



# INTERACTIVE HCP WITH JUPYTER

PRACE Training Course

2021-04-20..22 | JENS. H. GÖBBERT  
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# WELCOME

- Hello !
- Workshop information (live document)
  - [https://gitlab.version.fz-juelich.de/hedgedoc/2xL\\_vGsLQvyEwUg49sNAIA#](https://gitlab.version.fz-juelich.de/hedgedoc/2xL_vGsLQvyEwUg49sNAIA#)
- Workshop interaction
  - Zoom chat
- Workshop repository
  - <https://gitlab.version.fz-juelich.de/jupyter4jsc/prace-2021.04-jupyter4hpc>

<https://jupyter.org>

# 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

- day 2: Jupyterlab Customization for HPC

- 9:00 - 11:00
  - Welcome and Login
  - JupyterLab on HPC resources
  - Customizing your environment
- 11:00 - 11:30
  - Break
- 11:30 - 13:00
  - Using JupyterLab as Proxy
  - Remote visualization

- day 3: JupyterLab Optimization for HPC

- 9:00 - 11:00
  - Welcome and Login
  - Utilizing supercomputers with JupyterLab
- 11:00 - 11:30
  - Break
- 11:30 - 13:00
  - Extend/build/install your own JupyterLab
  - Jupyter-JSC under the hood
  - Workshop summary and feedback

## Resources:

HDF Cloud

JUSUF

F# JUWELS

<https://jupyter.org>

# PRE-WORKSHOP TODOS

## Register & Login

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

Join the training project

Wait to get joined

Sign usage agreement

→ **Connected Services:**

jupyter-jsc, unicore, HDFCloud

<https://jupyter.org>

The screenshot displays the user interface of the Jülich Supercomputing Centre. At the top, there is a navigation bar with the Jülich logo, 'Your account', 'Mentoring', a search bar, and 'Detailed Statistics'. Below this, the user's account information is shown, including 'Salutation', 'E-mail address', 'Telephone', and 'Address'. A section for 'Mentored projects' is visible. The 'Systems' section lists 'judac' (with a link to 'Manage SSH-keys') and 'jusuf' (with a link to 'JUSUF\_CPU: training2109'). A red circle highlights the text 'You need to sign the usage agreement to access this system' next to the 'jusuf' entry. Below the systems, the 'Projects' section shows 'Interactive High-Performance Computing with Jupyter' with a red circle around the 'Join a project' button. The 'Software' section is partially visible. At the bottom, the 'Connected Services' section shows a list of services: 'trac', 'lview', 'jards', 'gitlab', and 'jupyter-jsc', with a red circle around the 'jupyter-jsc' service.

# 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

The Jupyter logo, which consists of the word "jupyter" in a lowercase, sans-serif font, with a large, light gray smiley face underneath it. The logo is centered on the slide and surrounded by various programming language and technology icons in a light gray color, including Python, R, Julia, and others.

<https://jupyter.org>

Member of the Helmholtz Association

# MOTIVATION

## Rise of Jupyter's popularity

If popularity can be counted by

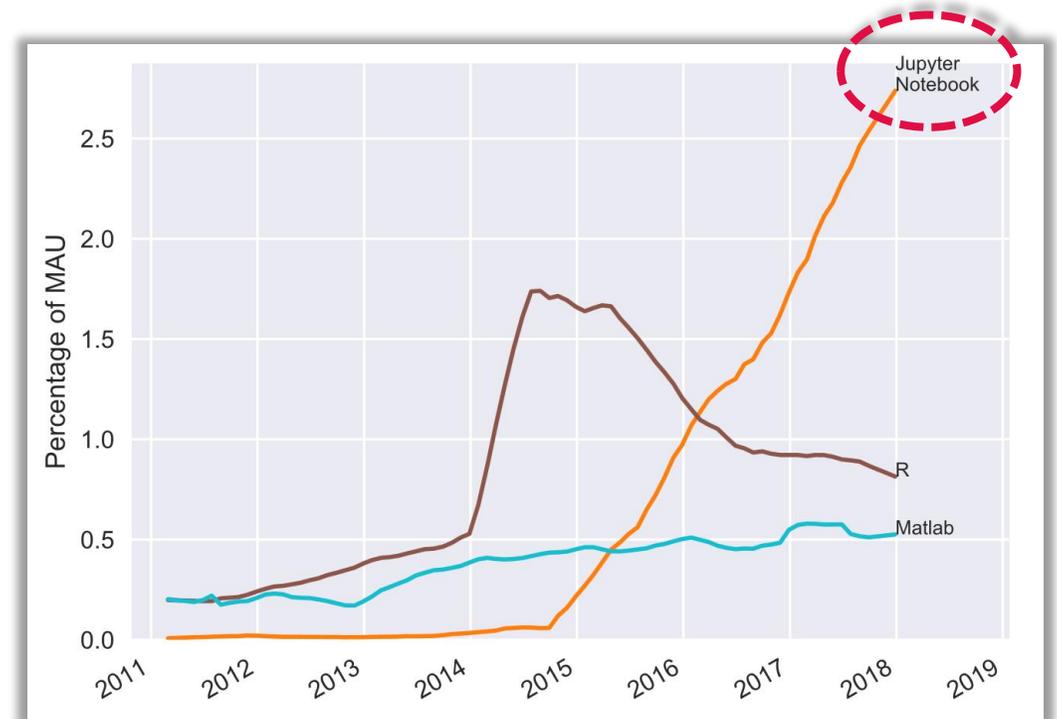
- Monthly aggregated number of user interactions with GitHub repos (= Monthly Active Users (MAU))

