



Interactive HPC with Jupyter

training course, 26+27.05.2021

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Jülich Supercomputing Centre (JSC)
Forschungszentrum Jülich (FZJ)



European
Commission

Horizon 2020
European Union funding
for Research & Innovation

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WELCOME

- Hello !
- Workshop information (live document)
 - <https://gitlab.version.fz-juelich.de/hedgedoc/oo2l4aZHSKO5eIJJOLPk3w?view>
- Workshop interaction
 - Zoom chat
- Workshop repository
 - <https://gitlab.version.fz-juelich.de/jupyter4jsc/CoE-2021.05-jupyter4hpc>

WELCOME

Agenda

- day 1: JupyterLab Introduction

- 9:00 - 11:00
 - Welcome and Login
 - Introducing JupyterLab
- 11:00 - 11:30
 - Break
- 11:30 - 13:00
 - JupyterLab extensions tour
 - Customizing your environment

- day 2: Jupyterlab for HPC

- 9:00 - 11:00
 - Welcome and Login
 - Build your own kernels
 - Using JupyterLab as Proxy
- 11:00 - 11:30
 - Break
- 11:30 - 13:00
 - Utilizing supercomputers with JupyterLab
 - Jupyter-JSC under the hood

Resources

HDF Cloud (OpenStack)

JUSUF (HPC cluster)

PRE-WORKSHOP TODOS

Register & Login

<https://judoor.fz-juelich.de>

Join the project „training2109“

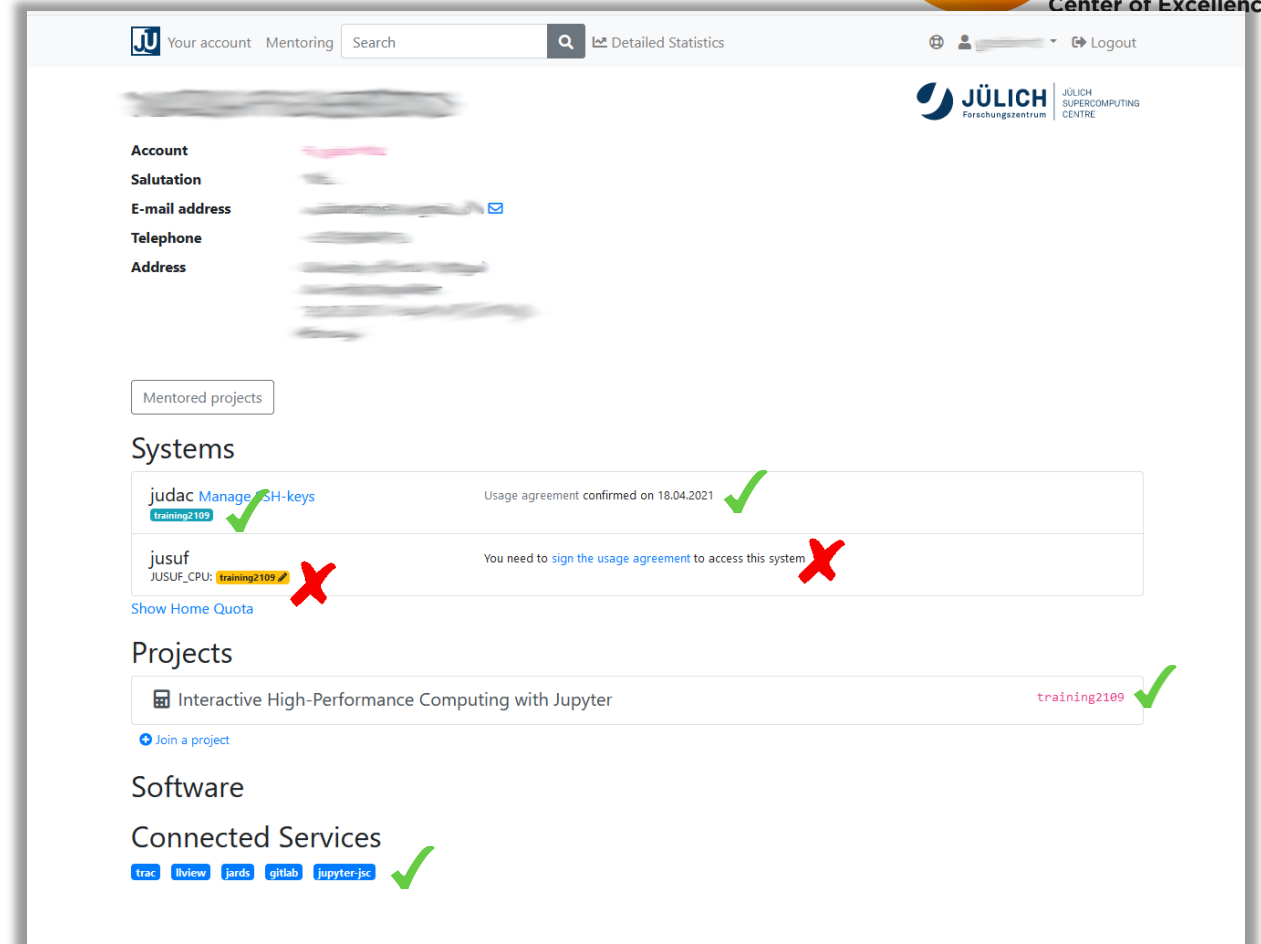
→ Wait to get joined by the project PI

Sign usage agreement

→ Wait for creation of HPC accounts

Check Connected Services:

jupyter-jsc



The screenshot shows the user interface of the Jülich Supercomputing Centre. At the top, there is a navigation bar with 'Your account', 'Mentoring', a search bar, and 'Detailed Statistics'. The user's name and a 'Logout' button are on the right. Below the navigation bar, the 'JÜLICH Forschungszentrum' logo is visible. The main content area is divided into several sections:

- Account:** Fields for Salutation, E-mail address (with a checkmark), Telephone, and Address.
- Mentored projects:** A button labeled 'Mentored projects'.
- Systems:** A table showing system status:

System	Status
judac Manage SH-keys training2109	Usage agreement confirmed on 18.04.2021 ✓
jusuf JUSUF_CPU: training2109	You need to sign the usage agreement to access this system ✗
- Projects:** A table showing project status:

Project	Status
Interactive High-Performance Computing with Jupyter	training2109 ✓
- Software:** A section for software management.
- Connected Services:** A list of services with status indicators: trac, lview, jards, gitlab, and jupyter-jsc (with a checkmark).

