

# EGI Tutorial at ISGC 2023

### Giuseppe La Rocca Community Support Team Lead.

TLP: GREEN Limited disclosure

ISGC 2023





### About me



### **Community Support Team Lead**. @ EGI Foundation Member of the EGI Foundation team since Dec. 2015 MSc in Computer Science Engineering from the University of Catania (Italy).

- EGI-ACE Community Manager
- Based on Catania, Italy

giuseppe.larocca@egi.eu https://www.egi.eu/people/giuseppe-la-rocca/





14:00	Intro about the EGI and the EGI infrastructure
	Auditorium, BHSS, Academia Sinica
	EGI VO for AP
	Auditorium, BHSS, Academia Sinica
	DEMO - How to use the EGI Cloud
15:00	Auditorium, BHSS, Academia Sinica
	DEMO - Getting started with the EGI Notebooks
	Auditorium, BHSS, Academia Sinica
16:00	Handa an with the FOI Natabasks and Danlay convises
10.00	Hands-on with the EGI Notebooks and Replay services
	Auditorium, BHSS, Academia Sinica
	Approach to reproducible data science with EGI and EOSC
	Auditorium, BHSS, Academia Sinica
	Overview of the hands-on - Full data lifecycle
17:00	
	Auditorium DUICC Academic Cinica
	Auditorium, BHSS, Academia Sinica

Giuseppe La Rocca

14:00 - 14:20

Giuseppe La Rocca

14:20 - 14:50

Giuseppe La Rocca

14:50 - 15:10

Giuseppe La Rocca

15:10 - 15:30

Giuseppe La Rocca

16:00 - 16:30

Giuseppe La Rocca

16:30 - 16:45

Giuseppe La Rocca

16:45 - 17:30

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# Introduction about the EGI and the EGI Infrastructure

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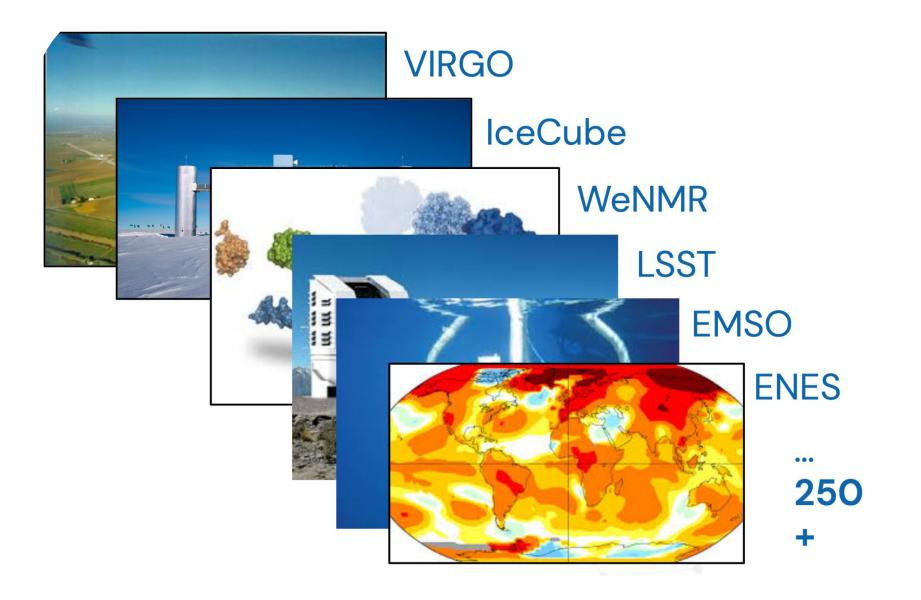




# The EGI Federation is an international e-infrastructure

We provide advanced computing and data analytics for research and innovation





### 2010

From the high-energy physics compute grid (WLCG)

