



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#
- 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, unicon, HDFCloud

<https://jupyter.org>

The screenshot displays the Jülich Supercomputing Centre user interface. At the top, there is a navigation bar with 'Your account', 'Mentoring', a search bar, and 'Detailed Statistics'. The main content area is divided into several sections:

- Account:** A sidebar on the left lists fields: Salutation, E-mail address (with an email icon), Telephone, and Address.
- Mentored projects:** A section with a button labeled 'Mentored projects'.
- Systems:** A table listing systems with their status and usage agreements.

System	Status / Action
judac Manage SSH-keys	Usage agreement confirmed on 18.04.2021
jusuf	You need to sign the usage agreement to access this system
- Projects:** A section with a button labeled 'Join a project' and a project entry: 'Interactive High-Performance Computing with Jupyter'.
- Software:** A section with a button labeled 'Join a project'.
- Connected Services:** A section with buttons for 'trac', 'lview', 'jards', 'gitlab', and 'jupyter-jsc'.

Red circles highlight the 'sign the usage agreement' text in the Systems section and the 'jupyter-jsc' button in the Connected Services section. A green circle highlights the 'Join a project' button in the Projects section.

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>

Member of the Helmholtz Association

MOTIVATION

Rise of Jupyter's popularity

If popularity can be counted by

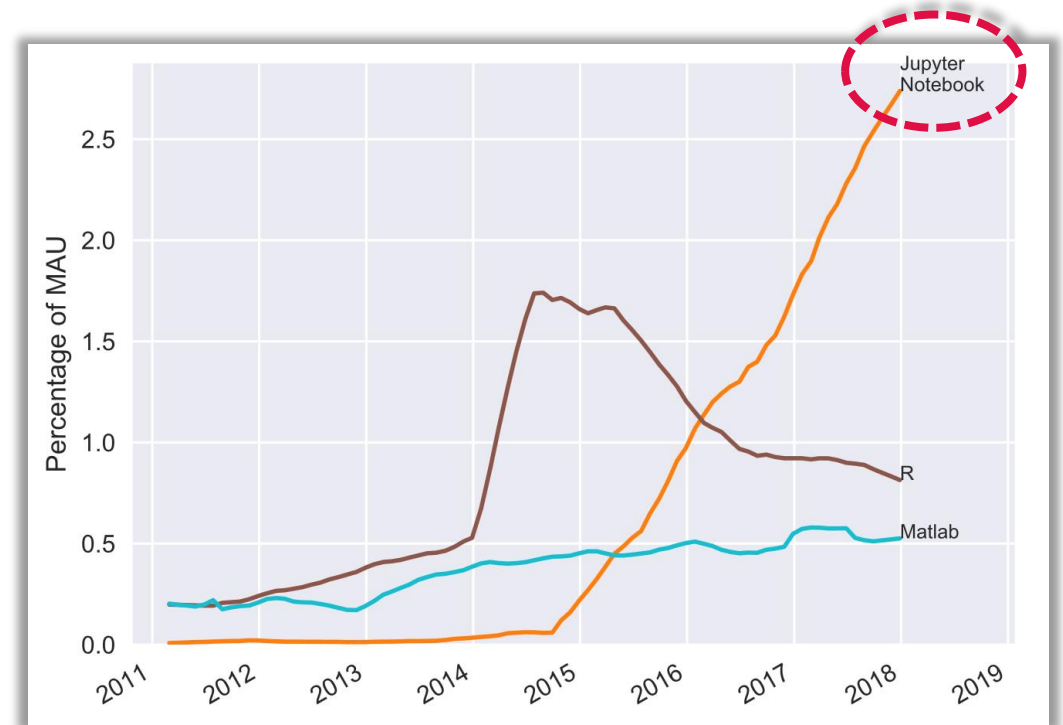
- Monthly aggregated number of user interactions with GitHub repos (= Monthly Active Users (MAU))

