JUPYTERLAB - SUPERCOMPUTING IN YOUR BROWSER

Introduction to Jupyter-JSC at Jülich Supercomputing Centre

2024-11-12 I JENS H. GÖBBERT (J.GOEBBERT@FZ-JUELICH.DE)
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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

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JUPYTER NOTEBOOK

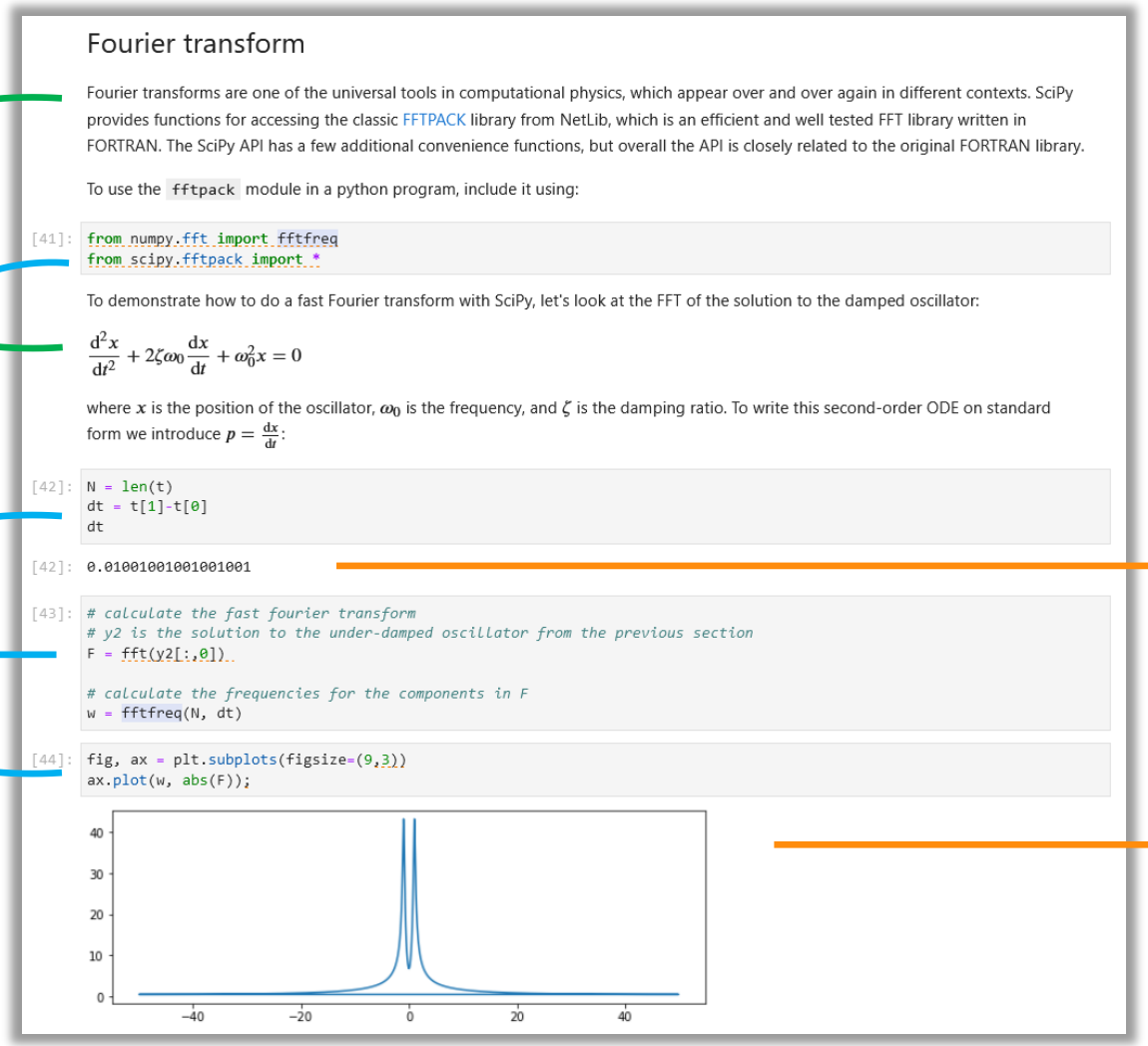
creating reproducible computational narratives

Markdown Cells

Code Cells

Output

Output

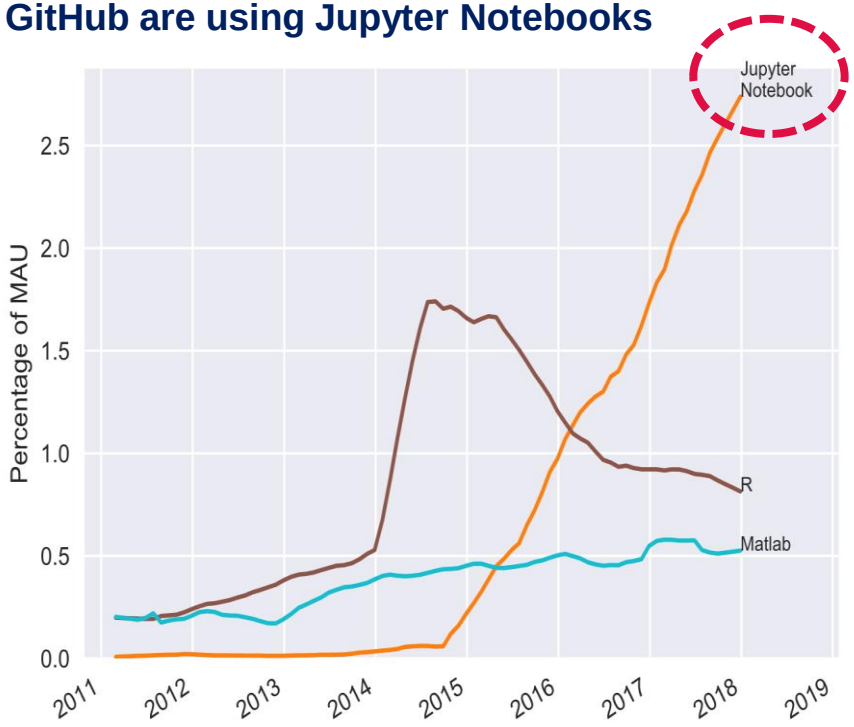


MOTIVATION

Rise of Jupyter´s popularity

- In 2007, Fernando Pérez and Brian Granger announced
  „**Ipython**: a system for interactive scientific computing“ [1]
- In 2014, Fernando Pérez announced
  a spin-off project from IPython called **Project Jupyter**.
  - IPython continued to exist as a Python shell and a kernel for Jupyter, while the Jupyter notebook moved under the Jupyter name.
- In 2015, GitHub and the Jupyter Project announced
  native rendering of Jupyter notebooks file format (.ipynb files) on the **GitHub**
- In 2017, the **first JupyterCon** was organized by O'Reilly in New York City.
  Fernando Pérez opened the conference with an inspiring talk. [2]
- In 2018, **JupyterLab** was announced
  as the next-generation web-based interface for Project Jupyter.
- In 2019, JupyterLab 1.0 …
  In 2020, JupyterLab 2.0 …
  In 2021, JupyterLab 3.0 …
  In 2023, JupyterLab 4.0 …

Counting how many Monthly Active Users (MAU) on GitHub are using Jupyter Notebooks



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

[1] Pérez F, Granger BE (2007) Ipython: a system for interactive scientific computing. Comput Sci Eng 9(3):21–29
[2] Pérez F, Project Jupyter: From interactive Python to open science -> https://www.youtube.com/watch?v=xuNj5paMuow

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HISTORY OF JUPYTERLAB AT JSC

2018 → 2019 → 2020 → 2021 → 2022 → 2023 → 2024

Initial Basis

JupyterLab modules
Authentication via Unity/IdM
Authorization via UNICORE
Orchestration Docker Swarm
Synchronization of User-DBs
Basic Data Protection Regulation
Fulfill Safety Requirements

Usage

Inplace Dokumentation
R, Julia, C++, Octave, Ruby
JupyterLabs on OpenStack
Dashboard Development
JupyterLab Usability
Kernel for Vis, DL
Testing & Benchmarking

Features

Remote Desktop Integration
Optional 2-Factor Auth.
Use for Workshops
Specialized Functionalities
Enhanced Data Access
Extended Logging
Cross-Side Demonstration

Redesign

Switch to **Kubernetes**
Redesign Management
Switch to **JupyterLab 3**
GPFS through UFTP
Support for User Extensions
Easybuild Modularization

Customization

Project/Community JHubs
Upgrade JHub Entrance-UI
Comp. Resource Permissions
Maintenance Improvements
Upgrade of Load Balancer
Modularization of Backend
External Clouds & HPC

JLab Beta → JLab 1 → JLab 2 → JLab 3 → JLab3+X → JLab4

HISTORY OF JUPYTERLAB AT JSC

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Orchestration
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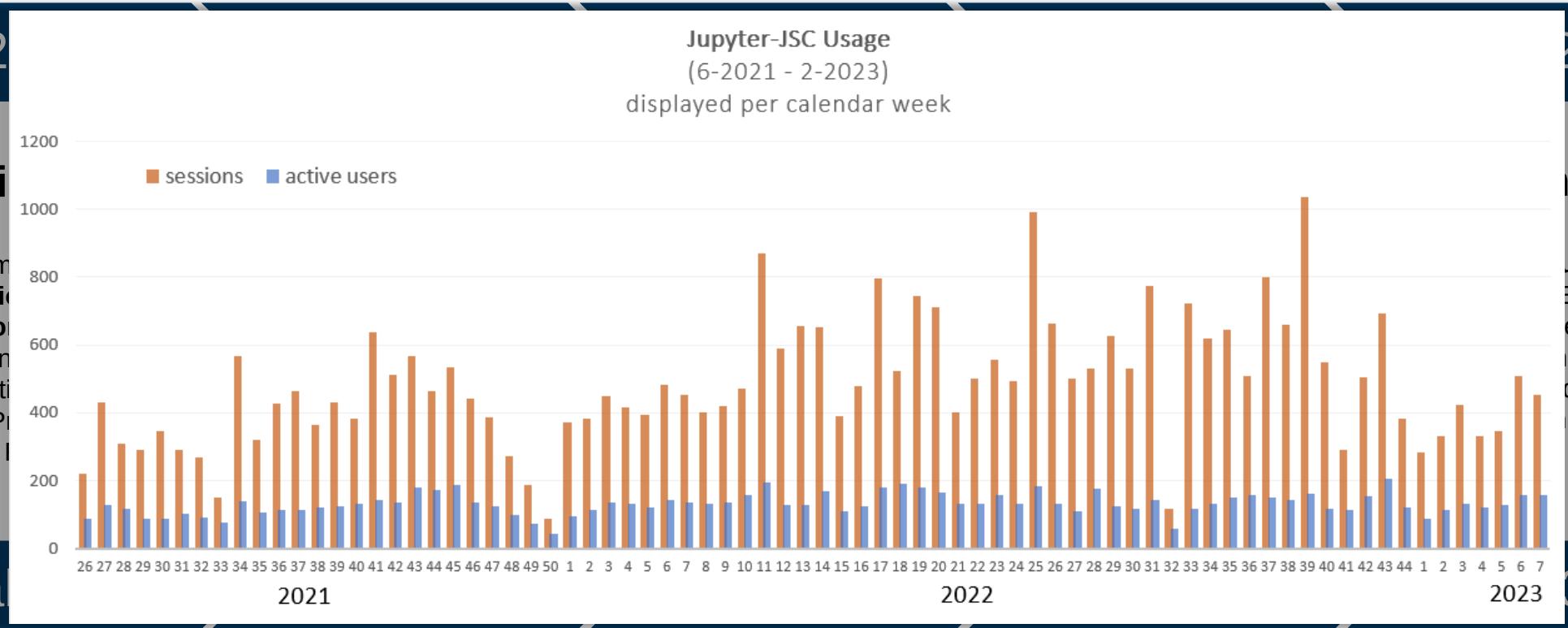
Basic Data P
Fulfill Safety



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unity JHubs
Entrance-UI
e Permissions
provements
d Balancer
of Backend

JLa

3+X

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TERMINOLOGY

TERMINOLOGY

What is JupyterLab

JupyterLab

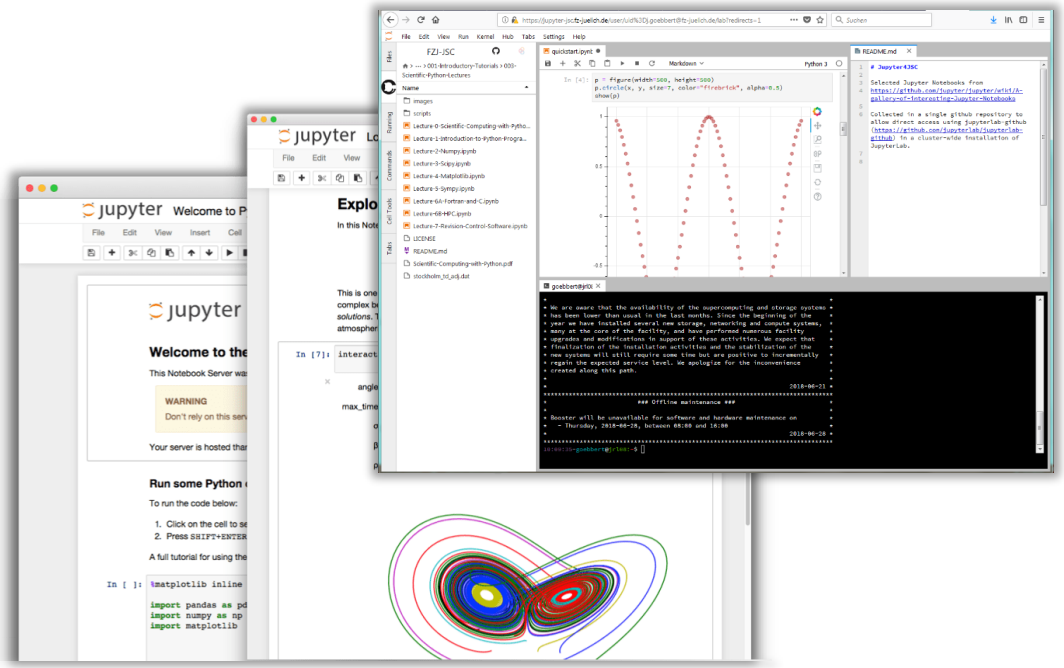
- **Interactive** working environment in the web browser
- For the creation of **reproducible** computer-aided narratives
- Very **popular** with researchers from all fields
- Jupyter = Julia + Python + R

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

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What is a Jupyter Notebook?

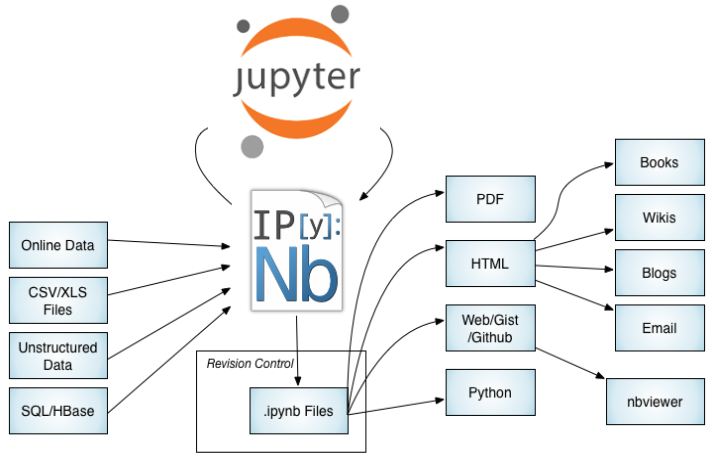
Jupyter Notebook

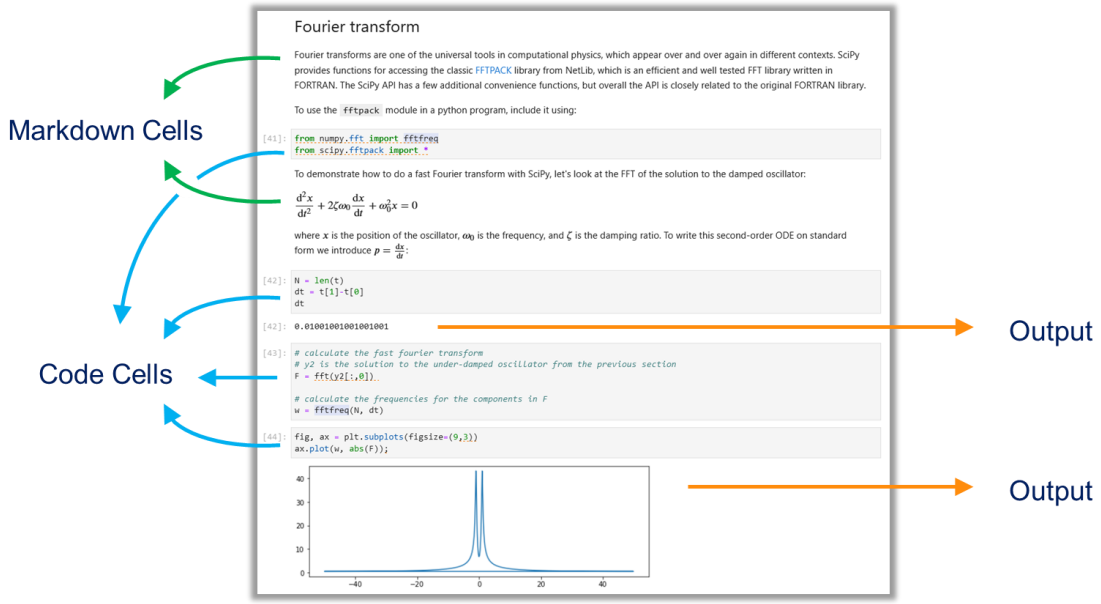
A notebook document (file extension .ipynb)
is a document that can be rendered in a web browser

- 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

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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, quantum-computing

- 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

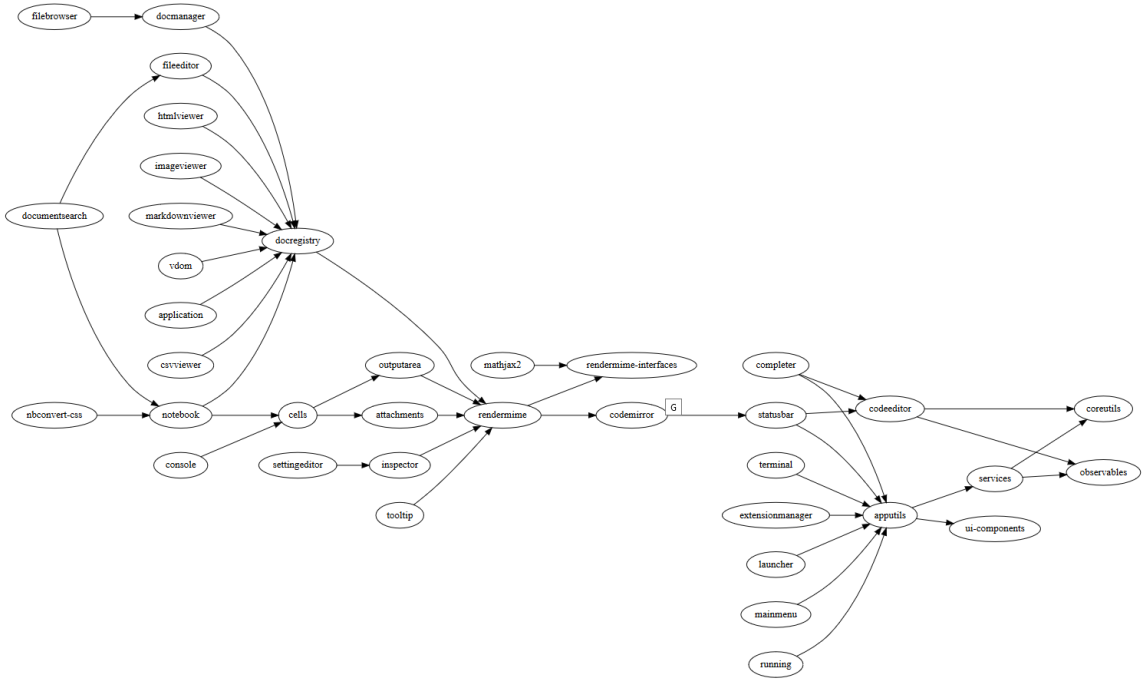
JupyterLab extensions can customize or enhance any part of JupyterLab.

