

# EXPANDS

**European Open Science Cloud Photon  
and Neutron Data Services**

## **Jupyter Kernel Validations as Photon Neutron Use Case**

Contribution to EOSC-Synergy Workshop

Presenter: Jason Brudvik, Patrick Fuhrmann

With contributions by: Zdeněk Matěj and Michael Schuh



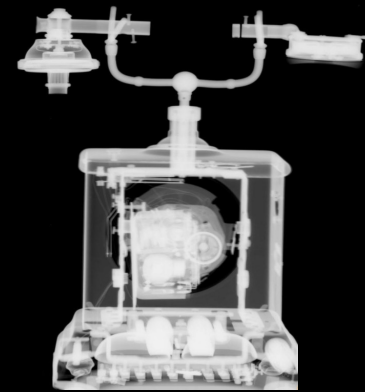
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# Introduction

## What is Photon and Neutron Science about?

### Photon

Beam interacts with **molecule hull**



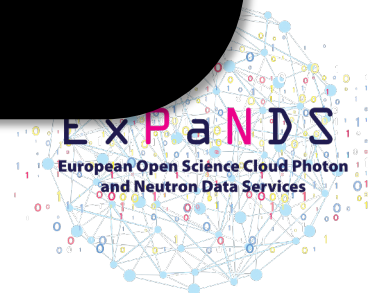
Energy

### Neutron

Beam interacts with **molecule nucleus**



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# Some typical PaN facilities!

Petra III



Soleil



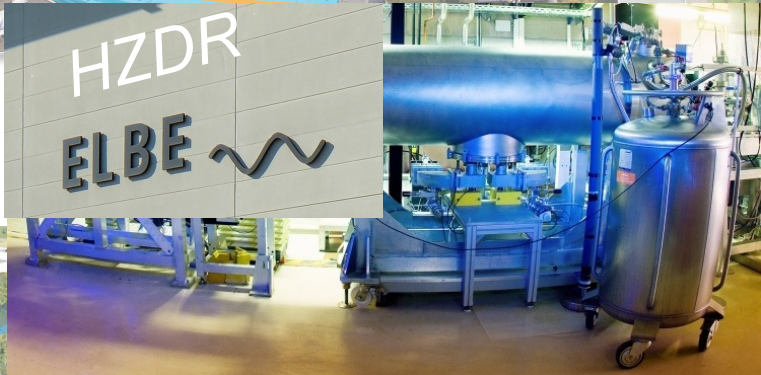
Max IV



ALBA



SwissFEL



Diamond



Bessy , HZB



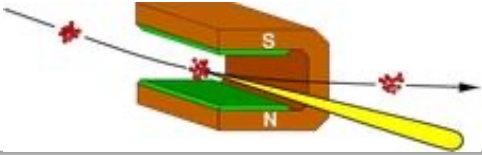
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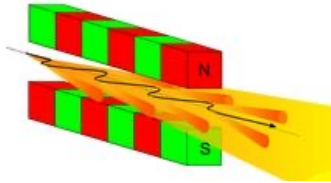
# From Beam Generation to Domain Science!

## Beam Generation

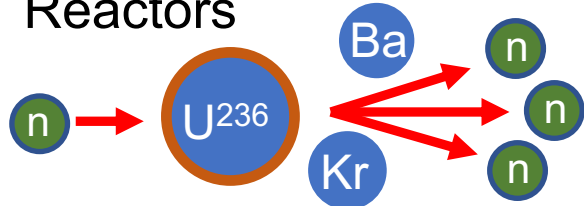
### Bending



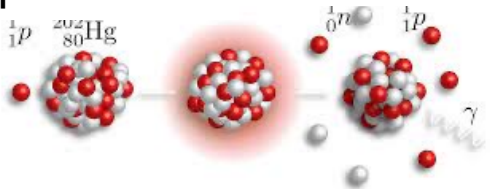
### Undulators



### Reactors



### Spallation



## Instrument Technique

Full field tomography



Single crystal X-ray diffraction



Serial crystallography



Ptychography



Small angle X-ray scattering



Neutron diffraction and tomography



Reflectometry



Terahertz spectroscopy



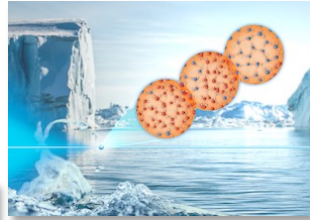
Scanning electron imaging



And many more ....