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

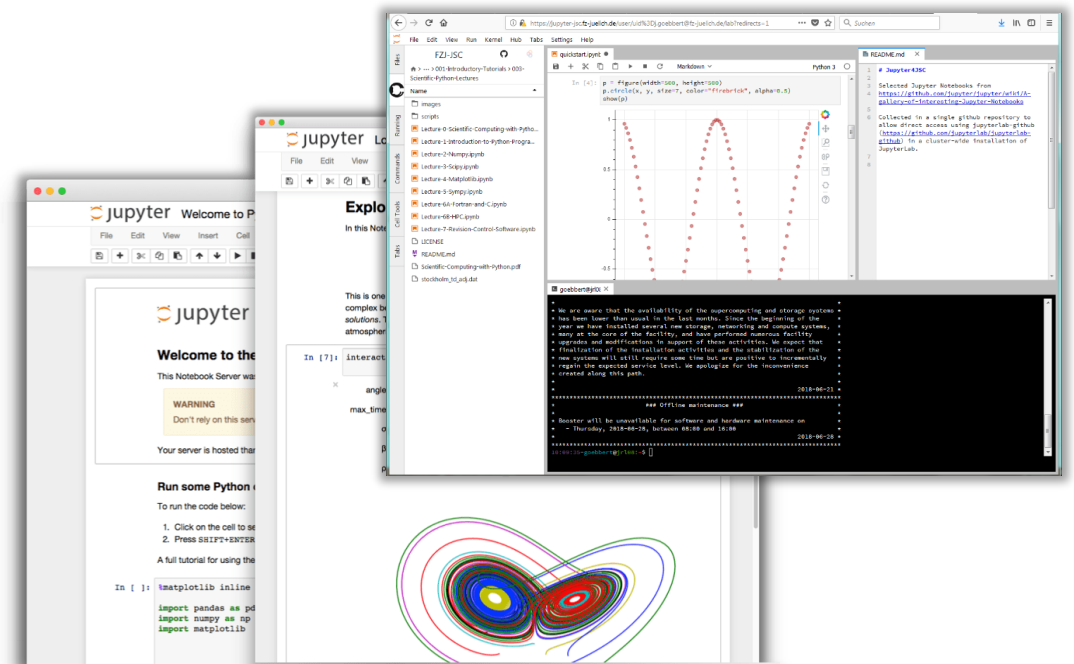
- **Interactive** working environment in the web browser
- For the creation of **reproducible** computer-aided narratives
- Very **popular** with researchers from all fields
- Jupyter = Julia + Python + R