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

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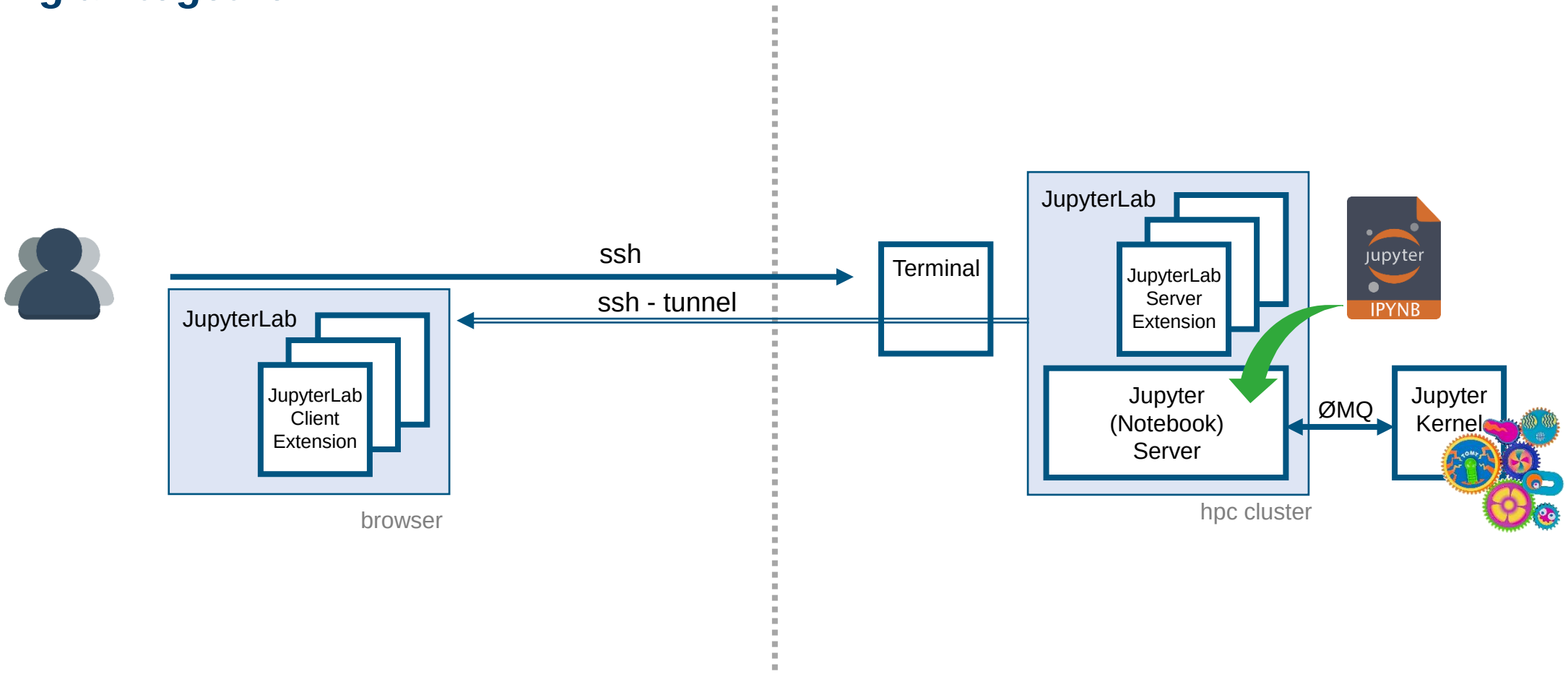
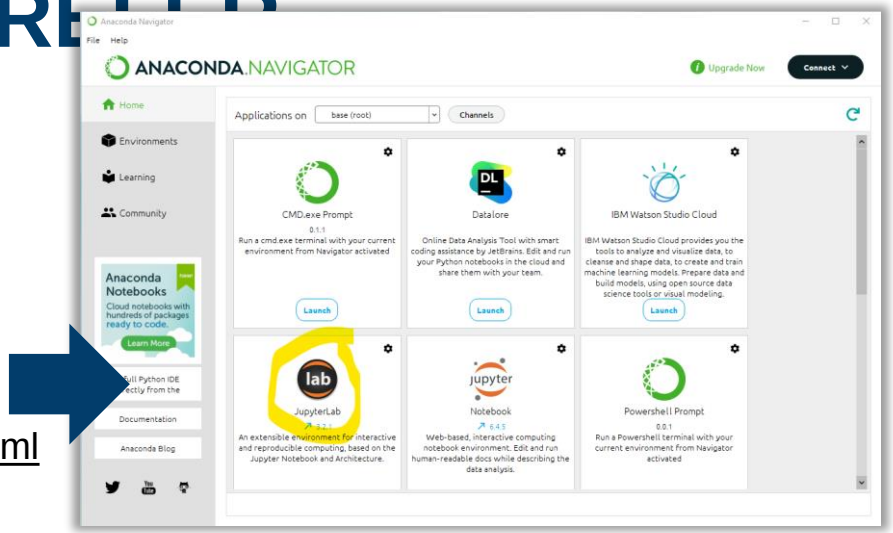
Bringing all together



INSTALLATION

JUPYTERLAB - WHEREVER YOU PREFER

Local, Remote, Browser-only



Local installation:

- **JupyterLab** installed using conda, mamba, pip, pipenv or docker.
  ➔ https://jupyterlab.readthedocs.io/en/stable/getting_started/installation.html

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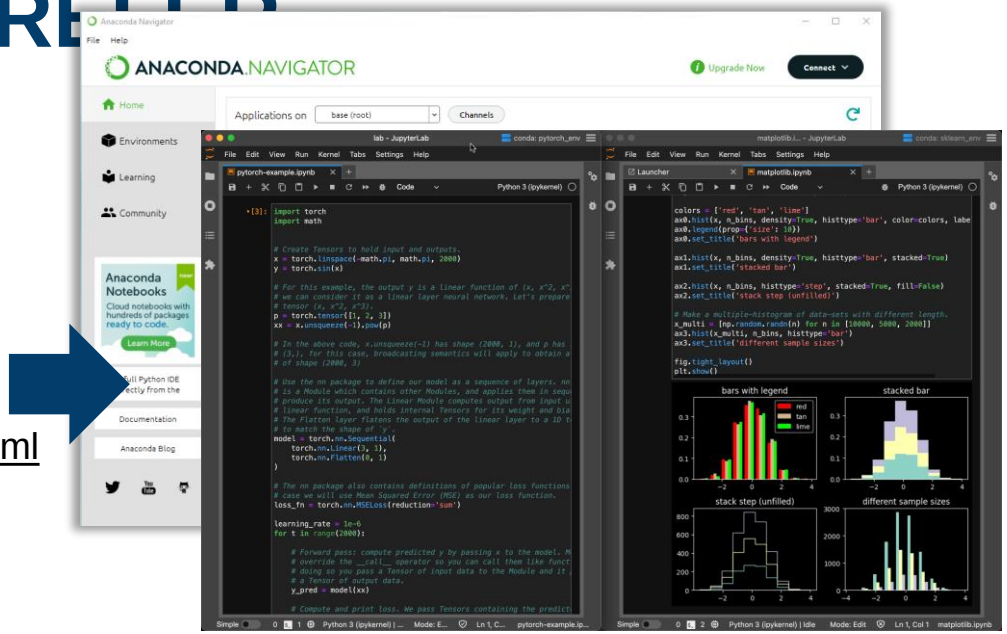

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- **JupyterLab** installed as normal desktop application **= JupyterLab Desktop**
  ➔ https://github.com/jupyterlab/jupyterlab-desktop/releases

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JUPYTERLAB - WHEREVER YOU PREFER

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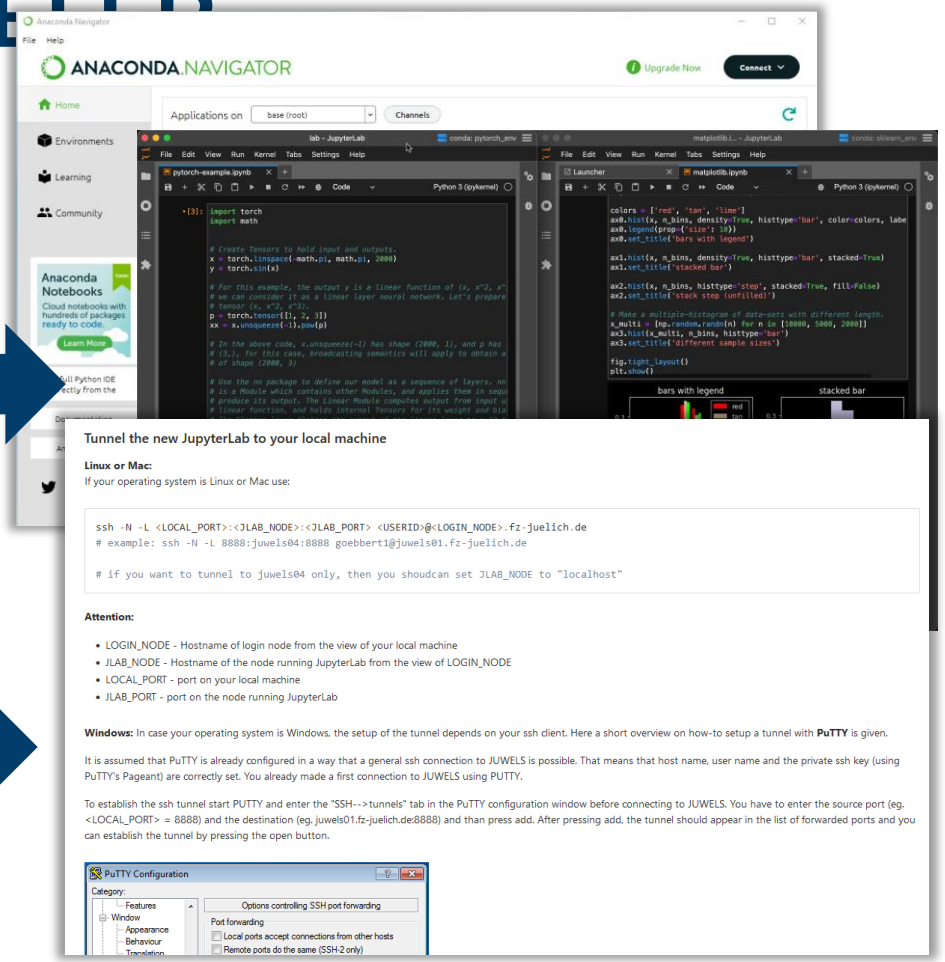

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Remote (cluster) installation:

- **JupyterLab** installed on a remote server and accessed through the browser
  - in $HOME (e.g. using pip or miniconda)
  - system-wide (e.g. with Easybuild, Spark) by the admins.

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JUPYTERLAB - WHEREVER YOU PREFER

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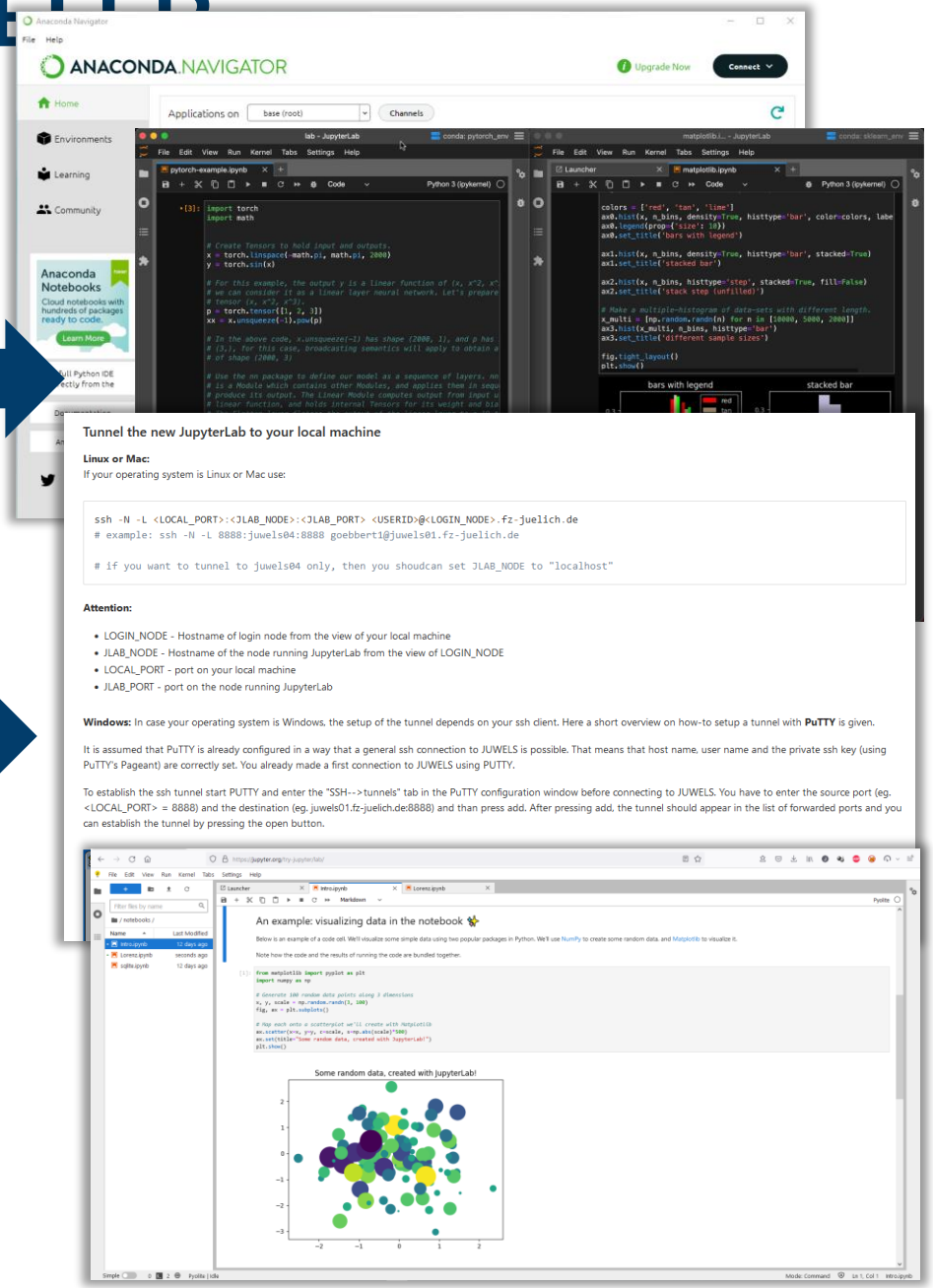
Browser-only installation (limited feature set):

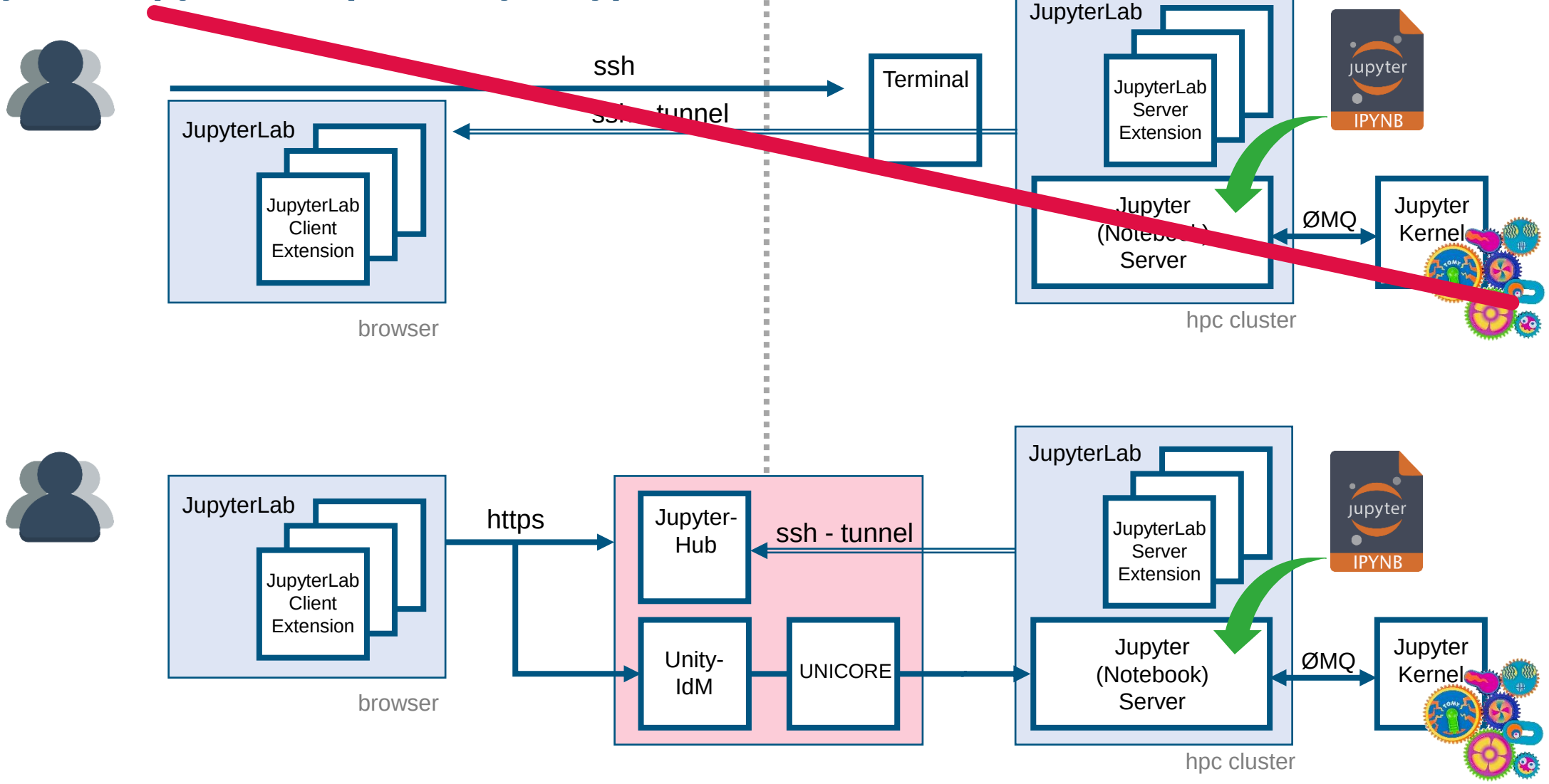
- **JupyterLab** local with server + client in your browser **= JupyterLite**
  Includes a browser-ready Python environment named Pyodide.
  ➔ https://jupyter.org/try-jupyter/lab



START & LOGIN

JUPYTER-JSC WEBSERVICE

Start your JupyterLab (the easy way)



PRE-ACCESS TODOS

1) Register & Login

- ✓ https://judoor.fz-juelich.de

2) Join a project

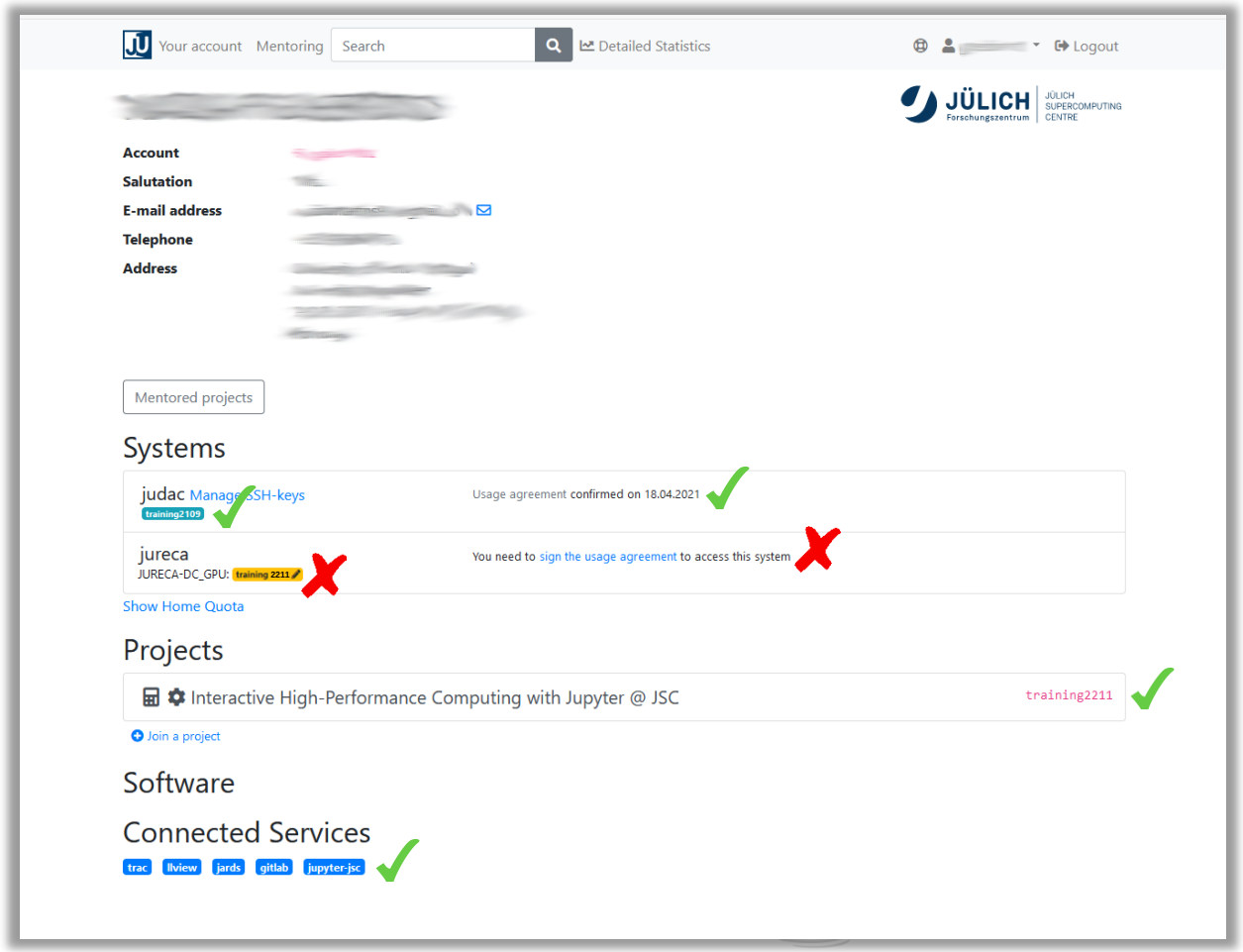
- ✓ Wait to get joined by the project PI

3) Sign usage agreement

- ✓ Wait for creation of HPC accounts

4) Check Connected Services:

- ✓ jupyter-jsc



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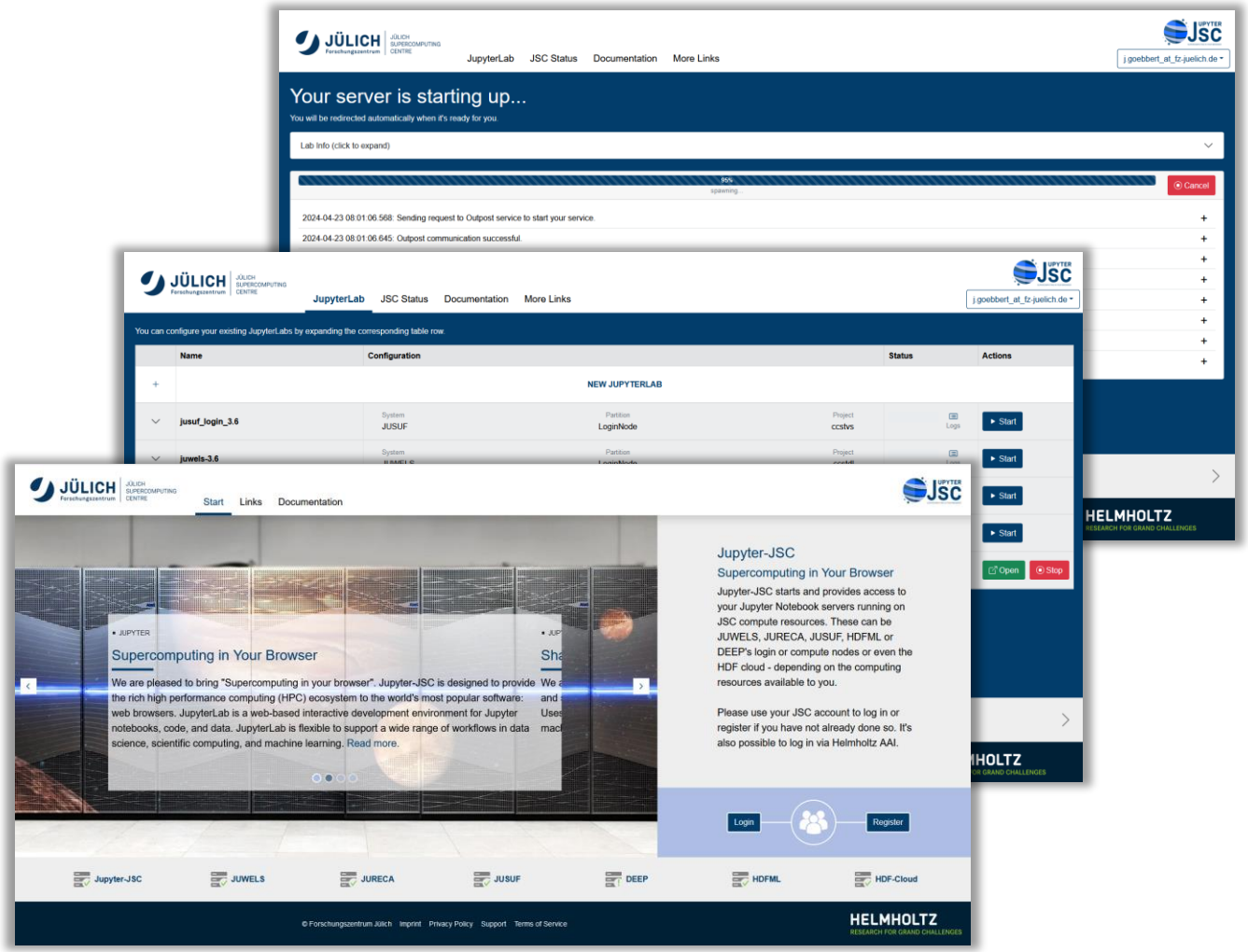
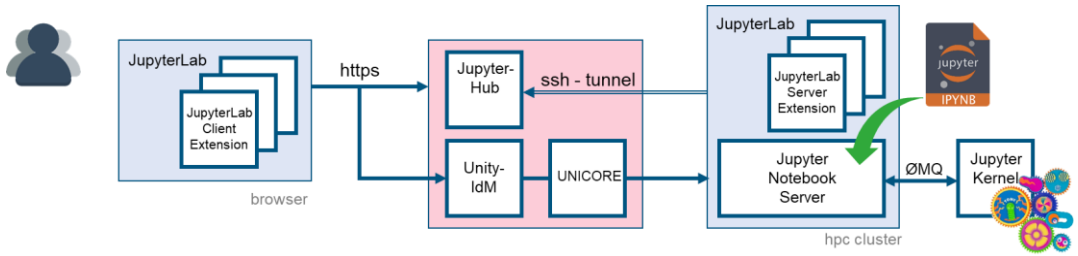
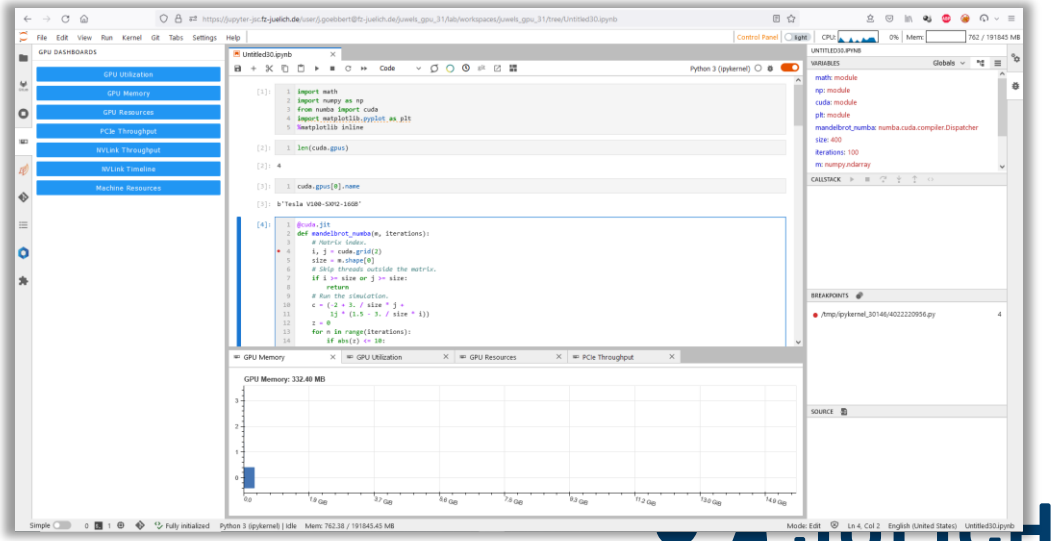
JUPYTER-JSC WEBSERVICE

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







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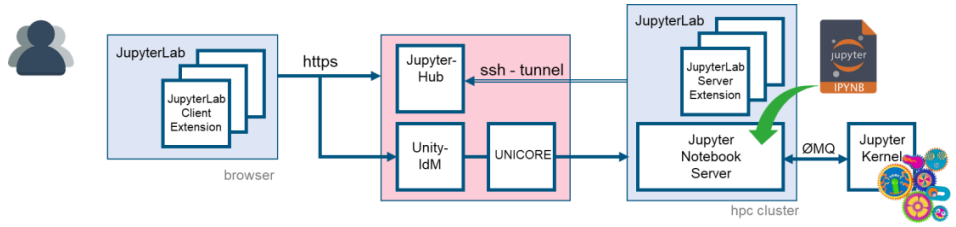
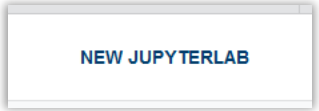
JUPYTER-JSC WEBSERVICE

Control Panel



A. New JupyterLab

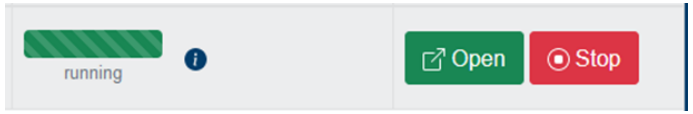


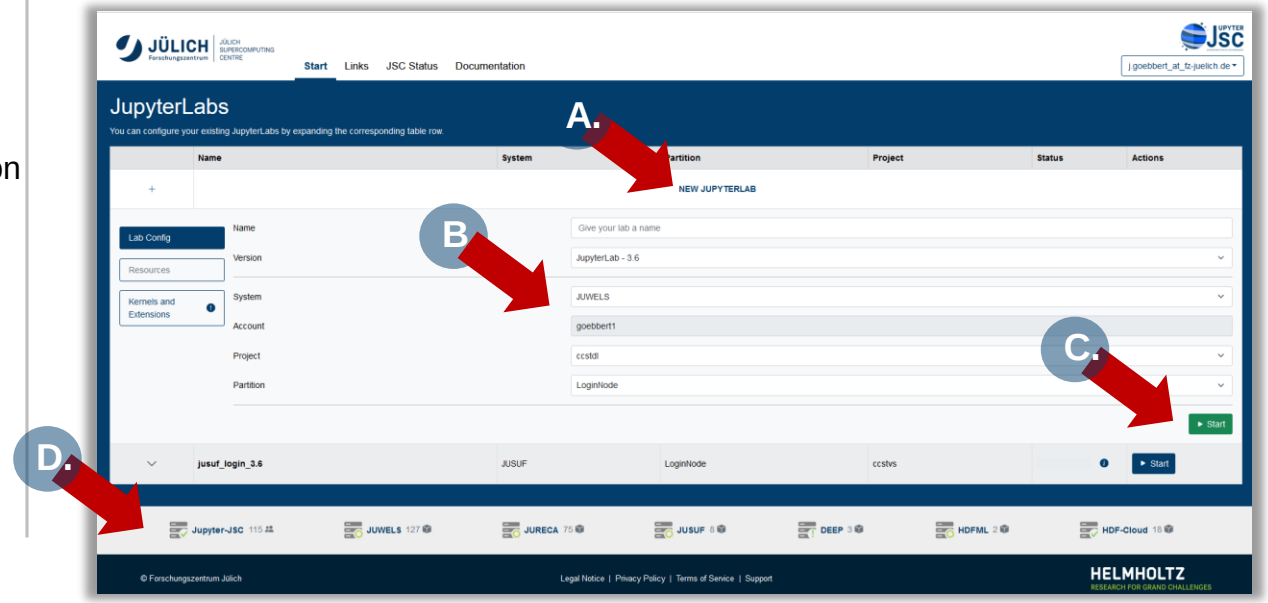
B. Configuration Dialog

- Lab Config: set Name, Version, System, Account, Project, Partition
- Resources: if running on a compute node
- Kernels and Extensions: Optional addons

C. Actions

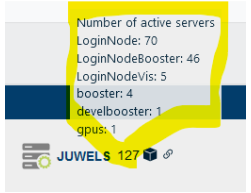
- Start/Open/Stop a JupyterLab
- Change/Delete **configuration**





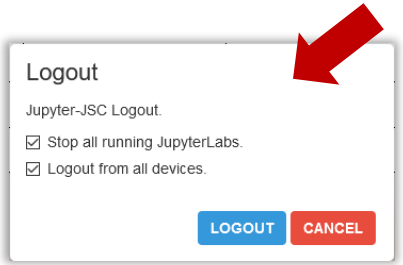
D. Statusbar

- Shows, (hover to get more details)
  - Number of active users in the last 24h
  - Number of running JupyterLabs
- Click to see system status page



E. Logout

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



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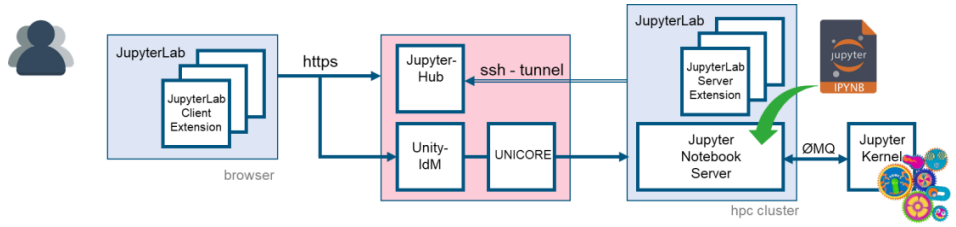
JUPYTER-JSC WEBSERVICE

JupyterLab Configuration



Jupyter-JSC – Configuration

Available options **depend on**

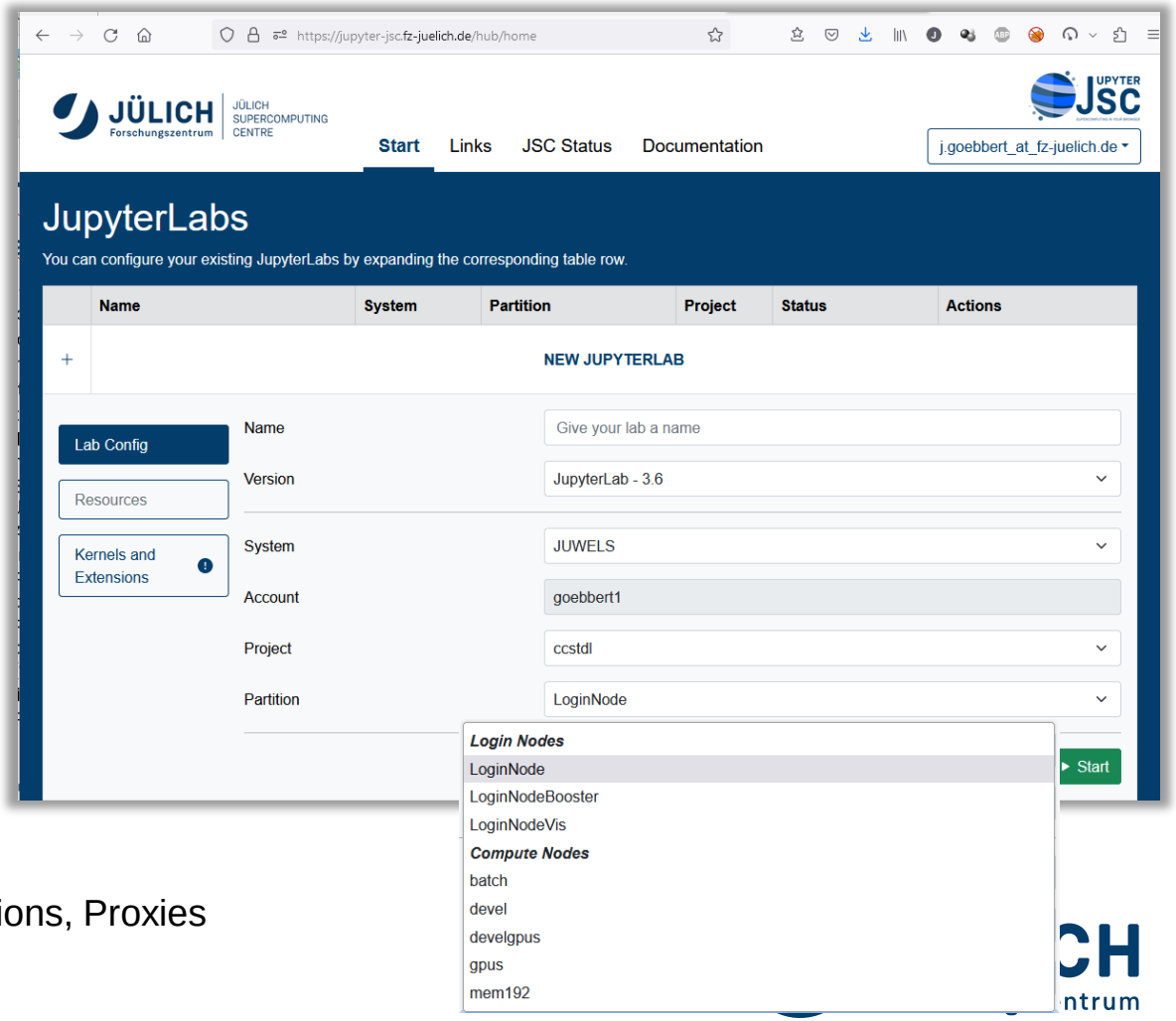
- user account settings visible in **judoor.fz-juelich.de**
- system specific usage agreement on JuDoor is signed (!!!)
- currently available systems in all of your projects

Basic options

- Version:
  multiple versions of JupyterLab are installed
- System:
  JUWELS, JURECA, JUSUF, DEEP, JSC-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)

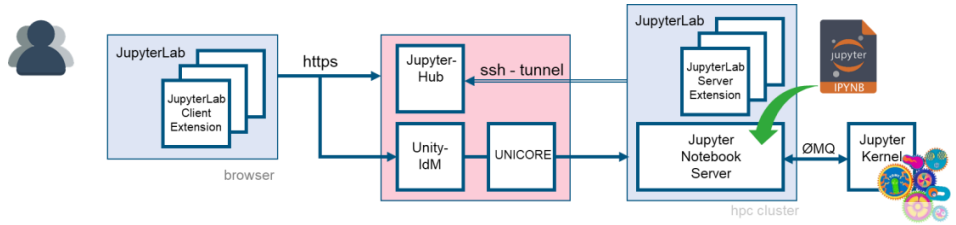
Extra options

- Partition == compute Resources
- Kernel and Extensions non-default JupyterKernel, Extensions, Proxies



JUPYTER-JSC WEBSERVICE

JupyterLab Configuration



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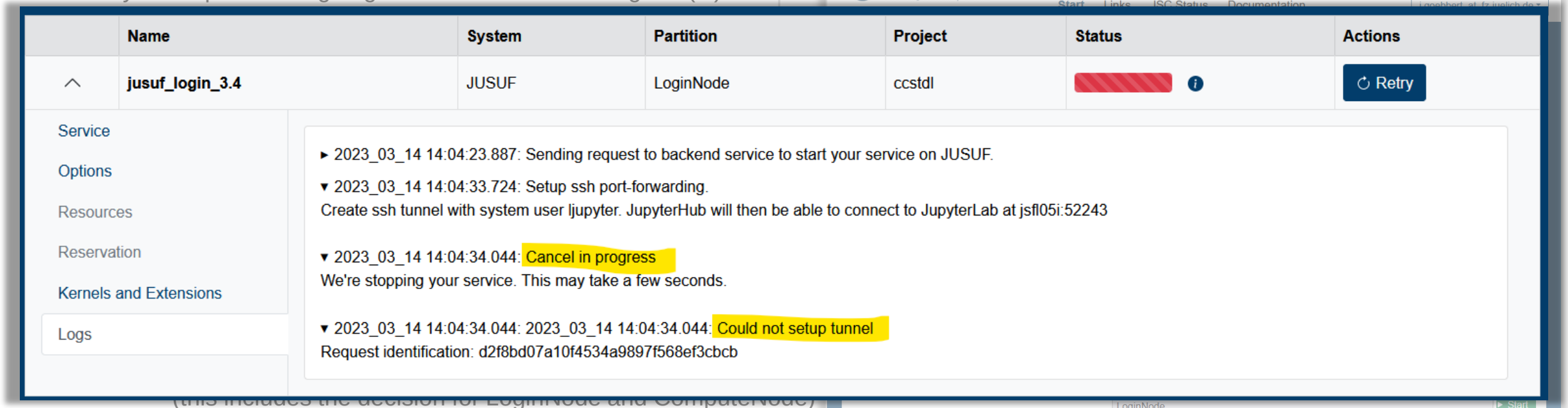
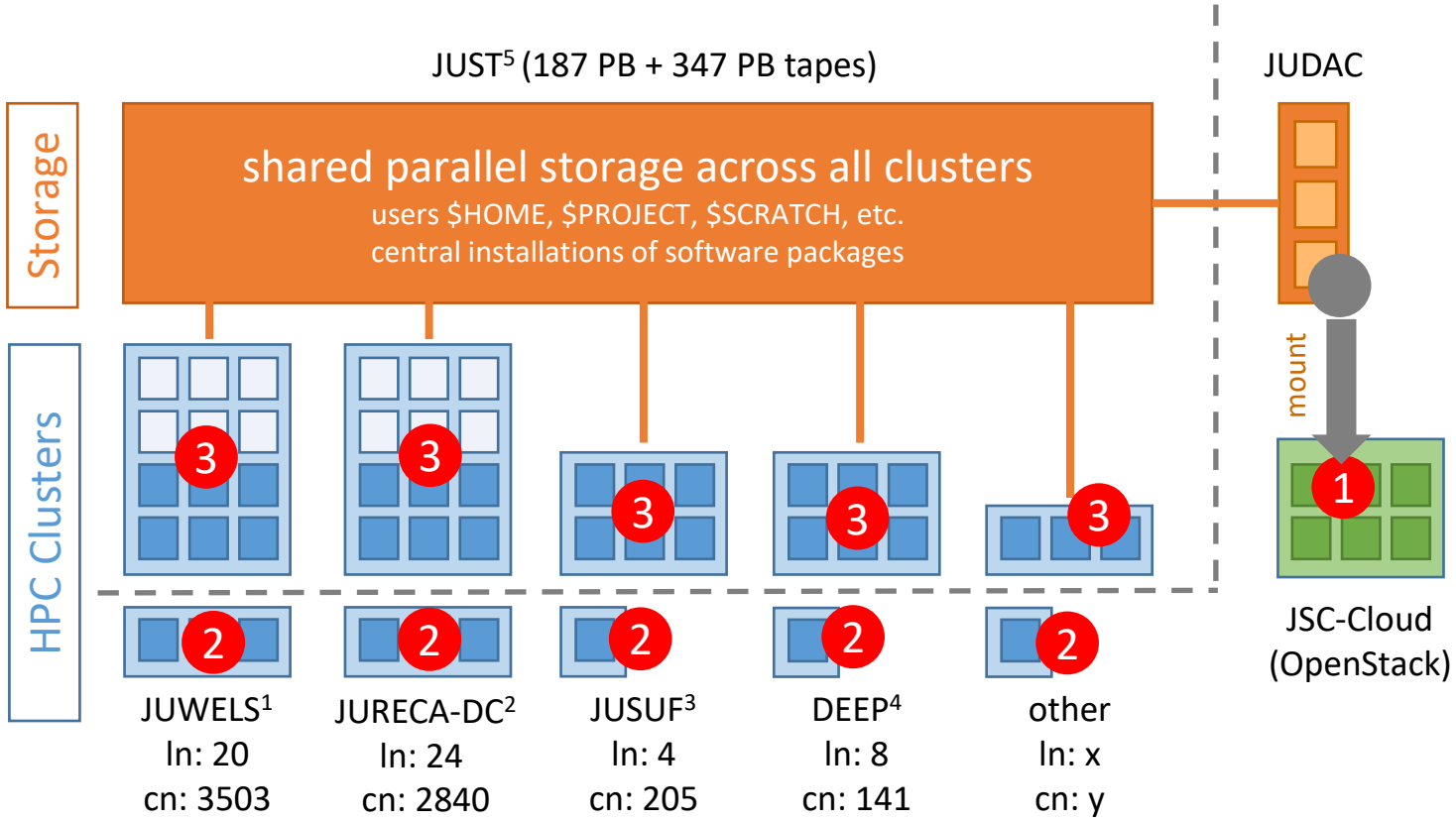


Extra options

- Partition == compute — Resources
- Kernel and Extensions — non-default JupyterKernel, Extensions, Proxies

JUPYTERLAB EVERYWHERE



JupyterLab everywhere

1. JupyterLab on cloud
2. JupyterLab on login nodes
3. JupyterLab on compute nodes

no. login nodes = ln
no. compute nodes = cn

[1] https://apps.fz-juelich.de/jsc/hps/juwels/configuration.html
[2] https://apps.fz-juelich.de/jsc/hps/jureca/configuration.html
[3] https://apps.fz-juelich.de/jsc/hps/jusuf/configuration.html
[4] https://www.fz-juelich.de/en/ias/jsc/systems/prototype-systems/deep_system
[5] https://apps.fz-juelich.de/jsc/hps/just/configuration.html

