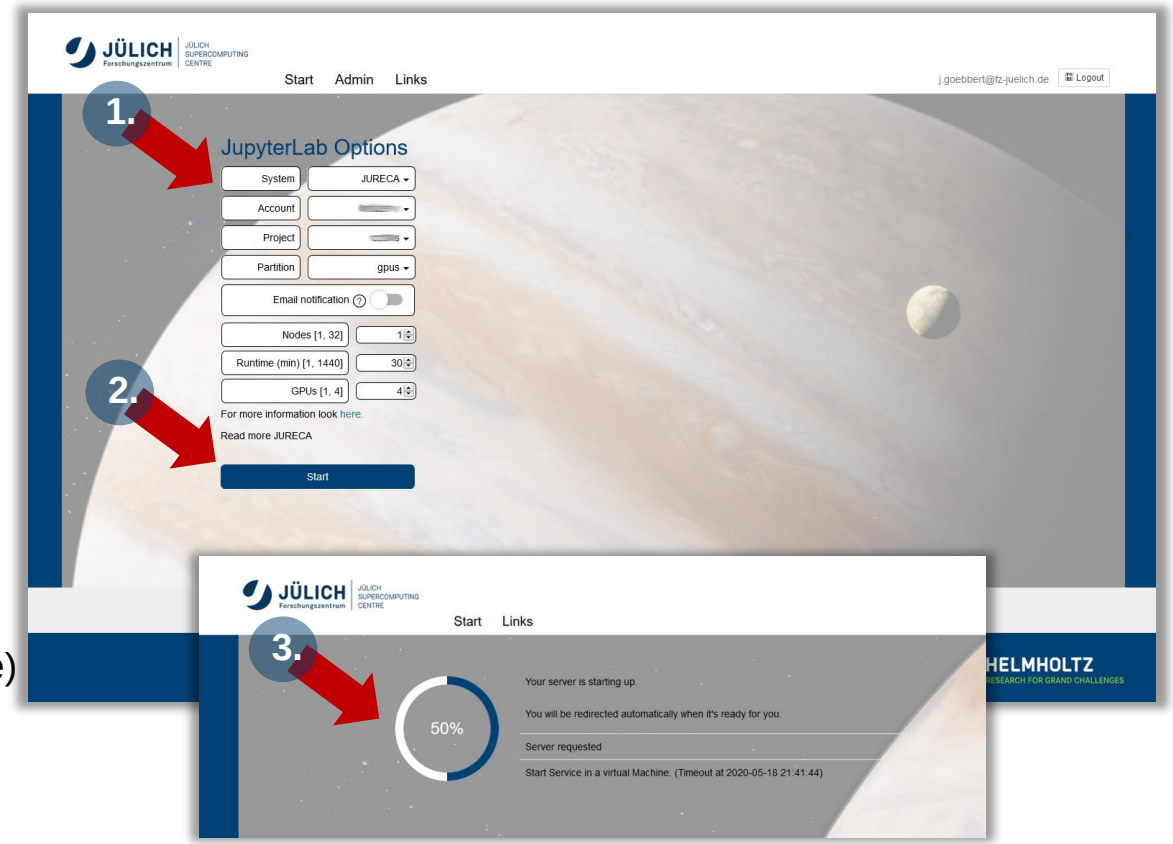
- user account settings visible in **judoor.fz-juelich.de**
- currently available systems in all of your projects
  - system specific usage agreement on JuDoor is signed

Basic options

- System:
  JUWELS, JURECA, JUSUF, DEEP, HDFML, HDF-Cloud
- Account:
  In general users only have a single account
- Project:
  project which have access to the selected system
- Partition:
  partition which are accessible by the project
  (this includes the decision for LoginNode and ComputeNode)
- Email notification:
  Send an email when the JupyterLab has started
  (useful if the JupyterLab starts on a compute node)

Extra options

- Partition == compute Nodes, Runtime, GPUs, …
- System == HDF-Cloud Image



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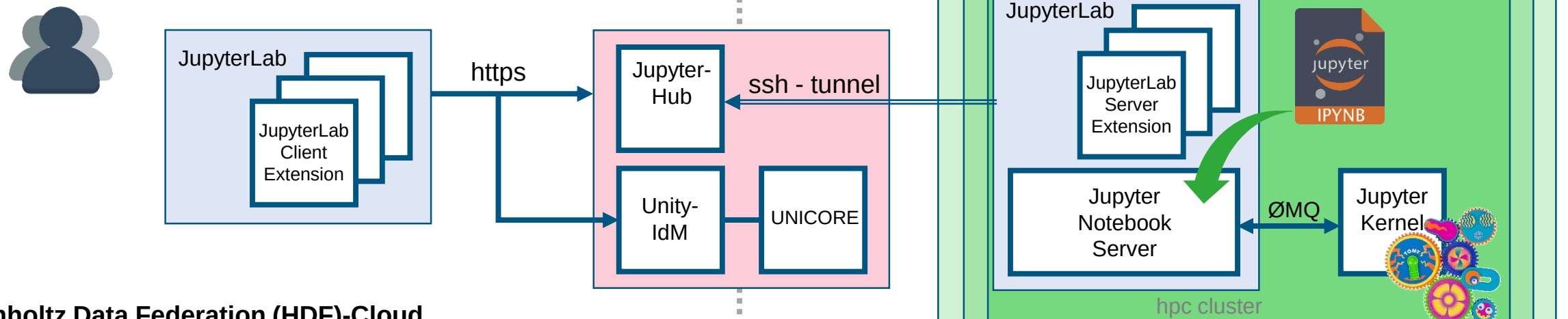
JUPYTER-JSC WEBSERVICE

System: HDF-Cloud



Helmholtz Data Federation (HDF)-Cloud

Any user having

- a JSC account **(judoor.fz-juelich.de)**
- the Connected Service “jupyter-jsc” enabled (default for HPC accounts)

can start

- Jupyter-JSC container images (containing JupyterLab) on the HDF-Cloud
  - **“base-notebook”** – close to the installation on the clusters
  - The Core Images of the Jupyter Docker Stacks
    - https://jupyter-docker-stacks.readthedocs.io
    - https://github.com/jupyter/docker-stacks

https://www.fz-juelich.de/ias/jsc/EN/Expertise/SciCloudServices/HDFCloud/_node.html

JUPYTER-JSC WEBSERVICE

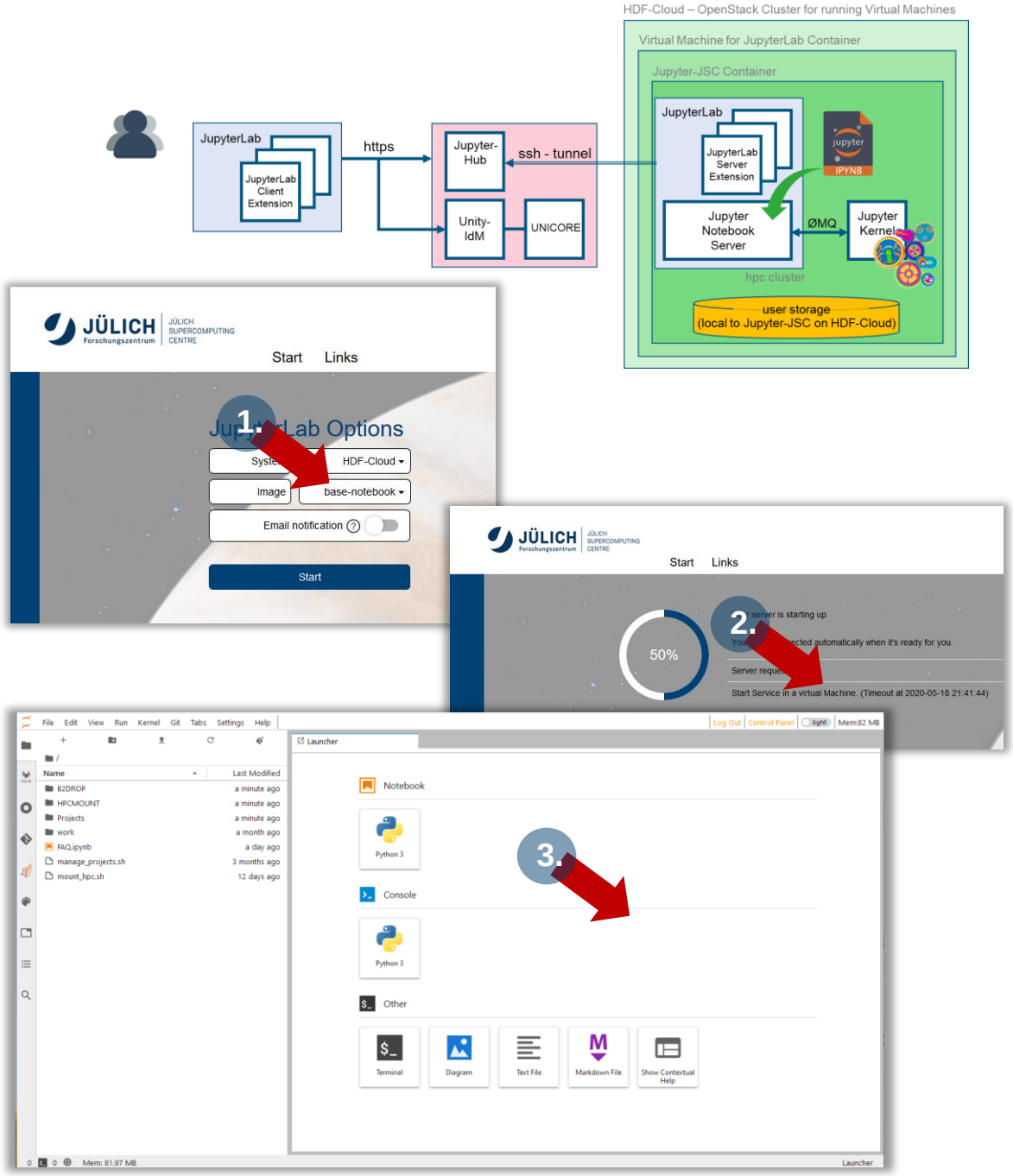
System: HDF-Cloud

Start JupyterLab on HDF-Cloud

- Requirements:
  - Registered JSC account at judoor.fz-juelich.de
  - Logined in to Jupyter-JSC at jupyter-jsc.fz-juelich.de
  - Named a new JupyterLab configuration

- Start a JupyterLab:
  - System == “HDF-Cloud”
  - Select Image == “base-notebook”
  - Click “Start”
  - Wait for JupyterLab to be started

JupyterLab is running in a container on the HDF-Cloud

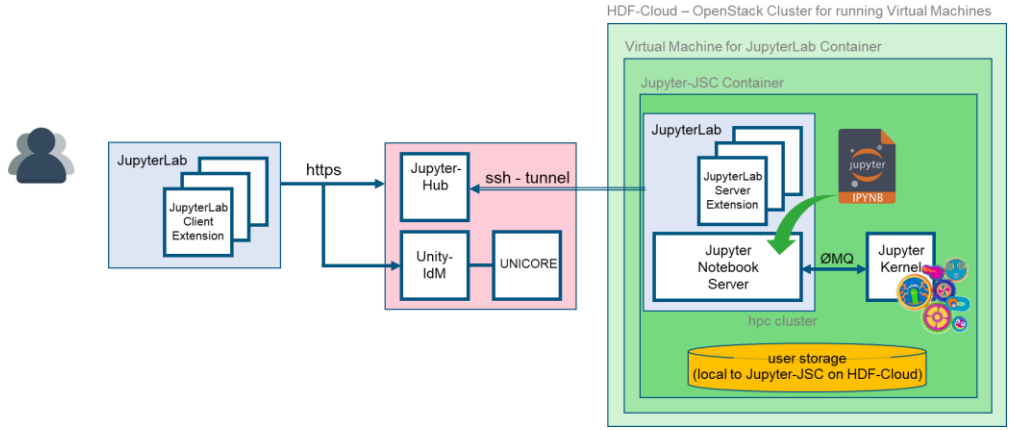


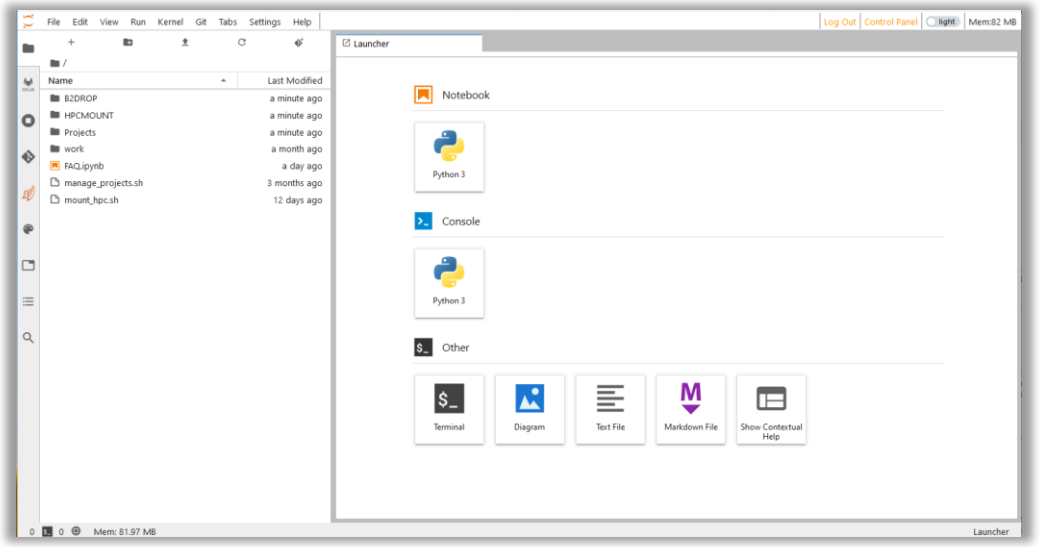
JUPYTER-JSC WEBSERVICE

System: HDF-Cloud

Limitations on JupyterLab on HDF-Cloud

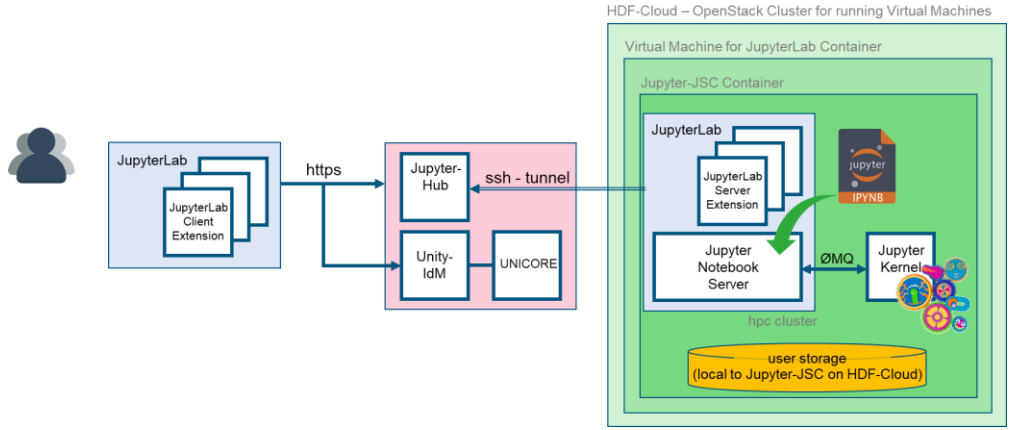
- max. **2 GB** memory
- Installed Jupyter Kernel limited
- Storage in Jupyter-JSC container
  - **is local** to the HDF-Cloud
  - only accessible from a Jupyter-JSC container
  - stored persistently in a personal data container if in
    - `~/work` (max. 10 GB)
    - `~/Projects` (max. 10 GB)
  - backup of ~/work and ~/Projects every day to tape
- Depending on the load of the OpenStack you might be limited in the **number of** simultaneous running JupyterLab containers
- HDF-Cloud has at the moment **no GPUs**