## Domain Science

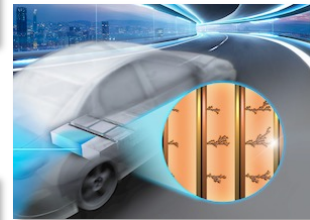
With high significance for bringing society forward.



Role of Water



Fine Dust



Battery

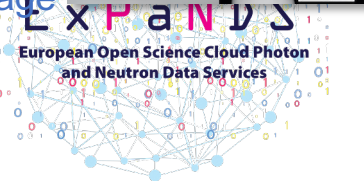


Superconductors



Cultural Heritage

Stolen from Petra IV TDR.



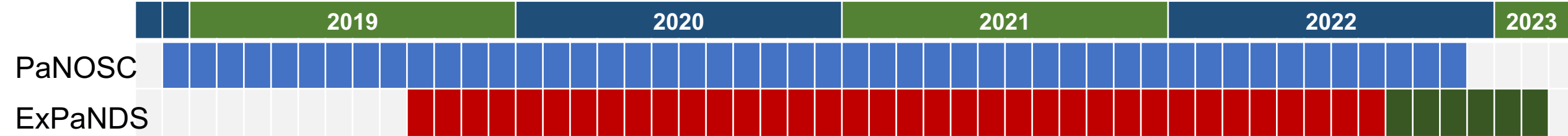
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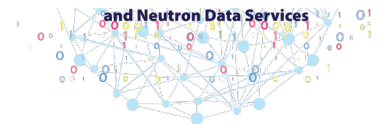
# The usual Project Cheat Sheet!



EU Call	HORIZON 2020 INFRA-EOSC-04		HORIZON 2020 INFRA-EOSC-5B
Description	Cluster of ESFRI PaN Sources		EOSC PaN Data Services
Partners	ESRF, ILL, ESS, EU-XFEL, CERIC-ERIC, ELI-DC, EGI		DESY, ALBA, DLS, ELETTRA, EGI, HZB, HZDDR, Max IV, PSI, Soleil, UKRI
Observers	GEANT EU-DAT National RI's		
Linked 3 <sup>rd</sup> Party	DESY STFC CESNET		
Start – End (Duration)	2018-12-01 – 2022-11-30 [4 Years]		2019-09-01 – 2023-02-28 [ 3 ½ Years]
Coordinators	A. Götz, G. Boderà		P. Fuhrmann, S. Servan
Budget	12 M Euros		6 M Euros
Home Page	PaNOSC.EU		ExPaNDS.EU
Twitter	@PaNOSC_eu #PaNOSC		@ExPaNDS_eu #ExPaNDS
GitHub	github.com/panosc-eu		Github.com/expands-eu



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# PaN facilities covered by PaNOSC/ExPaNDS



## Photon (LEAPS)



## Neutron (LENS)



ExPaNDS  
European Open Science Cloud Photon  
and Neutron Data Services



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# And now to our testing framework ....

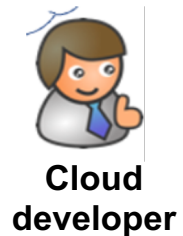
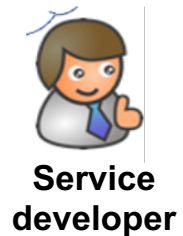
## .... and introducing Jason



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# Clarifying Roles: from Cloud Expert to Scientist!