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

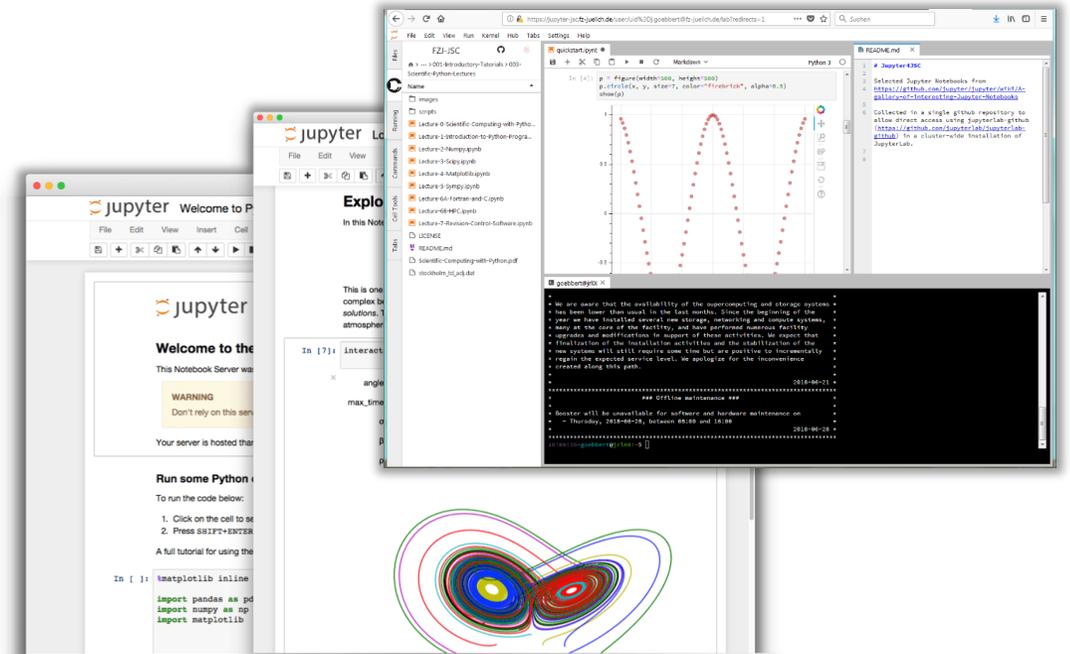
- **Interactive** working environment in the web browser
- For the creation of **reproducible** computer-aided narratives
- Very **popular** with researchers from all fields
- Jupyter = Julia + Python + R