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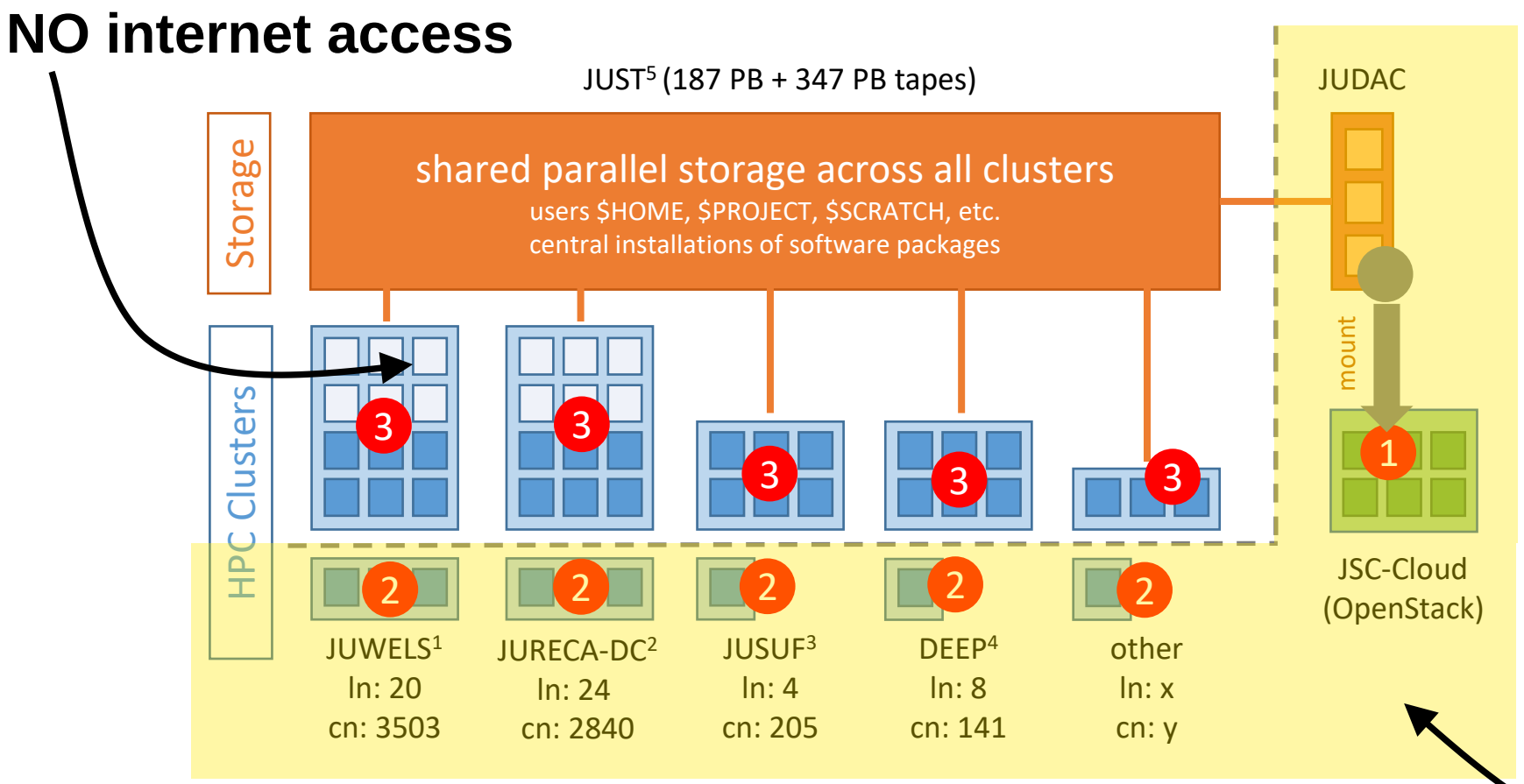
JUPYTERLAB EVERYWHERE



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[3] https://apps.fz-juelich.de/jsc/hps/jusuf/configuration.html
[4] https://www.fz-juelich.de/en/ias/jsc/systems/prototype-systems/deep_system
[5] https://apps.fz-juelich.de/jsc/hps/just/configuration.html

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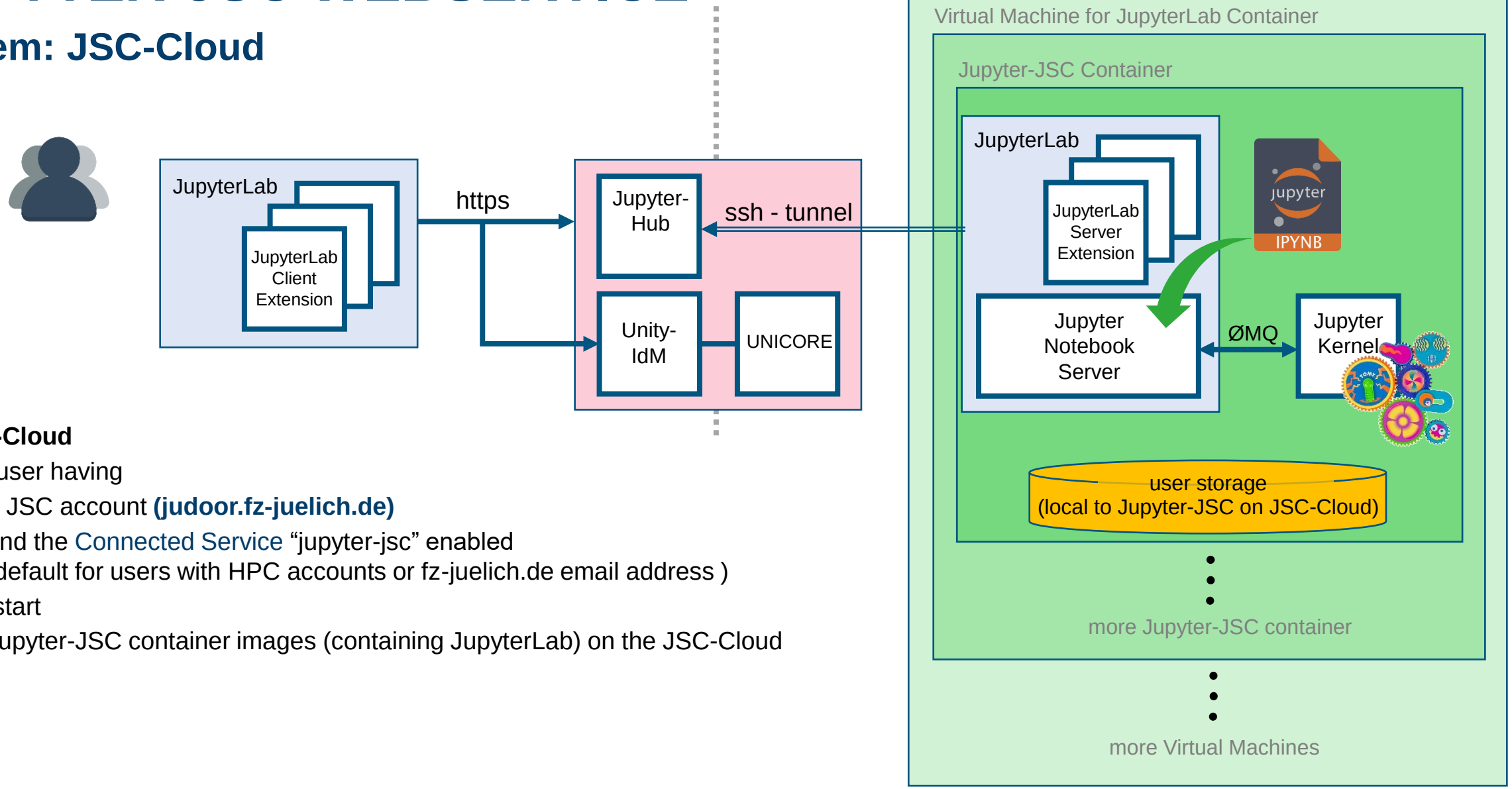
JUPYTER-JSC WEBSERVICE

System: JSC-Cloud



JSC-Cloud

Any user having

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

can start

- Jupyter-JSC container images (containing JupyterLab) on the JSC-Cloud

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

JUPYTER-JSC WEBSERVICE

System: JSC-Cloud

JSC-Cloud

Any user h

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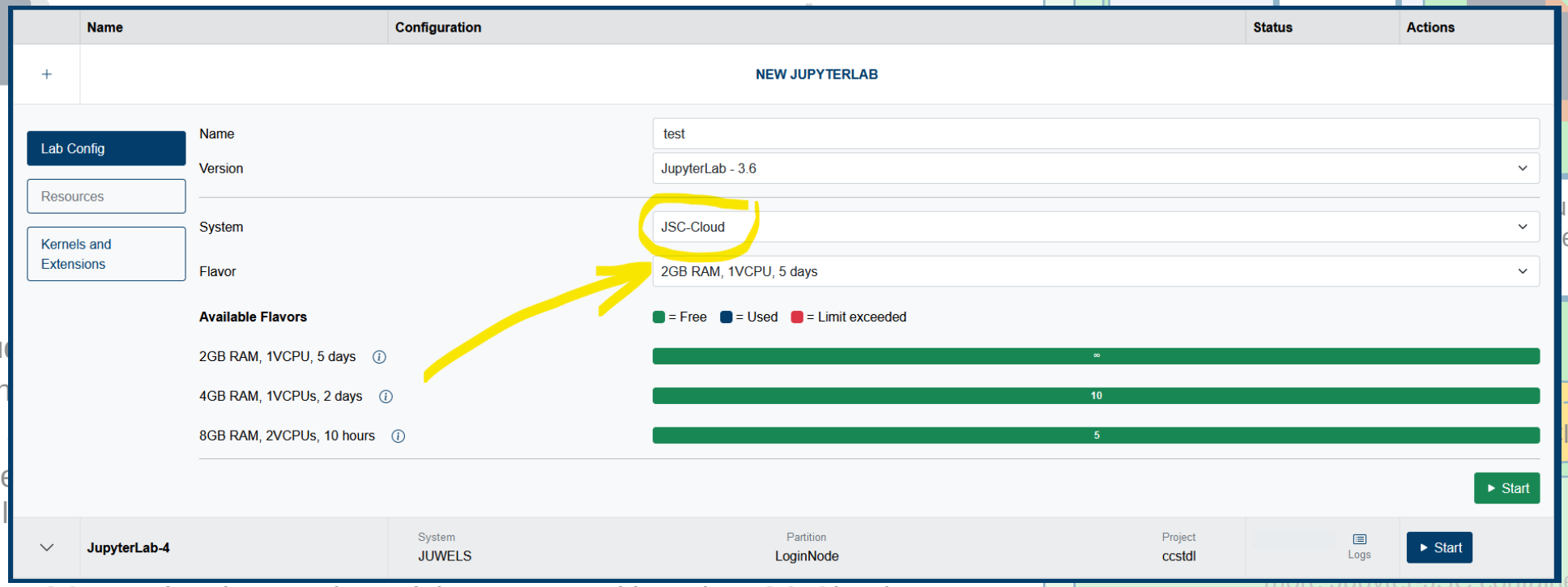
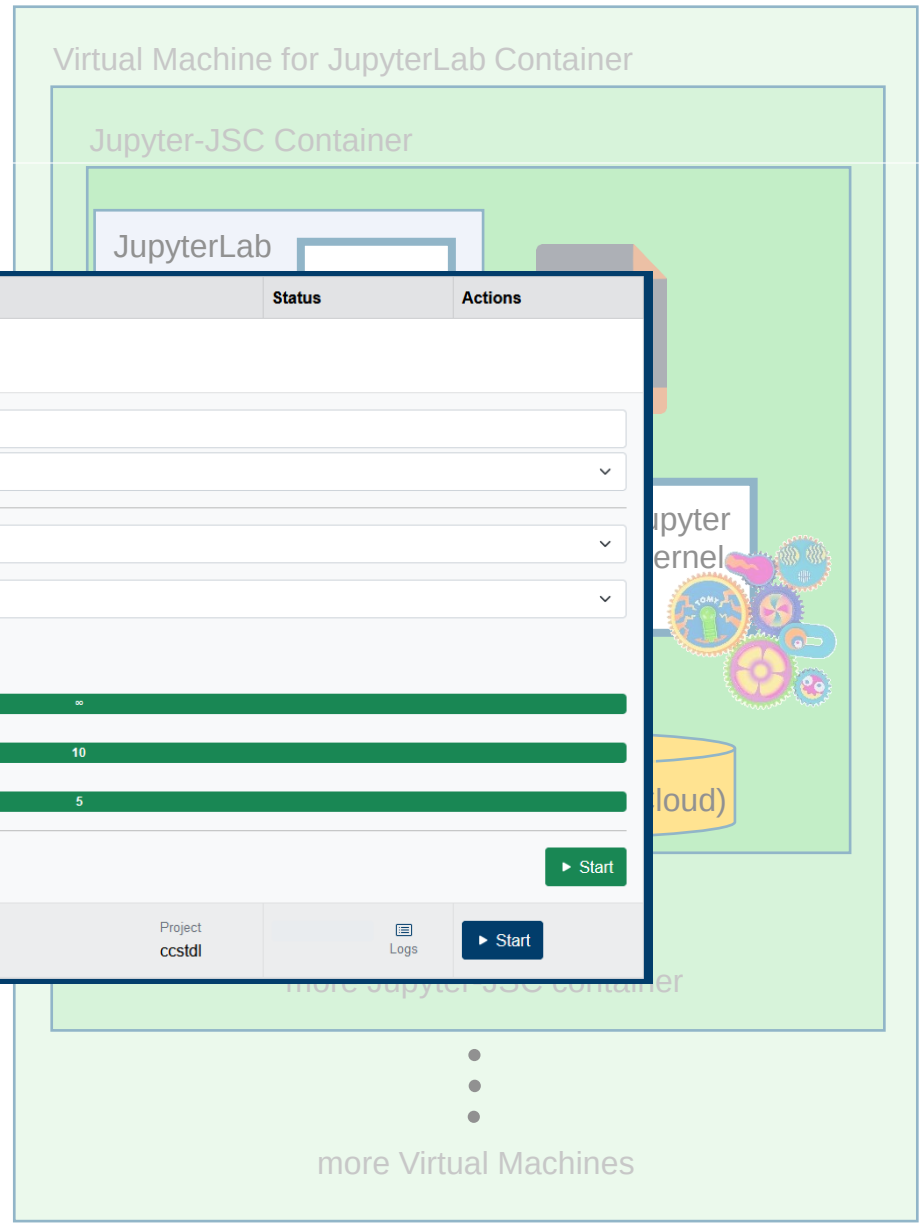
- and the (defaul

can start

- Jupyter-JSC container images (containing JupyterLab) on the JSC-Cloud





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

JUPYTER-JSC WEBSERVICE

System: JSC-Cloud

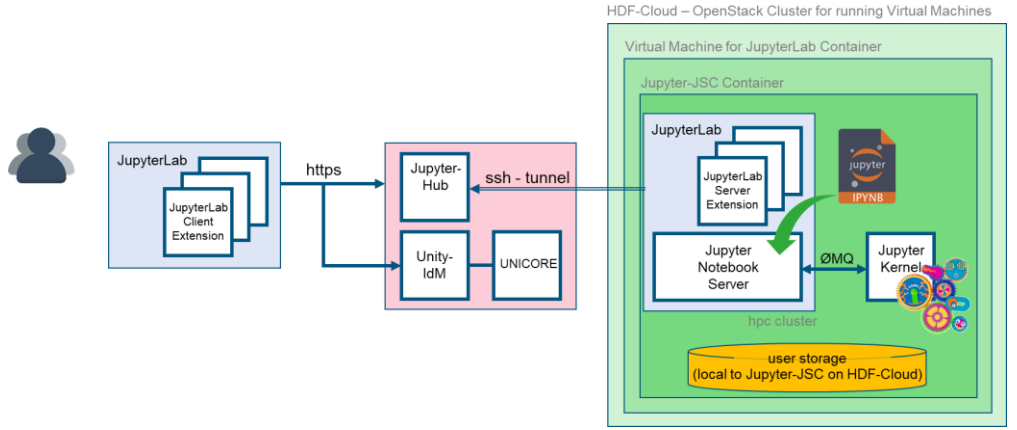
Start JupyterLab on JSC-Cloud

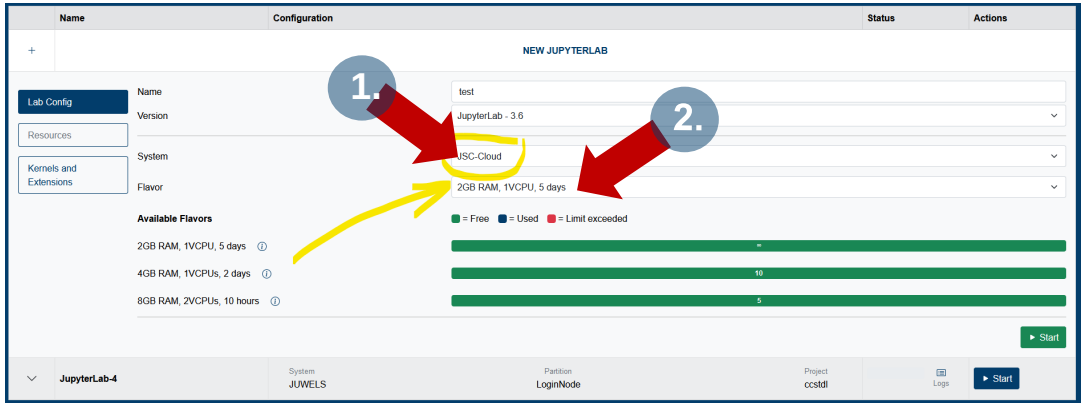
- Requirements:
  - Registered JSC account at https://judoor.fz-juelich.de
  - Logged in to Jupyter-JSC at https://jupyter-jsc.fz-juelich.de
  - Named a new JupyterLab configuration

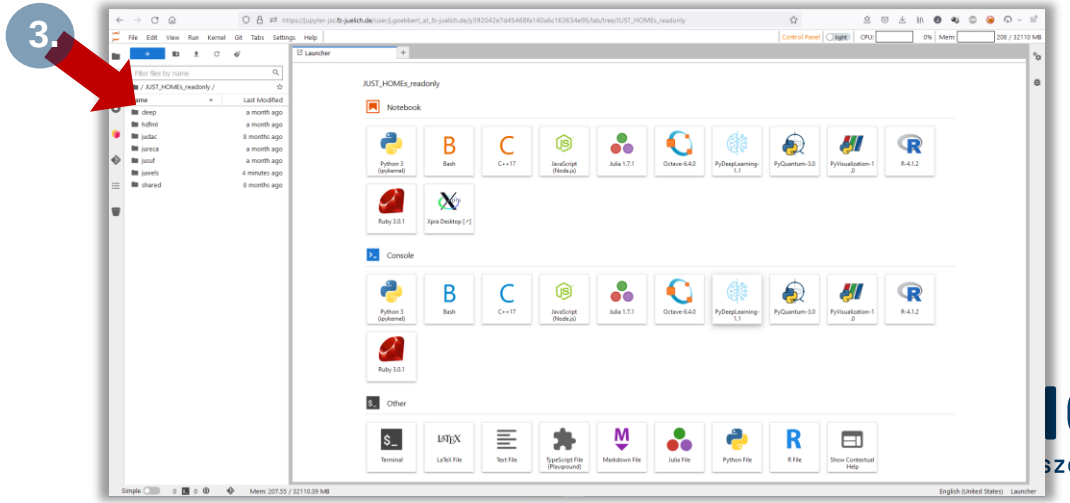
- Start a JupyterLab:
  - Version == “JupyterLab 4.2”
  - System == “JSC-Cloud”

Limitations on JupyterLab on JSC-Cloud

- max. memory depends on chosen flavor
  - ATTENTION:
    the container automatically stops,
    when more memory is used
- Storage in Jupyter-JSC container
  - **is local** to the JSC-Cloud and persistent
  - HPC $HOMEs are mounted read-only
    (but can be mounted read-write)
- **There is no flavor with GPUs, yet**







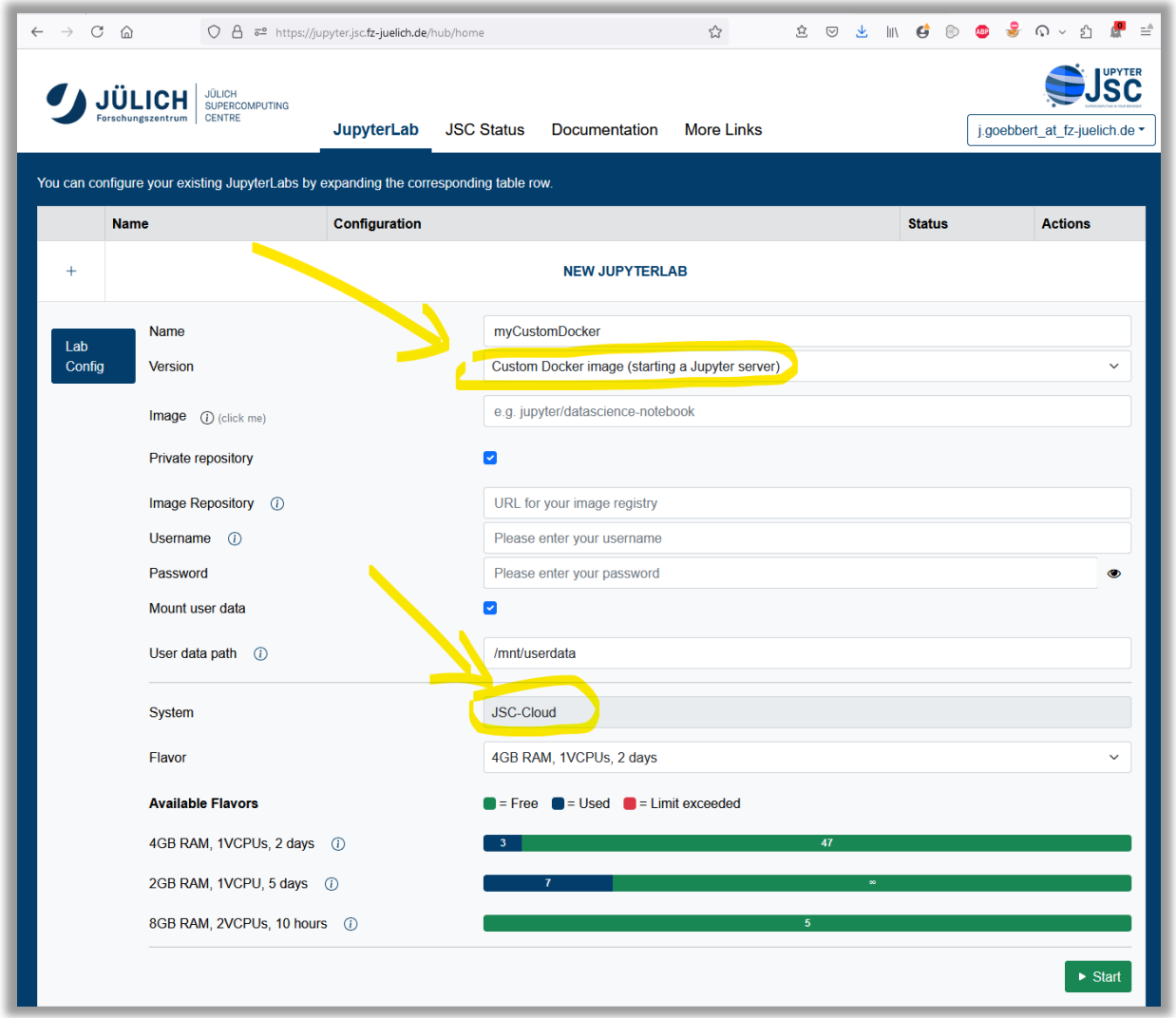
JUPYTER-JSC WEBSERVICE

System: JSC-Cloud

Custom Docker image on the JSC-Cloud

- Requirements:
  - Custom docker image must start a Jupyter server

- Examples:
  - https://jupyter-docker-stacks.readthedocs.io/en/latest/using/selecting.html