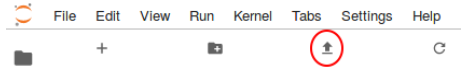
JUPYTER-JSC WEBSERVICE

System: HDF-Cloud



How can I share/backup my work from JupyterLab?

1. Download the file

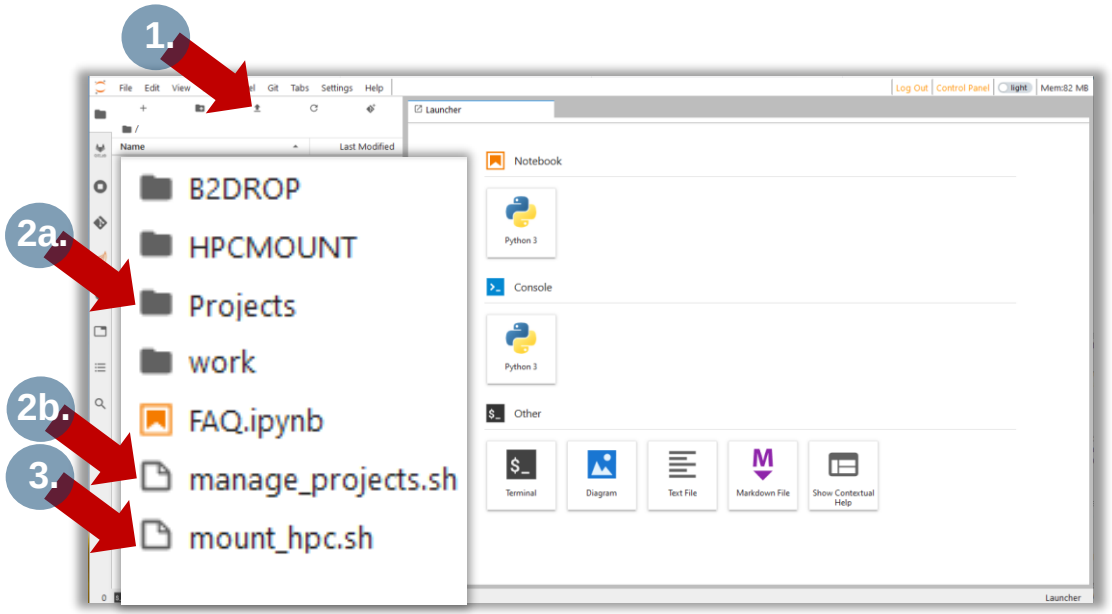


2. `~/Projects`
   for sharing data between JupyterLab-users on HDF-Cloud
3. Mount your HPC cluster directory with sshfs

- B2Drop – https://b2drop.eudat.eu
- Git / GitHub / GitLab

NEVER forget:

- Data is **ONLY** persistent in `~/Projects` and `~/work`

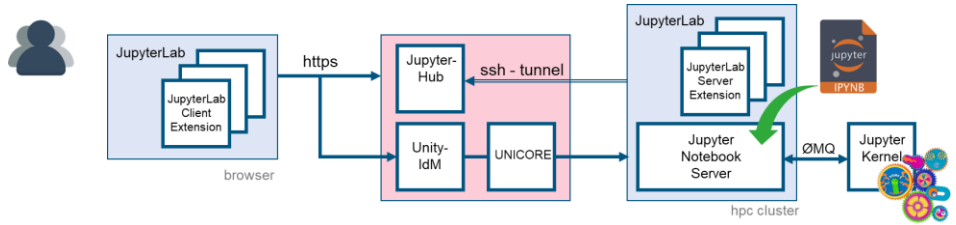


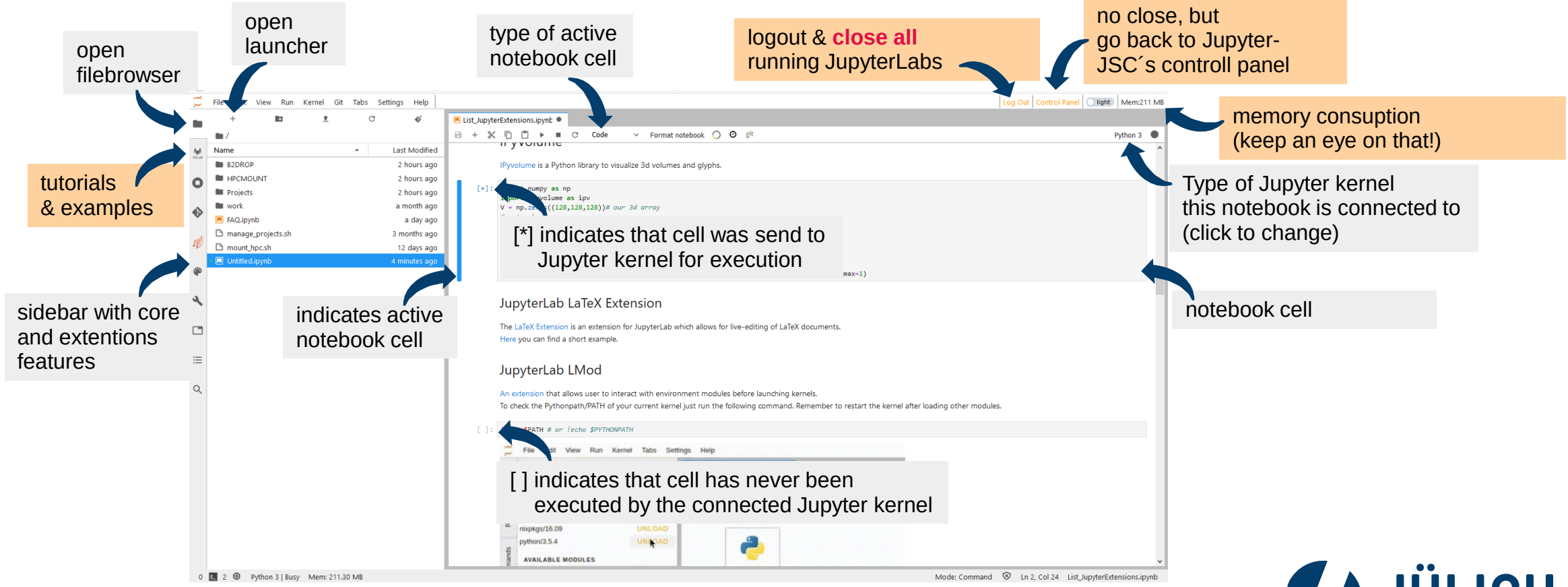
For more details please visit:

https://gitlab.version.fz-juelich.de/jupyter4jsc/j4j_notebooks/-/blob/master/FAQ_HDFCloud.ipynb

JUPYTER-JSC WEBSERVICE

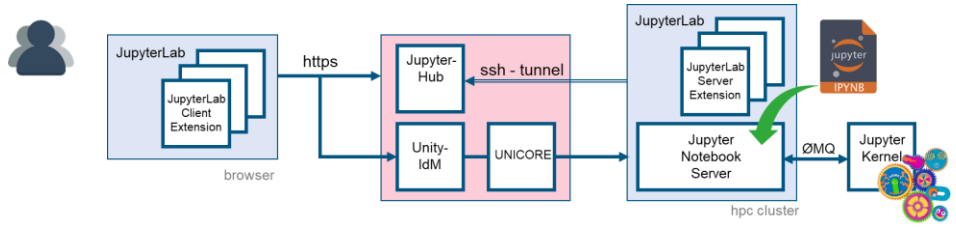
Some comments about the UI





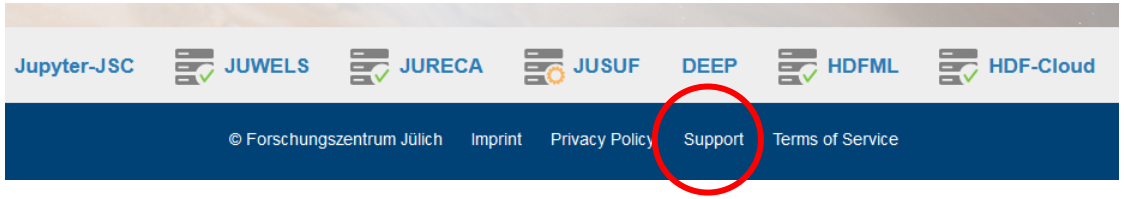
JUPYTER-JSC SECRETS

Very important to know



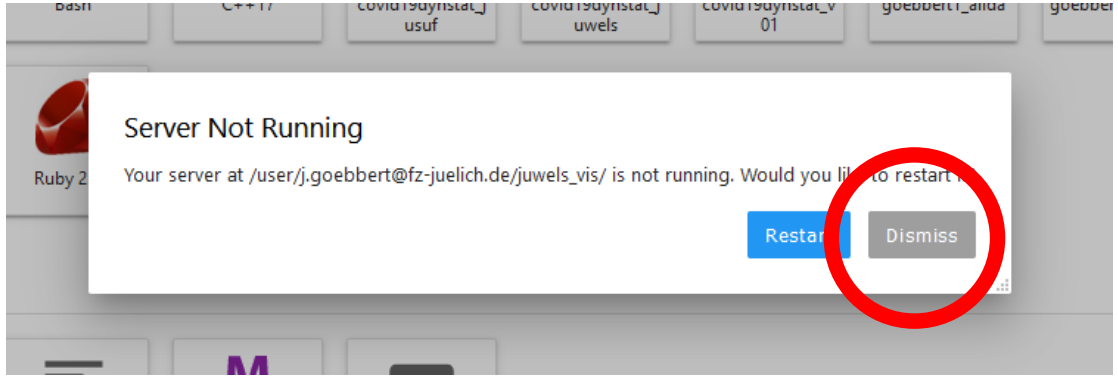
Secret 1: Support button

- Let us know, if something does not work.
  We can only fix it, if we know it.



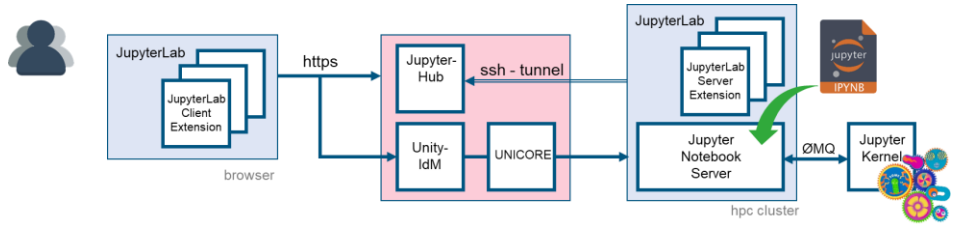
Secret 2: Reload on connection loss

- "Server Not Running" means, that your browser just lost connection => **Just hit "Dismiss" !!!**
- You can safely hit the "Reload" button of your browser, if the connection to JupyterLab ever gets lost.
  (but that takes more time)



JUPYTER-JSC SECRETS

For experts only ☺



Secret 3: Jupyter-JSC logs

- Jupyter-Lab gets started by UNICORE on our HPC systems
- On startup UNICORE created the directory `$SCRATCH_<project>/unicore-jobs/<random-hash>/`
  - In the terminal of a running JupyterLab, this directory is `$JUPYTER_LOG_DIR`
- In this directory you find
  - `stdout` -> terminal output of jupyterlab messages
  - `stderr` -> terminal output of jupyterlab error messages
  - `.start` -> details how your JupyterLab got started

Secret 4: change to a different JupyterLab version

- In .start you can see, that
  - `$HOME/.jupyter/start_jupyter-jsc.sh`

  is used to load JupyterLab if available.