### 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>

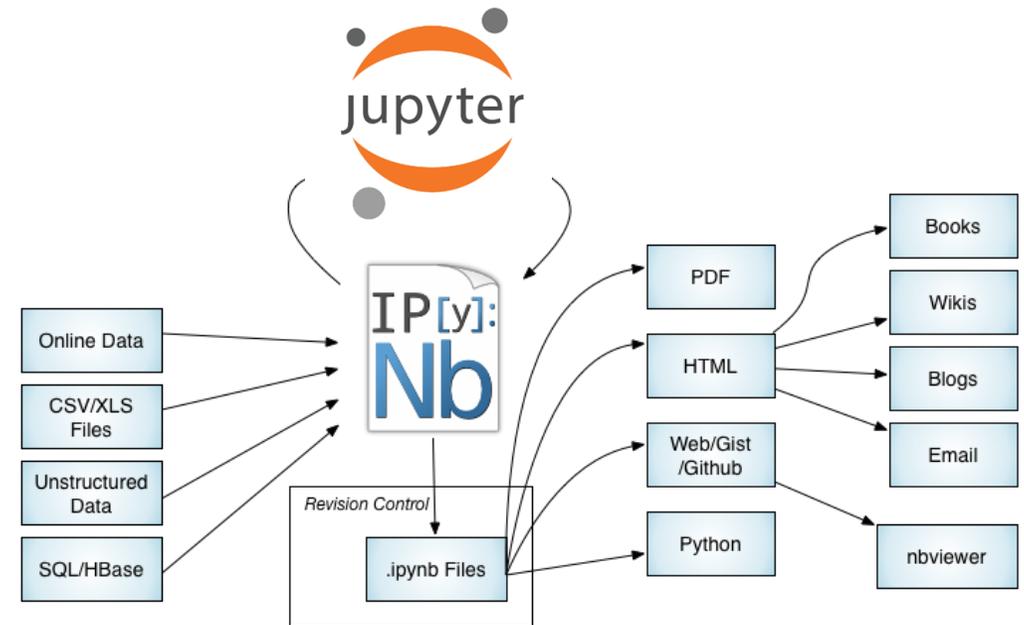
# TERMINOLOGY

## 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?

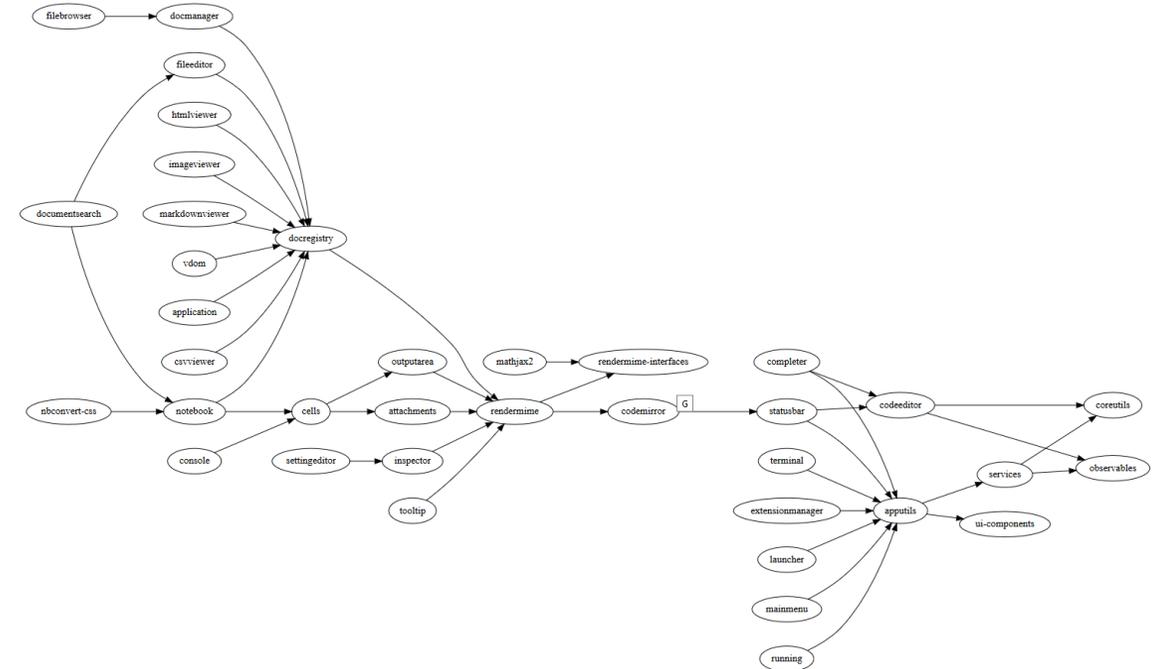
### JupyterLab Extension

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.

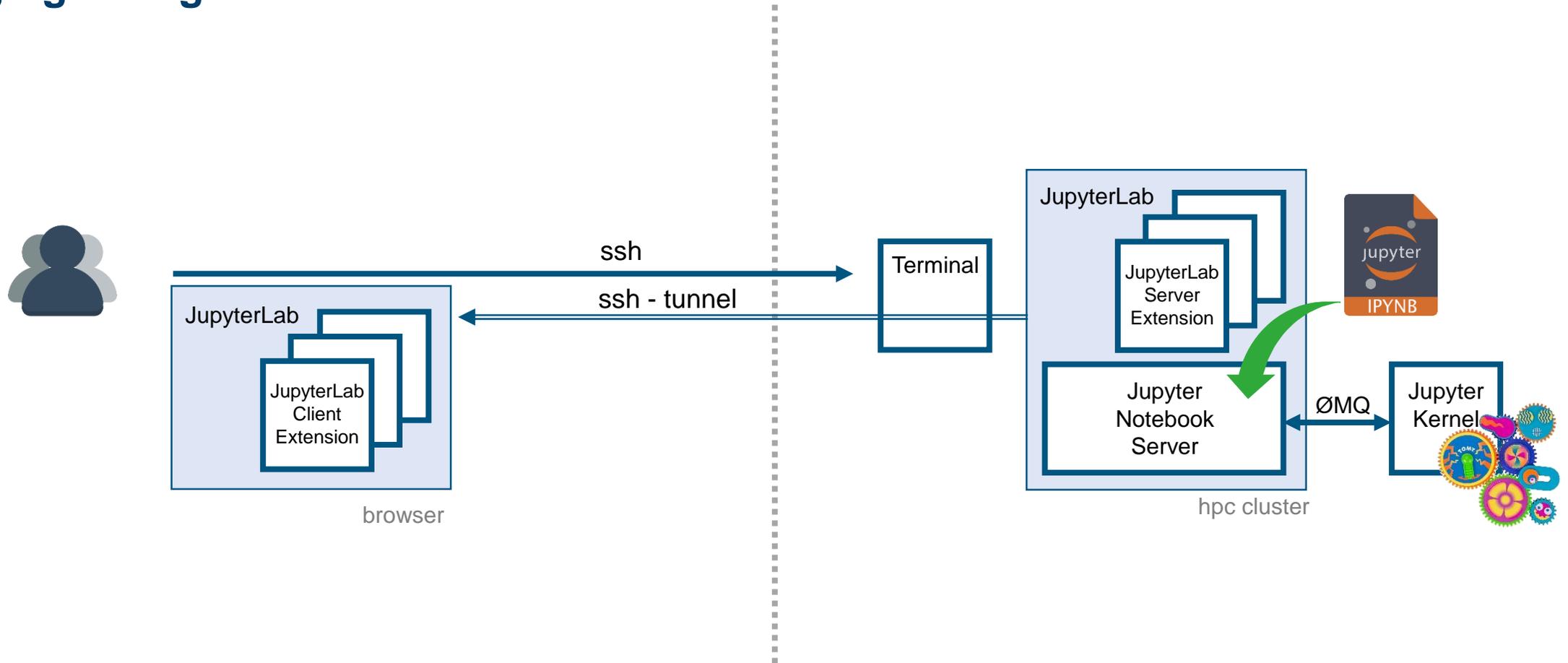
The whole JupyterLab itself is simply a **collection of extensions** that are no more powerful or privileged than any custom extension.