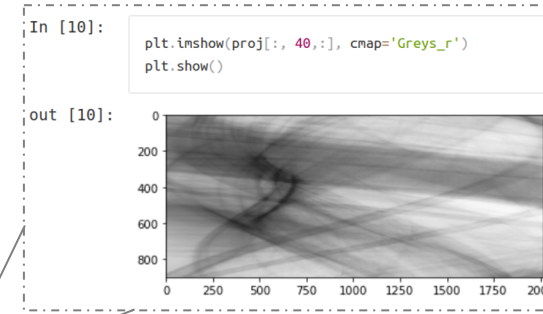


**Notebooks**  
FAIR Research Artifacts

**Servers and Kernels**  
Research Software as a Service

**Jupyter Hub**  
Data Analysis Platform

Open Science Commons



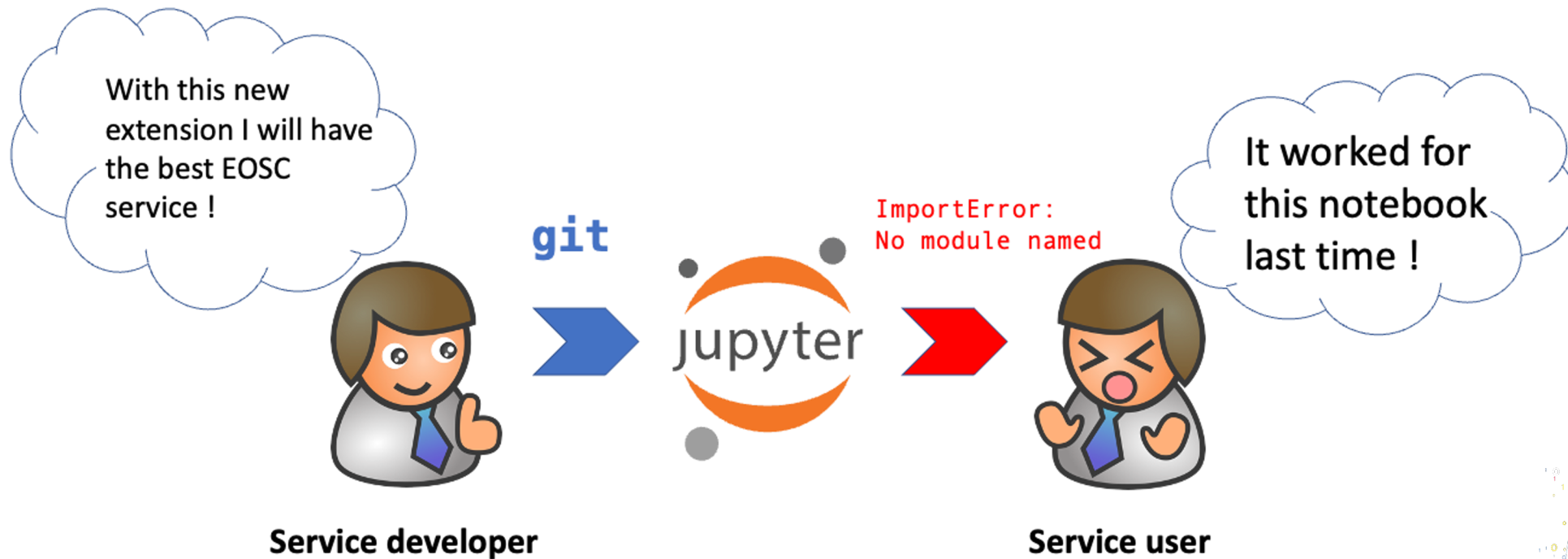


# SQAaaS I: Service Validation

**Description:** Test Jupyter service against reference scientific use cases

**Details:** Triggers as soon as something changes on the infrastructure or the Jupyter service  
(e.g. upgrading JupyterLab Version)

**Why:** *Improved user experience - things work when service users return to them*



# SQAaaS II: Scientific Use Case Validation

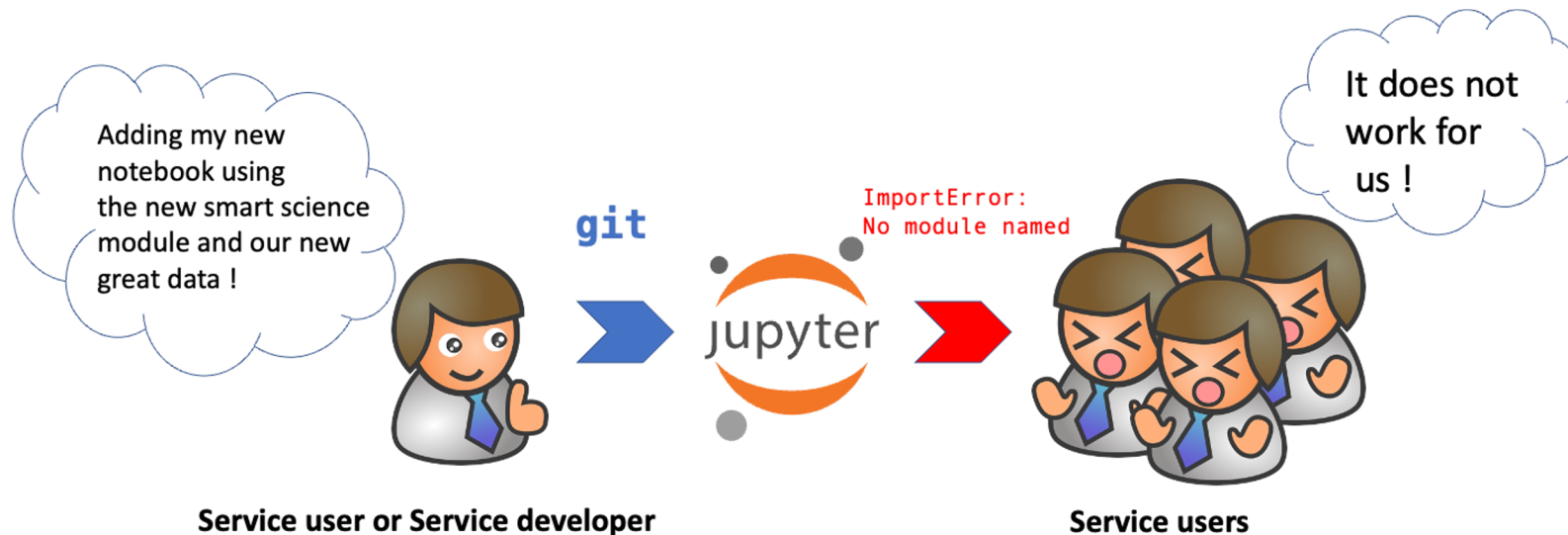
**Description:** Testing new use\_case = [Jupyter\_notebooks, envs, data] against the JupyterService