### 2022

To a multi-disciplinary, multi-technology infrastructure







#### Vision

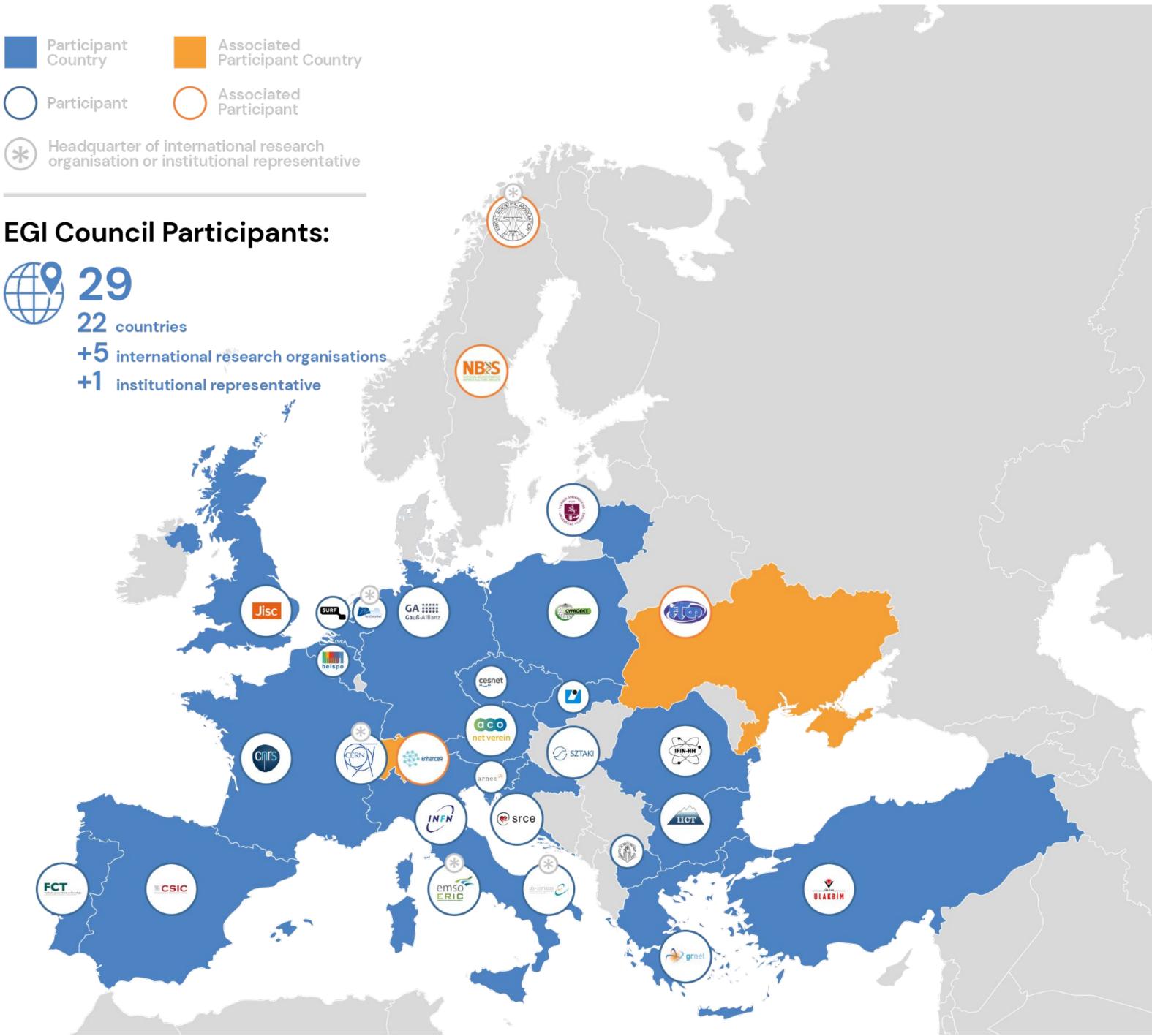
All researchers have seamless access to services, resources and expertise to collaborate and conduct world-class research and innovation

#### **Mission of the EGI Federation**

Deliver open solutions for advanced computing and data analytics in research and innovation

Mission of the EGI Foundation

Enable the EGI Federation to serve international research and innovation together



# International Partnerships



GEANT Association RENAM (Moldova) GRENA (Georgia) IMCS UL (Latvia)

CSIR Meraka Institute (South Africa)