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

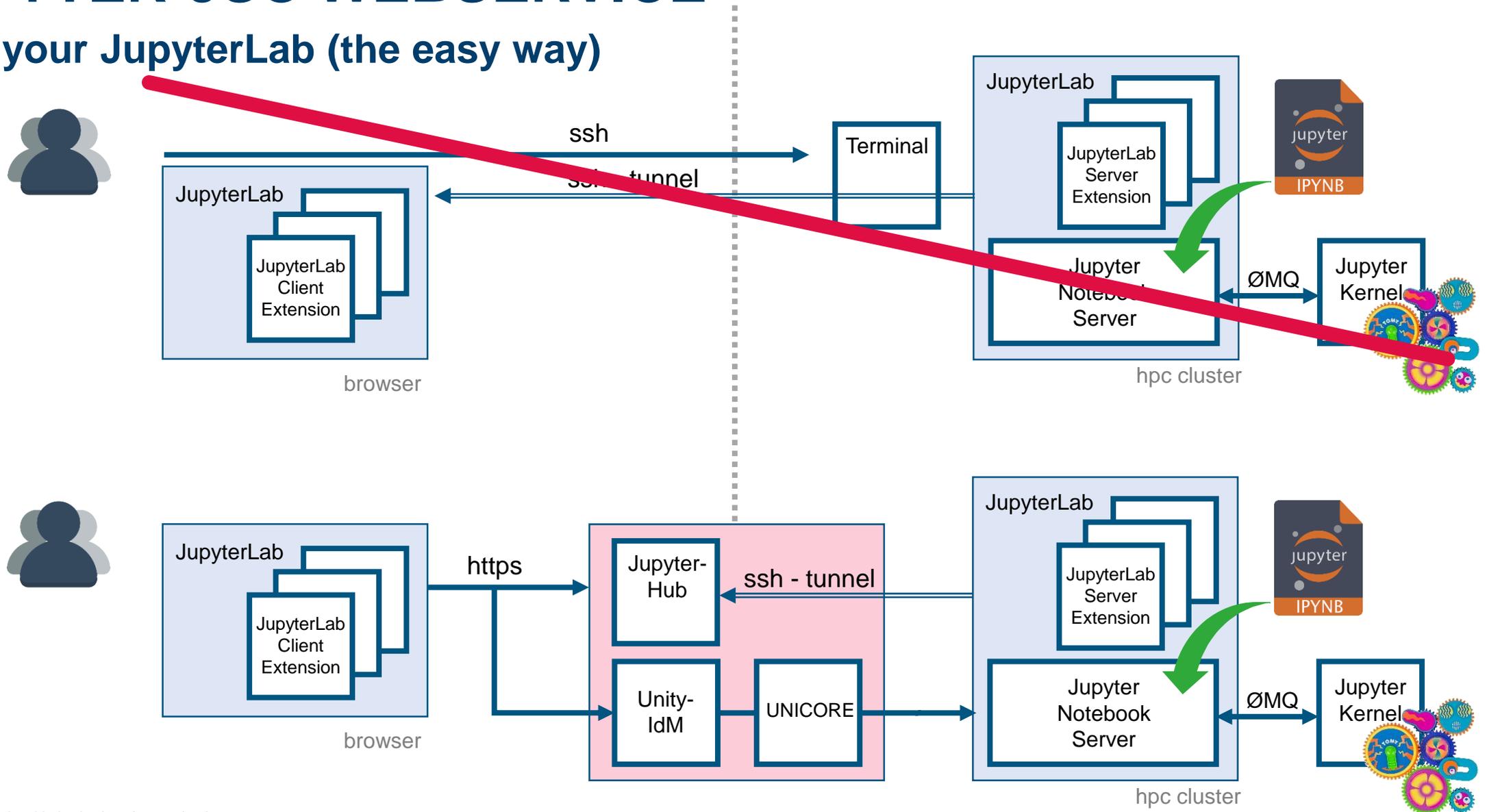
# TERMINOLOGY

## Bringing all together



# JUPYTER-JSC WEBSERVICE

## Start your JupyterLab (the easy way)



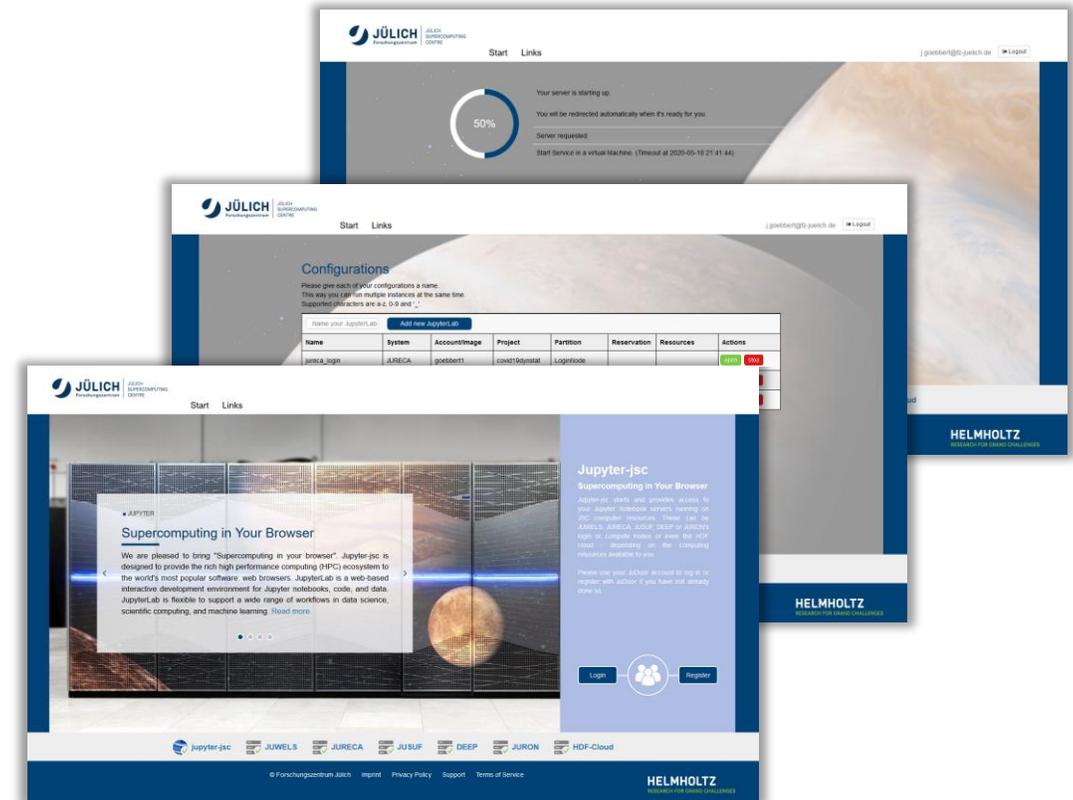
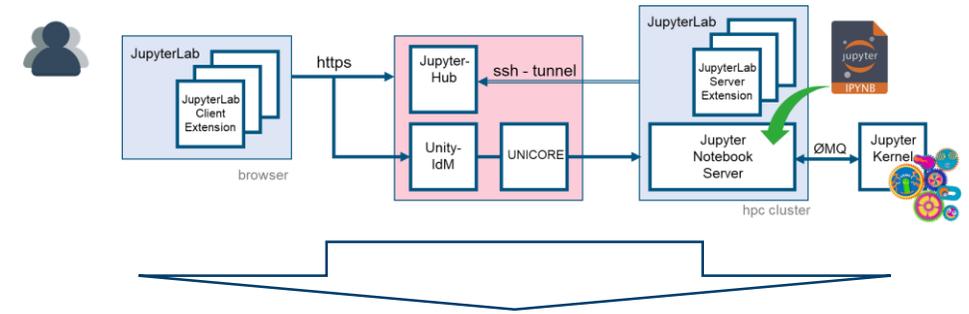
# JUPYTER-JSC WEBSERVICE