Here you can switch to an older/newer/other version of JupyterLab,
if the new one gives you trouble

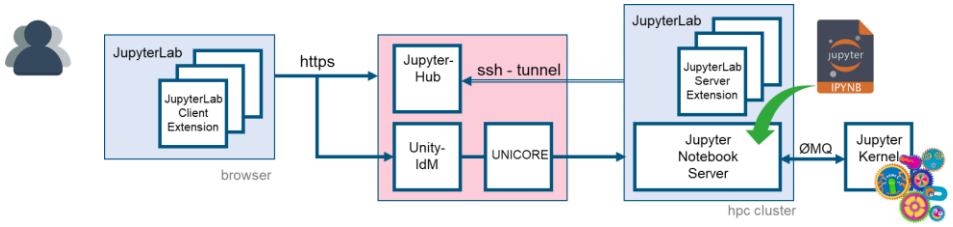
```
#!/bin/bash

module purge
module use $OTHERSTAGES
module load Stages/Devel-2019a
module load GCC/8.3.0
module load JupyterCollection/2019a.2.3
```

Switch to a different JupyterLab with
`$HOME/.jupyter/start_jupyter-jsc.sh`

JUPYTERLAB EXTENSIONS

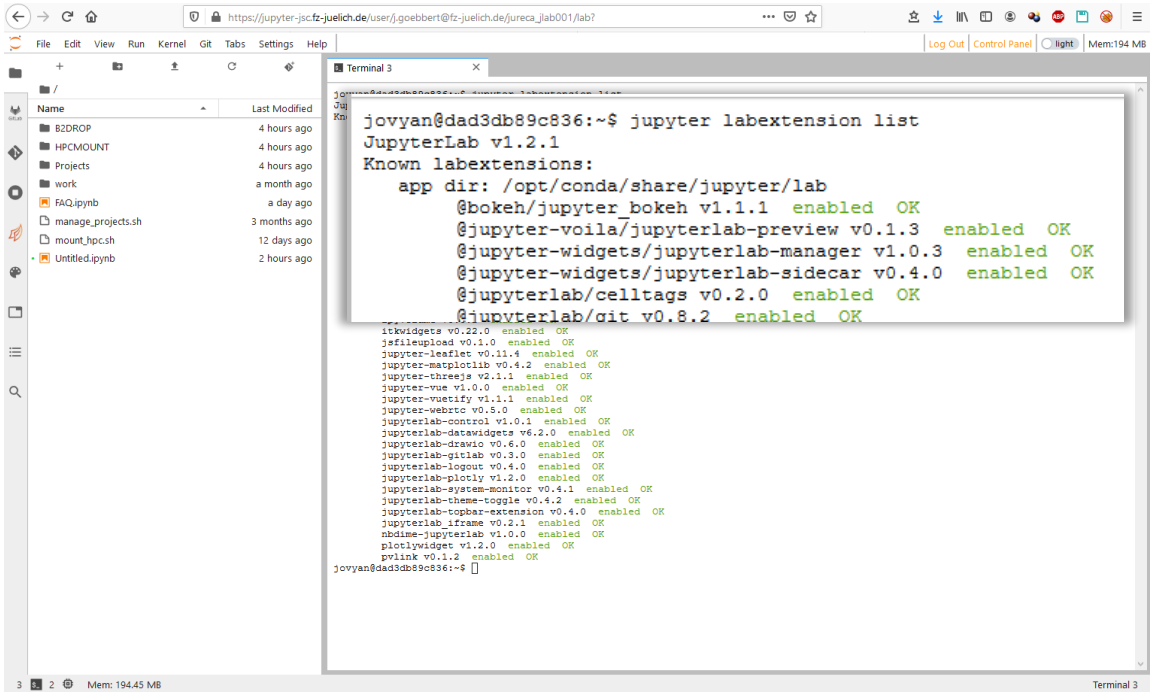
JUPYTER EXTENSIONS

Some general information



List the installed JupyterLab extensions

- Open the Launcher
- Start a Terminal
- Run command `jupyter labextension list`



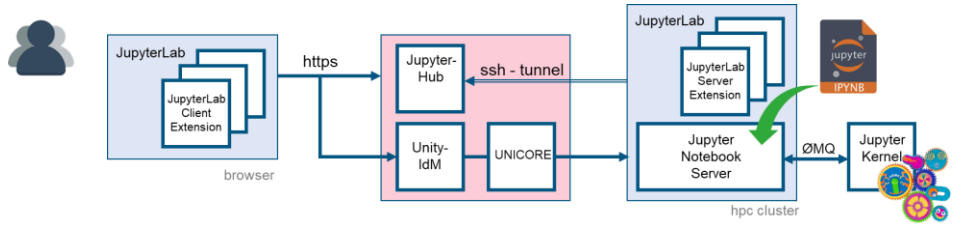
Extensions are installed in JupyterLab´s Application Directory, which

- stores any information that JupyterLab persists
  - including settings and built assets of extensions
- default location is `<sys-prefix>/share/jupyter/lab`
- can be relocated by setting $JUPYTERLAB_DIR
- is immutable
  - **any change requires a rebuild** of the whole JupyterLab to take effect!
  - contains the JupyterLab static assets
    - (e.g. `static/index.html`)

https://jupyterlab.readthedocs.io/en/stable/user/extensions.html

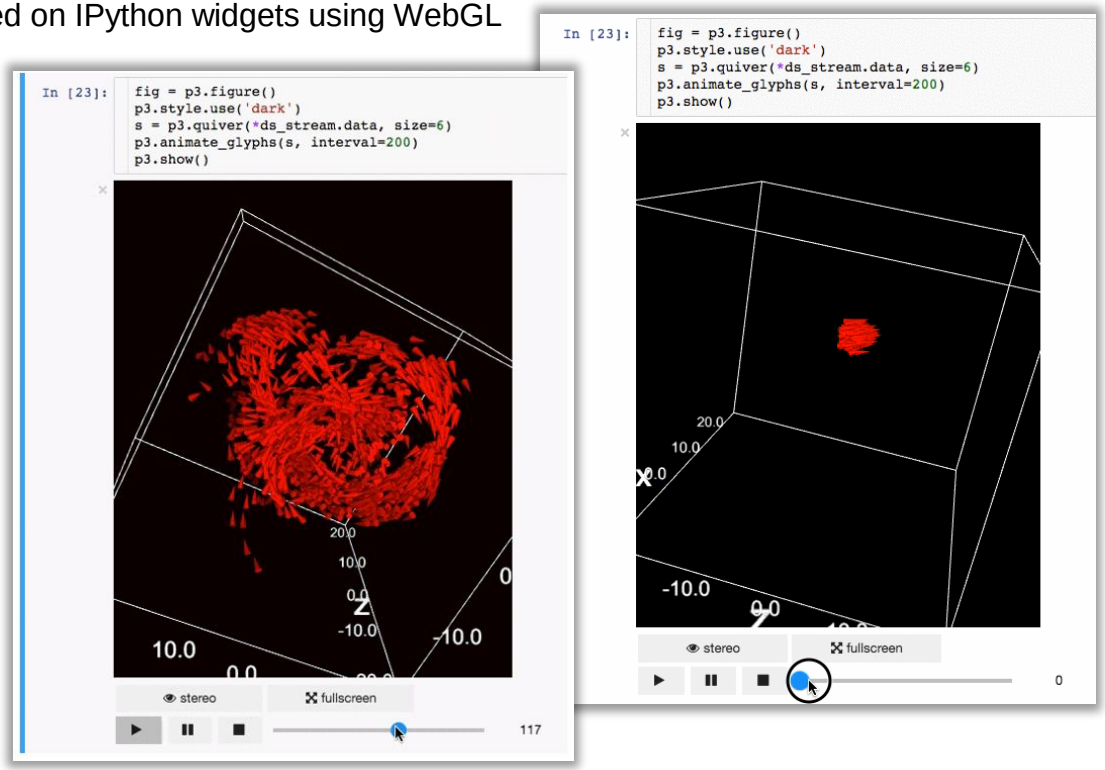
JUPYTER-JSC EXTENSIONS

Installed by default



IPyVolume

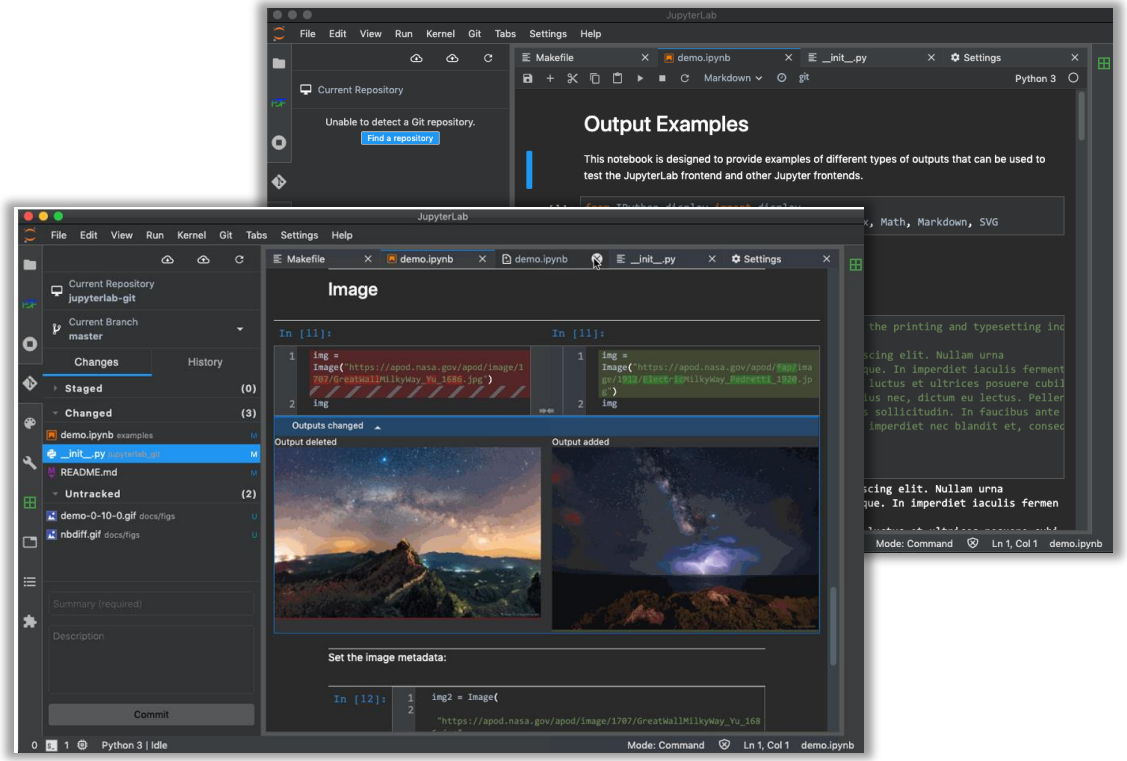
3d plotting for Python in the Jupyter notebook based on IPython widgets using WebGL



https://github.com/maartenbreddels/ipyvolume

JupyterLab-Git

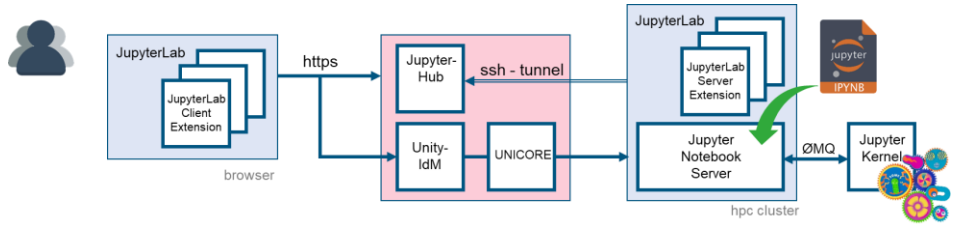
JupyterLab extension for version control using Git



https://github.com/jupyterlab/jupyterlab-git

JUPYTER-JSC EXTENSIONS

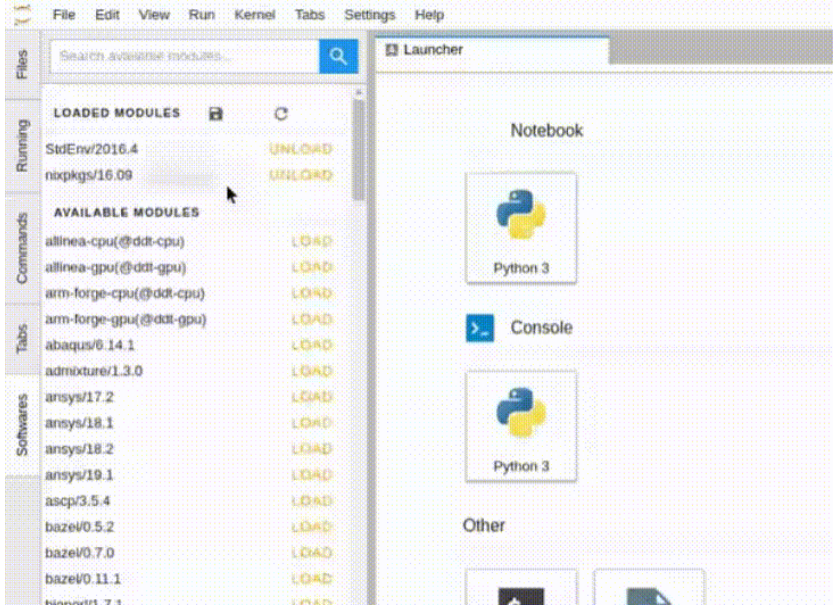
Installed by default



JupyterLab-Lmod

JupyterLab extension that allows user to interact with environment modules before launching kernels.