For more details, please visit

<https://gitlab.version.fz-juelich.de/hedgedoc/oo2I4aZHSKO5eIJJOLPk3w?view#Pre-Workshop-Todos>
or <https://gitlab.version.fz-juelich.de/jupyter4jsc/CoE-2021.05-jupyter4hpc/-/tree/master/preparation>

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



MOTIVATION

Rise of Jupyter's popularity

If popularity can be counted by

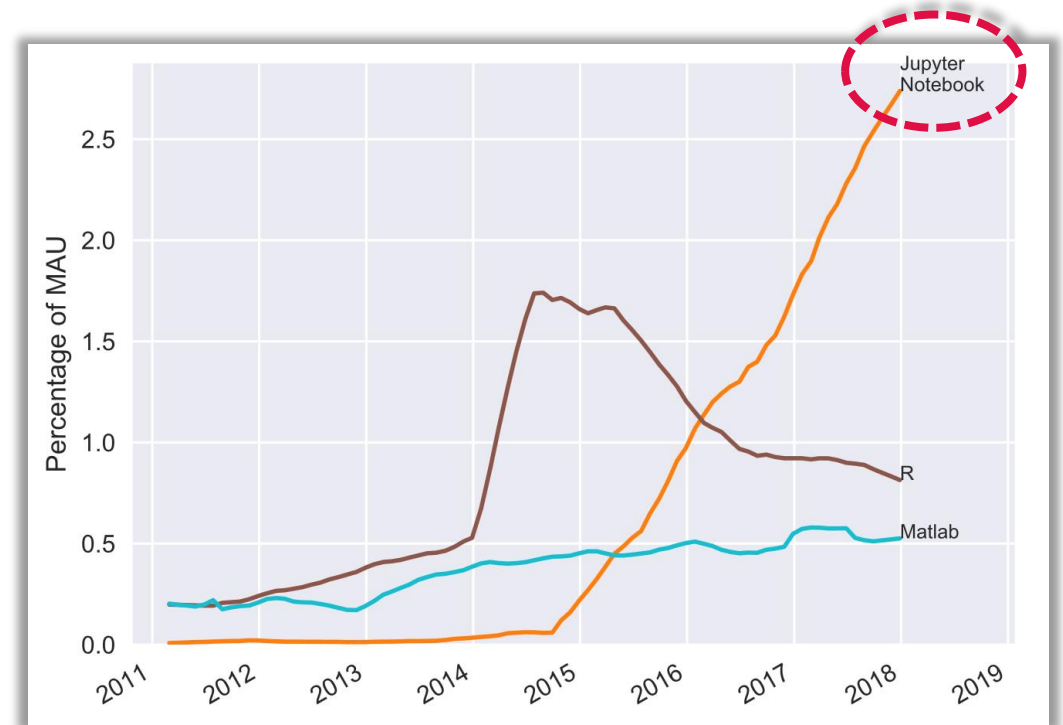
- Monthly aggregated number of user interactions with GitHub repos (= Monthly Active Users (MAU))

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

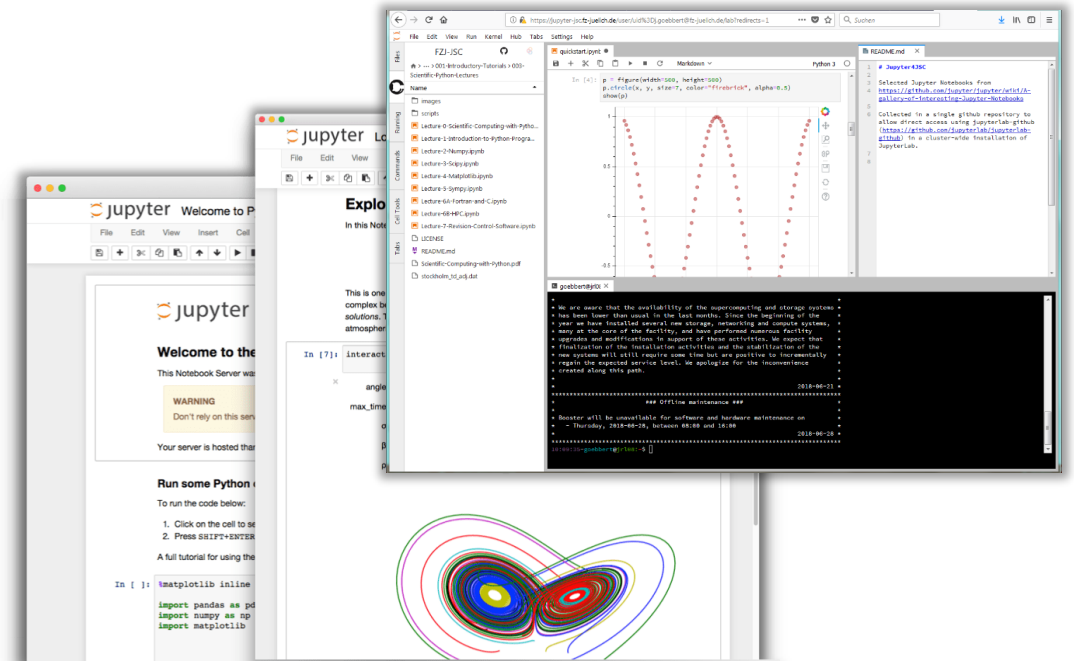
- **Interactive** working environment in the web browser
- For the creation of **reproducible** computer-aided narratives
- Very **popular** with researchers from all fields
- Jupyter = Julia + Python + R