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>

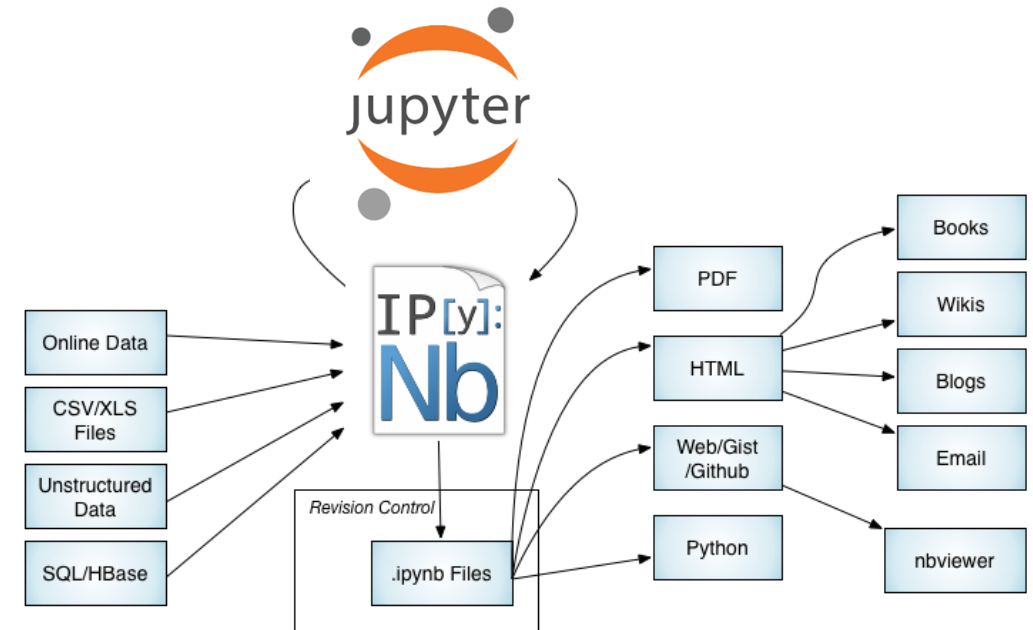
TERMINOLOGY

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

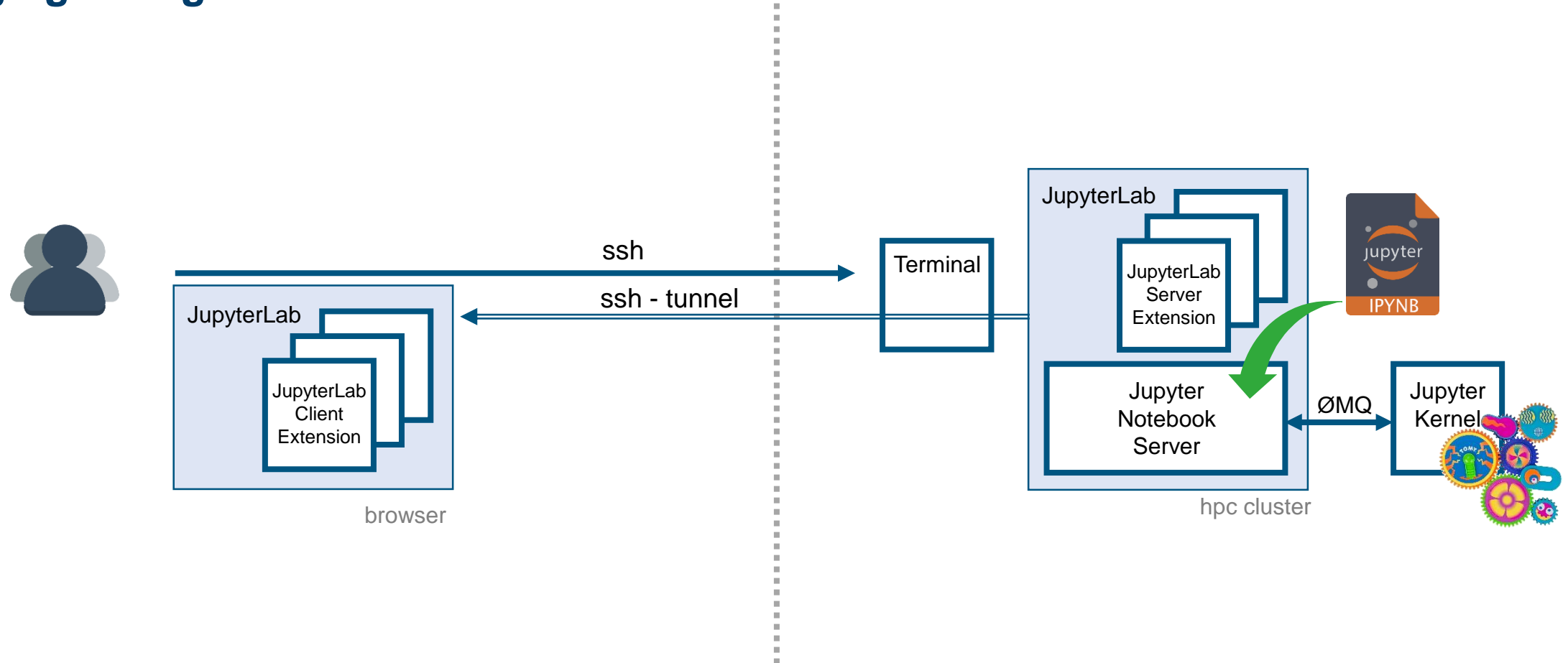
- **run code** in different programming languages and environments.
- can be **connected to** a notebook (one at a time).
- **communicates** via ZeroMQ with the JupyterLab.
- Multiple **preinstalled** Jupyter Kernels can be found on our clusters
 - Python, R, Julia, Bash, C++, Ruby, JavaScript
 - Specialized 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>