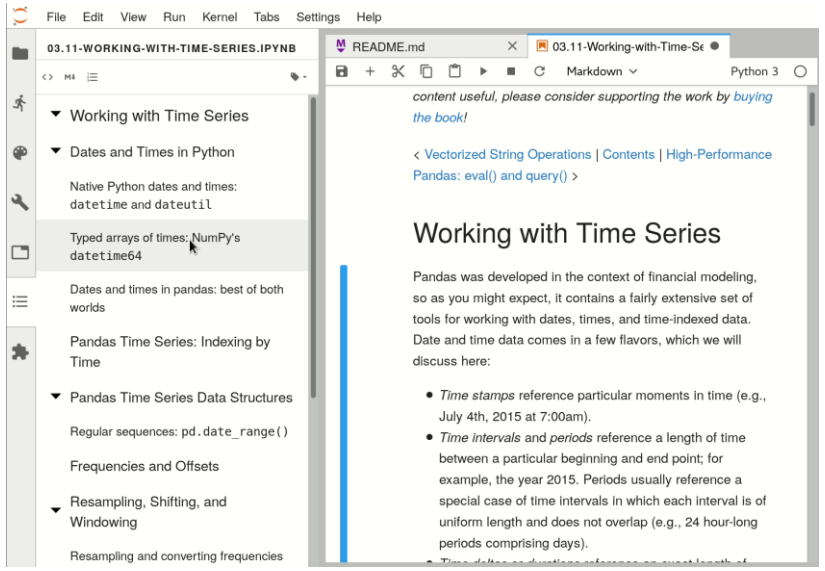
- **Remember** to restart the kernel after loading other modules.



https://github.com/cmd-ntrf/jupyter-lmod

JupyterLab-toc

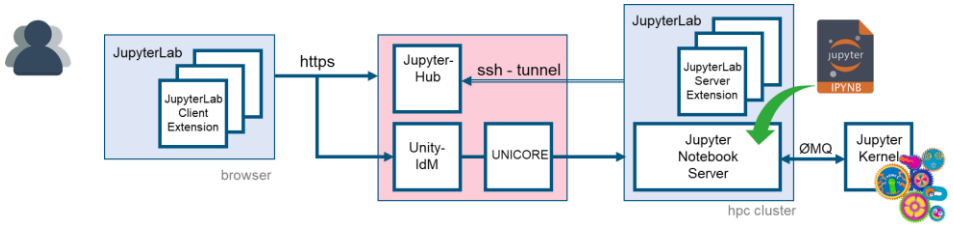
A Table of Contents extension for JupyterLab.
This auto-generates a table of contents in the left area when you have a notebook or markdown document open.The entries are clickable, and scroll the document to the heading in question.



https://github.com/jupyterlab/jupyterlab-toc

JUPYTER-JSC EXTENSIONS

Installed by default



PyThreeJS

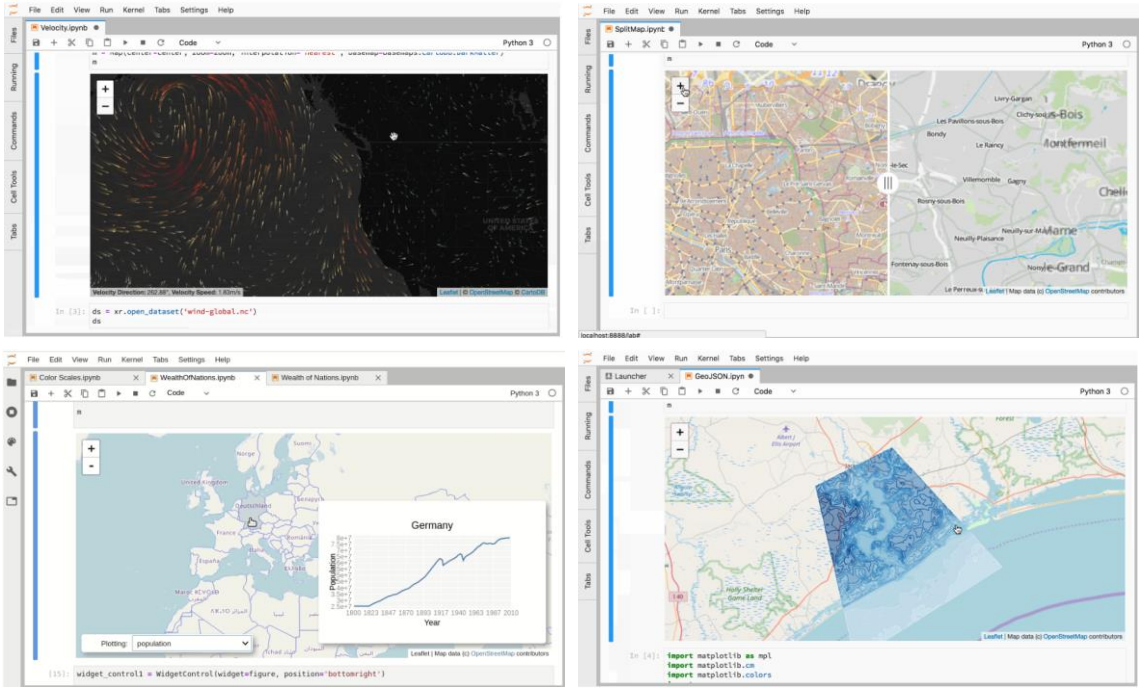
A Python / ThreeJS bridge utilizing the Jupyter widget infrastructure.
https://threejs.org - lightweight, 3D library with a default WebGL renderer.

```
In [9]: f = """
function f(origu,origv) {
    // scale u and v to the ranges I want: [0, 2*pi]
    var u = 2*Math.PI*origu;
    var v = 2*Math.PI*origv;

    var x = Math.sin(u);
    var y = Math.cos(v);
    var z = Math.cos(u+v);

    return new THREE.Vector3(x,y,z)
}
"""
surf_g = ParametricGeometry(func=f);

surf = Mesh(geometry=surf_g, material=LambertMaterial(color='green', side='FrontSide'))
surf2 = Mesh(geometry=surf_g, material=LambertMaterial(color='yellow', side='BackSide'))
scene = Scene(children=[surf, surf2, AmbientLight(color='#777777')])
c = PerspectiveCamera(position=[5, 5, 3], up=[0, 0, 1],
                      children=[DirectionalLight(color='white',
                                                 position=[3, 5, 1],
                                                 intensity=0.6)])
renderer = Renderer(camera=c, scene=scene, controls=[OrbitControls(controlling=c)])
display(renderer)
```

https://github.com/jupyter-widgets/pythreejs

IPyLeaflet

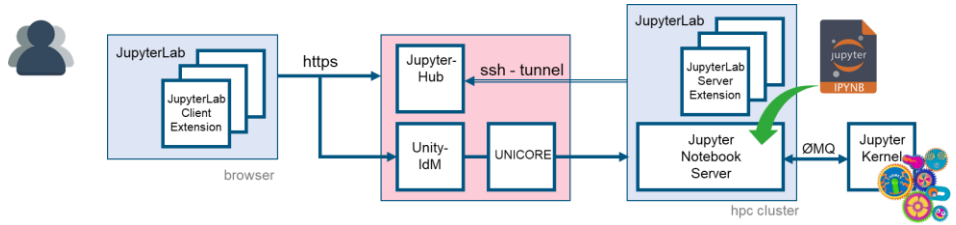
A Jupyter / Leaflet bridge enabling interactive maps in the Jupyter notebook.



https://github.com/jupyter-widgets/ipyleaflet

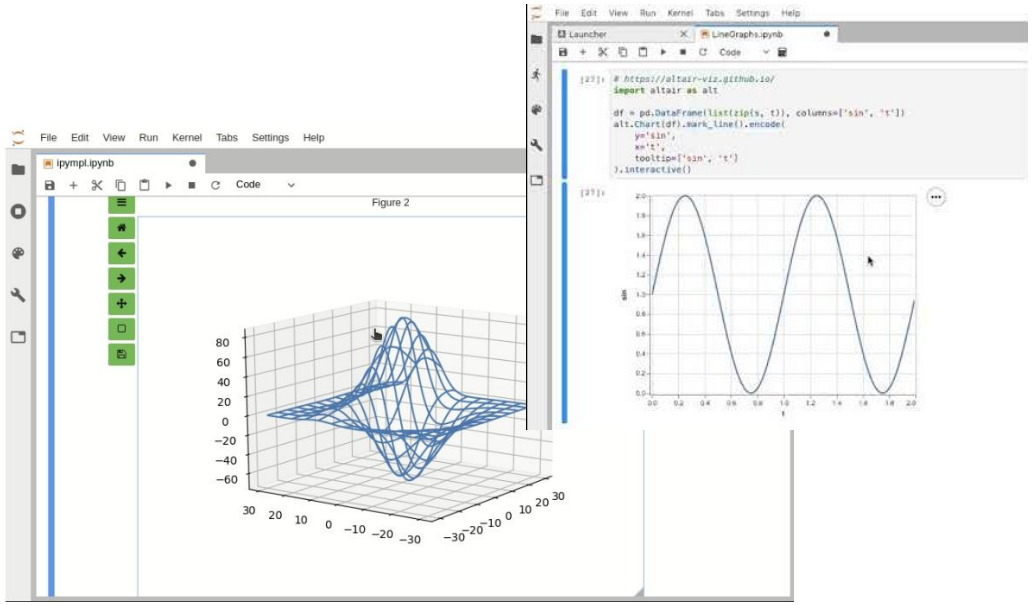
JUPYTER-JSC EXTENSIONS

Installed by default



IPyMPL - matplotlib

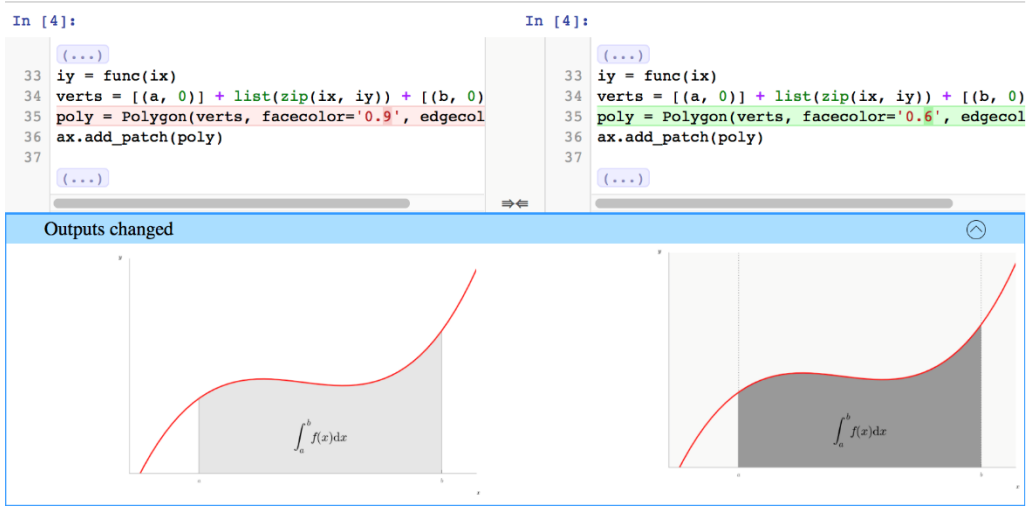
Leveraging the Jupyter interactive widgets framework, ipympl enables the interactive features of matplotlib in the Jupyter notebook and in JupyterLab.



https://github.com/matplotlib/ipympl

NBDime

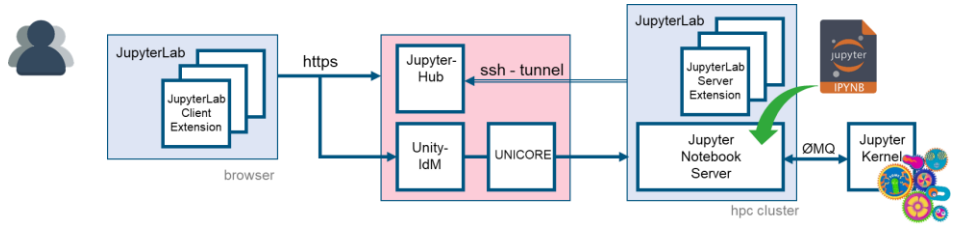
Tools for diffing and merging of Jupyter notebooks.



https://github.com/jupyter/nbdime

JUPYTER-JSC EXTENSIONS

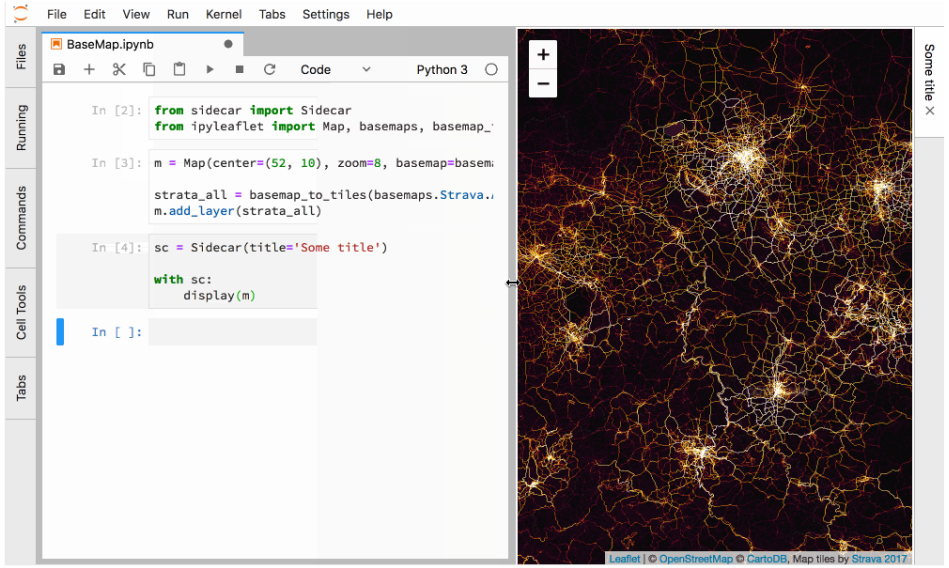
Installed by default



Plotly
JupyterLab extension for the interactive and browser-based graphing library Plotly.
https://plotly.com/python/

https://github.com/plotly/plotly.py

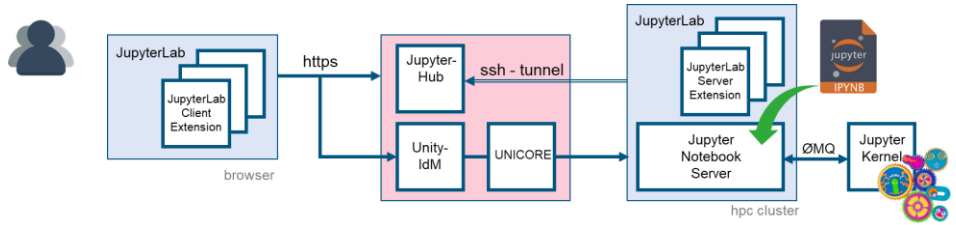
JupyterLab-Sidecar
A sidecar output widget for JupyterLab.