**Details:** When user adds data, envs and Jupyter notebooks, all is tested against the Jupyter service

**Why:** *reproducibility - scientific use cases work for all service users*

## Black-Box testing

More than 200 use cases expected, numerous environments with many python modules + user code in notebooks

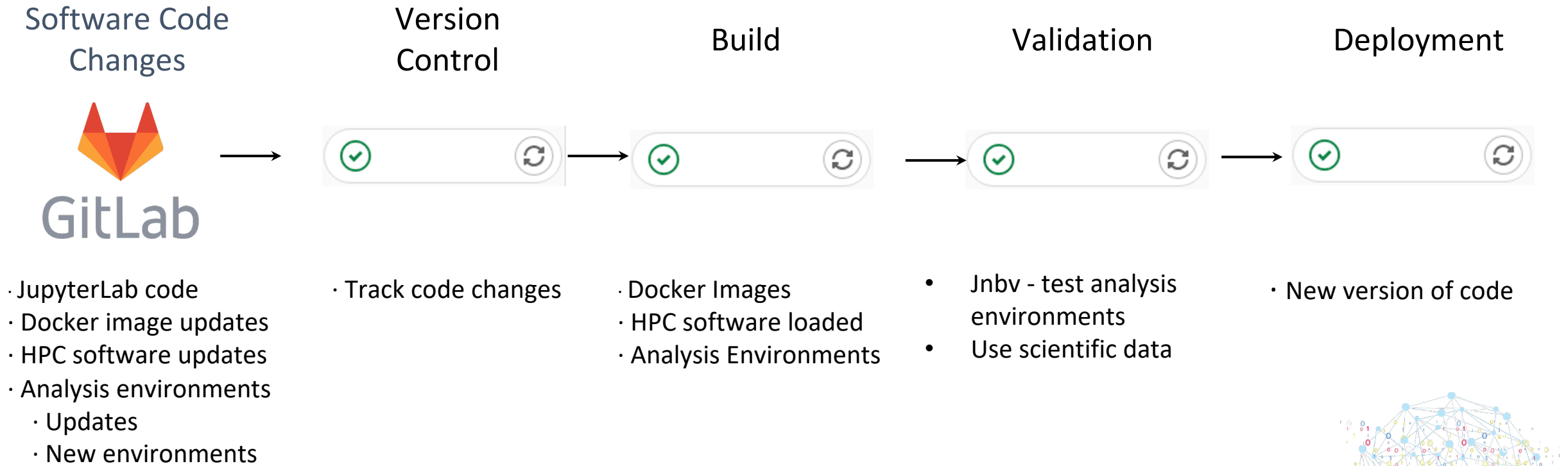




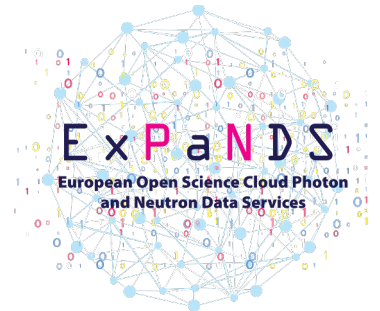
# MAX IV: JupyterHub Service QA

Using Jupyter kernel validation tests

## Production Validation Pipeline at MAX IV



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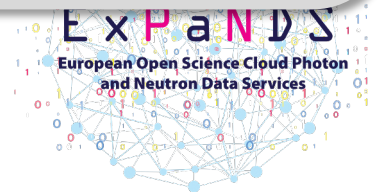
# Validation Tools used in Validation Stage