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>

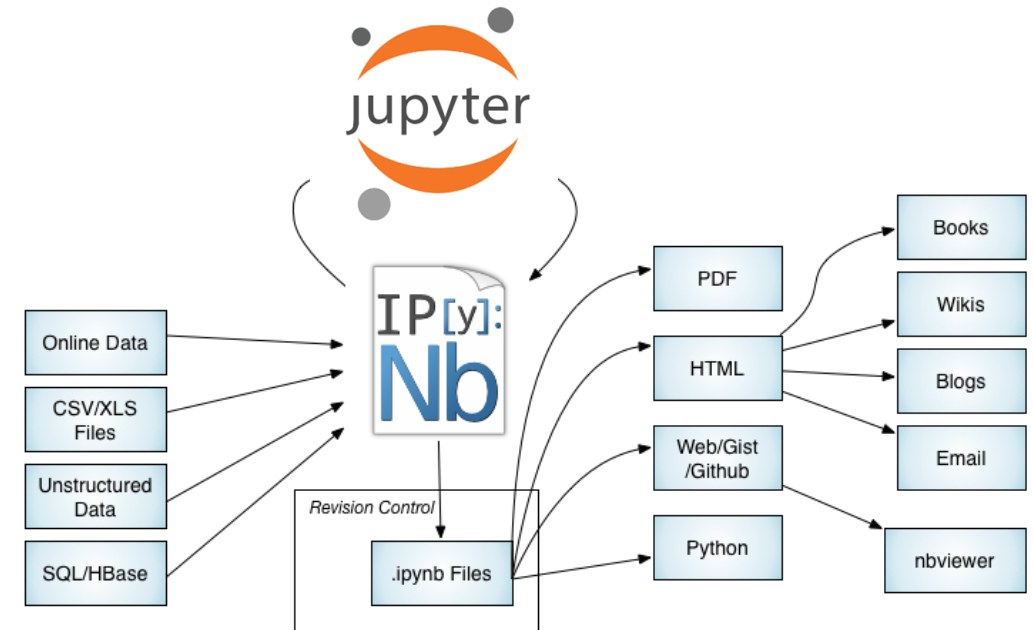
TERMINOLOGY

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?

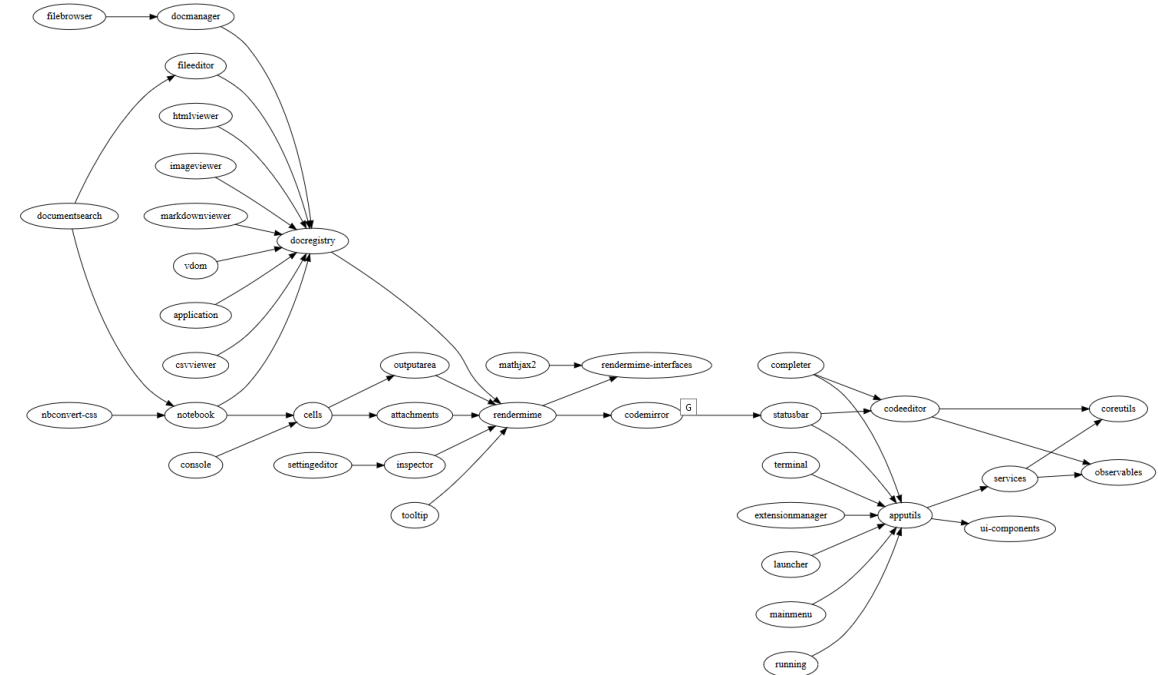
JupyterLab Extension

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.