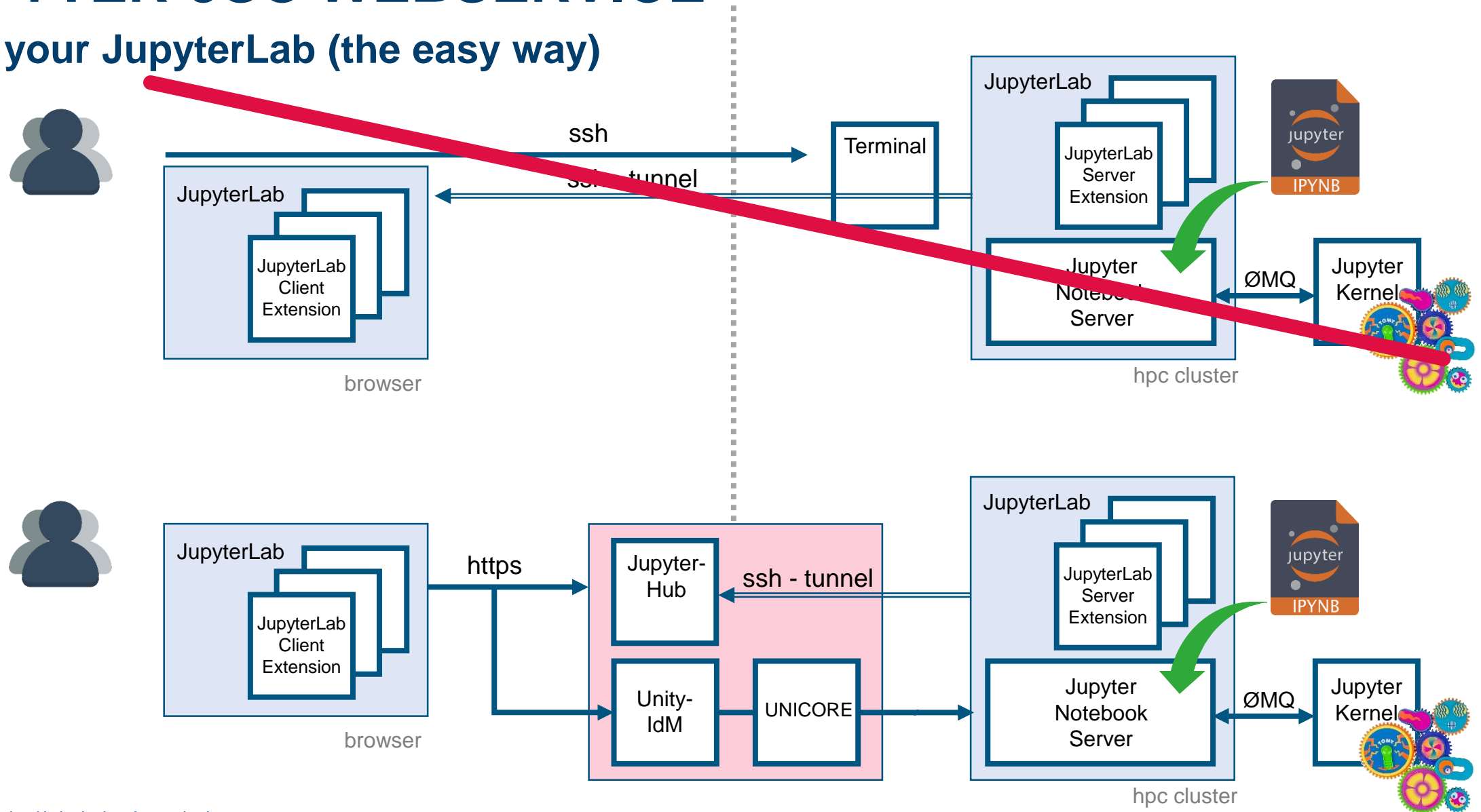
TERMINOLOGY

Bringing all together



JUPYTER-JSC WEBSERVICE

Start your JupyterLab (the easy way)



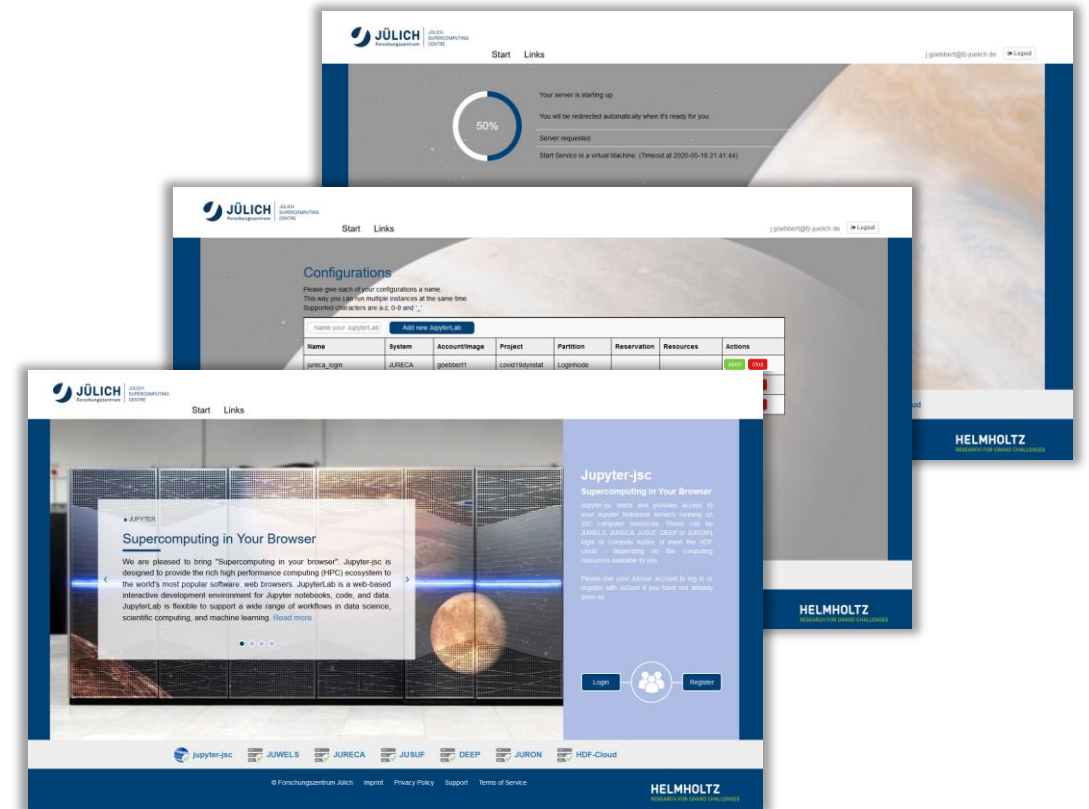
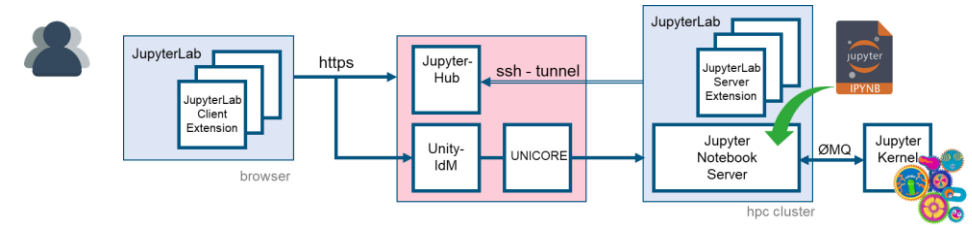
JUPYTER-JSC WEBSERVICE