## Jnbv

- Python package
- Execute, Test, Compare Jupyter notebooks
- Selection of Jupyter Kernels
- Logging of results
- Repository, see [1]

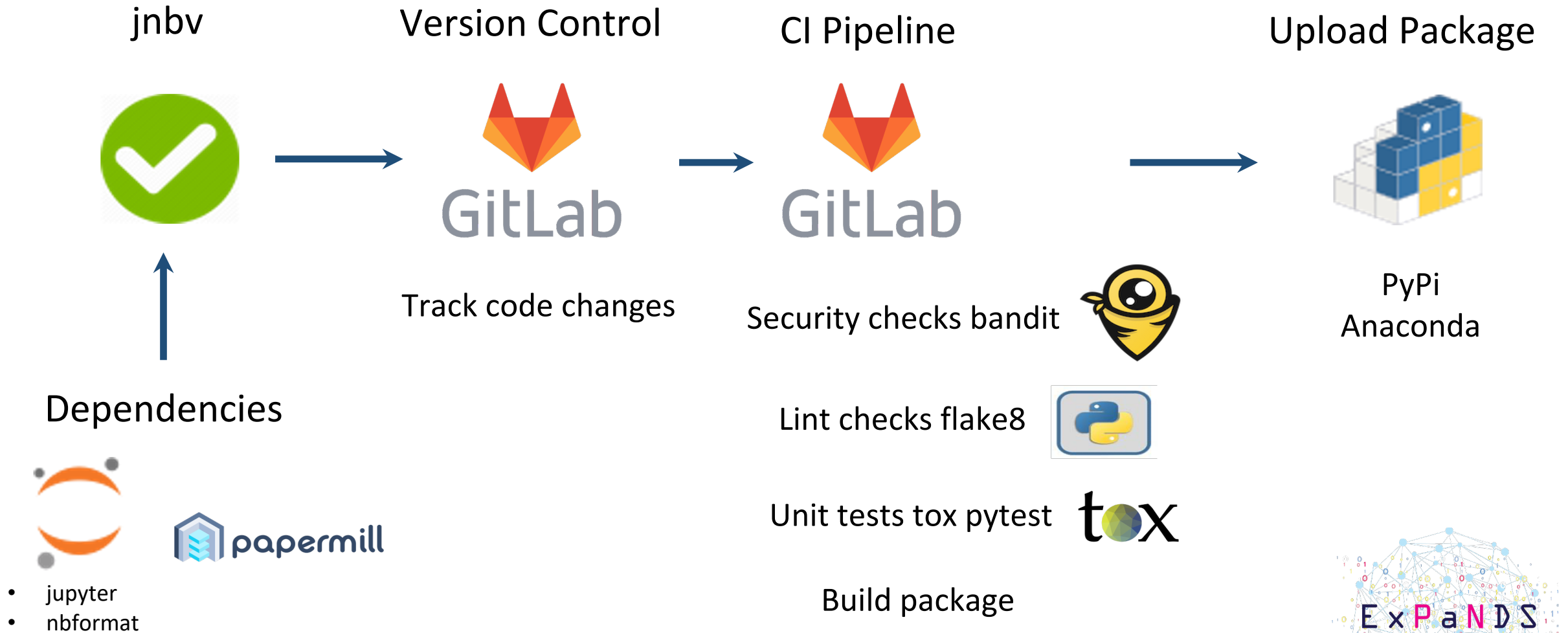
## Jupyter-notebook-validation

- Collection of >50 Jupyter notebooks for testing Jupyter Kernels at MAX IV Laboratory
- Makefile and SLURM scripts to simplify execution via docker images & SLURM jobs
- Repository, see [2]





# jnbv - Software Development QA



# jupyter-notebook-validation - Usage

Collection of notebooks associated with each kernel.