## 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

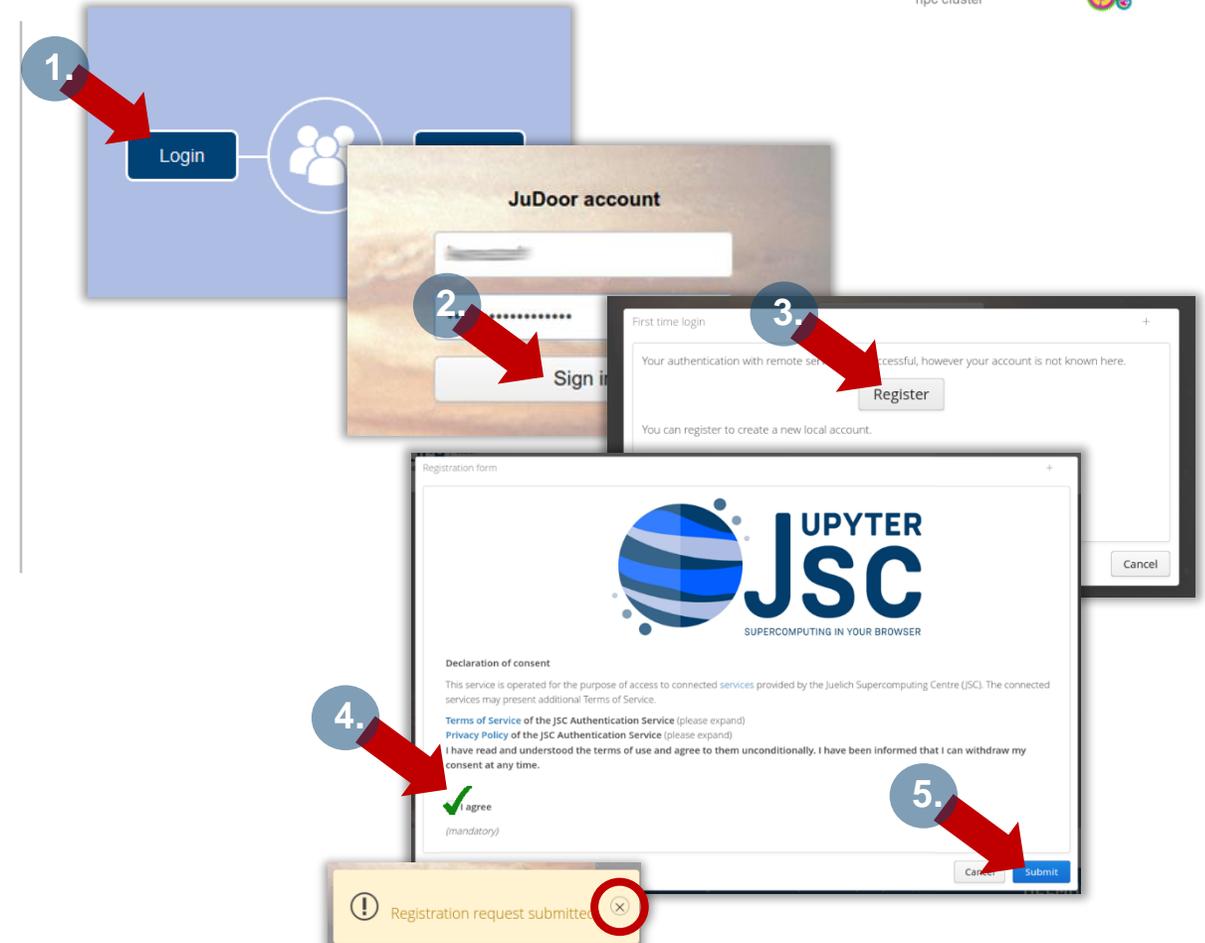
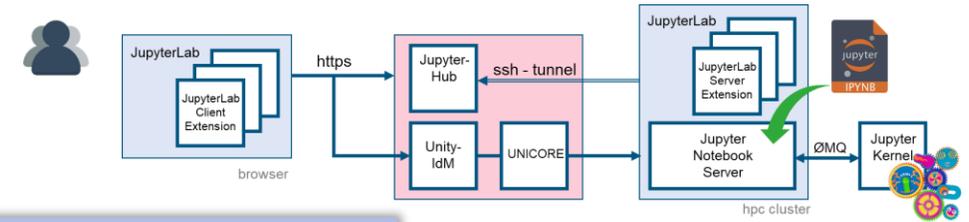
## First time login