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JUPYTER-JSC WEBSERVICE

System: JSC-Cloud

Custom Docker image on the JSC-Cloud

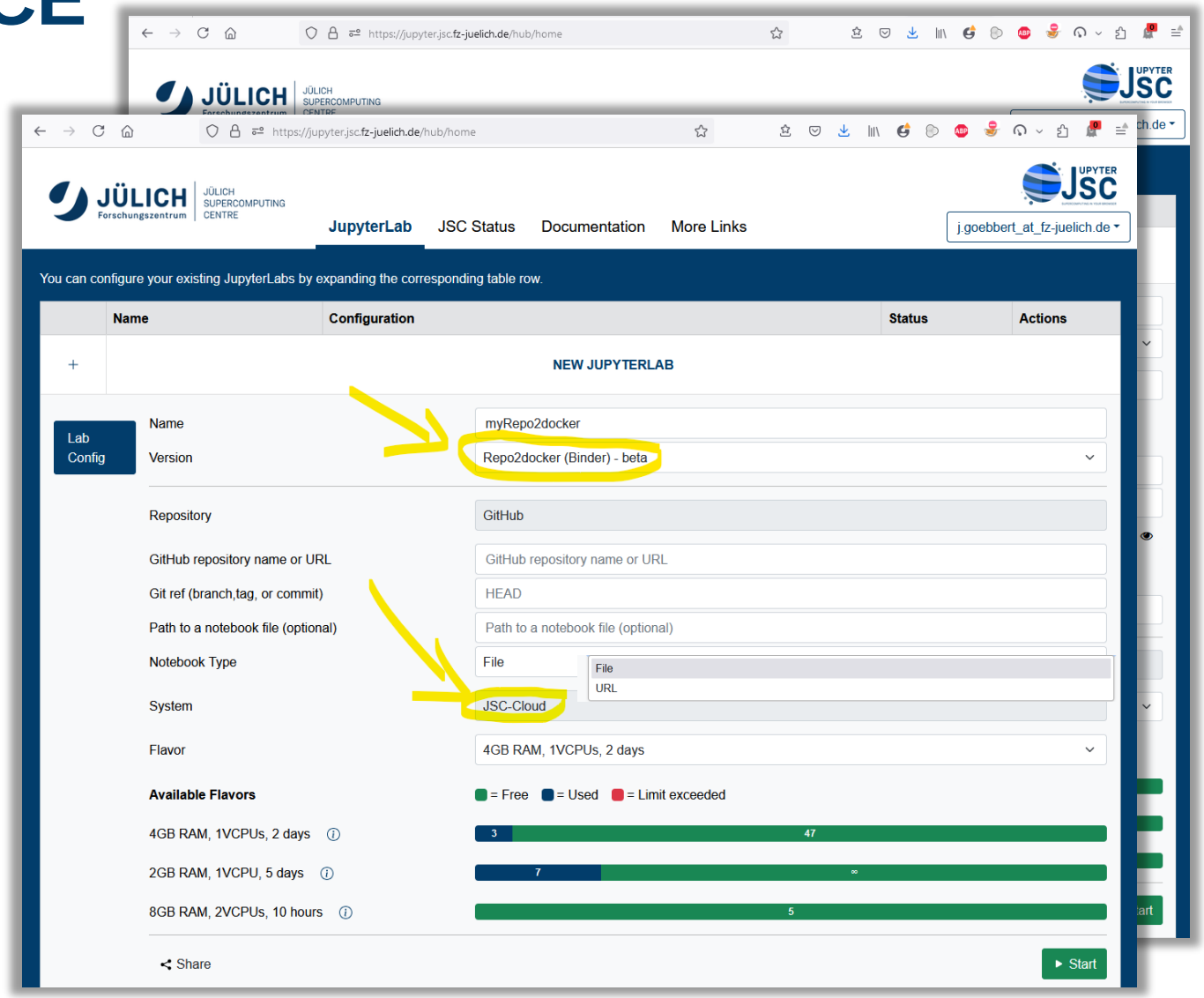
- Requirements:
  - Custom docker image must start a Jupyter server

- Examples:
  - https://jupyter-docker-stacks.readthedocs.io/en/latest/using/selecting.html

Repo2Docker (Binder) on the JSC-Cloud

- Requirements:
  - Repository compatible with repo2docker

- Details:
  - https://repo2docker.readthedocs.io/en/latest/configuration/index.html



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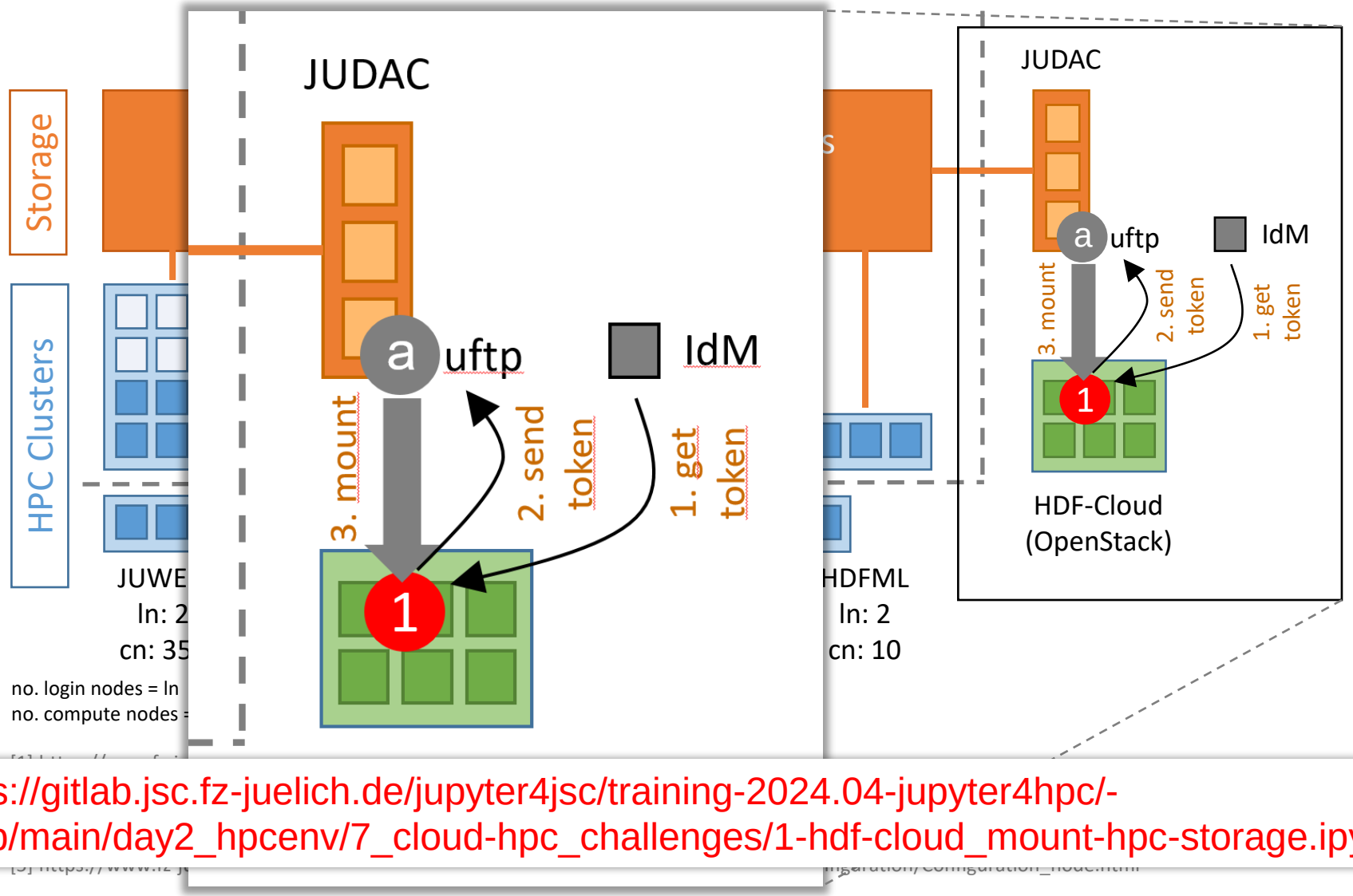
HOW TO MOUNT GPFS ON HDF-CLOUD



https://gitlab.jsc.fz-juelich.de/jupyter4jsc/training-2024.04-jupyter4hpc/-/blob/main/day2_hpcenv/7_cloud-hpc_challenges/1-hdf-cloud_mount-hpc-storage.ipynb

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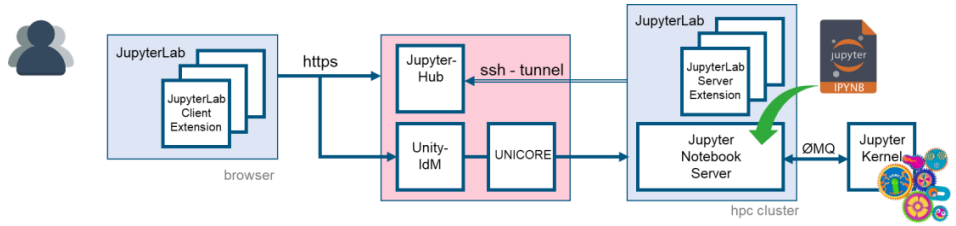
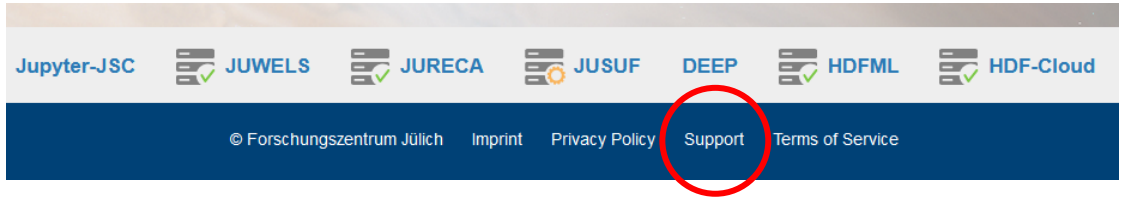
JUPYTER-JSC SECRETS

Very important to know



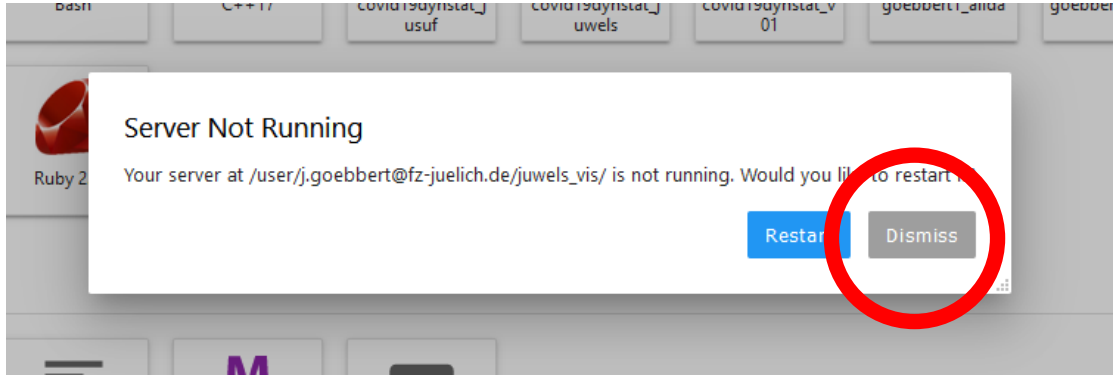
Secret 1: Support button

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

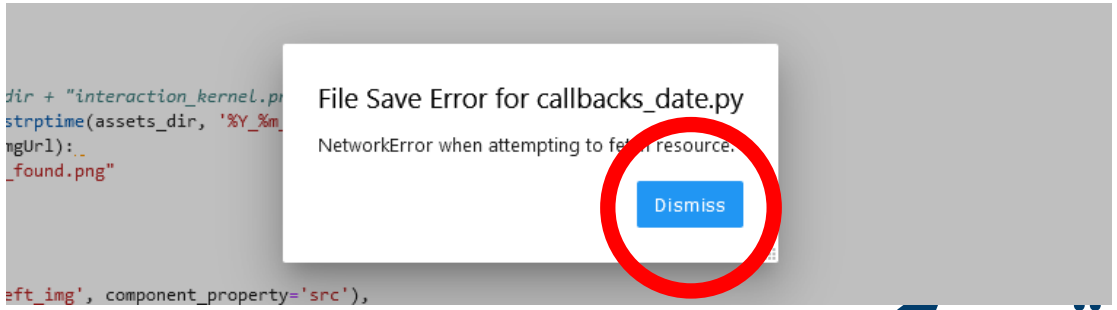


Secret 2: Reload on connection loss

- "Server Not Running"
  means, that your browser just lost connection
  => **Just hit "Dismiss" !!!**
  (as soon as you are online again)



- "File Save Error for <…>"
  means, that your browser just lost connection
  => **Just hit "Dismiss" !!!**
  (as soon as you are online again)



You can **always** safely hit the "Reload" button of your browser, if the connection to JupyterLab ever gets lost.
(it will just restart JupyterLab on the browser-site)

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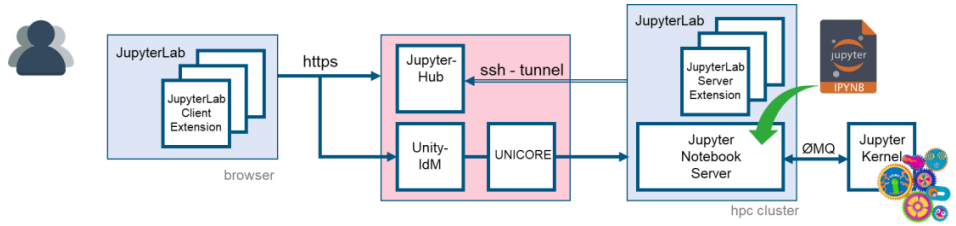
JUPYTER-JSC SECRETS

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 prepare the environment for JupyterLab.
  This script must ensure that the command `jupyter` is available in $PATH.

```
#!/bin/bash

module purge
module load Stages/2024
module load GCCcore/.12.3.0
module load Jupyter-bundle/20240520
```

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

It enables you to switch to an older/newer/other version of JupyterLab,
if the default one gives you trouble or is missing features.

https://gitlab.jsc.fz-juelich.de/jupyter4jsc/j4j_notebooks/-/blob/documentation/03-HowTos/Create_JupyterKernel_general.ipynb

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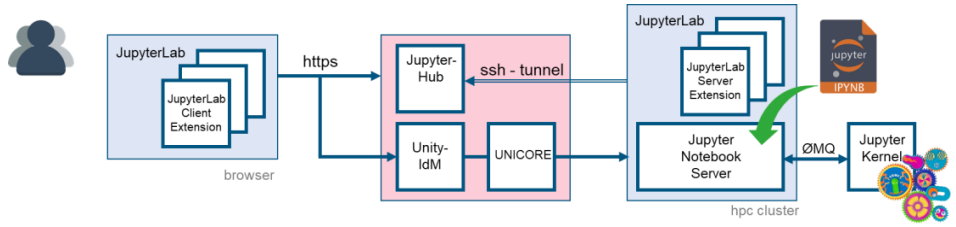
JUPYTER-JSC WEBSERVICE

Some comments about the UI



open filebrowser

open launcher

type of active notebook cell

no close, but go back to Jupyter-JSC´s controll panel

memory consuption (keep an eye on that!)

tutorials & examples

Type of Jupyter kernel this notebook is connected to (click to change)

sidebar with core and extentions features

[*] indicates that cell was send to Jupyter kernel for execution

notebook cell

indicates active notebook cell

[ ] indicates that cell has never been executed by the connected Jupyter kernel

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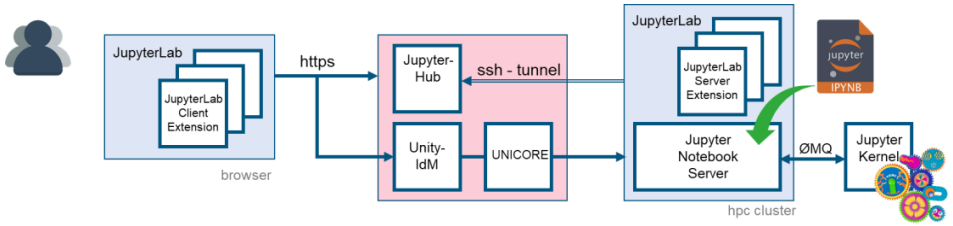
JUPYTERLAB EXTENSIONS

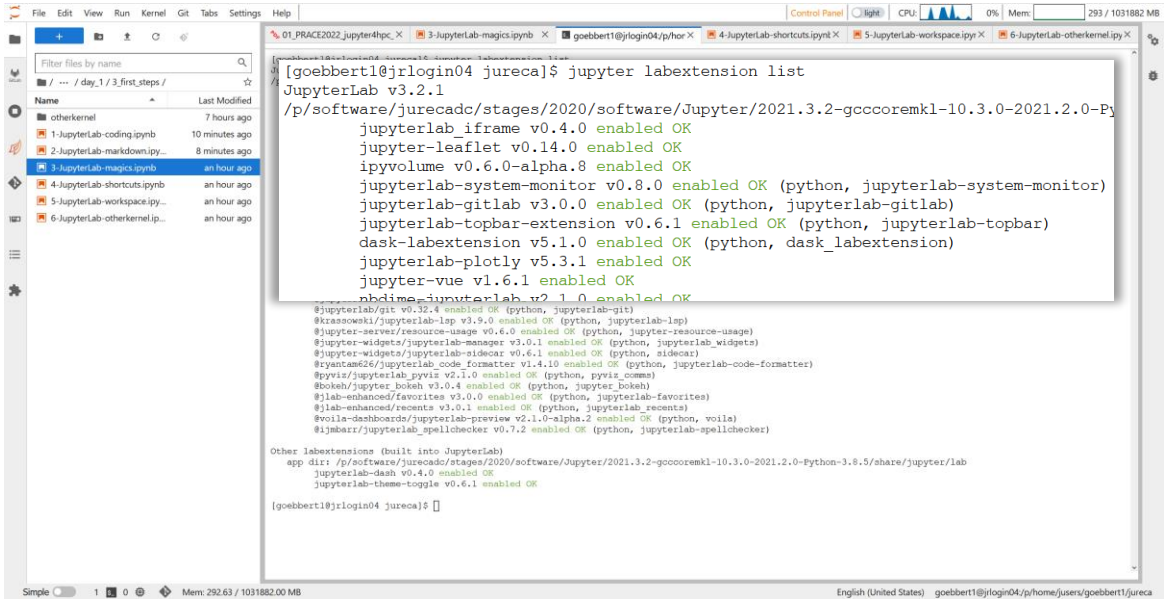
JUPYTERLAB EXTENSIONS

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
  - contains the JupyterLab static assets
    - (e.g. `static/index.html`)
  - **JupyterLab < 3:**
    any change requires a rebuild of the whole JupyterLab to take effect!
  - **JupyterLab >= 3:**
    introduced prebuild extensions, which are loaded at startup time

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

Hint: JupyterLab Playground

A JupyterLab extension to write and load simple JupyterLab plugins inside JupyterLab.

https://github.com/jupyterlab/jupyterlab-plugin-playground

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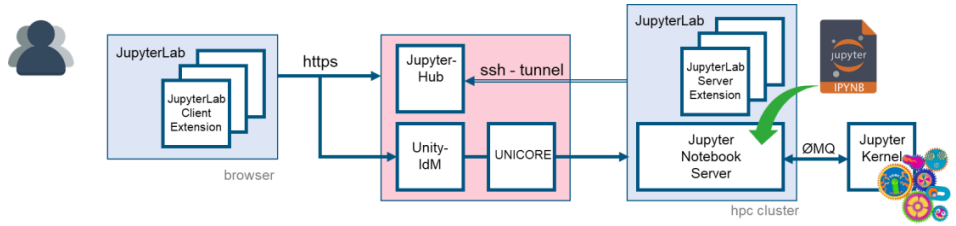
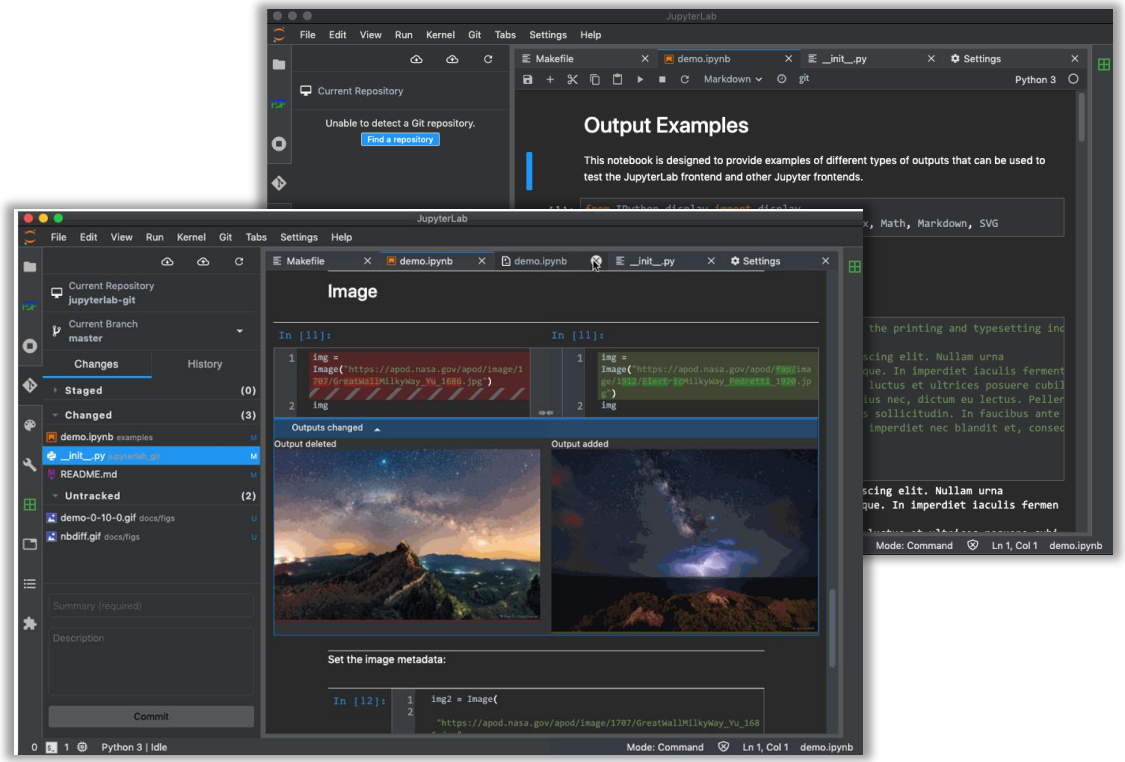
JUPYTERLAB EXTENSIONS