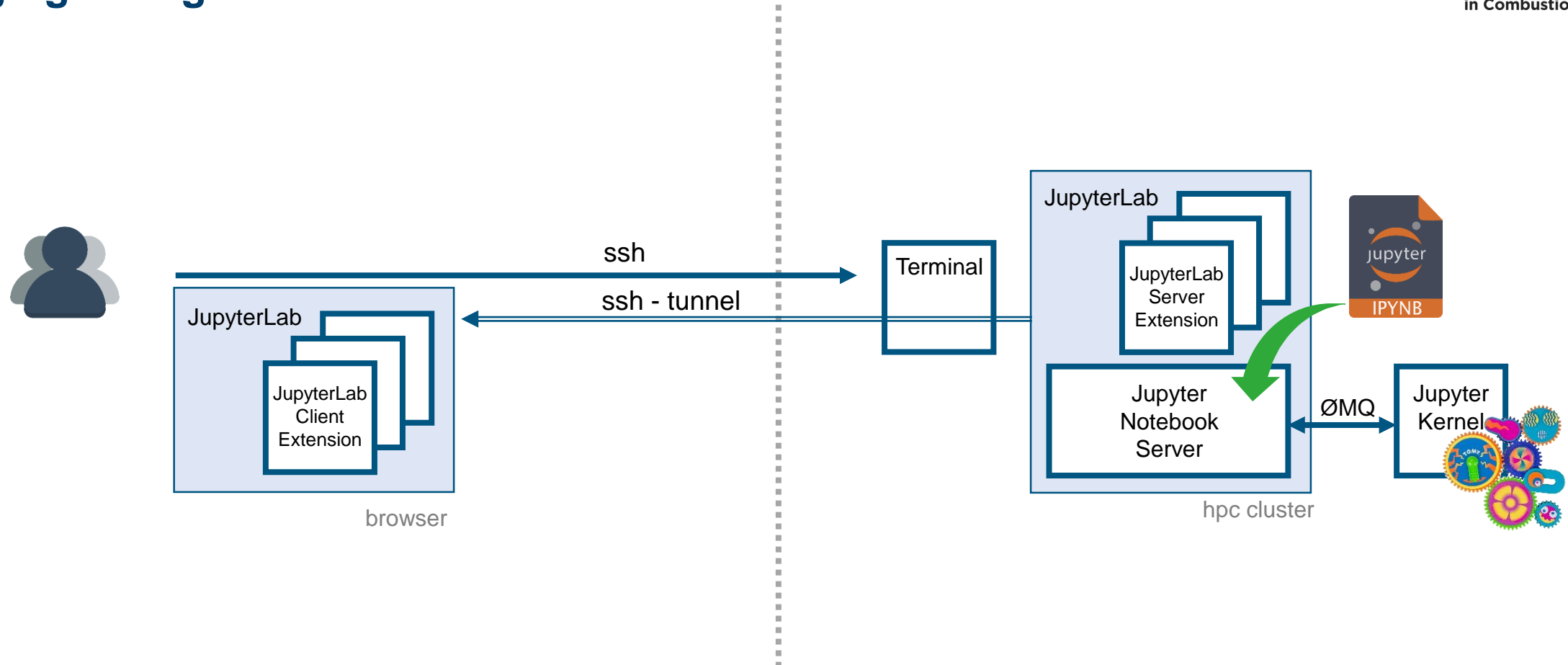
The whole JupyterLab itself is simply a **collection of extensions** that are no more powerful or privileged than any custom extension.