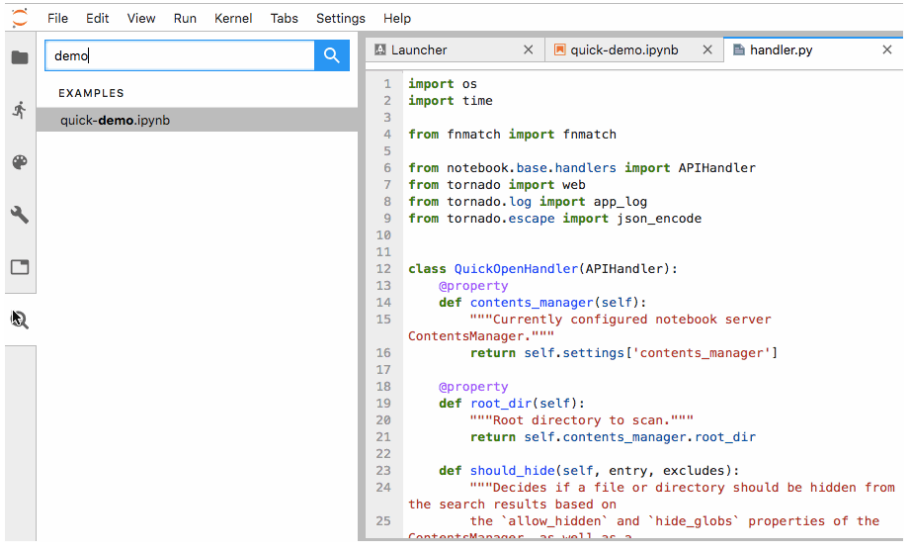
https://github.com/jupyter-widgets/jupyterlab-sidecar

JUPYTER-JSC EXTENSIONS

Installed by default

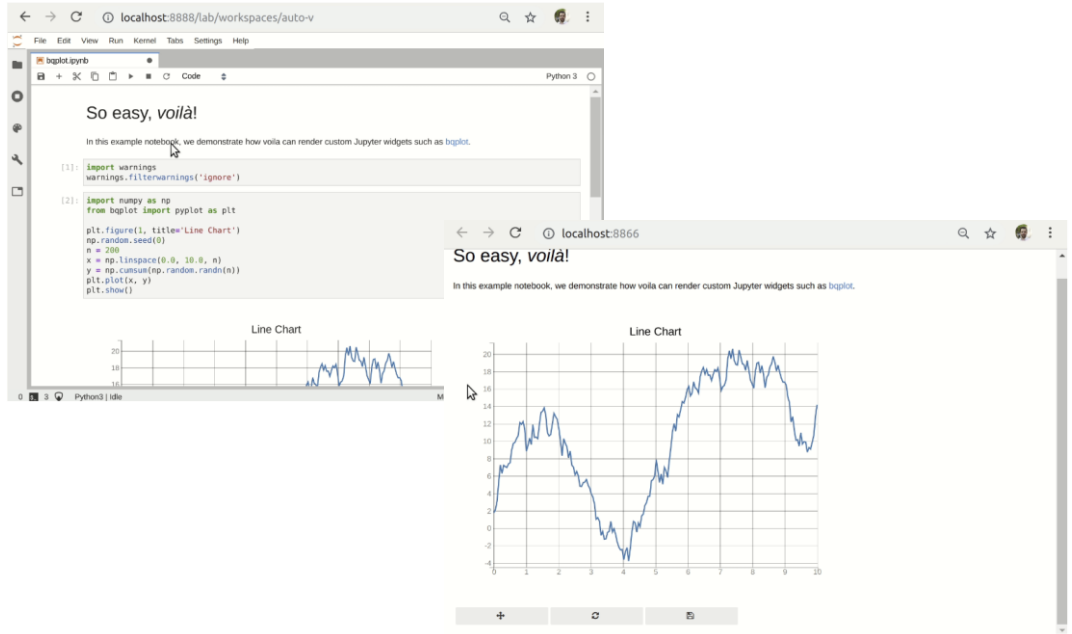


JupyterLab-Quickopen
Quickly open a file in JupyterLab by typing part of its name



https://github.com/parente/jupyterlab-quickopen

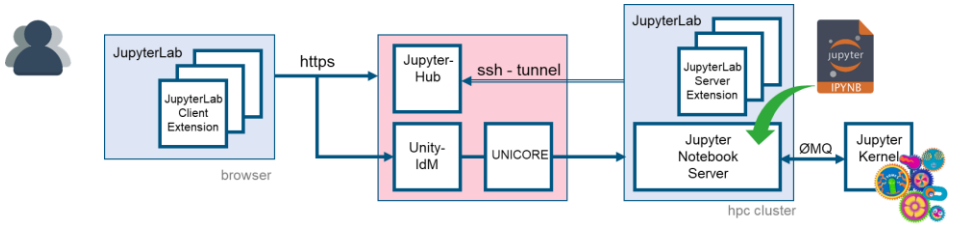
Voilà
Voilà turns Jupyter notebooks into standalone web applications.



https://github.com/voila-dashboards/voila

JUPYTER-JSC EXTENSIONS

Installed by default



Presented JupyterLab extensions

- ipyvolume
- @jupyterlab/git
- **jupyterlab-lmod**
- @jupyterlab/toc
- jupyter-threejs
- jupyter-leaflet
- jupyter-matplotlib
- jupyterlab-plotly
- @jupyter-widgets/jupyterlab-sidecar
- @parente/jupyterlab-quickopen
- @jupyter-voila/jupyterlab-preview

More installed JupyterLab extensions

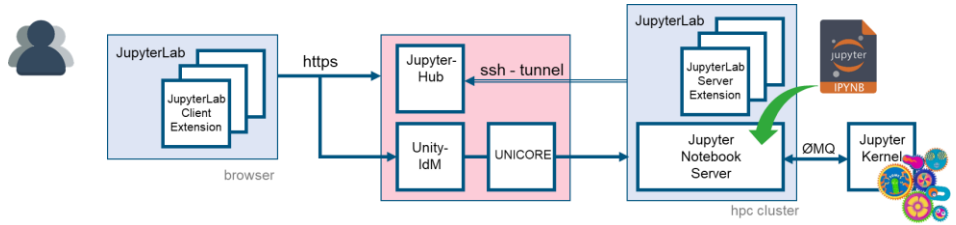
- @bokeh/jupyter_bokeh
- **dask-labextension**
- jupyterlab-gitlab
- bqplot
- @jupyterlab/latex
- @krassowski/jupyterlab_go_to_definition
- @pyviz/jupyterlab_pyviz
- @ryantam626/jupyterlab_code_formatter
- **@jupyterlab/server-proxy**
- itkwidgets
- jupyter-vue
- @jupyterlab/celltags
- jupyterlab-drawio

https://gitlab.version.fz-juelich.de/jupyter4jsc/j4j_notebooks/-/blob/master/001-Jupyter/List_JupyterExtensions.ipynb
https://npmjs.com

JUPYTER KERNEL

JUPYTER KERNEL

How to create your own Juypter Kernel



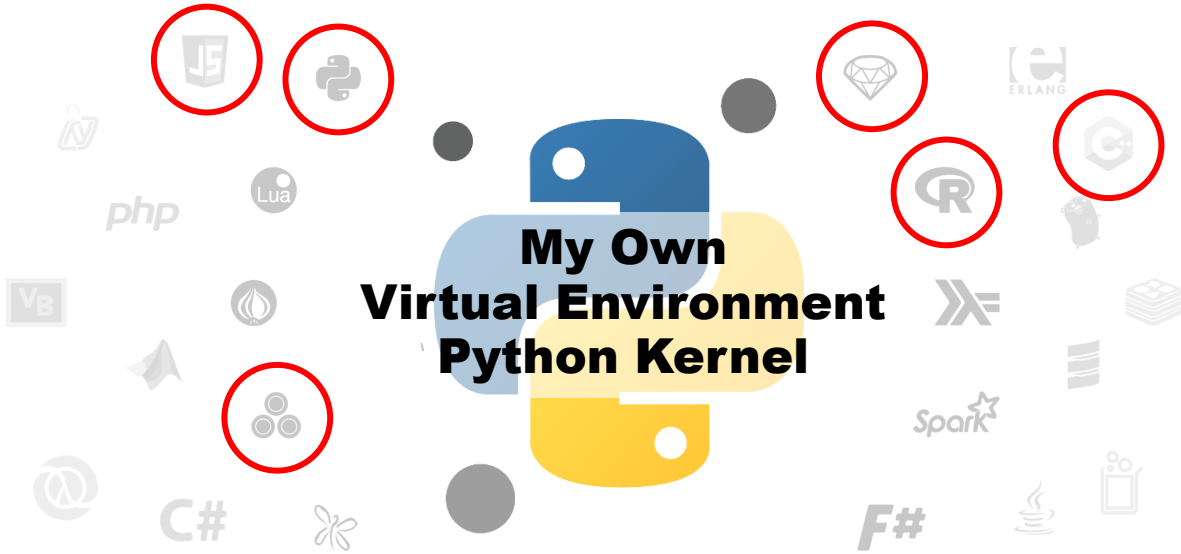
Jupyter Kernel

A “kernel” refers to the separate process which executes code cells within a Jupyter notebook.

Jupyter Kernel

- run code in different programming languages **and environments**.
- can be connected to a notebook (one at a time).
- communicates via ZeroMQ with the JupyterLab.

- Multiple **preinstalled** Jupyter Kernels can be found on our clusters
  - Python, R, Julia, Bash, C++, Ruby, JavaScript
  - Specialized kernels for visualization, quantumcomputing

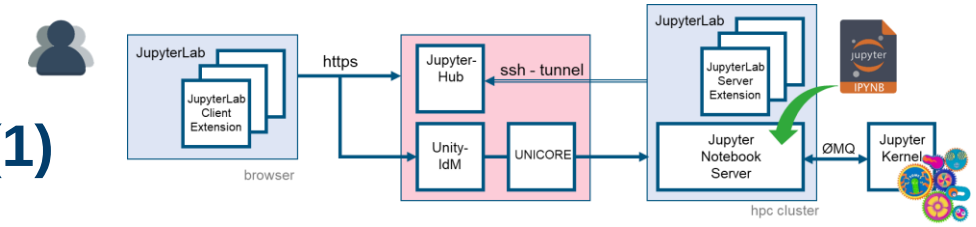


You can easily **create your own kernel** which for example runs your specialized virtual Python environment.

https://github.com/jupyter/jupyter/wiki/Jupyter-kernels

JUPYTER KERNEL

1. Create/Pimp new virtual Python environment (1)



1. **Login to JupyterLab and open terminal**

2. **Load required modules**

```
Lnode:> module purge
Lnode:> module use $OTHERSTAGES
Lnode:> module load Stages/Devel-2019a
Lnode:> module load GCC/8.3.0
Lnode:> module load Jupyter
```

3. **Load extra modules you need for your kernel**

```
Lnode:> module load <module you need>
```

Building your own Jupyter kernel is a three step process

1. Create/Pimp new **virtual Python environment**
   `venv`
2. Create/Edit **launch script** for the Jupyter kernel
   `kernel.sh`
3. Create/Edit Jupyter **kernel configuration**
   `kernel.json`

1. **Create a virtual environment named <venv_name> at a path of your choice:**

```
Lnode:> python -m venv --system-site-packages <your_path>/<venv_name>
```

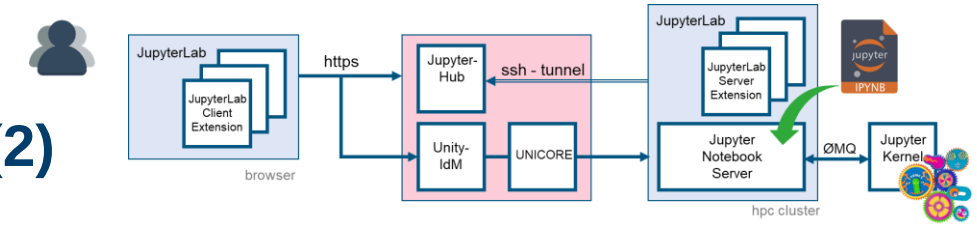
2. **Activate your environment**

```
Lnode:> source <your_path>/<venv_name>/bin/activate
```

https://gitlab.version.fz-juelich.de/jupyter4jsc/j4j_notebooks/-/blob/master/001-Jupyter/Create_JupyterKernel_general.ipynb

JUPYTER KERNEL

1. Create/Pimp new virtual Python environment (2)



1. **Ensure python packages installed in the virtual environment are always prefered**

```
(<venv_name>) Lnode:> export PYTHONPATH=\
${VIRTUAL_ENV}/lib/python3.6/site-packages:${PYTHONPATH}
```

2. **Install Python libraries required for communication with Jupyter**

```
(<venv_name>) Lnode:>
        pip install --ignore-installed ipykernel
```

3. **Install whatever else you need in your Python virtual environment (using pip)**

```
(<venv_name>) Lnode:>
        pip install <python-package you need>
```

Building your own Jupyter kernel is a three step process

1. Create/Pimp new **virtual Python environment**
   `venv`
2. Create/Edit **launch script** for the Jupyter kernel
   `kernel.sh`
3. Create/Edit Jupyter **kernel configuration**
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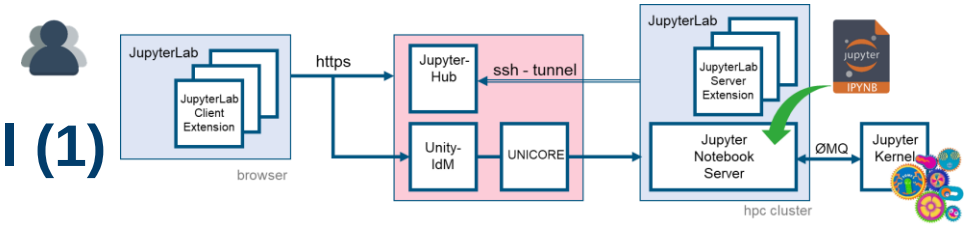
JUPYTER KERNEL