Installed by default at Jupyter-JSC



JupyterLab-Git

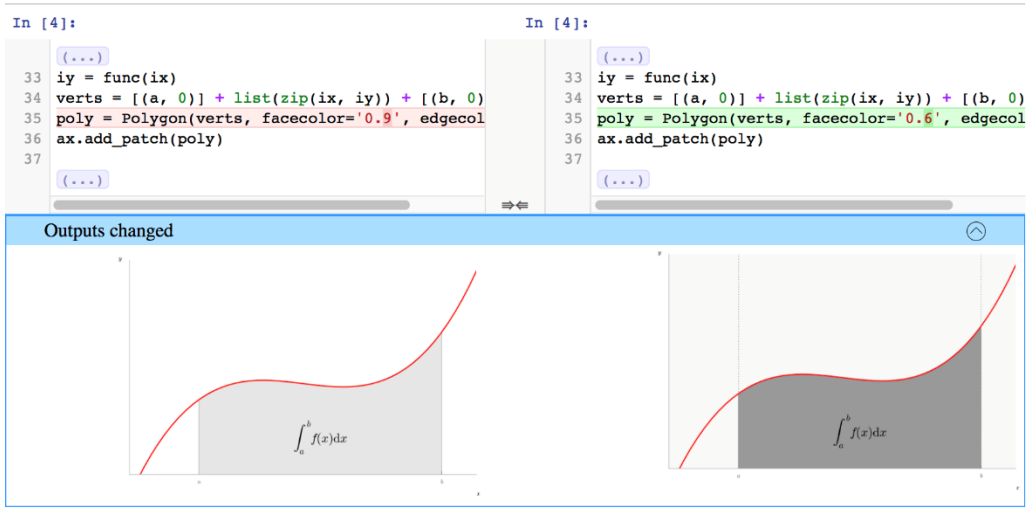
JupyterLab extension for version control using Git



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

NBDime

Tools for diffing and merging of Jupyter notebooks.



https://github.com/jupyter/nbdime

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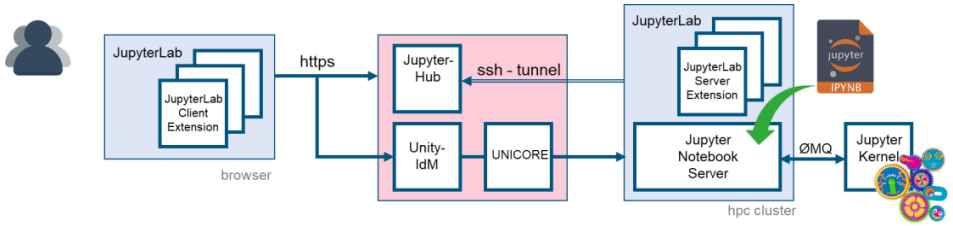
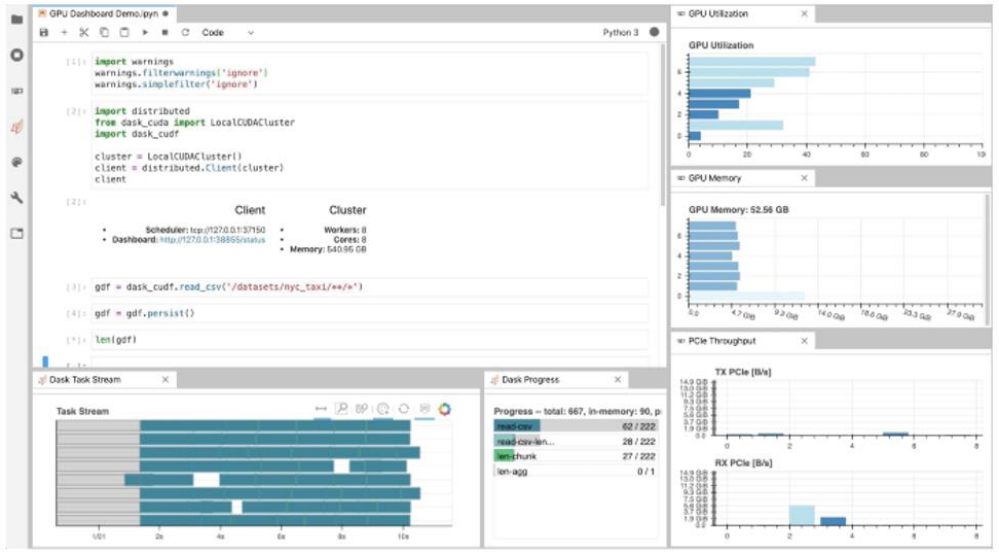
JUPYTERLAB EXTENSIONS

Installed by default at Jupyter-JSC



NVDashboard

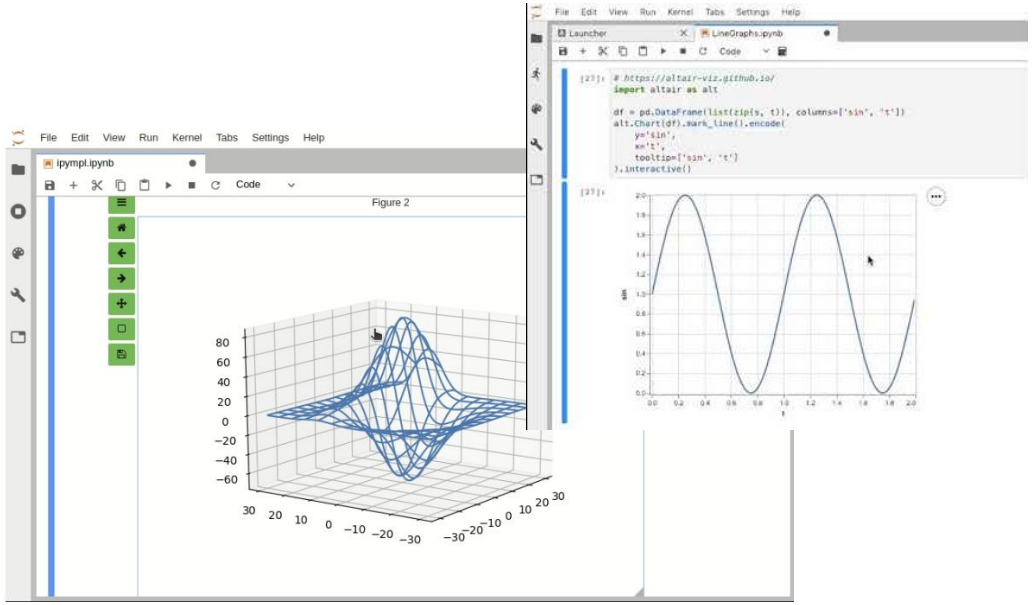
NVDashboard is an open-source package for the real-time visualization of NVIDIA GPU metrics in interactive Jupyter Lab environments.



https://github.com/rapidsai/jupyterlab-nvdashboard
https://developer.nvidia.com/blog/gpu-dashboards-in-jupyter-lab/

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

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JUPYTERLAB EXTENSIONS

Installed by default at Jupyter-JSC

Core packages	Version	Link	Description
jupyterlab	4.2.1	https://jupyterlab.readthedocs.io	-
notebook	7.2.0	https://jupyter-notebook.readthedocs.io	Jupyter Notebook as a Jupyter Server extension
jupyterlab_server	2.27.1	https://jupyterlab-server.readthedocs.io	Server components for JupyterLab applications
jupyterhub	4.1.5	https://jupyterhub.readthedocs.io	Multi-user server for Jupyter notebooks

Optional extension	Version	Link	Description
jupyterlab-nvdashboard	0.10.0	https://github.com/rapidsai/jupyterlab-nvdashboard , eb-file	A JupyterLab extension for displaying dashboards of GPU usage.
jupyter-slurm-provisioner	0.6.0	https://github.com/FZJ-JSC/jupyter-slurm-provisioner , eb-file	Allows to start Jupyter kernels as a SLURM job remote from the Jupyter server
nglview	3.1.2	http://nglviewer.org/nglview/latest/ , eb-file	Jupyter widget to interactively view molecular structures and trajectories
jupyter-ai	2.15.0	https://jupyter-ai.readthedocs.io/ , eb-file	A generative AI extension for JupyterLab

Core Kernels	Version	Link	Description
Bash	0.9.3	https://github.com/takluyver/bash_kernel , eb-file	A bash kernel for IPython
Cling (C++)	20231018	https://github.com/root-project/cling/ , eb-file	Jupyter kernel for the C++ programming language
Julia	1.9.5	https://github.com/JuliaPy/pyjulia , eb-file	python interface to julia
LFortran	0.30.0	https://lfortran.org/ , eb-file	Modern interactive LLVM-based Fortran compiler
Octave	8.4.0	https://www.octave.org/ , eb-file	Scientific Programming Language - Powerful mathematics-oriented syntax with built-in 2D/3D plotting and visualization tools
R	4.3.2	https://irkernel.github.io , eb-file	R kernel for Jupyter
Ruby	3.2.2	https://github.com/SciRuby/iruby , eb-file	Ruby kernel for Jupyter

Community Kernels	Version	Link	Description
DeepLearning	2024.3	eb-file	Python kernel incl. a collection of extra modules/packages for Deep Learning
PyEarthSystem	2024.3	eb-file	Python kernel incl. a collection of extra modules/packages for the Earth System community
QuantumComputing	2024.5	eb-file	Python kernel incl. a collection of extra modules/packages for the quantum computing community
Visualization	2024.3	eb-file	Python kernel incl. a collection of extra modules/packages for visualization

JupyterLab Applications	Version	Link	Description
Xpra	5.0.8	https://xpra.org eb-file	Remote desktop for X11 applications in the browser

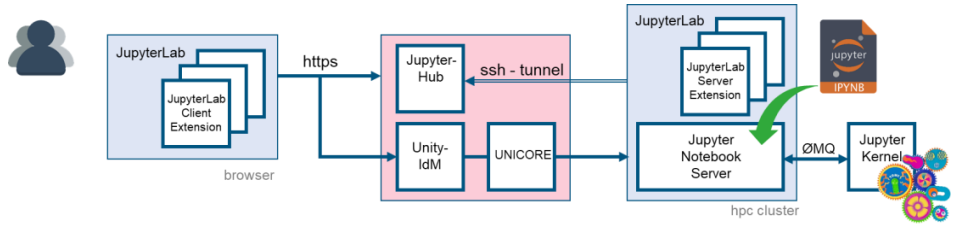
Core Extensions	Version	Link	Description
jupyter-server-proxy	4.1.2	https://jupyter-server-proxy.readthedocs.io	Jupyter notebook server extension to proxy web services.
jupyterlab-lsp	5.1.0	https://github.com/jupyter-lsp/jupyterlab-lsp	Coding assistance for JupyterLab using Language Server Protocol
ipympl	0.9.4	https://matplotlib.org/ipympl/	Interactive features of matplotlib in Jupyter
ipyleaflet	0.19.1	https://ipyleaflet.readthedocs.io	Interactive maps in the Jupyter notebook
bqplot	0.13.0rc0	https://bqplot.github.io/bqplot/	Plotting library for IPython/Jupyter notebooks
jupyterlab_gitlab	4.0.0	https://github.com/jupyterlab-contrib/jupyterlab-gitlab	A JupyterLab extension for browsing GitLab repositories
jupyterlab_git	0.50.1	https://github.com/jupyterlab/jupyterlab-git	A Git extension for JupyterLab
nbdime	4.0.1	https://nbdime.readthedocs.io/	Tools for diffing and merging of Jupyter notebooks.
jupyterlab_latex	4.0.0	https://github.com/jupyterlab/jupyterlab-latex	JupyterLab extension for live editing of LaTeX documents
plotly	5.22.0	https://plotly.com/python/	Python graphing library for interactive, publication-quality graphs.
jupyter_bokeh	4.0.4	https://github.com/bokeh/jupyter_bokeh	An extension for rendering Bokeh content in JupyterLab notebooks
panel	1.3.8	https://panel.holoviz.org/	The powerful data exploration & web app framework for Python
holoviews	1.18.3	https://holoviews.org/	With Holoviews, your data visualizes itself.
jupyterlab_h5web	12.1.0	https://github.com/silx-kit/jupyterlab-h5web	Open and explore HDF5 files in JupyterLab. Can handle very large (TB) sized files, and datasets of any dimensionality
ipyparallel	8.8.0	https://ipyparallel.readthedocs.io	IPython Parallel: Interactive Parallel Computing in Python
dask_labextension	7.0.0	https://github.com/dask/dask-labextension	JupyterLab extension for Dask
voila	0.5.7	https://voila.readthedocs.io	Voilà turns Jupyter notebooks into standalone web applications
nbdev	2.3.25	https://nbdev.fast.ai/	Create delightful software with Jupyter Notebooks
sidecar	0.7.0	https://github.com/jupyter-widgets/jupyterlab-sidecar	A sidecar output widget for JupyterLab
dash	2.17.0	https://plotly.com/dash	Data Apps & Dashboards for Python. No JavaScript Required.
jupyterlab-spellchecker	0.8.4	https://github.com/jupyterlab-contrib/spellchecker	Spellchecker for JupyterLab notebook markdown cells and file editor.
jupyterlab-favorites	3.2.1	https://github.com/NERSC/jupyterlab-favorites	Add the ability to save favorite folders to JupyterLab for quicker browsing
jupyterlab-resource-usage	1.0.2	https://github.com/jupyter-server/jupyter-resource-usage	JupyterLab extension to for monitoring your own resource Usage
jupyterlab-tour	4.0.1	https://github.com/jupyterlab-contrib/jupyterlab-tour	A JupyterLab UI tour built on jupyterlab-tutorial and react-joyride.
papermill	2.5.0	https://papermill.readthedocs.io	Parameterize, execute, and analyze notebooks
pyunicore	1.0.0	https://github.com/HumanBrainProject/pyunicore	UNICORE REST bindings for python

https://gitlab.jsc.fz-juelich.de/jupyter4jsc/j4j_notebooks/-/blob/documentation/05-News&Updates/Announcement-2024-06_JupyterLab4.2-Upgrade.ipynb

JUPYTER KERNEL

JUPYTER KERNEL

How to create your own Juypter Kernel



Jupyter Kernel

A “kernel” refers to the separate process wh

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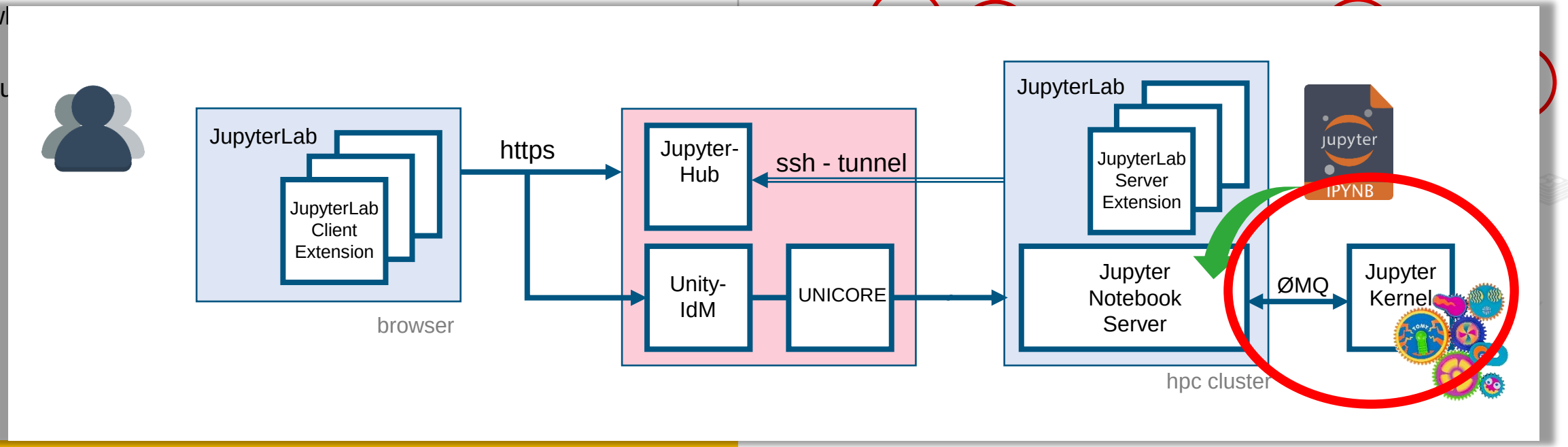

You can easily **create your own kernel** which for example runs your specialized virtual Python environment.

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

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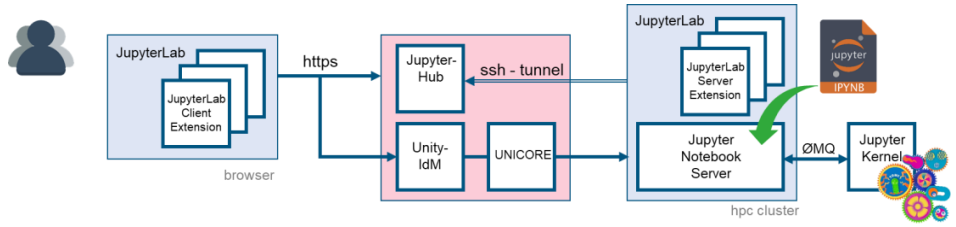
JUPYTER KERNEL

How to create your own Juypter Kernel



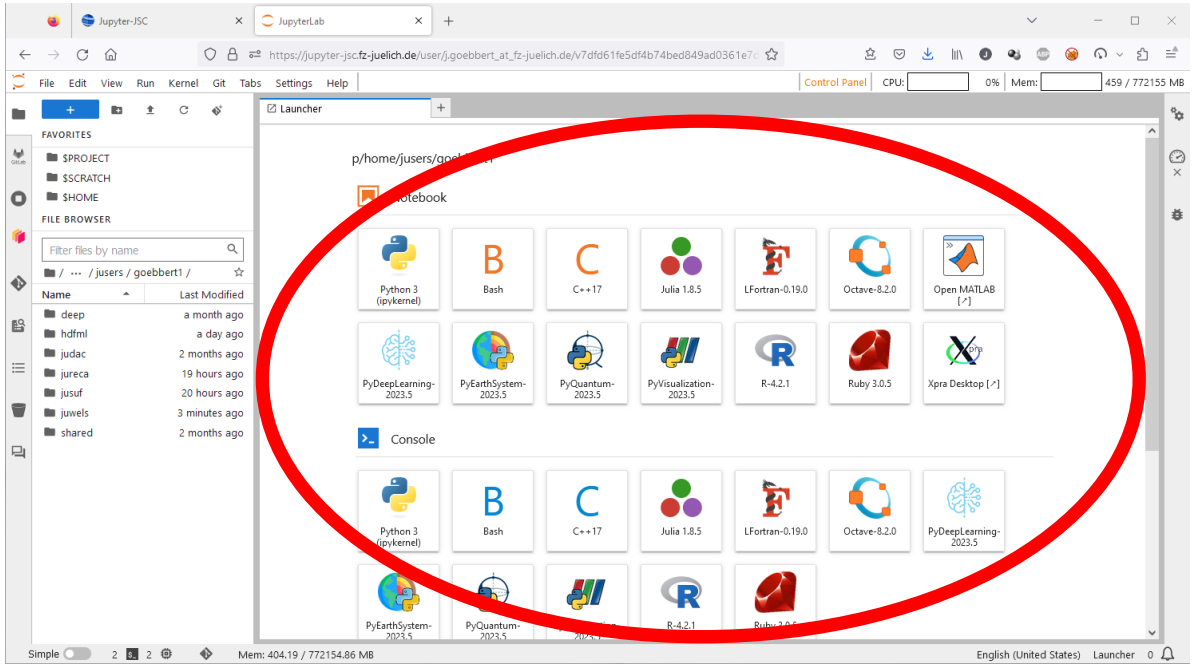
Jupyter Kernel

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, quantum computing



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JUPYTER KERNEL

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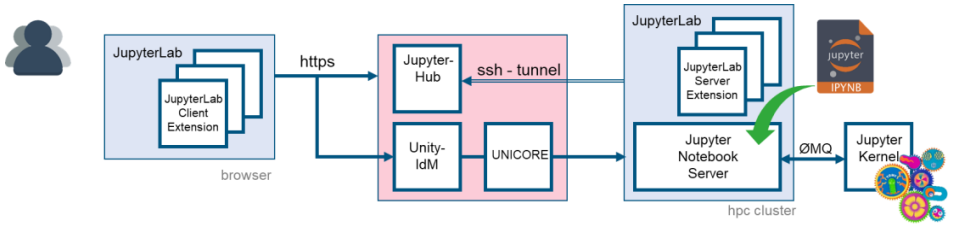

Jupyter Kernel

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, quantum computing

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

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

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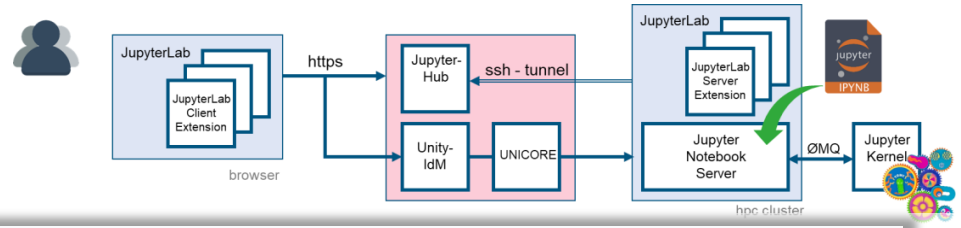
JUPYTER KERNEL

How to create your own Juypter Kernel



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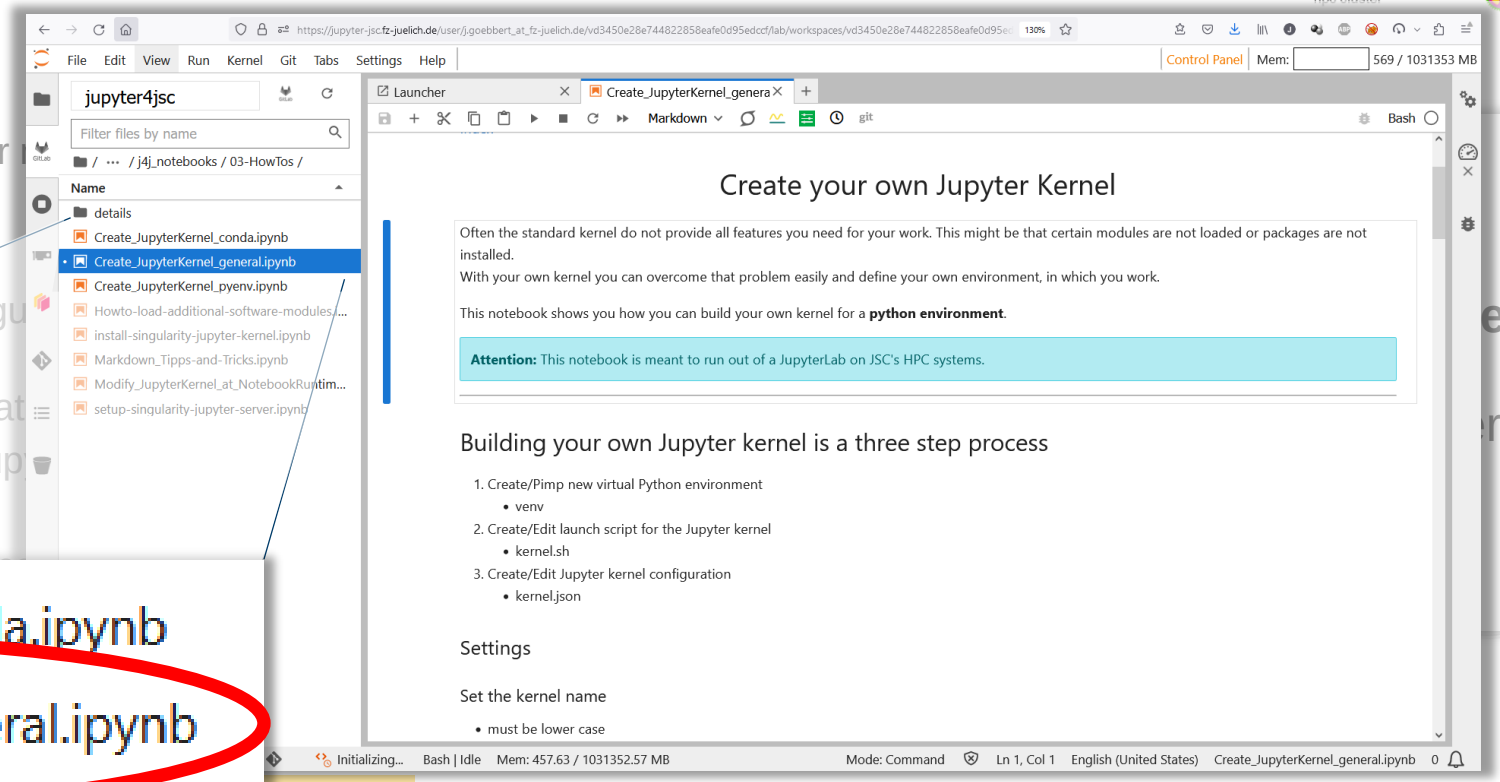

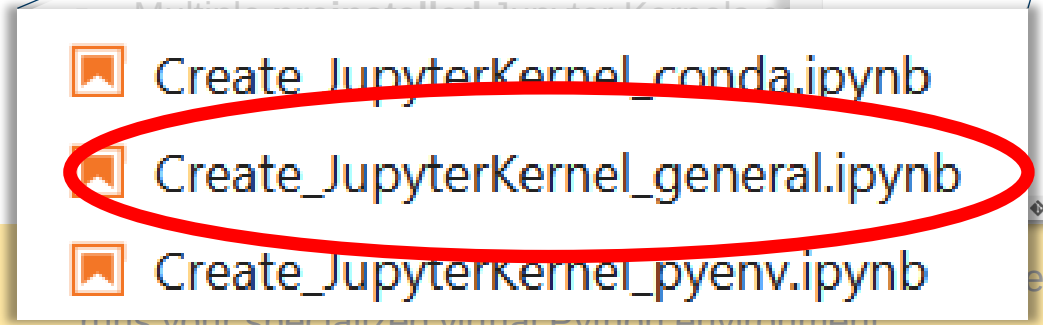

runs your specialized virtual Python environment.

