

ECMWF JupyterHub on Atos HPC and cloud

Introduction to ECMWF computing services

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Cloud and software support @ User Service Section

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What is JupyterHub

- Browser-based Jupyter Lab environment
- Users can use the service to launch an isolated server on any of the available backends
- Perform on-the-fly data processing close to data using the readily available software and tools (just like working on HPC*) on a shared resource
- It is not a replacement for all batch/HPC workflows, but provides interactive means to interact with data and software for building prototypes

*if you are using the HPC backend

JupyterHub at ECMWF - Timeline

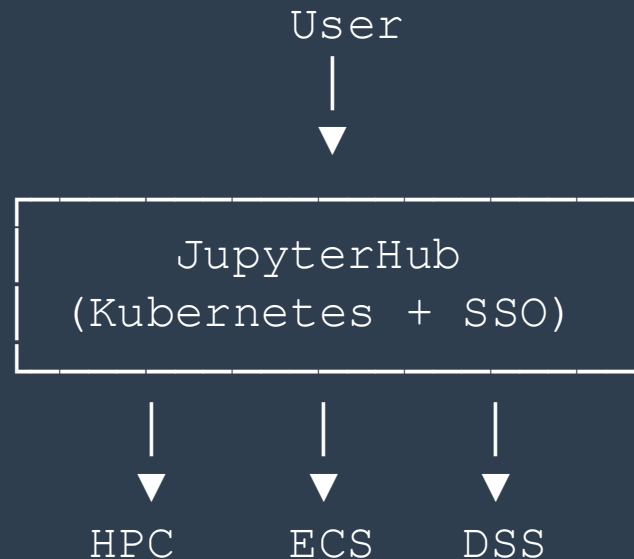
2025+	• GPU support testing
Mid 2025	• DSS backends access enabled, Upgrade to JupyterHub 5
Late 2024	• Ecosystem / software updates
Mid 2024	• HPC & ECS backends enabled
Early 2024	• Service becomes public
Late 2023	• Internal pilot

Architecture - one front door, many engines

JupyterHub orchestrates the service, while compute happens on the backend you choose:

- HPCF (Slurm) for larger/comprehensive workloads
- ECS (ecgate-class) for testing and smaller tasks
- DSS (near data) for lightweight, data-proximate tasks

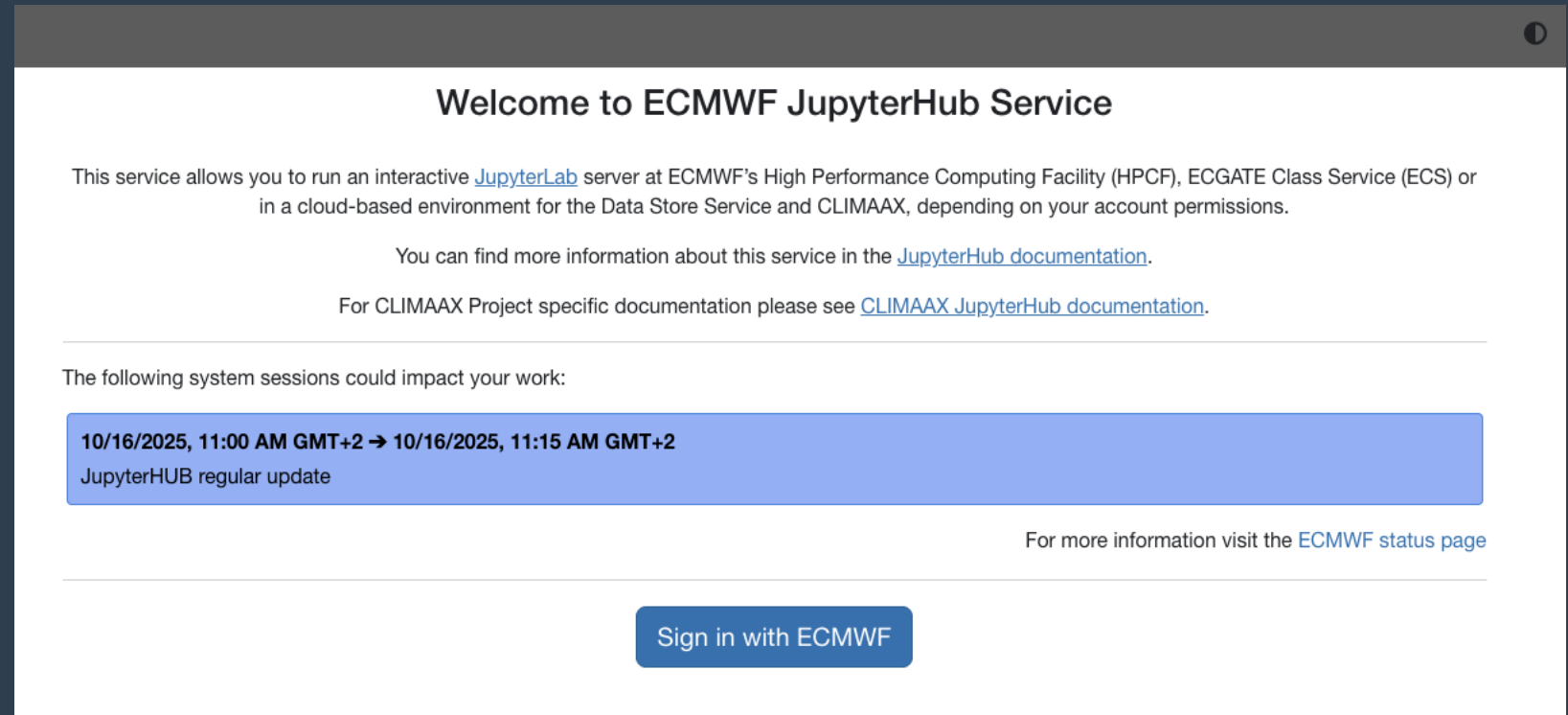
Backend decoupling brings flexibility, easy integration of new backends