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

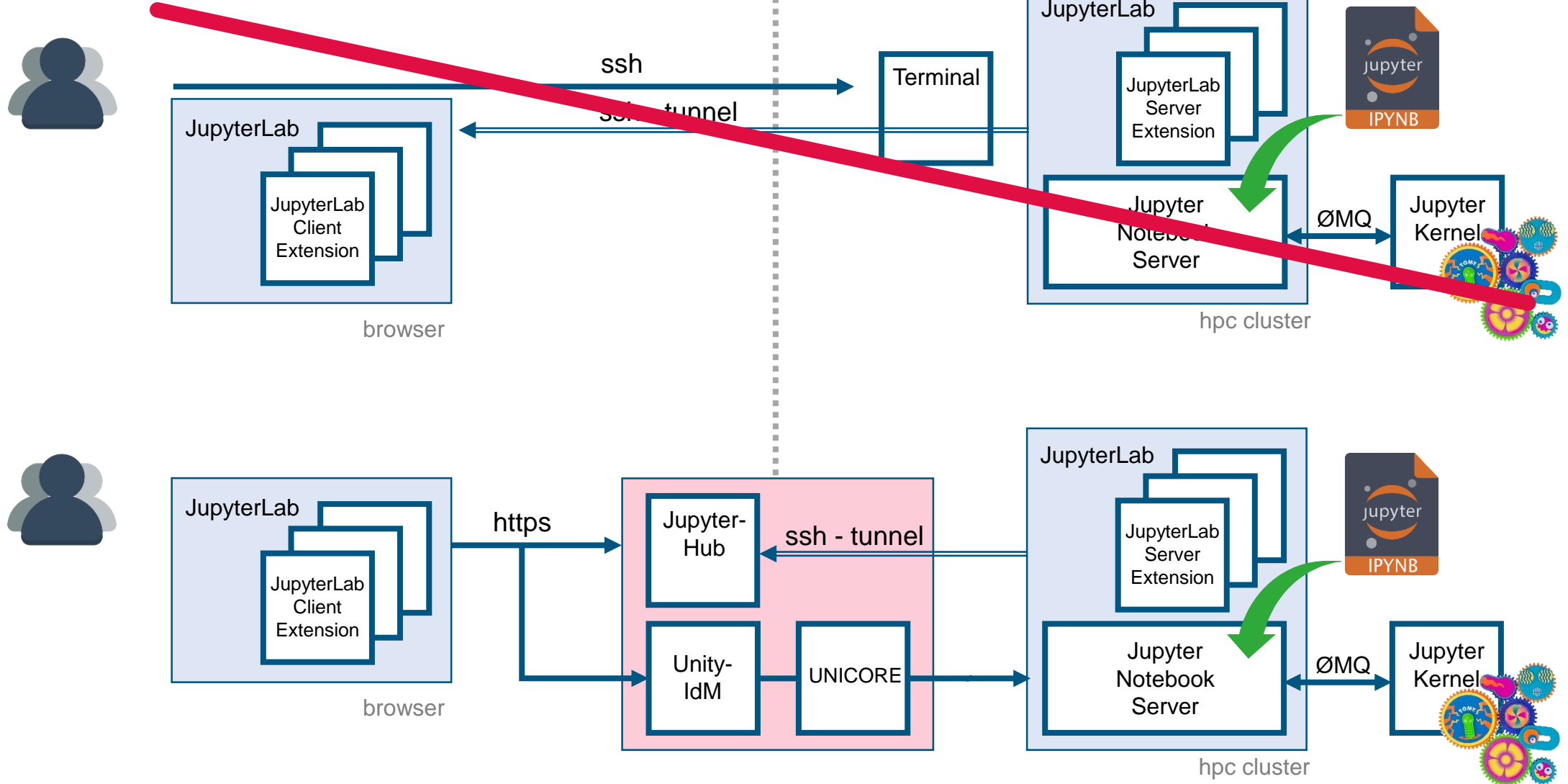
TERMINOLOGY

Bringing all together



JUPYTER-JSC WEBSERVICE

Start your JupyterLab (the easy way)



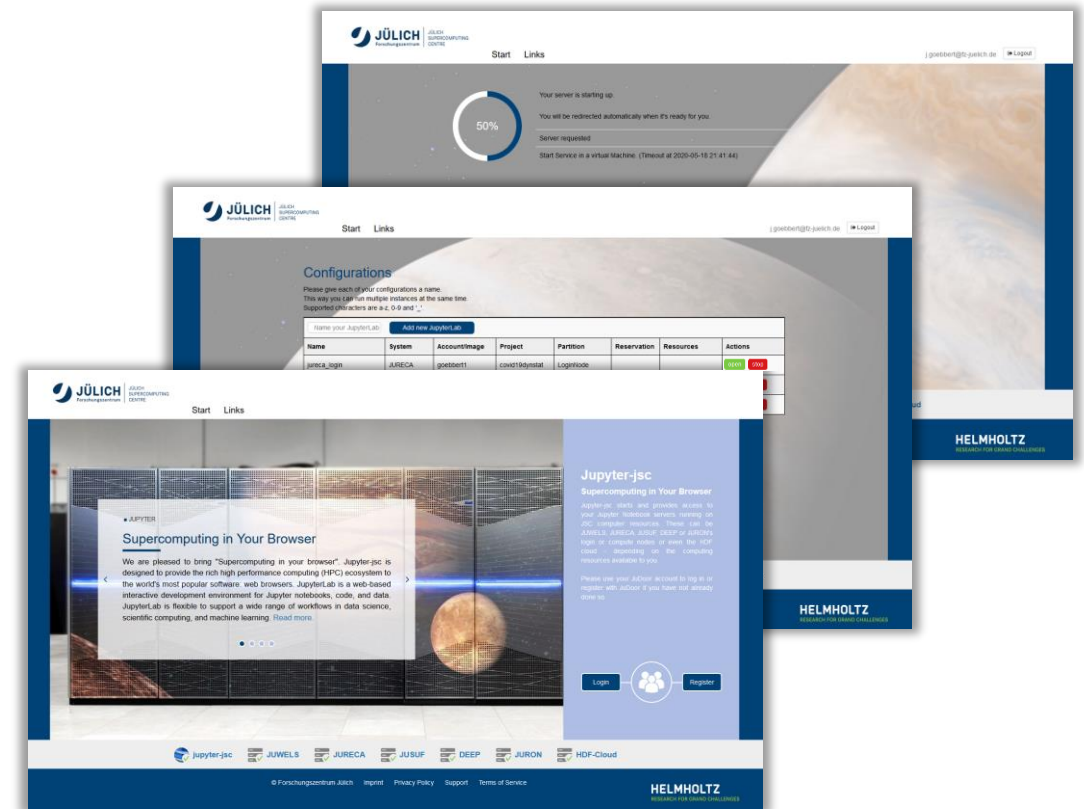
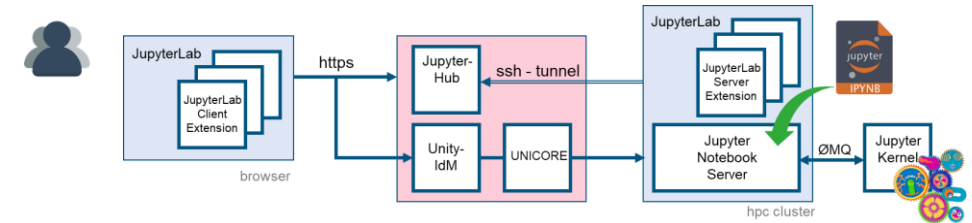
JUPYTER-JSC WEBSERVICE