2. Create/Edit launch script for the Jupyter kernel (1)



1. **Create launch script, which loads your Python virtual environment and starts the ipykernel process inside:**

```
(<venv_name>) Lnode:> touch ${VIRTUAL_ENV}/kernel.sh
```

2. **Make launch script executable**

```
(<venv_name>) Lnode:> chmod +x ${VIRTUAL_ENV}/kernel.sh
```

3. **Edit the launch script for your new Jupyter kernel**

```
(<venv_name>) Lnode:> vi ${VIRTUAL_ENV}/kernel.sh
```

Building your own Jupyter kernel is a three step process

1. Create/Pimp new **virtual Python environment**
   `venv`
2. Create/Edit **launch script** for the Jupyter kernel
   `kernel.sh`
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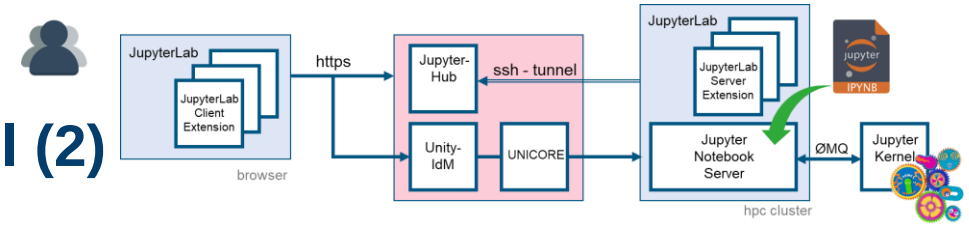
   `kernel.json`

https://gitlab.version.fz-juelich.de/jupyter4jsc/j4j_notebooks/-/blob/master/001-Jupyter/Create_JupyterKernel_general.ipynb

JUPYTER KERNEL

2. Create/Edit launch script for the Jupyter kernel (2)




```
#!/bin/bash

# Load required modules
module purge
module load $OTHERSTAGES
module load Stages/Devel-2019a
module load GCC/8.3.0
module load Jupyter

# Load extra modules you need for your kernel
#module load <module you need>

# Activate your Python virtual environment
source <your_path>/<venv_name>/bin/activate

# Ensure python packages installed in the virtual environment are always prefered
export PYTHONPATH=${VIRTUAL_ENV}/lib/python3.6/site-packages:${PYTHONPATH}

exec python -m ipykernel $@
```

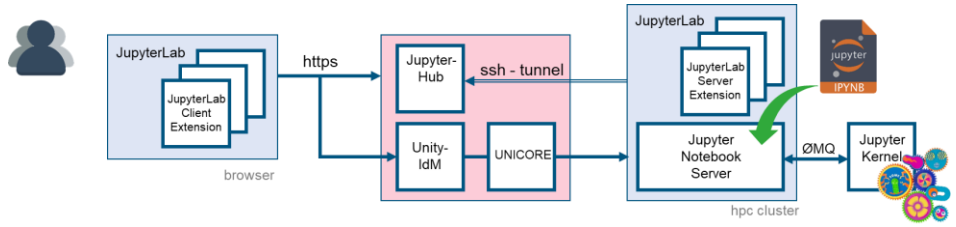
Building your own Jupyter kernel is a three step process

1. Create/Pimp new **virtual Python environment**
   `venv`
2. Create/Edit **launch script** for the Jupyter kernel
   `kernel.sh`
3. Create/Edit Jupyter **kernel configuration**
   `kernel.json`

https://gitlab.version.fz-juelich.de/jupyter4jsc/j4j_notebooks/-/blob/master/001-Jupyter/Create_JupyterKernel_general.ipynb

JUPYTER KERNEL

3. Create/Edit Jupyter kernel configuration (1)



1. **Create your Jupyter kernel configuration files**

```
(<venv_name>) Lnode:>
python -m ipykernel install --user --name=<my-kernel-name>
```

2. **Update your kernel file to use the lauch script**

```
(<venv_name>) Lnode:>
vi ~/.local/share/jupyter/kernels/<my-kernel-name>/kernel.json
{
 "argv": [
  "<your_path>/<venv_name>/kernel.sh",
  "-m",
  "ipykernel_launcher",
  "-f",
  "{connection_file}"
 ],
 "display_name": "<my-kernel-name>",
 "language": "python"
}
```

Building your own Jupyter kernel is a three step process

1. Create/Pimp new **virtual Python environment**
   `venv`
2. Create/Edit **launch script** for the Jupyter kernel
   `kernel.sh`
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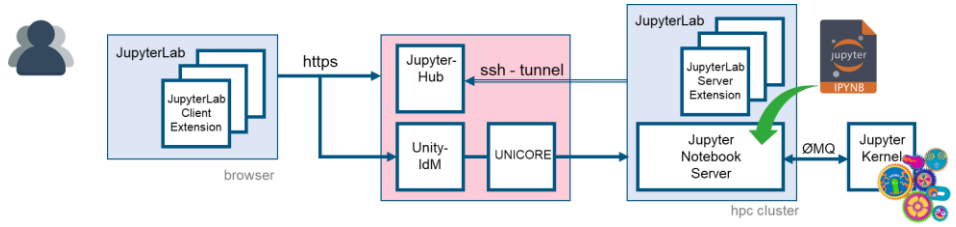
JUPYTER KERNEL

Run your Jupyter kernel configuration



Run your Jupyter Kernel

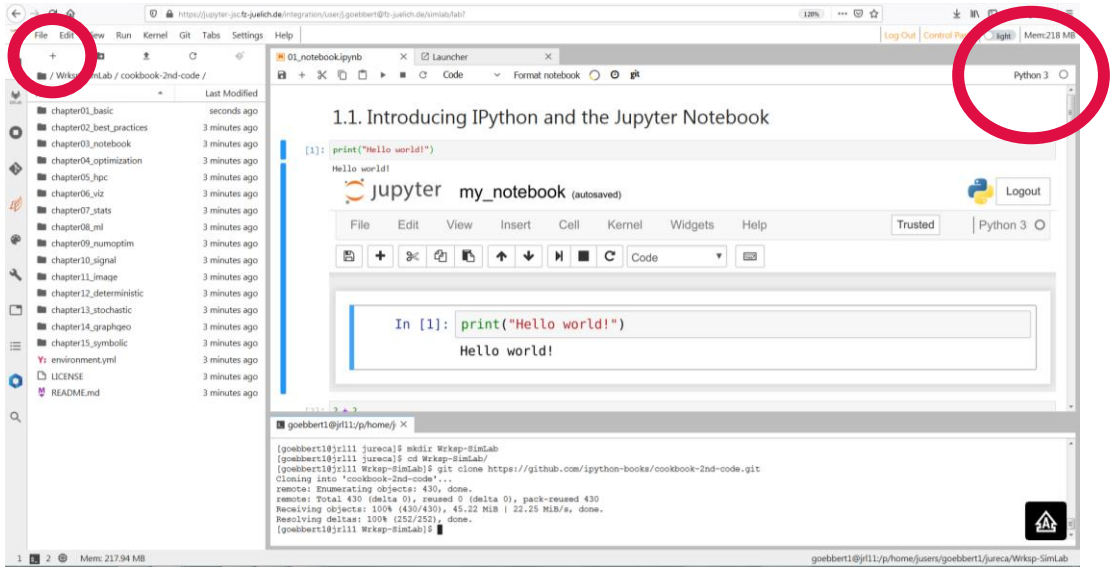
1. https://jupyter-jsc.fz-juelich.de
2. Choose system where your Jupyter kernel is installed in `~/.local/share/jupyter/kernels`
3. Select your kernel in the launch pad or click the kernel name.

Conda

How to base your Jupyter Kernel on a Conda environment:
https://gitlab.version.fz-juelich.de/jupyter4jsc/j4j_notebooks/-/blob/master/001-Jupyter/Create_JupyterKernel_conda.ipynb

Project kernel

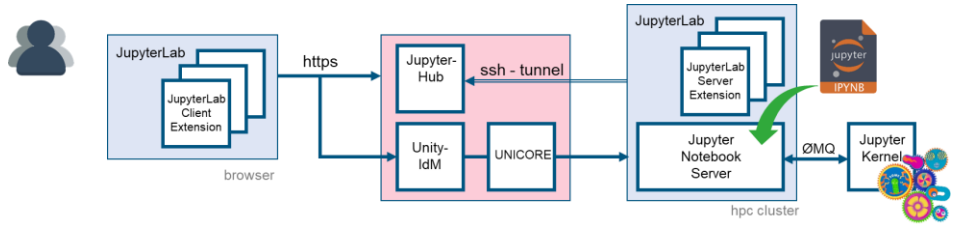
On request Jupyter kernel can be made available to a whole project. They are installed then to
`$PROJECT/.local/share/jupyter/kernels`



https://gitlab.version.fz-juelich.de/jupyter4jsc/j4j_notebooks/-/blob/master/001-Jupyter/Create_JupyterKernel_general.ipynb

JUPYTER KERNEL

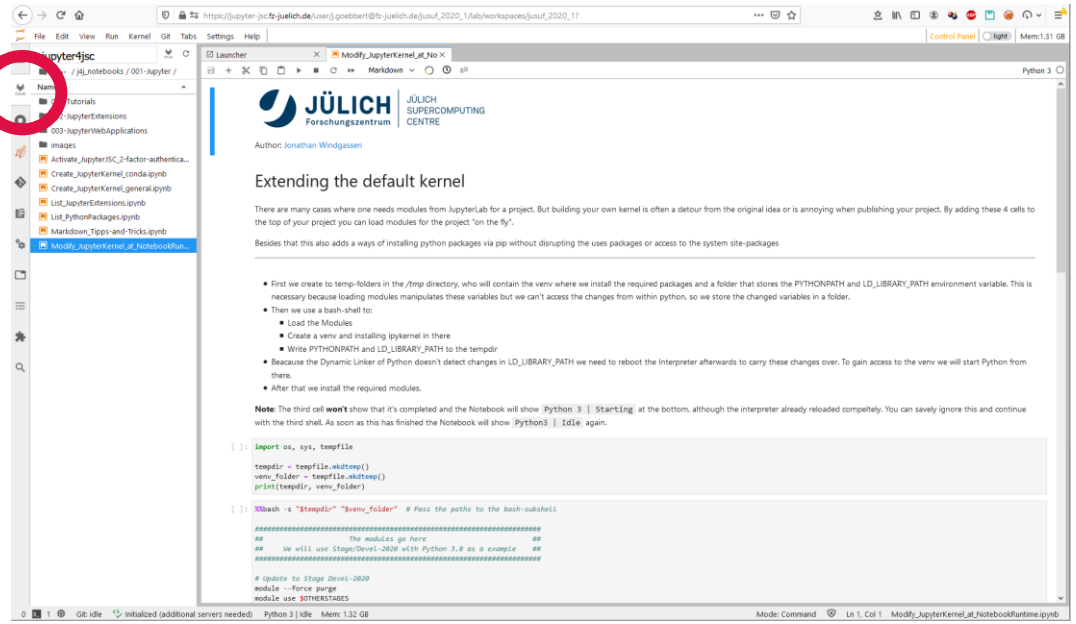
Shortcut!



You do NOT want to build your own kernel,
every time you QUICKLY need a package or module.

You are lucky – we can show you a workaround / hack(!):

1. https://jupyter-jsc.fz-juelich.de
2. Click on the Github-Icon in the sidebar
3. Go to “001-Jupyter”
4. Open Modify_JupyterKernel_at_NotebookRuntime.ipynb



What´s the trick

```
os.execve(f"{venv_folder}/bin/python", args, env)
```

Workflow

1. Create a Python virtual environment at any location.
2. **WITHIN** the notebook
   - restart the kernel´s python interpreter
   - of that Python virtual environment
   - with the correct environment variables set.

https://github.com/FZJ-JSC/jupyter-jsc-notebooks/blob/master/001-Jupyter/Modify_JupyterKernel_at_NotebookRuntime.ipynb

JUPYTER CAN DO MORE

JUPYTERLAB – REMOTE DESKTOP

Run your X11-Applications in the browser

Jupyter-JSC gives you easy access to a remote desktop

1. https://jupyter-jsc.fz-juelich.de
2. Click on “Xpra” (not available on JURECA, yet)

Xpra - X Persistent Remote Applications
is a tool which runs X clients on a remote host and directs their display to the local machine.