Access & first-use

Prerequisites:

- SSO + MFA with ECMWF account
- add JupyterHub's **SSH public key** to
`~/.ssh/authorized_keys`
- each user can have **one active** JupyterHub **session** at a time
- sessions are time limited and in case of inactivity they expire



The screenshot shows the 'Welcome to ECMWF JupyterHub Service' page. It includes a header with the service name, a paragraph explaining the service's purpose, and links to documentation. A section titled 'The following system sessions could impact your work:' contains a blue box with session details: '10/16/2025, 11:00 AM GMT+2 → 10/16/2025, 11:15 AM GMT+2' and 'JupyterHUB regular update'. At the bottom, there is a 'Sign in with ECMWF' button and a link to the 'ECMWF status page'.

Welcome to ECMWF JupyterHub Service

This service allows you to run an interactive [JupyterLab](#) server at ECMWF's High Performance Computing Facility (HPCF), ECGATE Class Service (ECS) or in a cloud-based environment for the Data Store Service and CLIMAAX, depending on your account permissions.

You can find more information about this service in the [JupyterHub documentation](#).

For CLIMAAX Project specific documentation please see [CLIMAAX JupyterHub documentation](#).

The following system sessions could impact your work:

10/16/2025, 11:00 AM GMT+2 → 10/16/2025, 11:15 AM GMT+2
JupyterHUB regular update

For more information visit the [ECMWF status page](#)

[Sign in with ECMWF](#)

User documentation covering the initial setup can be found here:

<https://confluence.ecmwf.int/display/UDOC/First+use%3A+enabling+access+to+your+HPCF+or+ECS+account+from+JupyterHub>

Starting a session (Backend Options)

- Pick engine/environment
- Set **CPUs** and **Memory**
- Choose **Duration** (auto-stop)
- Size of **TMPDIR** for temporary files
- Set **Project** for accounting
- Choose a **Version** (base stack)

Home Token

Compute Backend Options

Select an Environment

ECMWF ATOS HPCF

Run a JupyterLab session on the ECMWF Atos HPCF under your user account. You will have access to the standard software stack, environment and files in the HPCF computing service. Configurations selected below will be persisted and will be re-used the next time you use this profile.

Memory
8 GB RAM

CPU
2 CPU

Session Duration
12 Hours

Temporary Storage
3 GB

Project Account
ecus

Version
Default

Debug
No

Start

If startup misbehaves enable debug option and inspect the log.

This is helpful evidence and very useful for cases when you need further support, to help us replicate and investigate issue.