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



JUPYTER-JSC WEBSERVICE

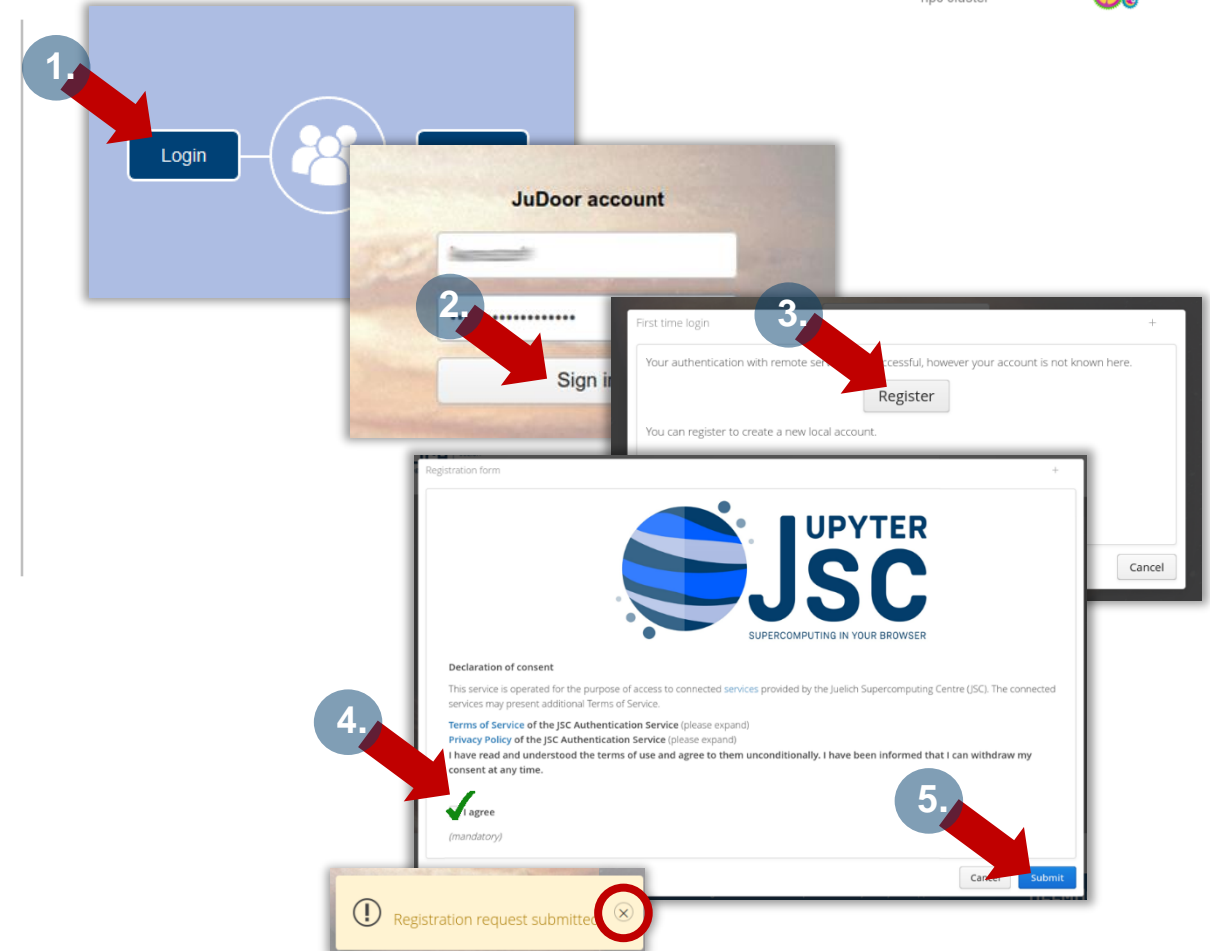
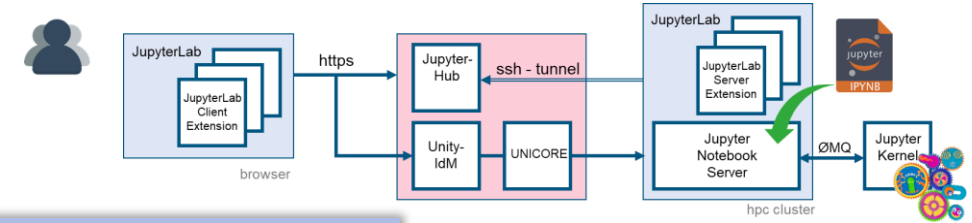
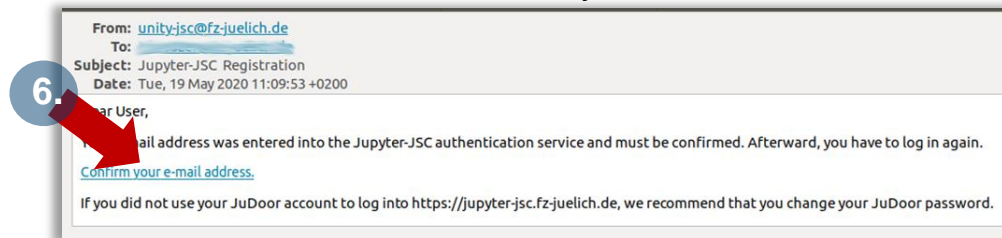
First time login