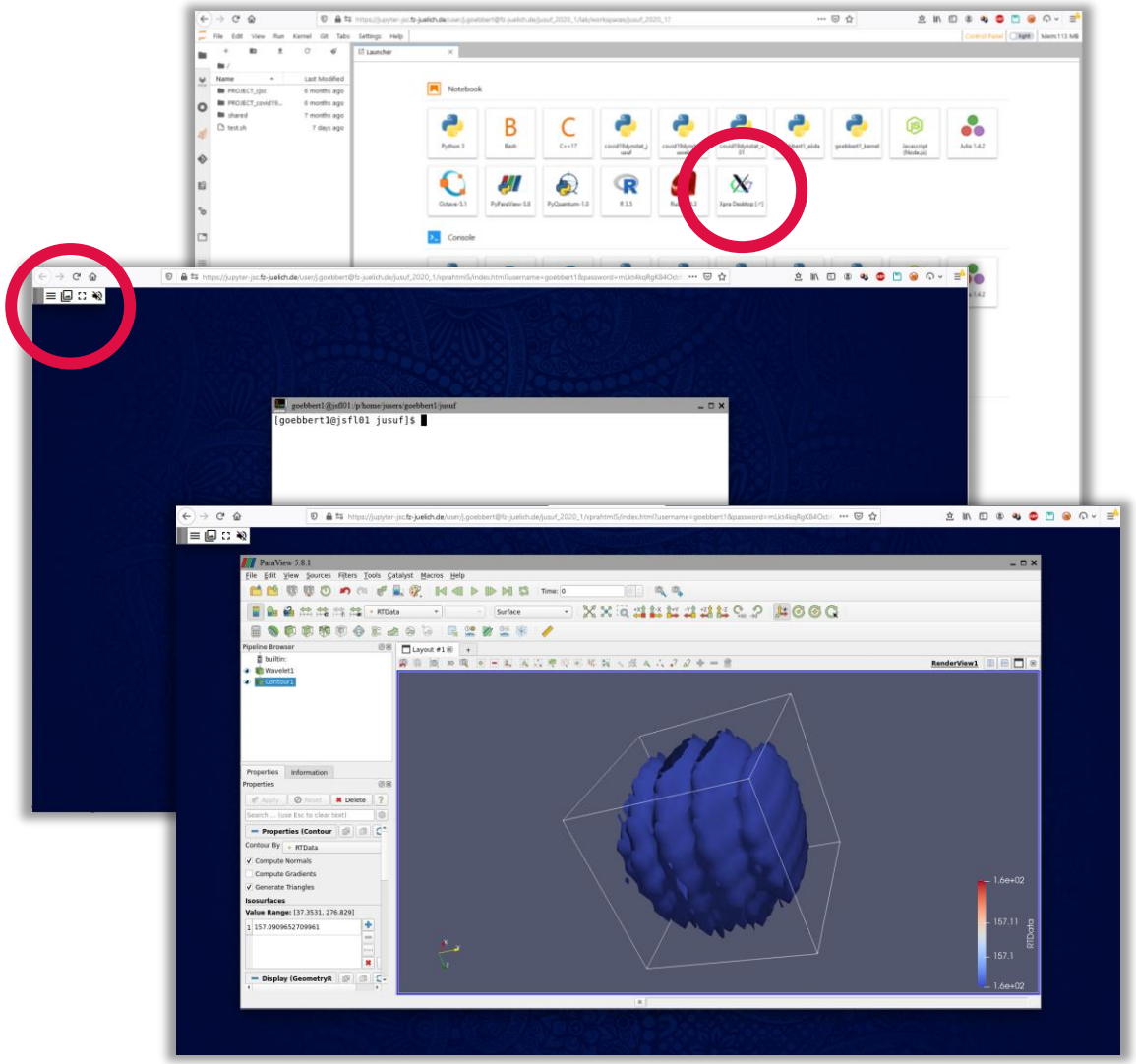
- Runs in a browser
- allows dis-/reconnection without disrupting the forwarded application
- https://xpra.org

The remote desktop will run on the same node as your JupyterLab does (this includes compute nodes).

It gets killed, when you stop your JupyterLab session.

Hint:

- `CTRL + C -> CTRL + Insert`
- `CTRL + V -> SHIFT + Insert`



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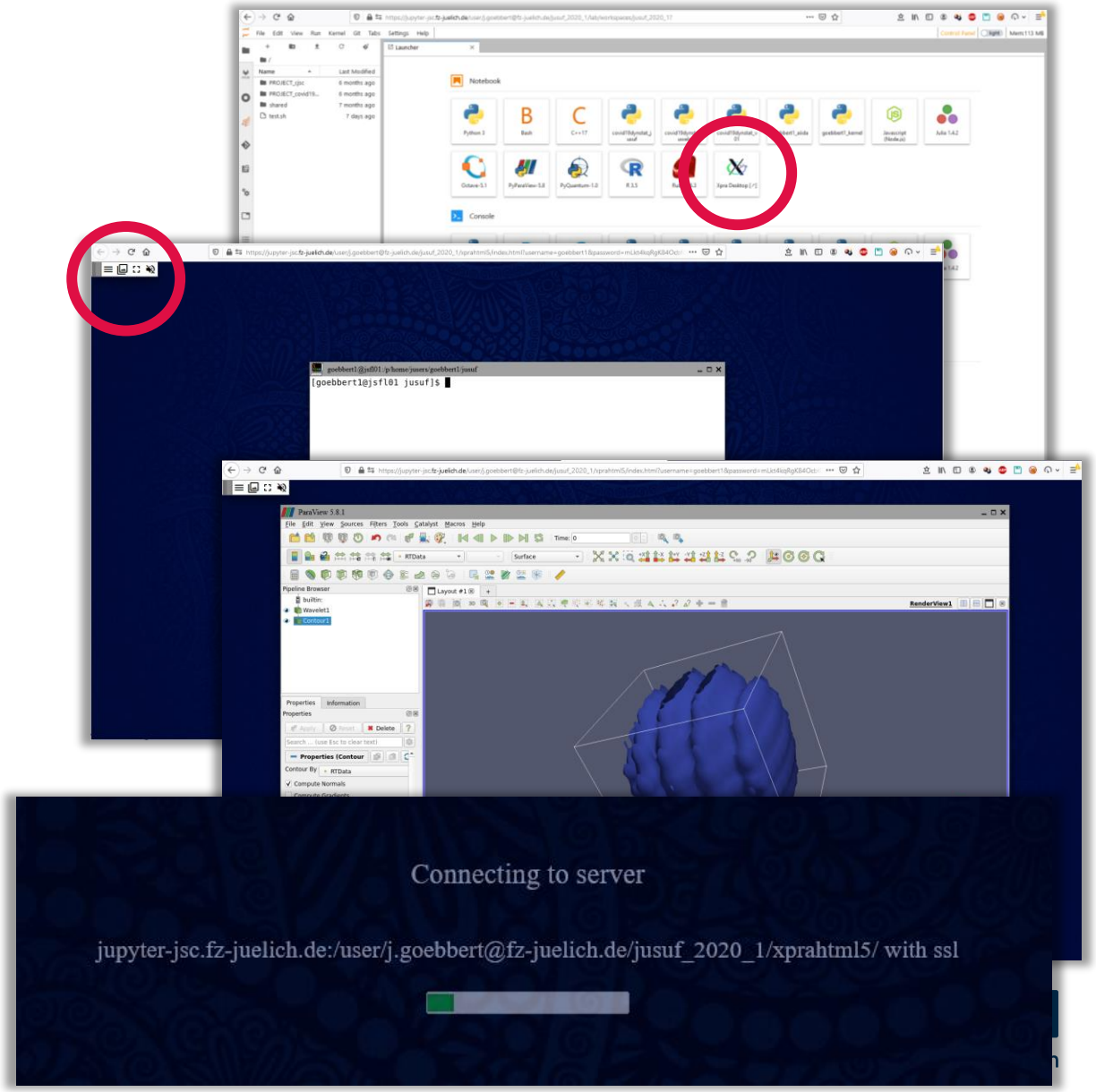
If the connection got lost at some point,
just hit the “reload” button of your browser.



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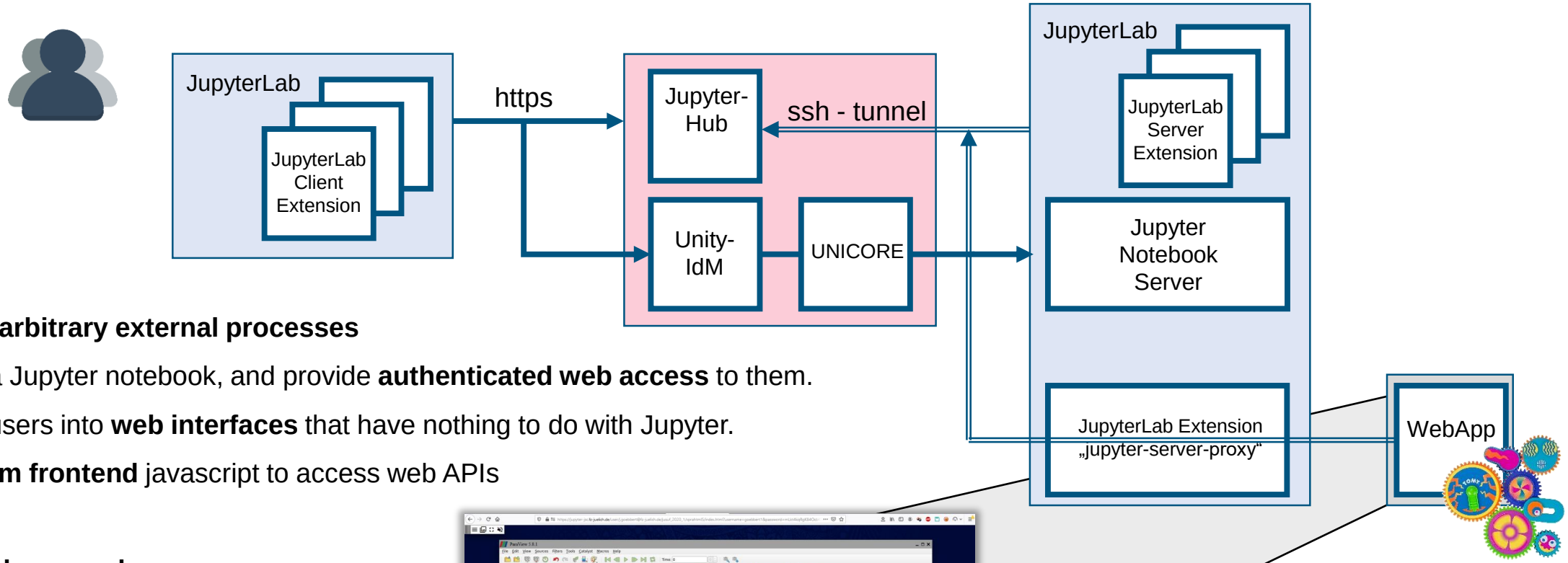
JUPYTERLAB – WEBSERVICE PROXY

Extension: jupyter-server-proxy

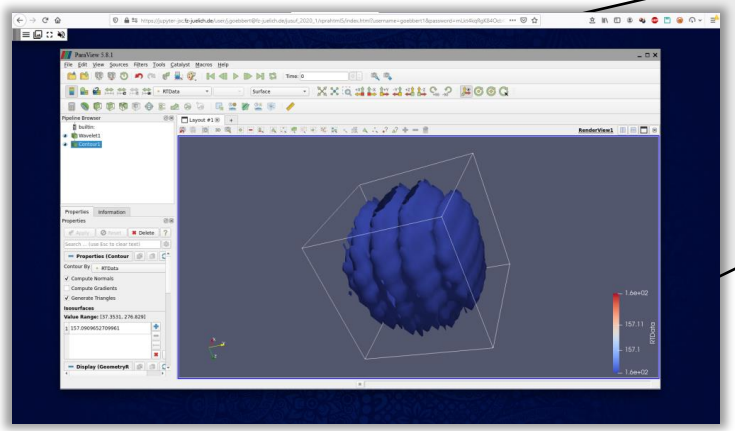


Allows to run **arbitrary external processes**

- alongside a Jupyter notebook, and provide **authenticated web access** to them.
- launching users into **web interfaces** that have nothing to do with Jupyter.
- **access from frontend** javascript to access web APIs

Other possible examples:

TensorBoard, RStudio, Shiny, OpenRefine, custom REST-APIs, …



https://github.com/jupyterhub/jupyter-server-proxy

JUPYTERLAB – WEBSERVICE PROXY

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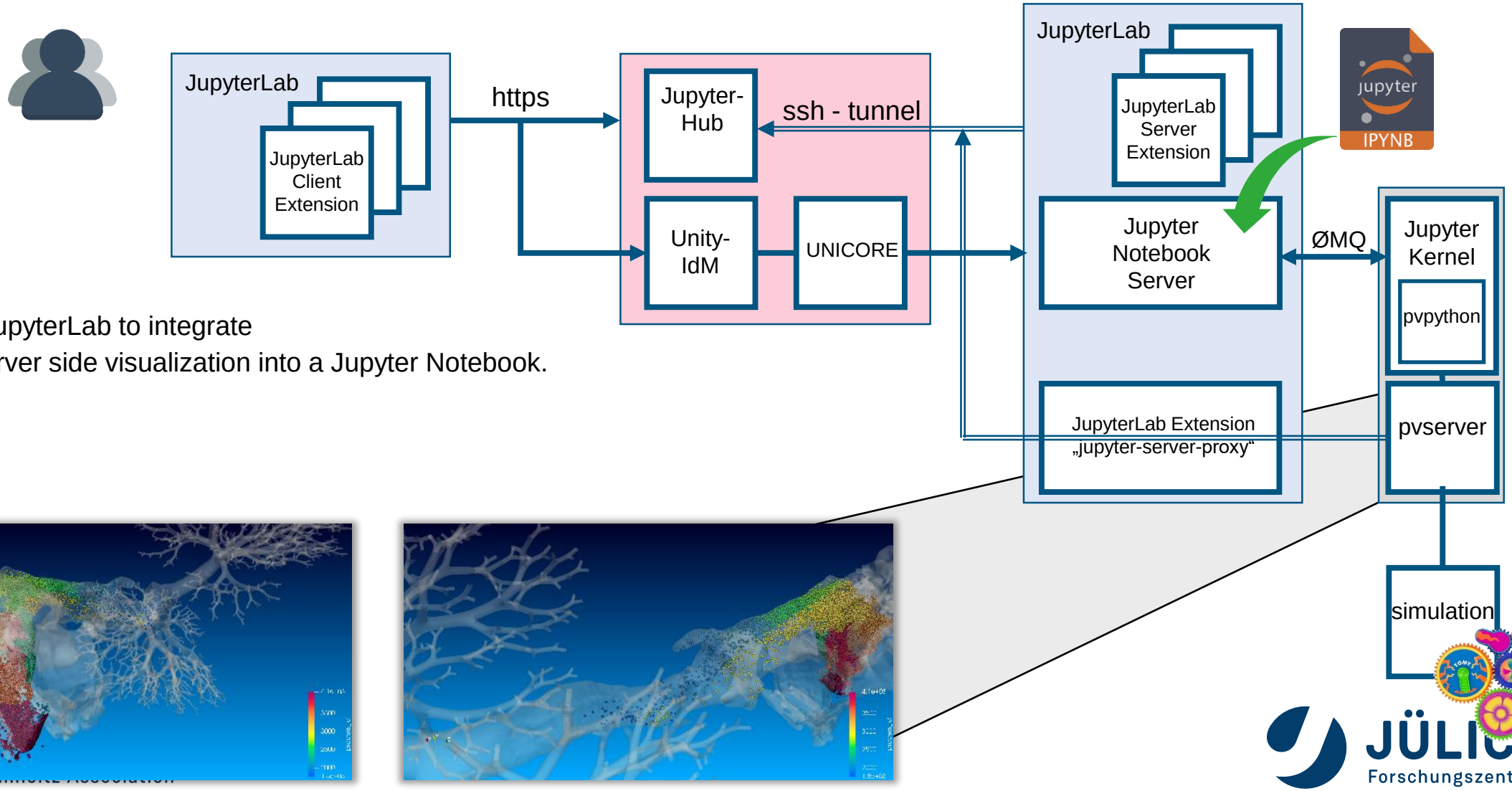

How to use JupyterLab to integrate
interactive server side visualization into a Jupyter Notebook.