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

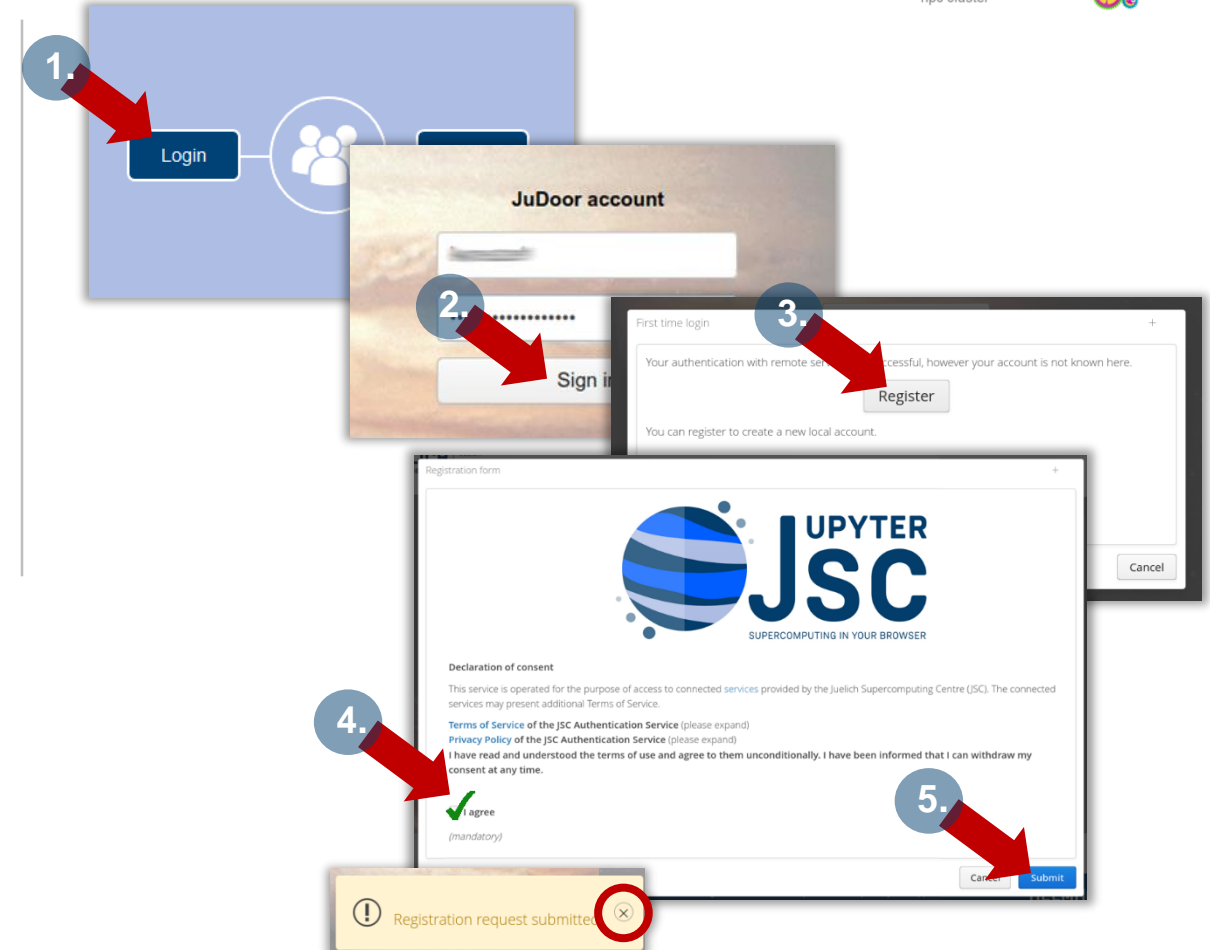
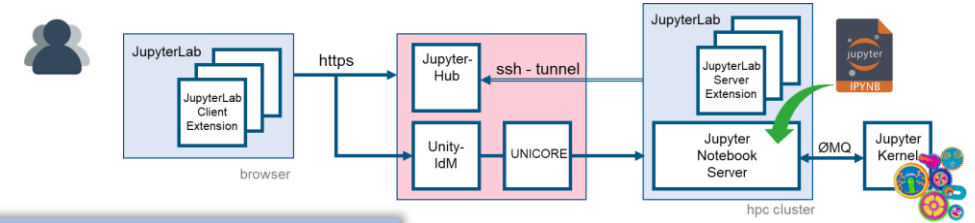
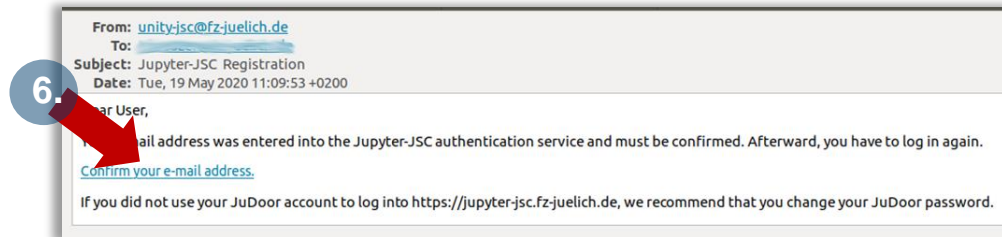
First time login