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

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

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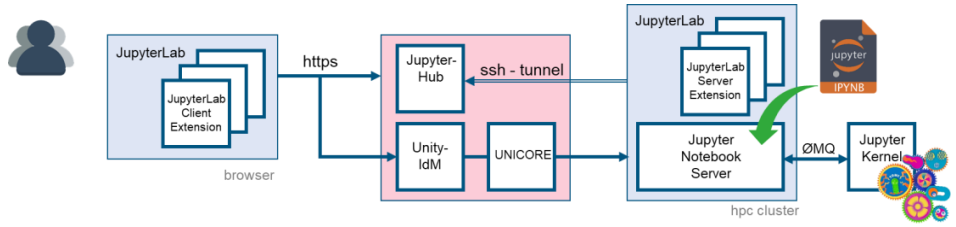
JUPYTER KERNEL

Run your Jupyter kernel configuration

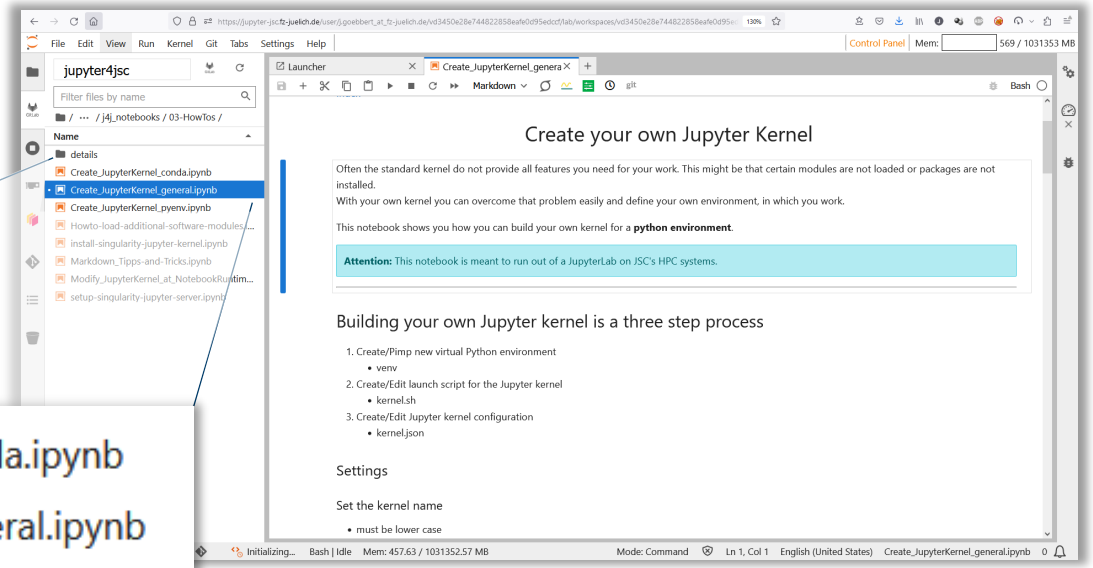


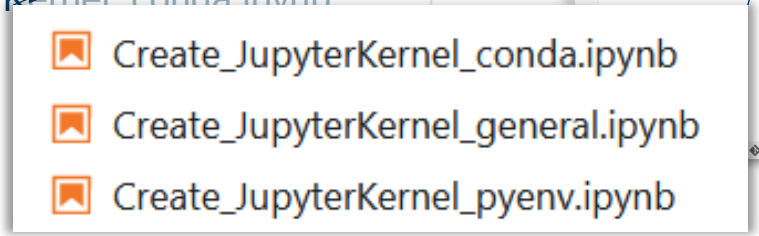
Run your Jupyter Kernel

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.

One of the many alternatives: Conda

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





Your kernel is
independent of the software stage
in which JupyterLab is located.

Jupyter kernel are **NOT limited** to Python at all!
The kernel-endpoint just needs to talk the Jupyter's kernel protocol (in general over ZeroMQ).
E.g.
- IRkernel for R (https://github.com/IRkernel/IRkernel)
- IJulia.jl (https://github.com/JuliaLang/IJulia.jl)

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SLURM WRAPPED KERNELS WITH SLURM-PROVISIONER

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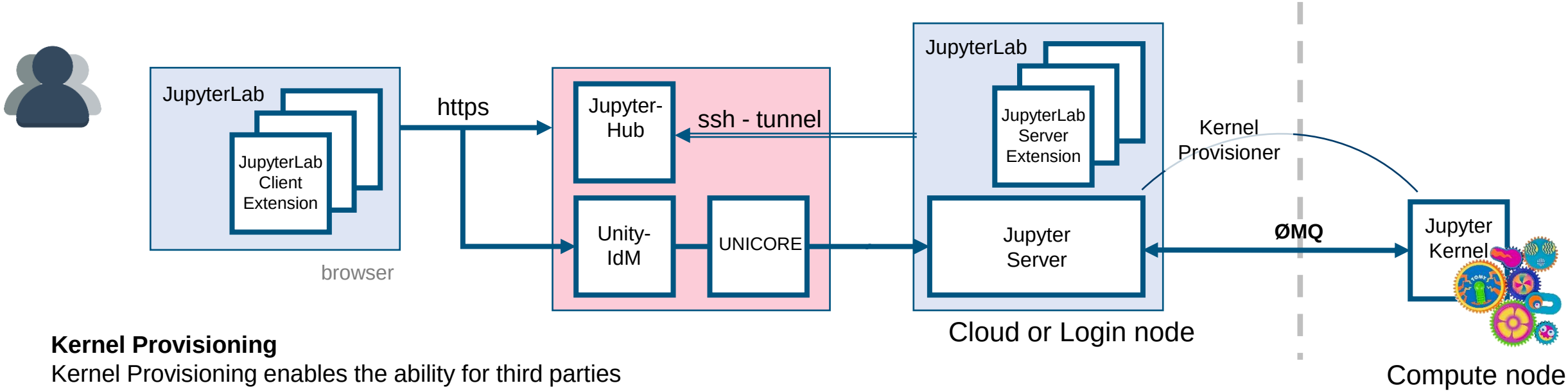
REMOTE JUPYTER KERNELS

Running multiple Jupyter kernels separate on the HPC system



Kernel Provisioning
Kernel Provisioning enables the ability for third parties
to **manage the lifecycle of a kernel's runtime environment**.

By implementing and configuring a *kernel provisioner*,
third parties have the ability to **provision kernels for different environments**,
typically managed by resource managers like Kubernetes, Hadoop YARN, Slurm, etc.

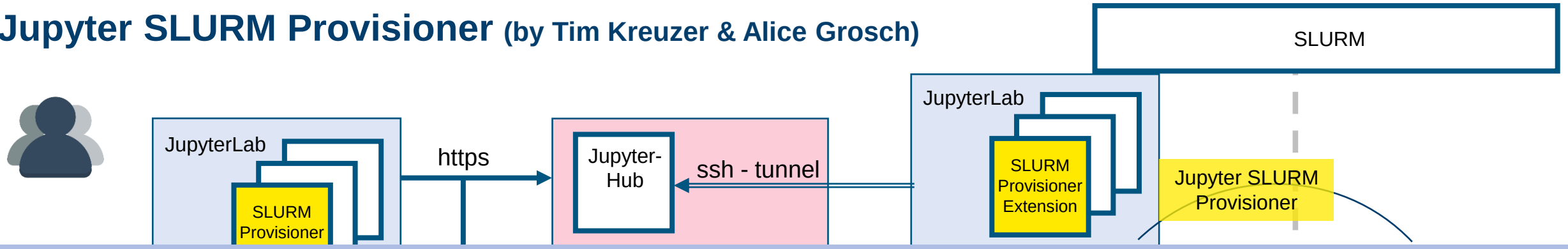
The kernel provisioner optionally extends the current **metadata stanza within the kernel.json**
to include the specification of the kernel provisioner name, along with an optional config stanza

```
[..]
"metadata": {
    "kernel_provisioner": {
        "provisioner_name": "slurm-provisioner",
        "config": {
            "kernel_argv": "Python",
            "project": "zam",
            "partition": "batch",
            "nodes": 1,
            "runtime": 3600,
        }
    }
},
```

https://jupyter-client.readthedocs.io/en/stable/provisioning.html

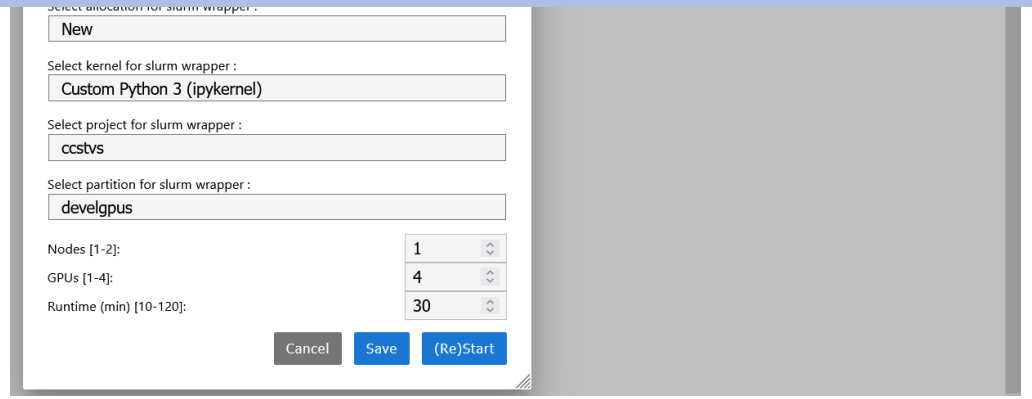
REMOTE JUPYTER KERNELS

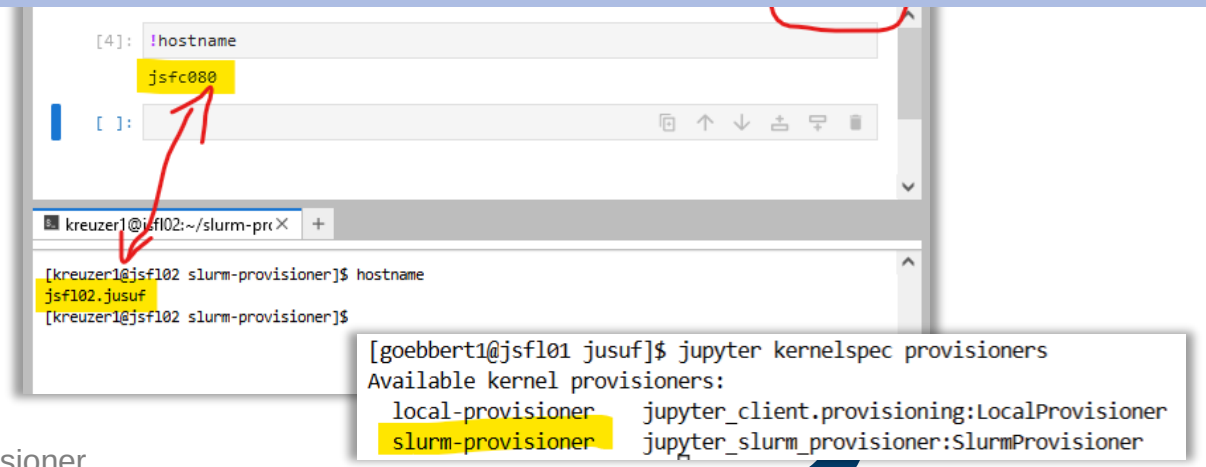
Jupyter SLURM Provisioner (by Tim Kreuzer & Alice Grosch)



Slurm wrapped kernels allow you to run kernels on compute nodes while your Jupyter Server runs on a login node.

This has the advantage that when your allocation on the compute node(s) ends, **only the kernel is stopped**, but your JupyterLab server keeps running. You will only have to restart the kernel, not your entire JupyterLab instance.





https://github.com/FZJ-JSC/jupyter-slurm-provisioner
https://github.com/FZJ-JSC/jupyter-slurm-provisioner-extension

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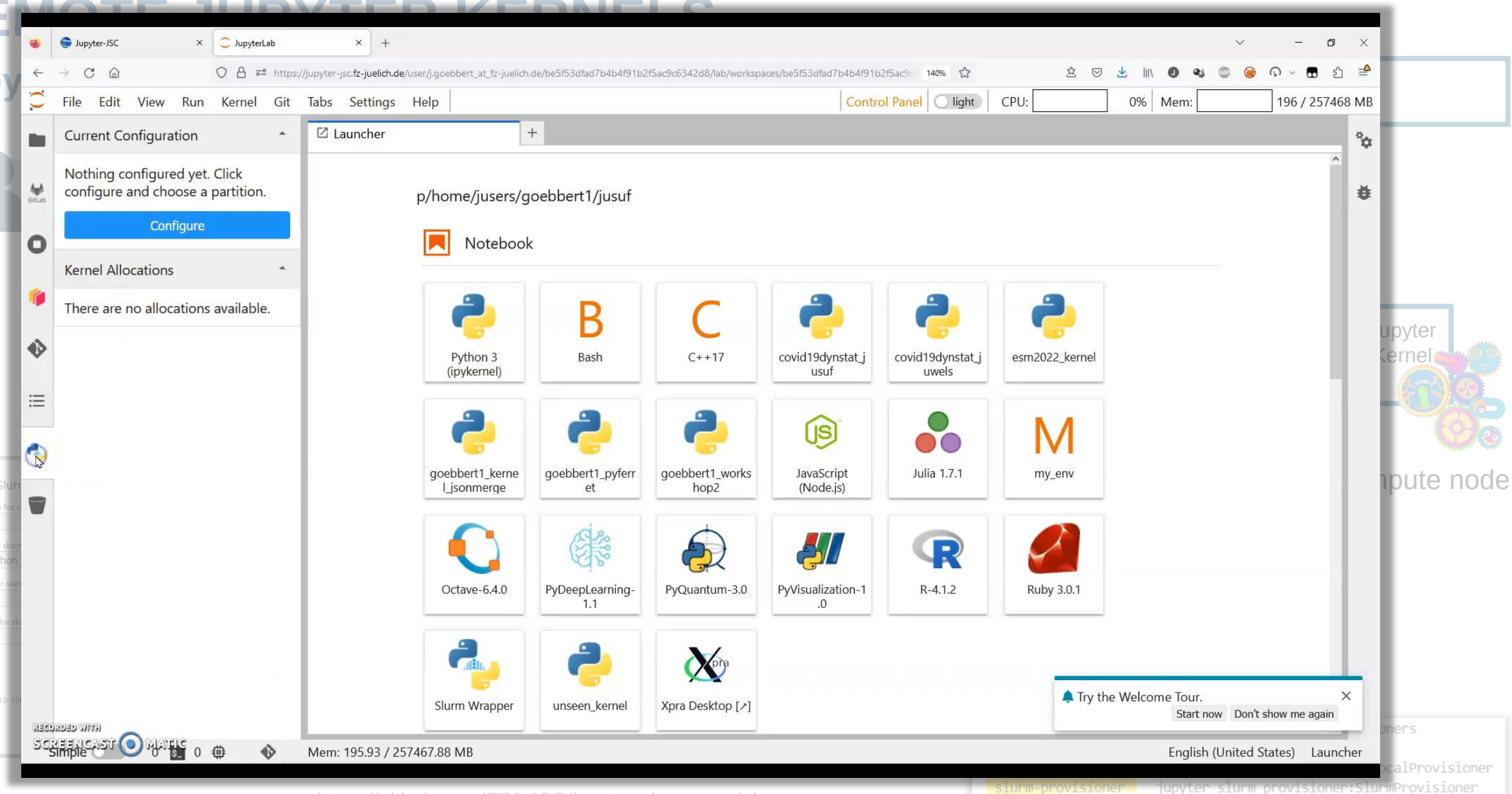
REMOTE JUPYTER KERNELS

Jupy



upyter
Kernel

mpute node

https://github.com/FZJ-JSC/jupyter-slurm-provisioner
https://github.com/FZJ-JSC/jupyter-slurm-provisioner-extension

slurm-provisioner jupyter_slurm_provisioner:SlurmProvisioner

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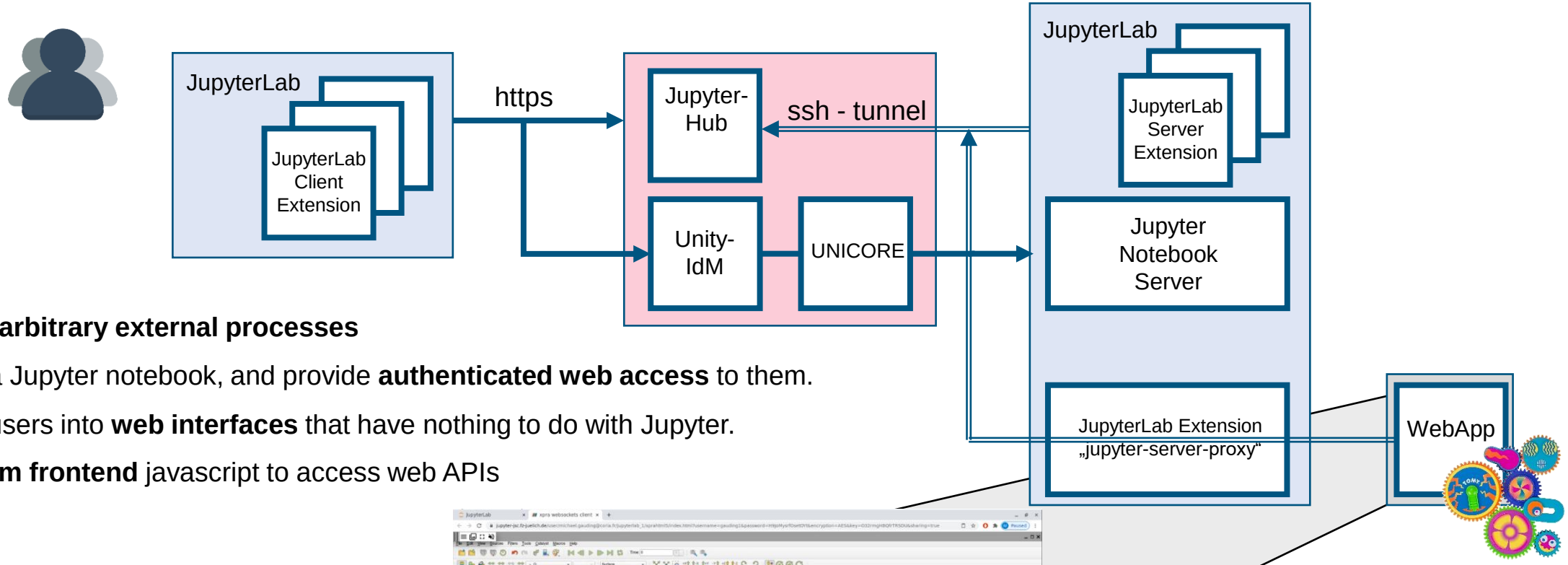
JUPYTER SERVER PROXY

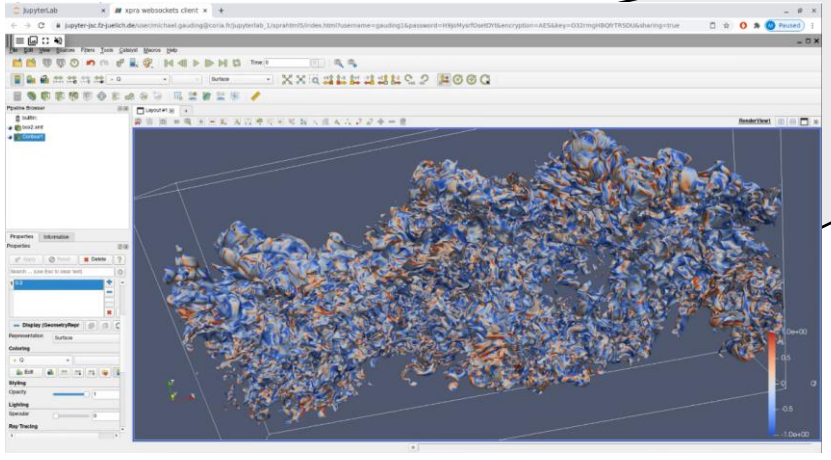
JUPYTERLAB – WEBSERVICE PROXY

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



Turbulent mixing with variable density,
subset of 1939x600x3584 grid points, Michael Gauding, CORIA