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

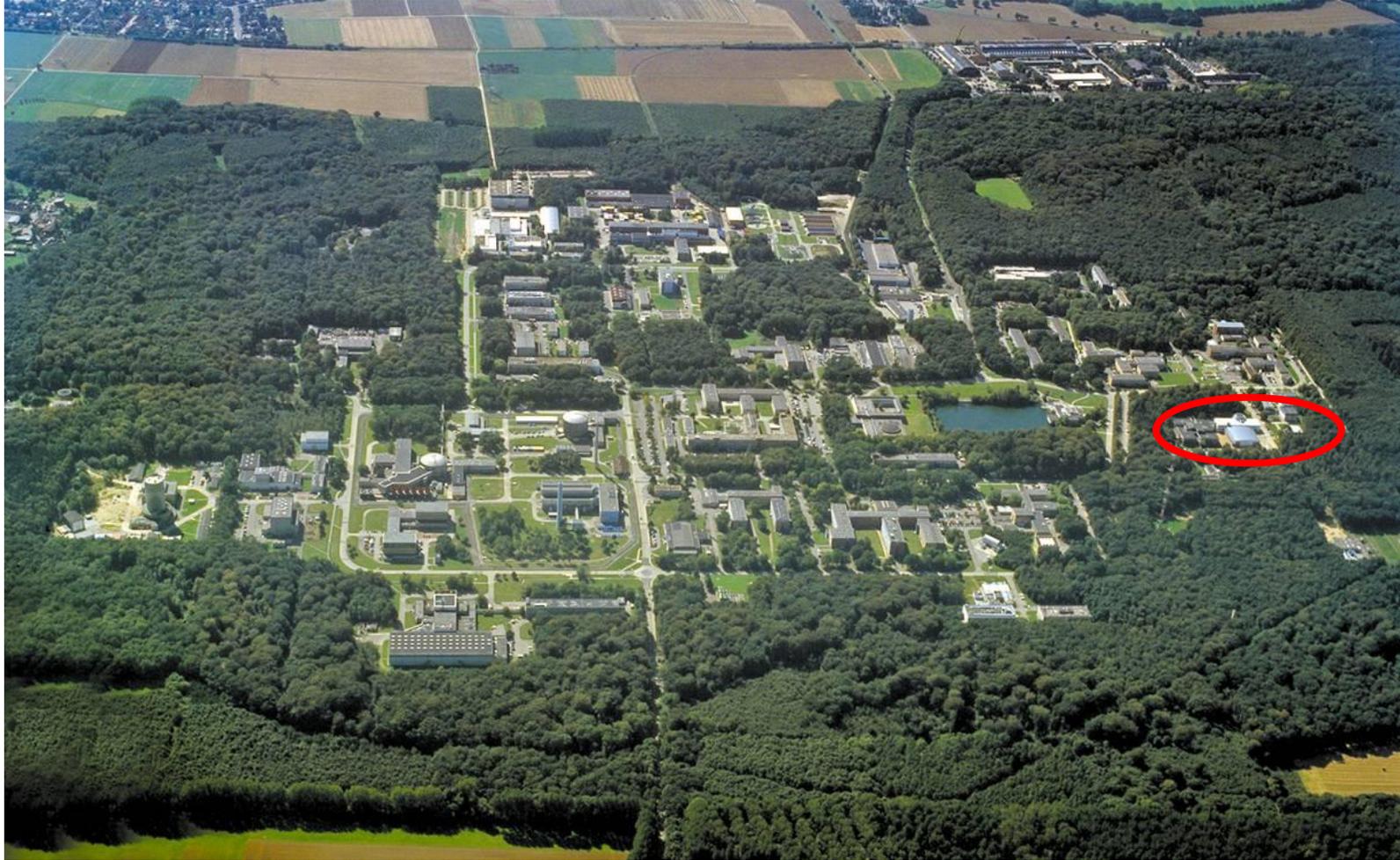
### Jupyter-JSC first time login

- Requirements:
  - Registered at [judoor.fz-juelich.de](https://judoor.fz-juelich.de)
    - (with "Connected Services" = jupyter-jsc)