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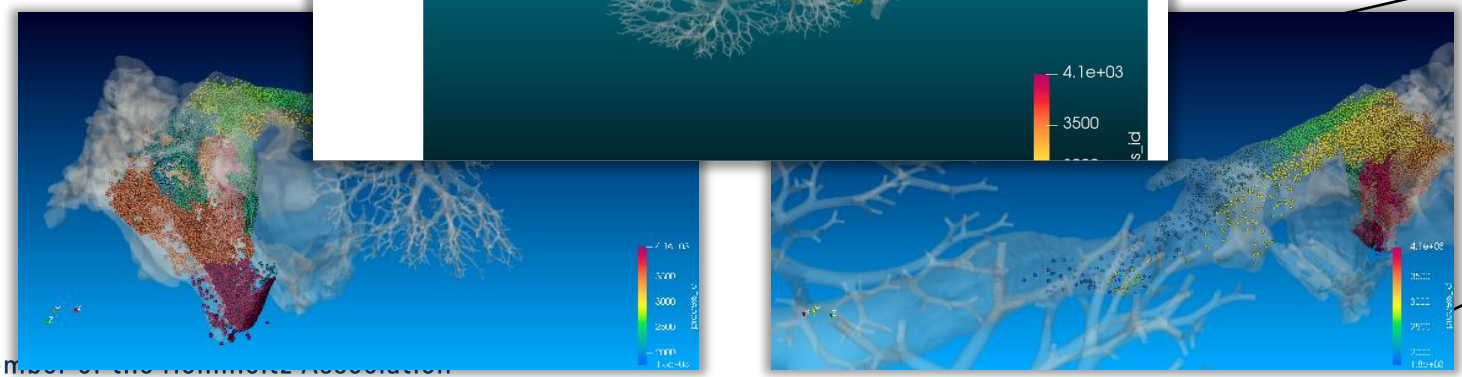
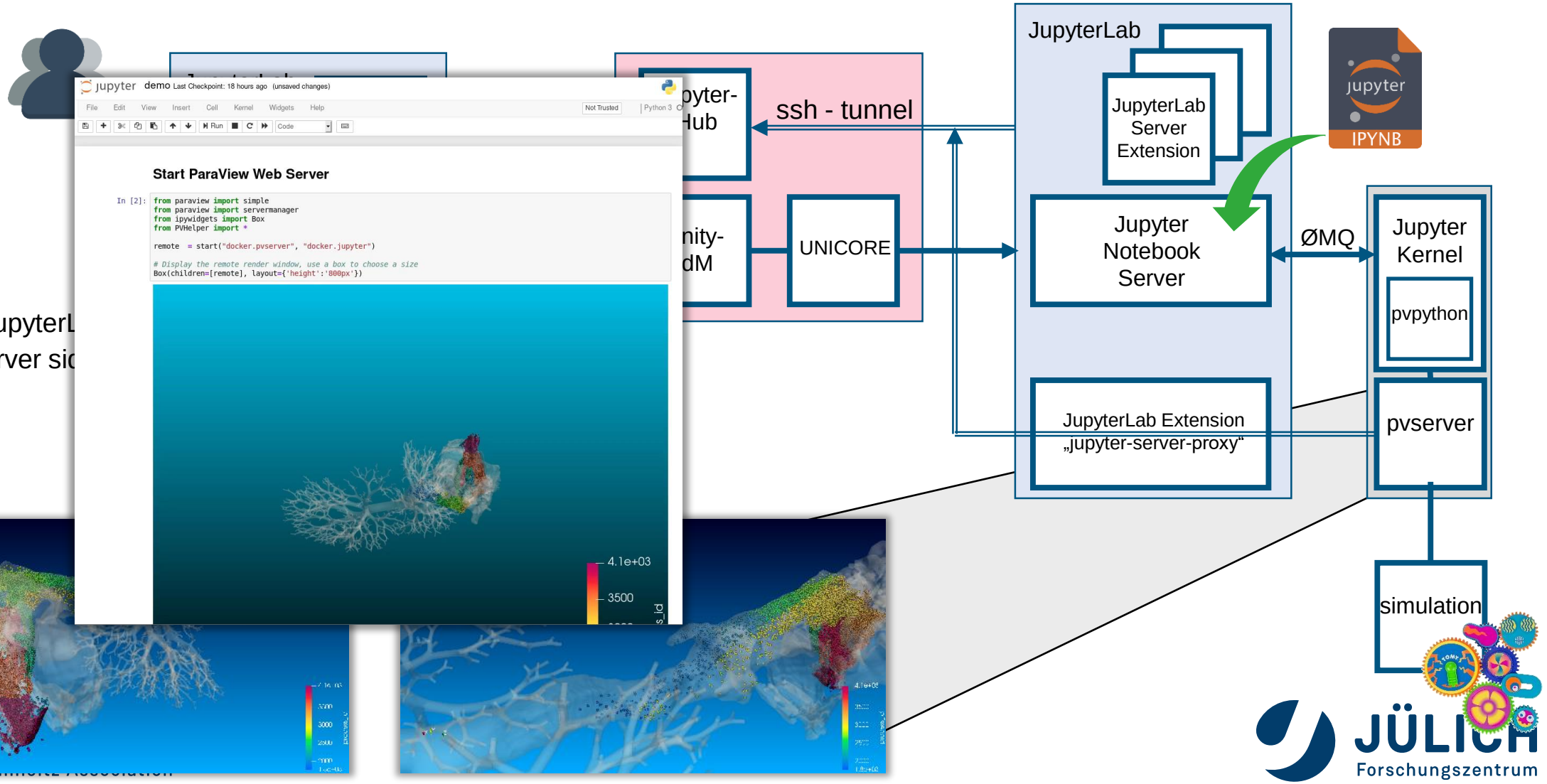
JUPYTERLAB – WEBSERVICE PROXY

Extension: jupyter-server-proxy

How to use JupyterL
interactive server sic





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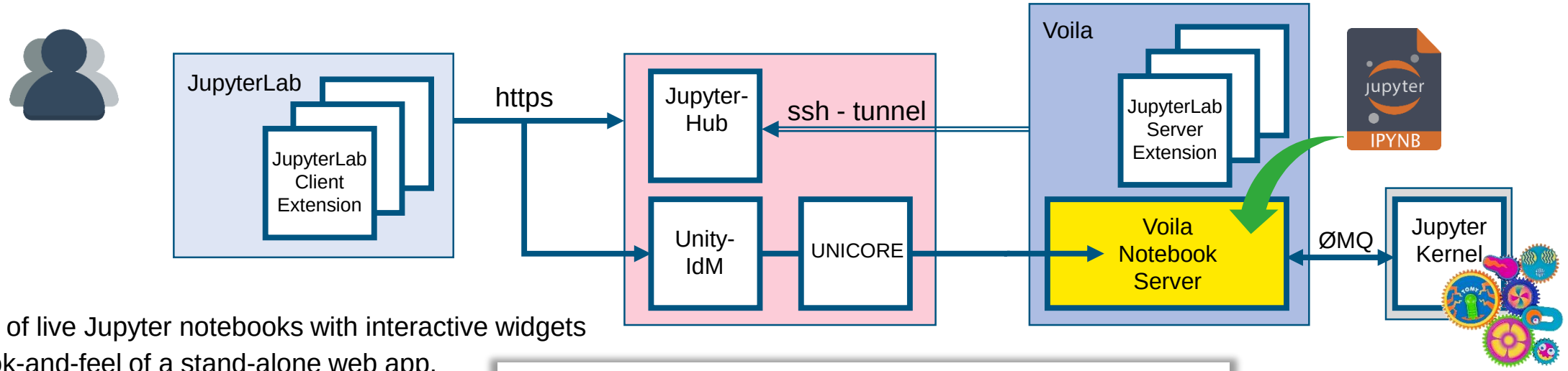
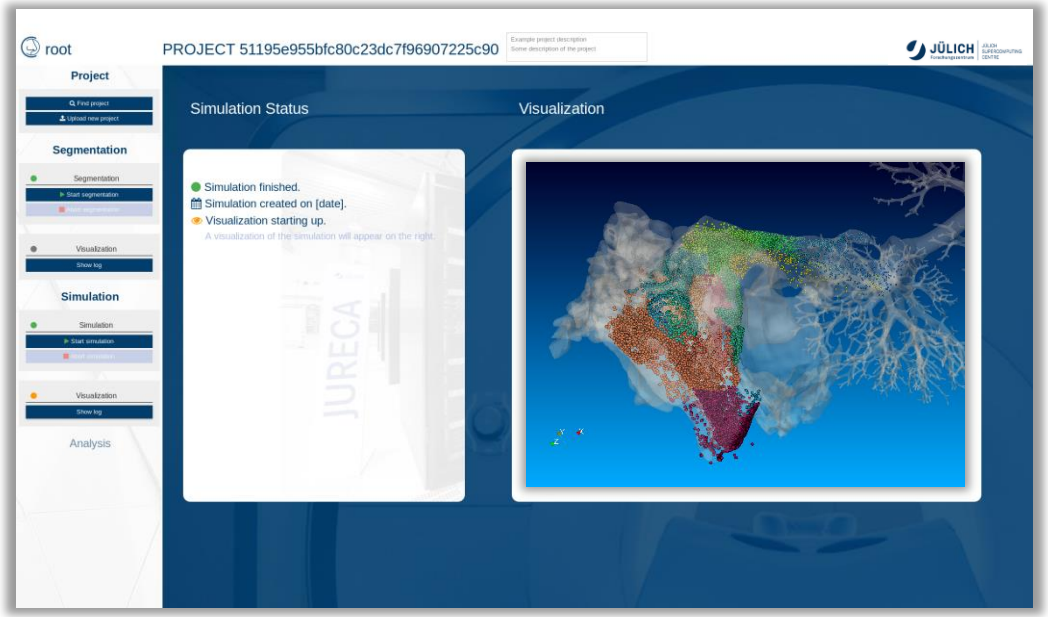
DASHBOARDS WITH JUPYTER/VOILA

Voilà turns Jupyter notebooks into standalone web applications



- **Rendering** of live Jupyter notebooks with interactive widgets with the look-and-feel of a stand-alone web app.
- Voilà disallows execute requests from the front-end, **preventing** execution of arbitrary code.
- **Enables** HPC users to develop easly web applications from their Jupyter notebooks.



https://github.com/voila-dashboards/voila
https://voila-gallery.org

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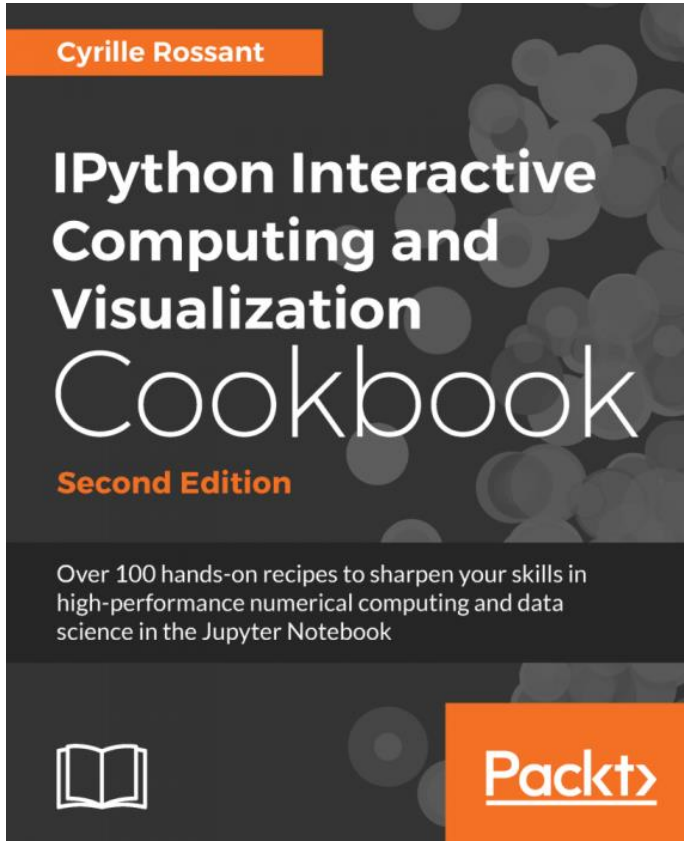
TUTORIALS

Get started with Jupyter

Possible start to enter the world of interactive computing with IPython in Jupyter:

- Leverage the Jupyter Notebook for interactive data science and visualization
- High-performance computing and visualization for data analysis and scientific modeling
- A comprehensive coverage of scientific computing through many hands-on, example-driven recipes with detailed, step-by-step explanations



https://ipython-books.github.io
https://github.com/ipython-books/cookbook-2nd

BENEFITS

Why Jupyter is so popular among Data Scientists

Some of the reasons …

- Jupyter allows to view the results of the code in-line without the dependency of other parts of the code.
- Jupyter mixes easy for users who extend their code line-by-line with feedback attached all along the way
- Jupyter Notebooks support visualization and include rendering data in live-graphics and charts.
- Jupyter is maintaining the state of execution of each cell automatically.
- Supports IPyWidget packages, which provide standard user interface for exploring code and data interactively.
- Platform and language independent because of its representation in JSON format.

QUESTIONS?

https://jupyter-jsc.fz-juelich.de