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

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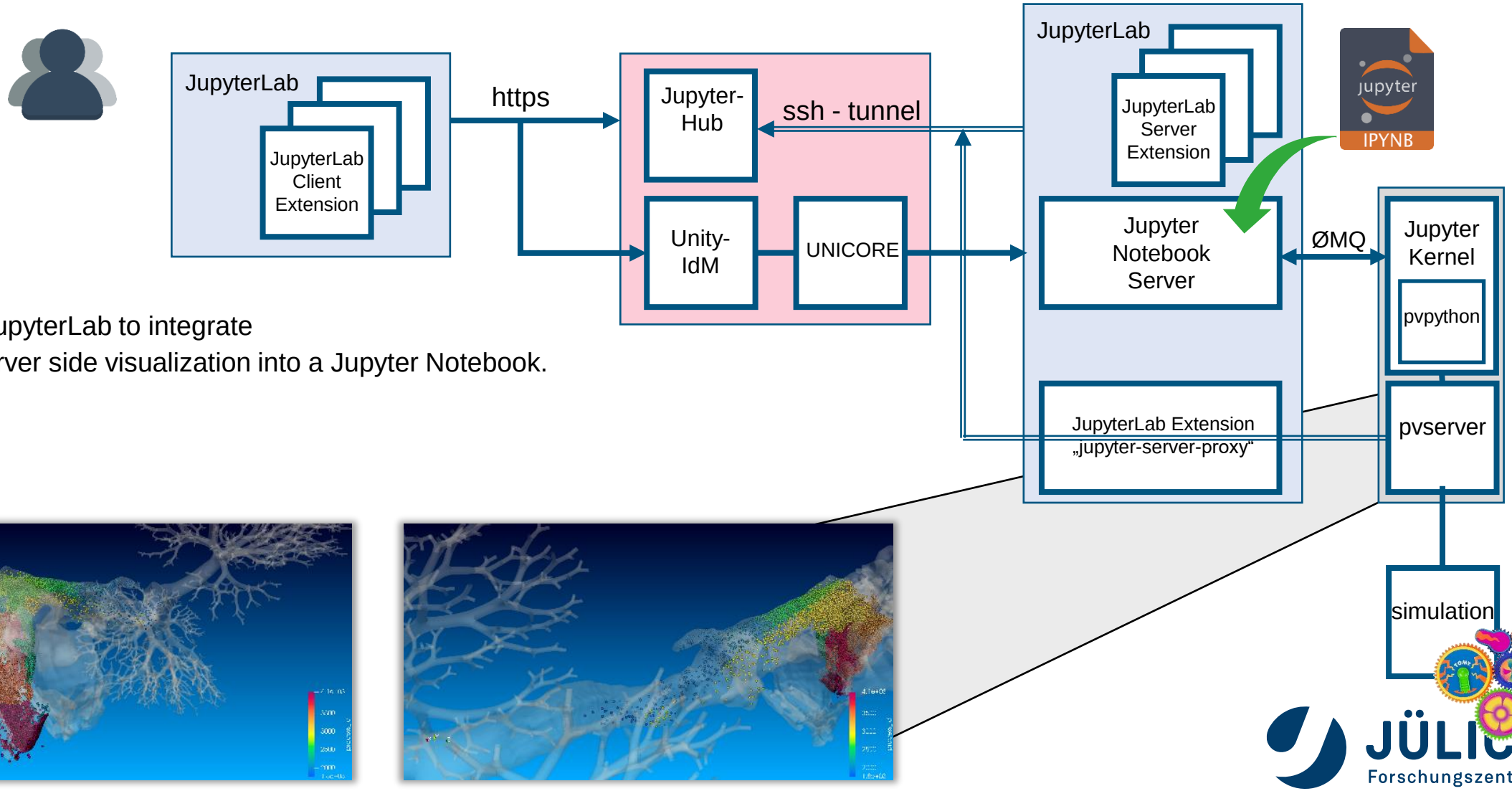
JUPYTERLAB – WEBSERVICE PROXY

Extension: jupyter-server-proxy



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

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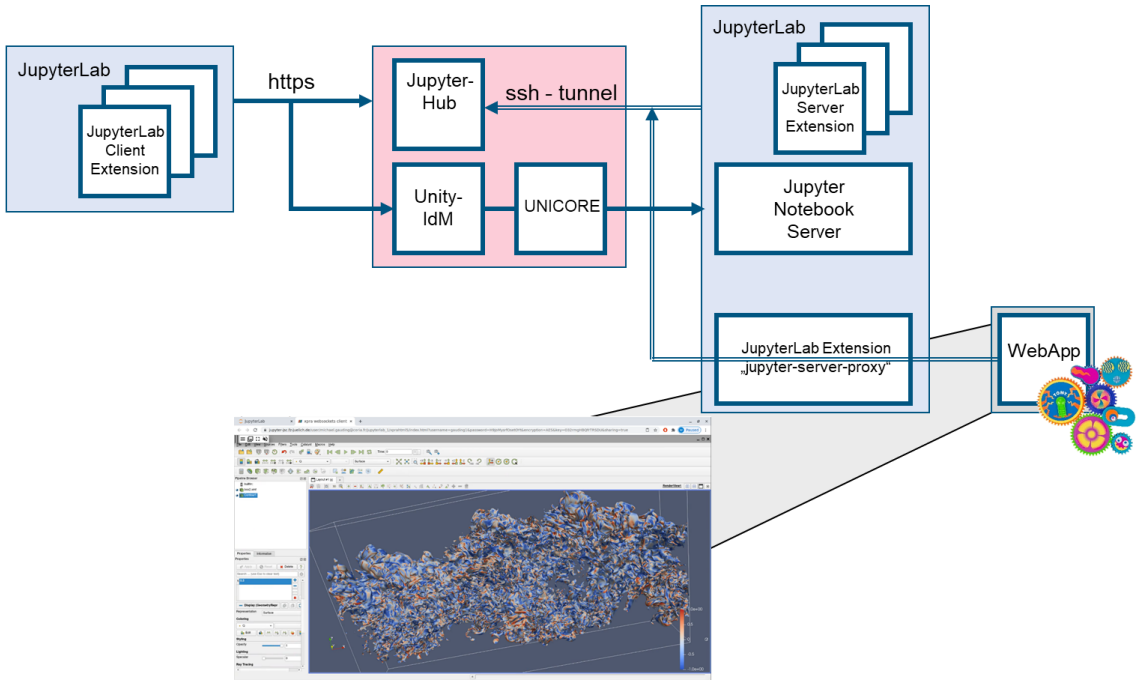
PORT TUNNELING – WEBSERVICE PROXY

Extension: jupyter-server-proxy



Accessing Arbitrary Ports or Hosts from the Browser

If you have a web-server running on the server
listening on <port>, you can access it through the notebook at
<notebook-base>/proxy/<port>
The URL will be rewritten to remove the above prefix.

You can disable URL rewriting by using
<notebook-base>/proxy/absolute/<port>
so your server will receive the full URL in the request.

This works for all ports listening on the local machine.

Example:

https://jupyter-jsc.fz-juelich.de/user/j.goebbert@fz-juelich.de/juwels_login/**proxy/<port>**
https://jupyter-jsc.fz-juelich.de/user/j.goebbert@fz-juelich.de/juwels_login/**proxy/<host>:<port>**

Upcoming: Support proxying to a server process via a Unix socket (#337)

https://jupyter-server-proxy.readthedocs.io/en/latest/arbitrary-ports-hosts.html

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JUPYTER SERVER PROXY EXAMPLES

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”

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

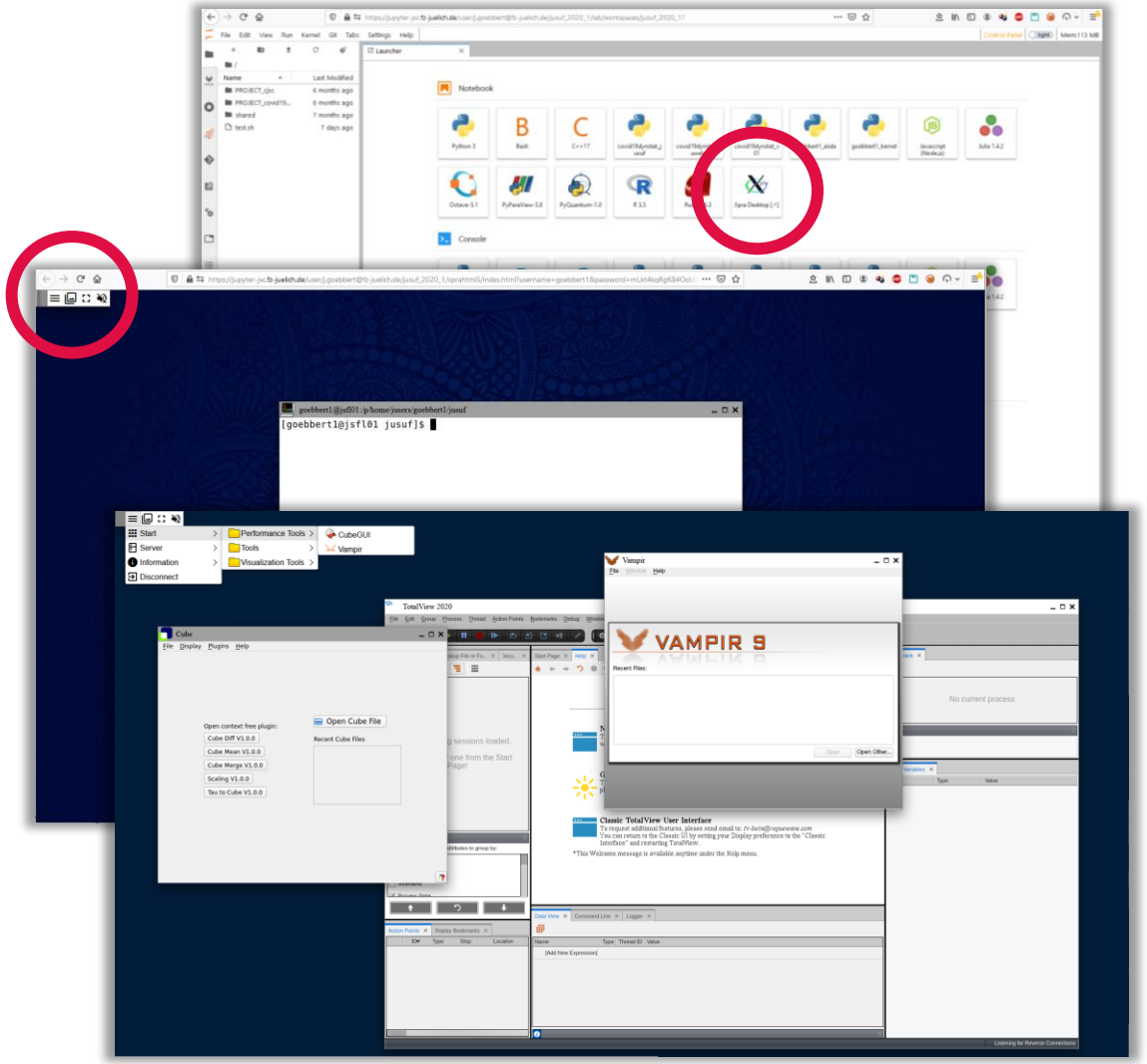
- Runs in a browser
- allows dis-/reconnection without disrupting the forwarded application
- https://xpra.org

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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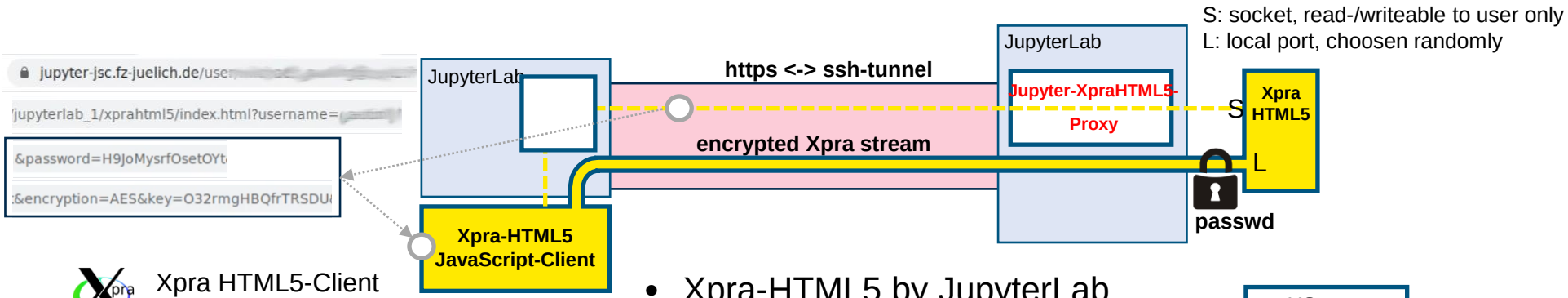
JUPYTERLAB – REMOTE DESKTOP

Run your X11-Applications in the browser



- Xpra-HTML5 by JupyterLab
  - Access through **JupyterLab-URL** by configurable https proxy
  - Auto-generated **one-time password & encryption key** is communicated through https-proxy

XServer (dummy driver)

https://github.com/FZJ-JSC/jupyter-xprahtml5-proxy

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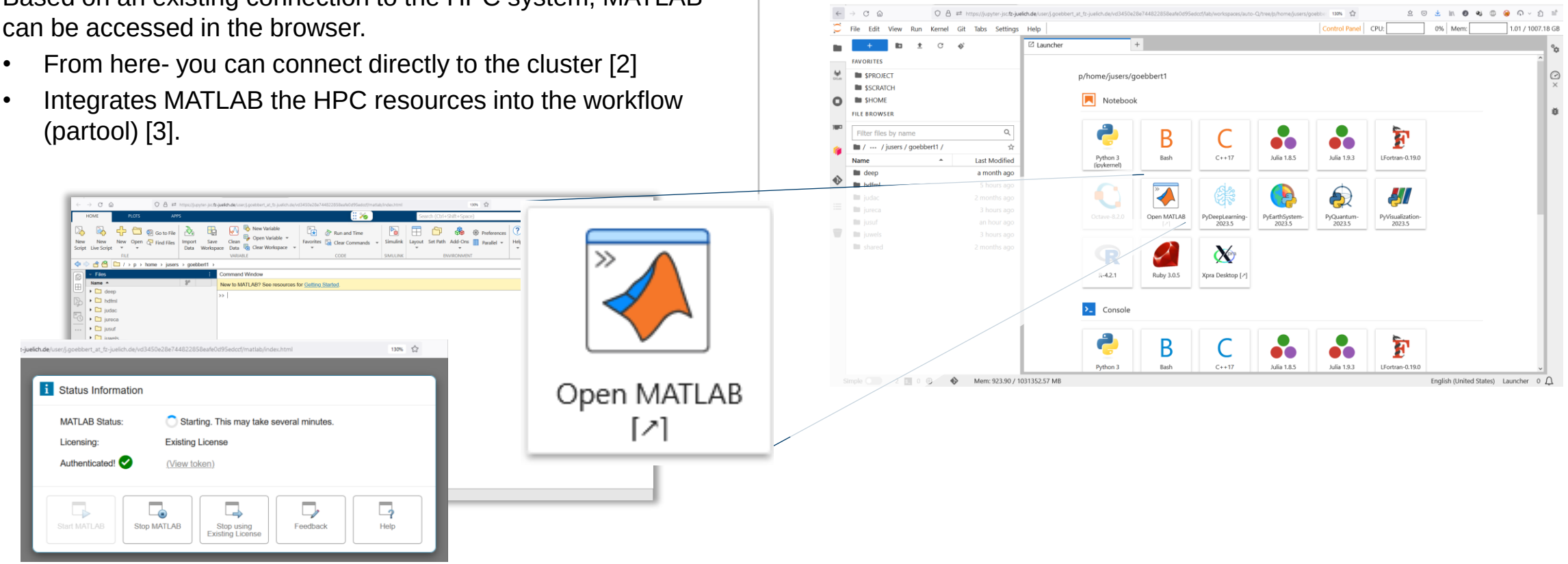
JUPYTERLAB – MATLAB

Web-based GUI for MATLAB

MATLAB – Web-based GUI

Based on an existing connection to the HPC system, MATLAB can be accessed in the browser.

- From here- you can connect directly to the cluster [2]
- Integrates MATLAB the HPC resources into the workflow (partool) [3].



[1] https://www.fz-juelich.de/en/ias/jsc/services/user-support/software-tools/matlab
[2] https://de.mathworks.com/help/parallel-computing/remoteclusteraccess.html
[3] https://de.mathworks.com/products/parallel-computing.html

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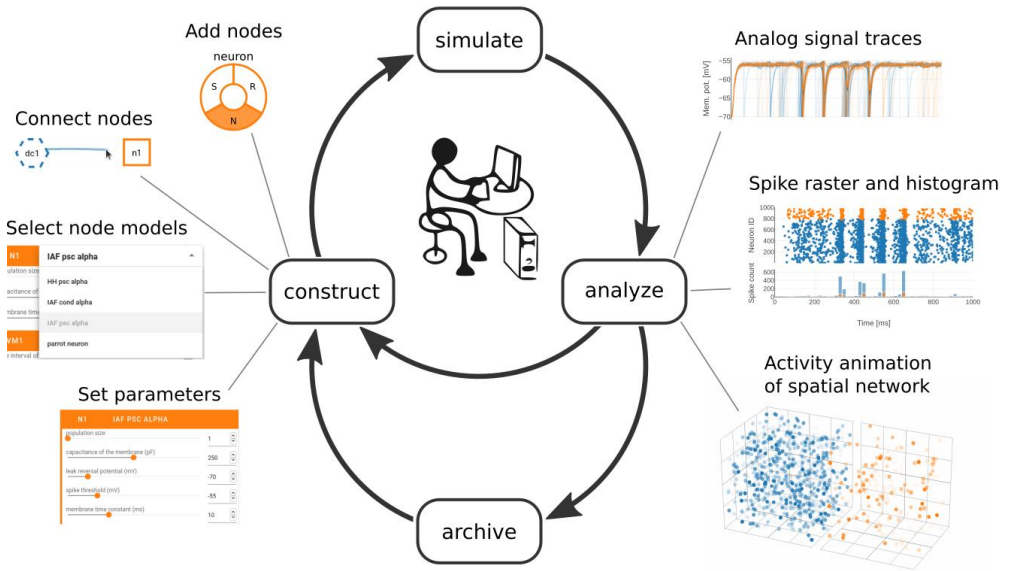
JUPYTERLAB – NEST DESKTOP

Web-based GUI for Neuroscientists using NEST

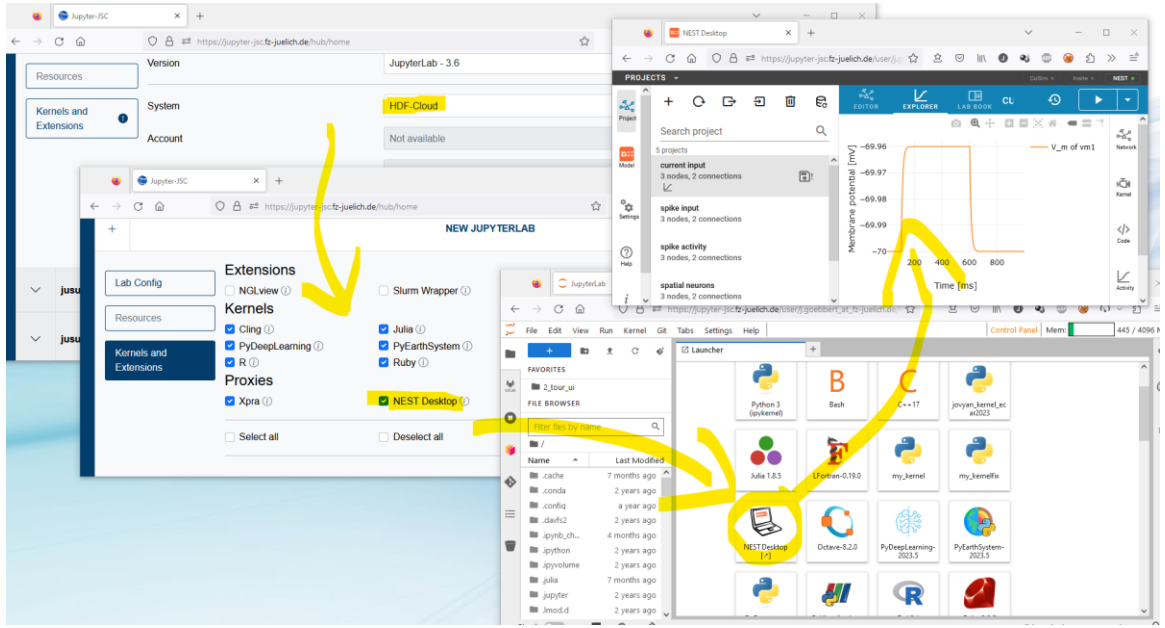
NEST-Desktop

NEST Desktop is a web-based GUI application for NEST Simulator, an advanced simulation tool for the computational neuroscience.



Jupyter-JSC gives you easy access to a NEST-Desktop

With Jupyter-JSC using Jupyter-Server-Proxy authenticated & authorized users get secure access to the WebUI of NEST-Desktop running NEST-simulations on HPC.



Plugin for Jupyter-Server-Proxy: jupyter-xprahtml5-proxy
https://github.com/jhgoebbert/jupyter-nestdesktop-proxy

[1] https://nest-desktop.readthedocs.io
[2] https://www.nest-simulator.org

CONCLUSION

Why Jupyter is so popular among Data Scientists

JupyterLab …

… is a **web-based platform for interactive computing and data analysis**
that is well-suited to the needs of research software engineers.

… provides researchers with a **comprehensive environment** for working with
code, text, multimedia, and data, making it an ideal tool for a wide range of research tasks.

… is designed to be **flexible and customizable**,
and can be modified to suit the specific needs and workflows of individual researchers.

… supports the creation of **reproducible research** through its support for Jupyter notebooks.

… supports **collaboration and sharing** of research work
through its support for sharing notebooks, dashboards, and other elements of a research project.

… provides a wide range of **extensions and plugins**
that can be used to integrate other tools and services into the environment.

… is an **open-source project**, which means that researchers
have access to the source code and can contribute to its development.

QUESTIONS?

Training course: https://gitlab.jsc.fz-juelich.de/jupyter4jsc/training-2024.04-jupyter4hpc