1. Login at [jupyter-jsc.fz-juelich.de](https://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

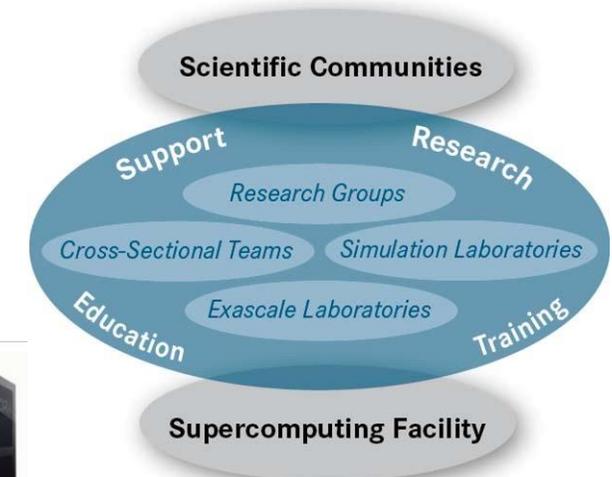
## Application support

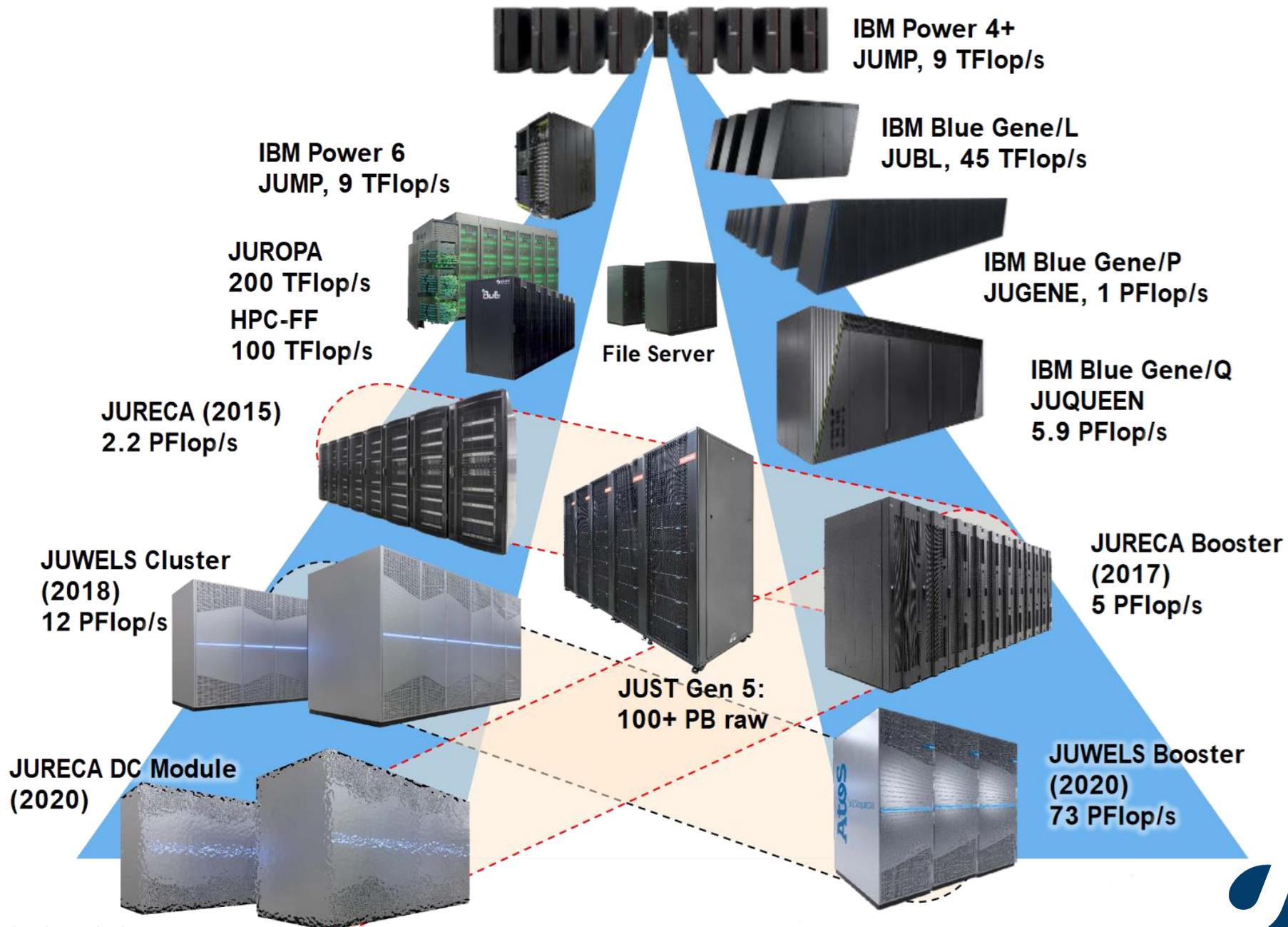
- Unique support & research environment at JSC
- Peer review support and coordination