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

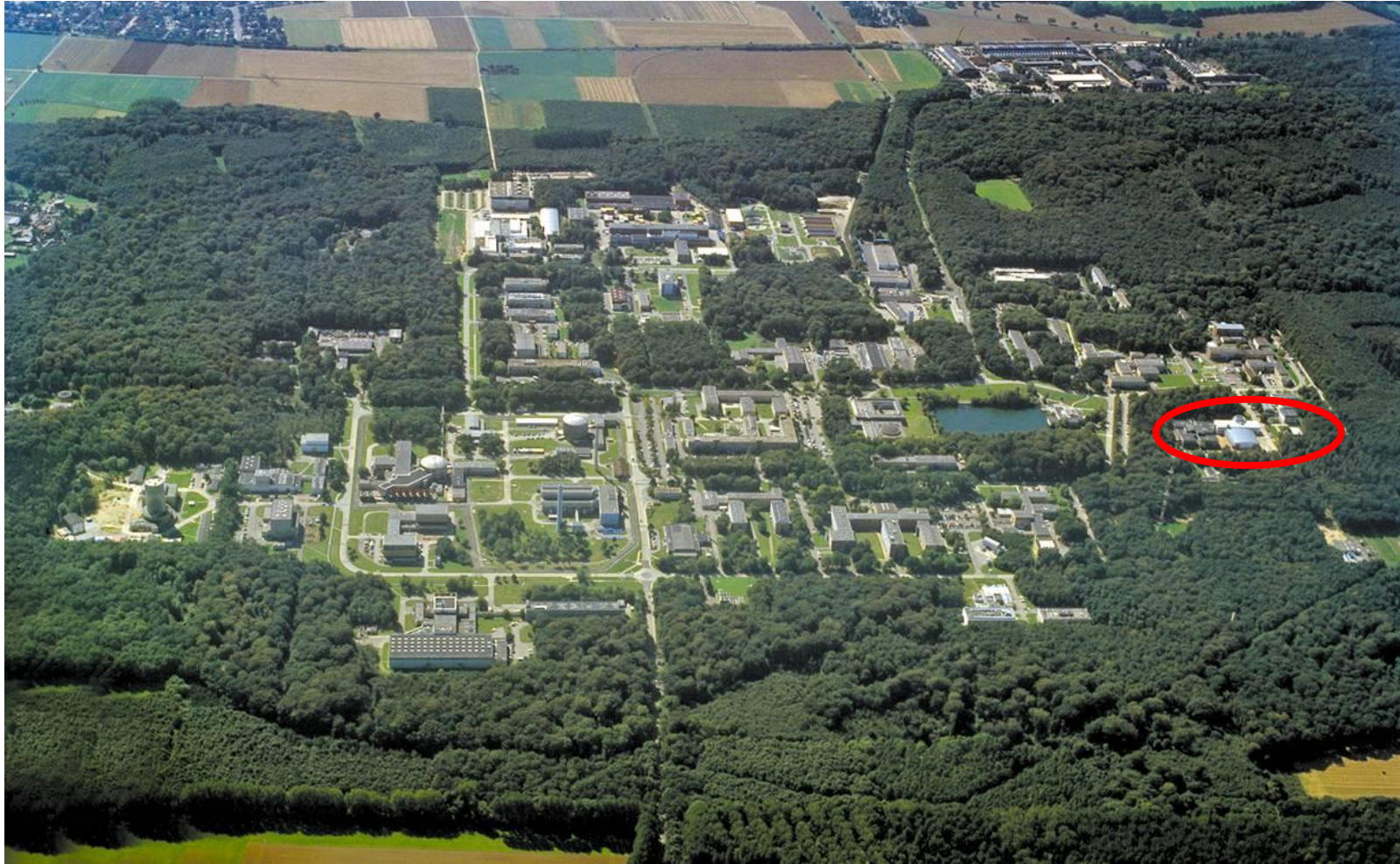
Jupyter-JSC first time login

- 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