- Around 13 kernels;
- 3 to 6 notebooks for each kernel;
- Production for 3 separate technologies, as we have different partners with a variety of

requirements:

- Docker Swarm
- Kubernetes
- HPC



# jnbv & jupyter-notebook-validation In Use at MAX IV Laboratory



## Jupyter-docker-stacks

- JupyterLab docker images in use at MAX IV
- Jnbv & Jupyter-notebook-validation
- Repository, see [3]



## Jupyterhub-HPC

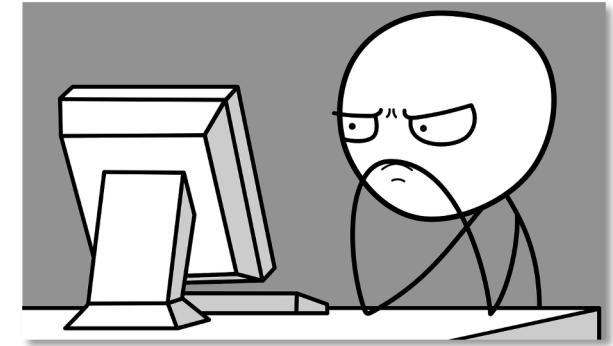
- Full installation of JupyterHub on HPC at MAX IV
- Jnbv & Jupyter-notebook-validation
- Repository, see [4]



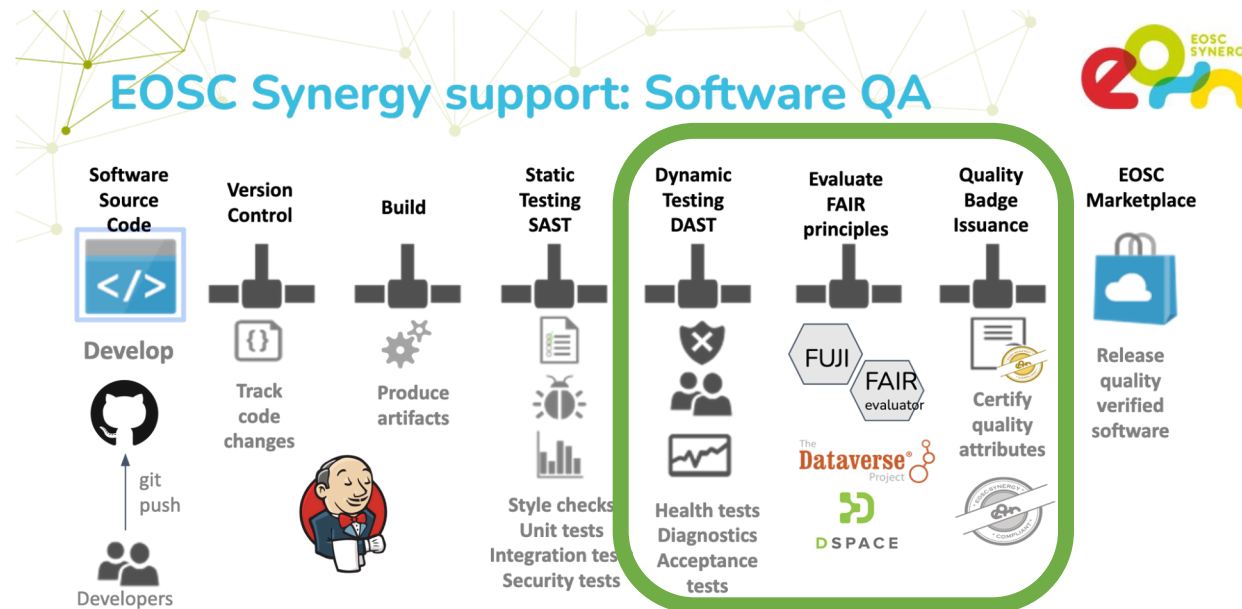


# In relation to EOSC-Synergy

- Jupyter Kernel Validations
  1. Service Validation
  2. Scientific Use-Case Validation
- “Data” FAIRness is not validated (e.g. access)



What is missing ?



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# References

- [1] [GitLab > MAXIV-SCISW > JUPYTERHUB > jnbv](#)
- [2] [GitLab > MAXIV-SCISW > JUPYTERHUB > jupyter-notebook-validation](#)
- [3] [GitLab > MAXIV-SCISW > JUPYTERHUB > jupyter-docker-stacks](#)
- [4] [GitLab > MAXIV-SCISW > JUPYTERHUB > jupyterhub-hpc](#)



# Thanks (Gracias)



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