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

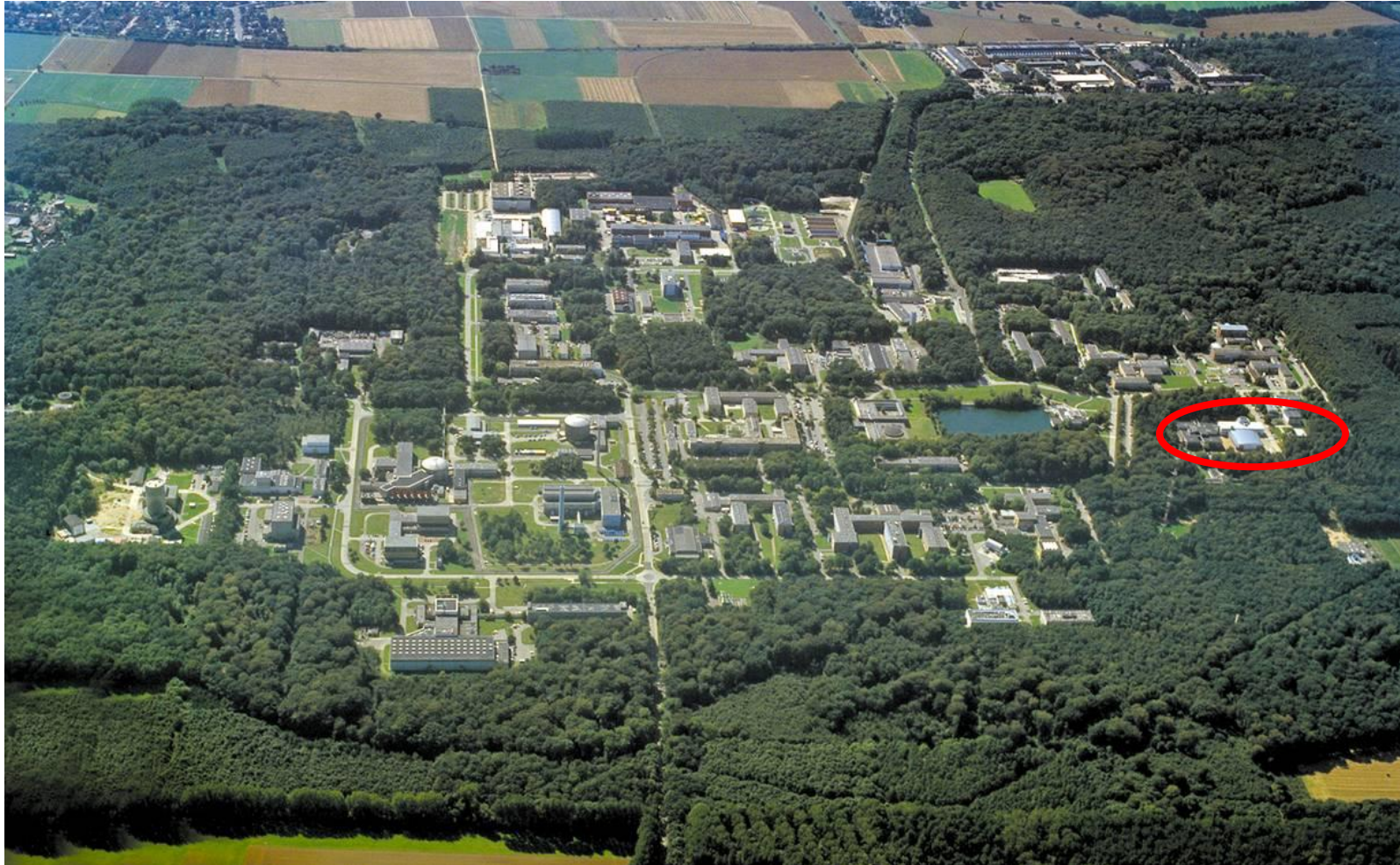
Jupyter-JSC first time login

- 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



FORSCHUNGSZENTRUM JÜLICH



JÜLICH SUPERCOMPUTING CENTRE



Supercomputer operation for:

- Centre – FZJ
- Region – RWTH Aachen University
- Germany – Gauss Centre for Supercomputing
John von Neumann Institute for Computing
- Europe – PRACE, EU projects

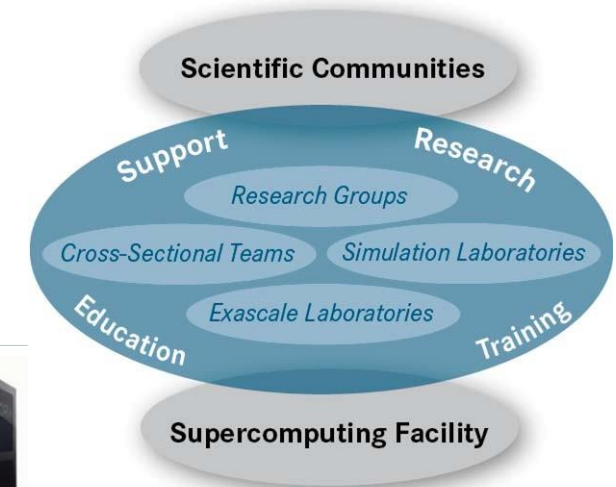
Application support

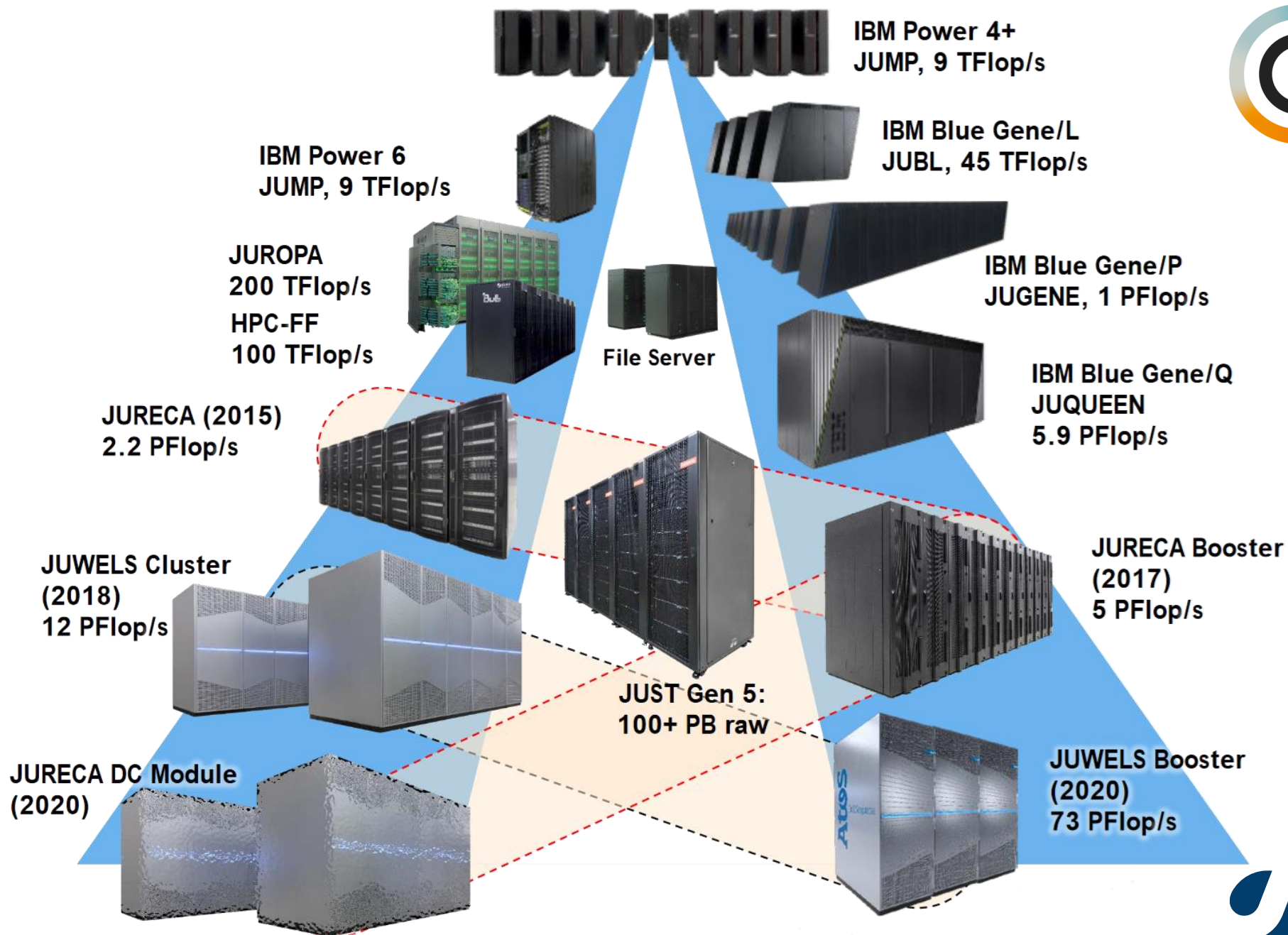
- Unique support & research environment at JSC
- Peer review support and coordination