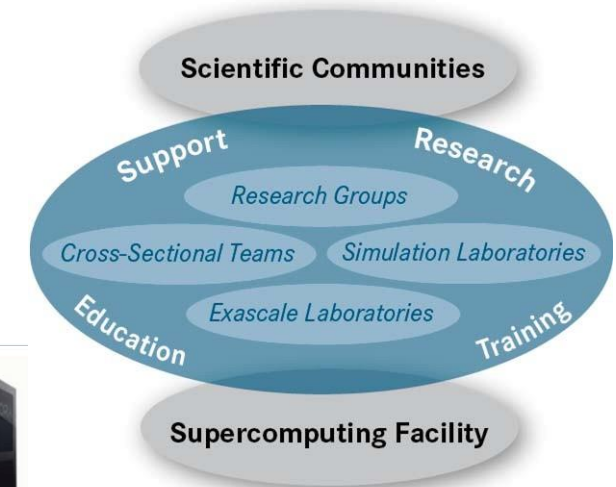
Application support

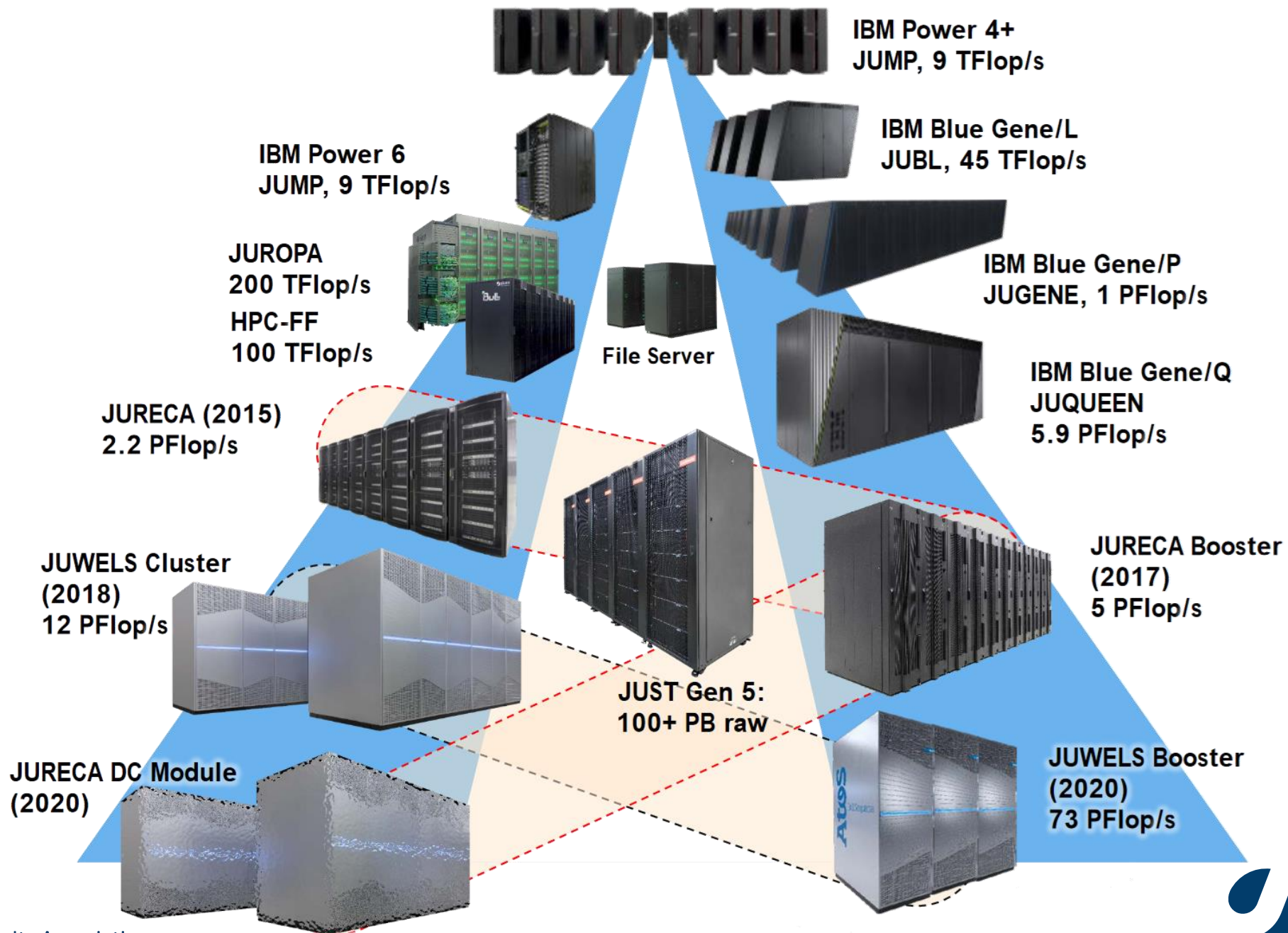
- Unique support & research environment at JSC
- Peer review support and coordination