## R&D work

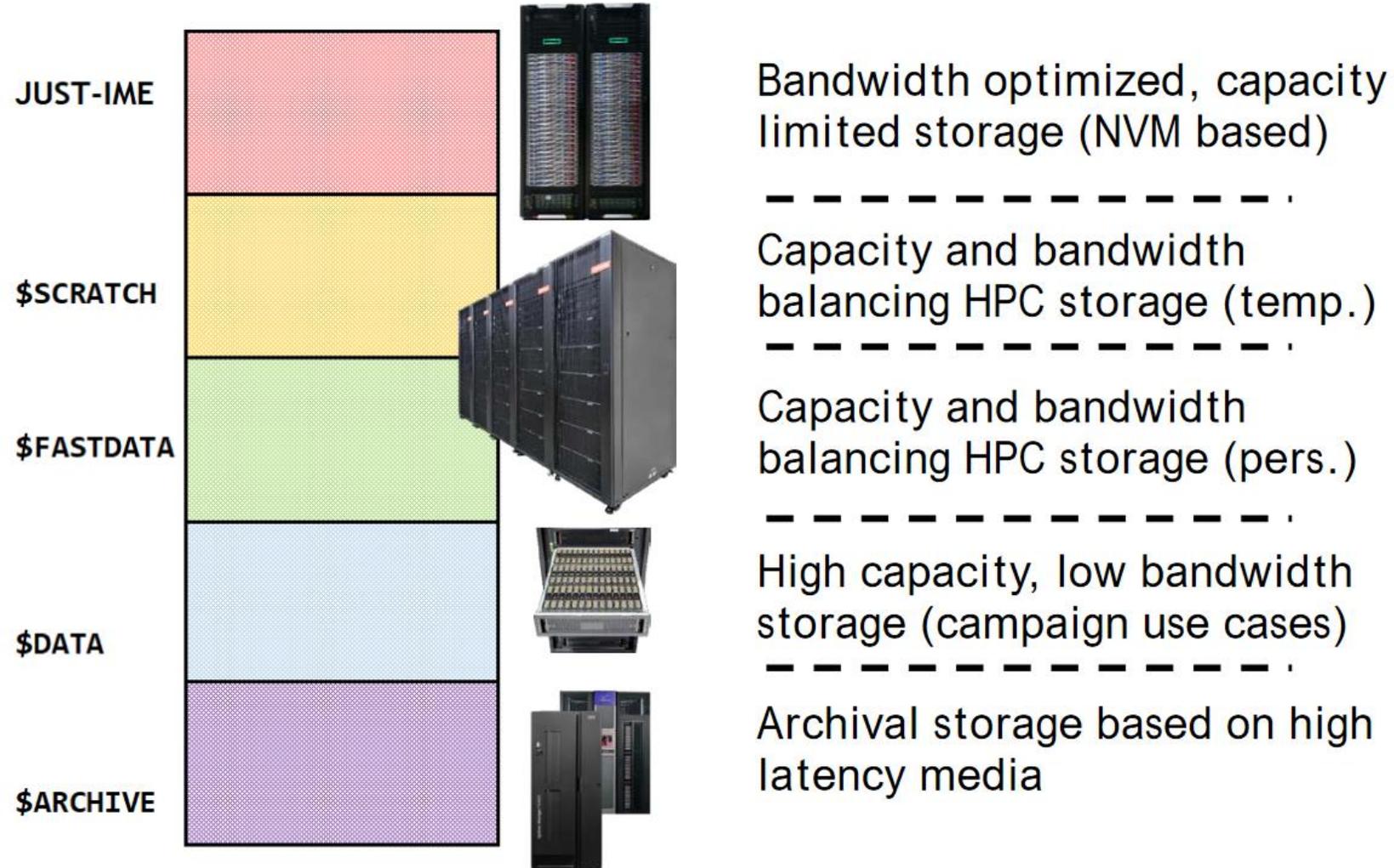
- Methods and algorithms, computational science, performance analysis and tools
- Scientific Big Data Analytics
- Computer architectures, Co-Design  
Exascale Laboratories: EIC, ECL, NVIDIA

## Education and Training





# JUST: MULTI-TIER STORAGE SYSTEM



# DOMAIN SPECIFIC SUPPORT