R&D work

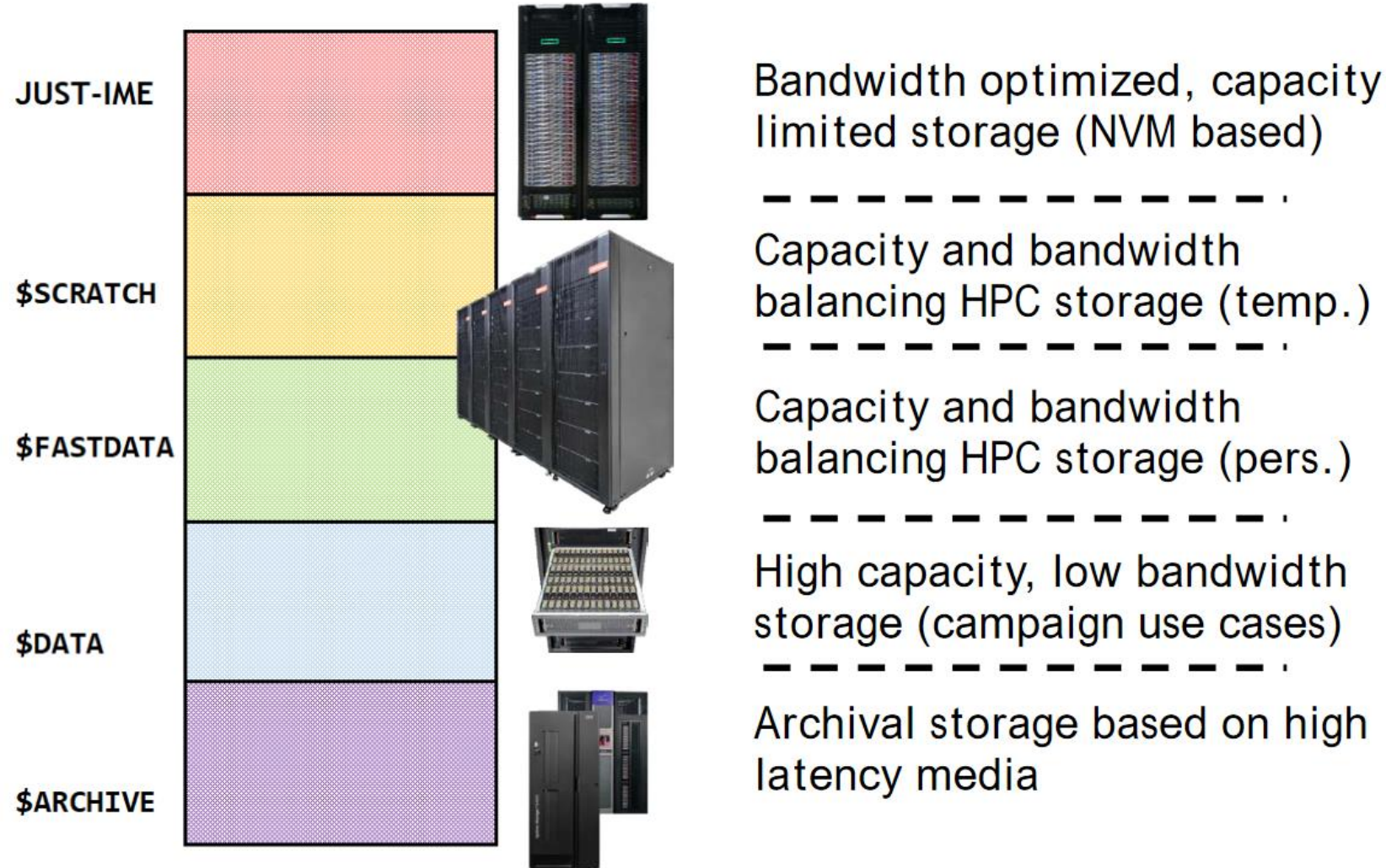
- Methods and algorithms, computational science, performance analysis and tools
- Computer architectures, Co-Design, Exascale Laboratories

Education and Training





JUST: MULTI-TIER STORAGE SYSTEM



DOMAIN SPECIFIC SUPPORT