JupyterLab tour

- **Launcher** →

Notebooks, Consoles, Terminal

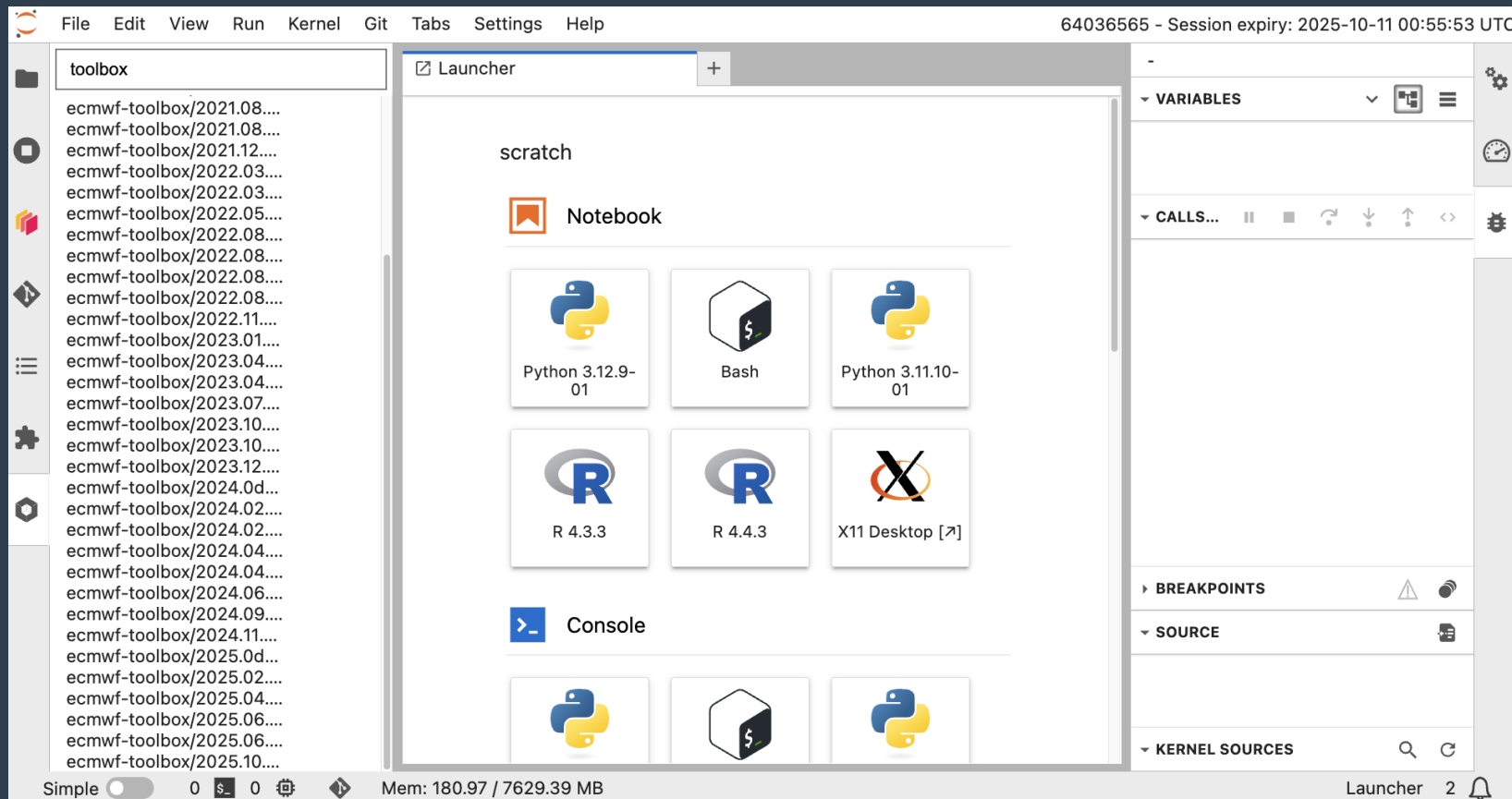
- **Left sidebar** →

File browser, Git (if enabled), Running, Commands

Kernel menu → restart/change kernel (environment captured at start)

- **Extensions** →

modules panel, Git, PyPI UI



Software stacks: modules, kernels and conda

- ECMWF software arrives via modules (eccodes, magics, ...)
- **Golden rule:** load modules **before** starting a kernel (or restart it).
- To use your own conda environment as a kernel for Jupyter notebook you will need to have *ipykernel* installed in the conda environment before starting your Jupyter instance.

ipykernel can be installed with:

```
conda activate myCondaEnv
conda install ipykernel
python3 -m ipykernel install --user --name=myCondaEnv --env PATH "$CONDA_PREFIX/bin:\$PATH"
```

- If you want to make your own Python *virtual env* visible in Jupyterlab, the steps are similar:

```
source /path/to/myVenv/bin/activate
pip3 install ipykernel
python3 -m ipykernel install --user --name=myVenv --env PATH "/path/to/myVenv/bin:\$PATH"
```

You can remove unnecessary personal kernels simply:

```
jupyter kernelspec uninstall myKernelName
```


Managing storage & best practices

- **HOME**: small, backed-up; default start location
- **PERM/HPCPERM**: used for long-term storage
- **SCRATCH**: high-capacity, temporary storage for big temporary files

You can add handy shortcuts in HOME:

```
for s in perm hpcperm scratch;  
do ln -snf /$s/$USER ~/ $s; done
```

FAVORITES

- hpcperm /
- perm /
- scratch /



Limits, etiquette & troubleshooting

- Sessions auto-end at the time you choose - save before that.
- One active Hub session by design; avoid parallel *ecinteractive* Jupyter.
- ‘No space’ usually means **TMPDIR** is too small—start with a bigger one.
- Startup failed? **Debug = Yes**, read the log, seek support.



Resources

- Login page: <https://jupyterhub.ecmwf.int/hub/login>
- User docs: <https://confluence.ecmwf.int/display/UDOC/JupyterHub>
- Support portal: <https://www.ecmwf.int/en/support>

Thank you!

Q&A