R&D work

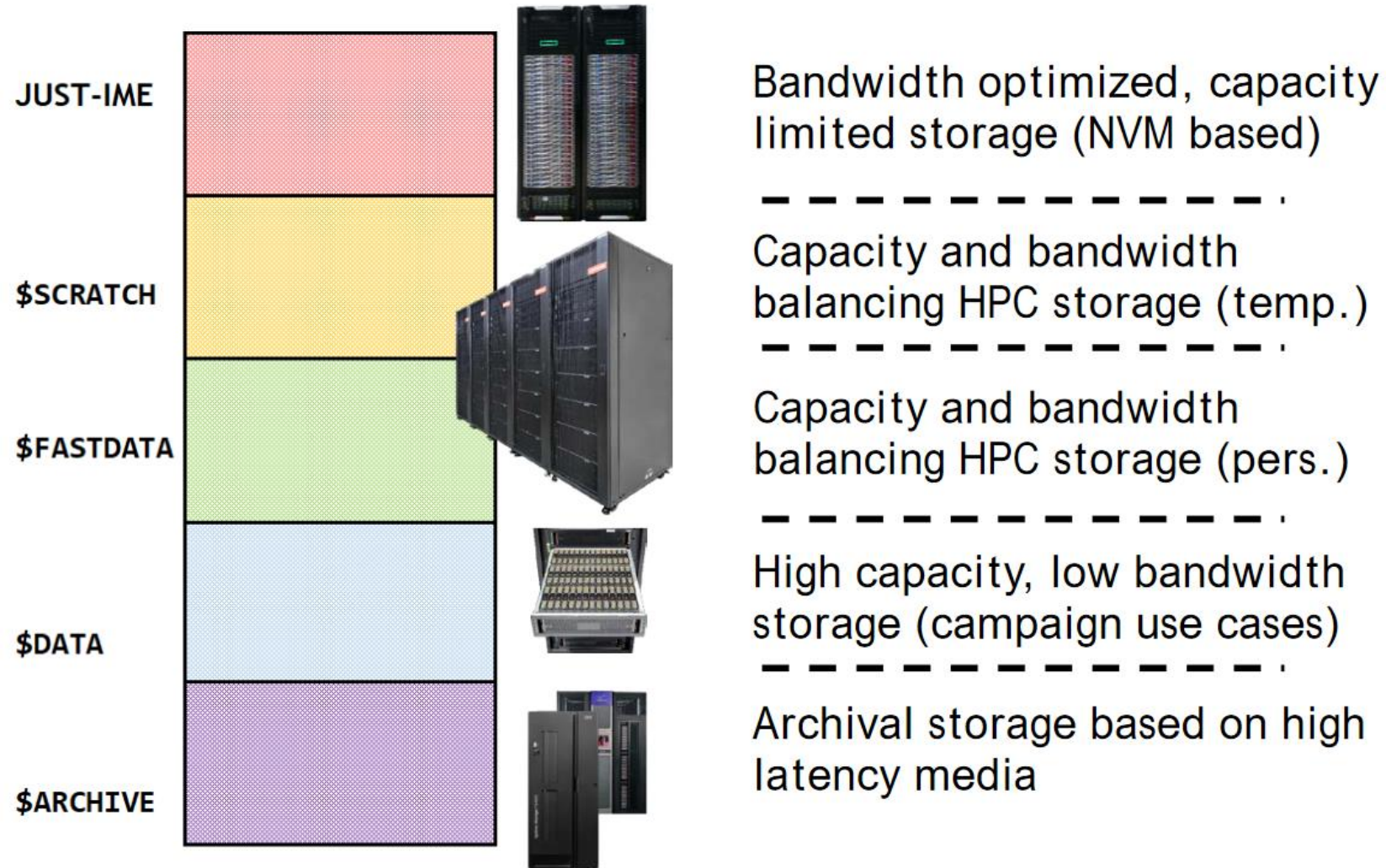
- Methods and algorithms, computational science, performance analysis and tools
- Scientific Big Data Analytics
- Computer architectures, Co-Design
Exascale Laboratories: EIC, ECL, NVIDIA

Education and Training





JUST: MULTI-TIER STORAGE SYSTEM



DOMAIN SPECIFIC SUPPORT