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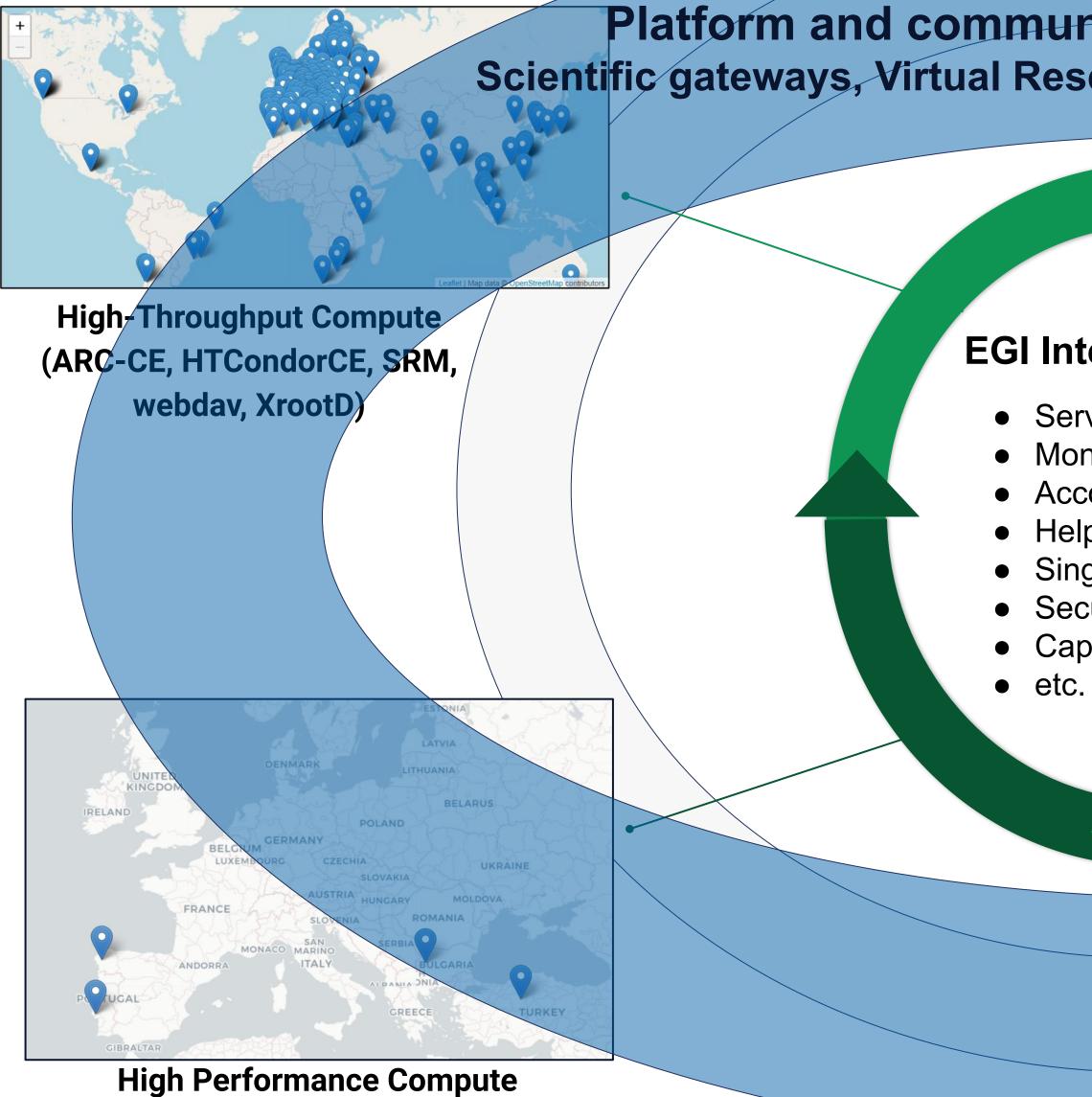
Open Science Grid (USA) CLAF (Latin America) Compute Canada

> SSTIR (China) CNIC (China) IHEP (China) ASGC (Taiwan)





### The EGI Infrastructure



21 March 2023 (since 2022)

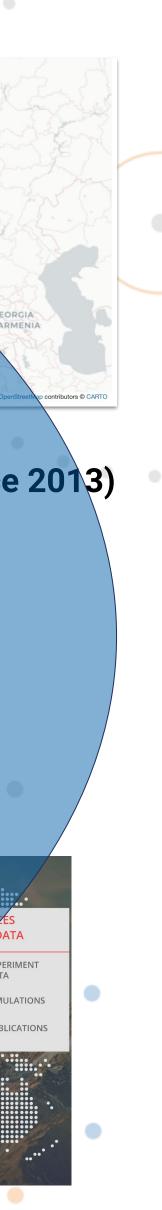
Platform and community specific services built on top: Scientific gateways, Virtual Research Environments, Application portals, etc.

#### **EGI Internal services**

- Service registry
  - Monitoring
  - Accounting
  - Helpdesk
  - Single sign-in
  - Security oversight
  - Capacity management

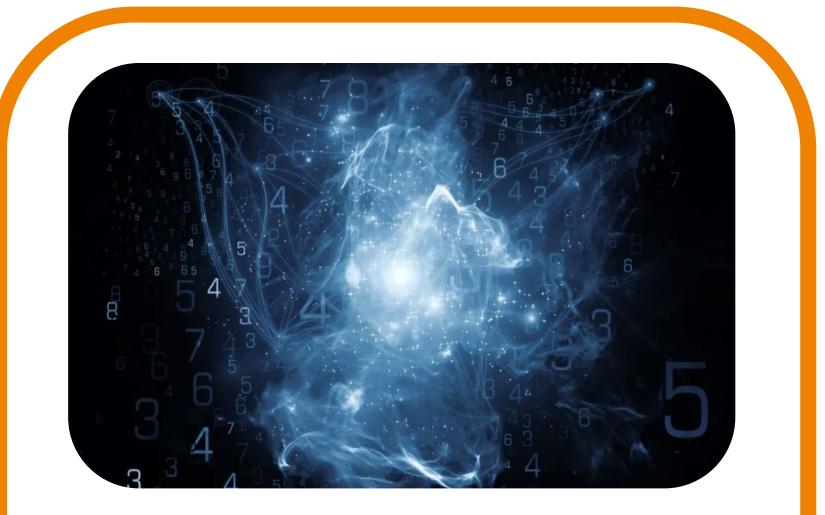
**Cloud Compute** (based on OpenStack. Since 2013)

Data (based on OneData), egi.eu |



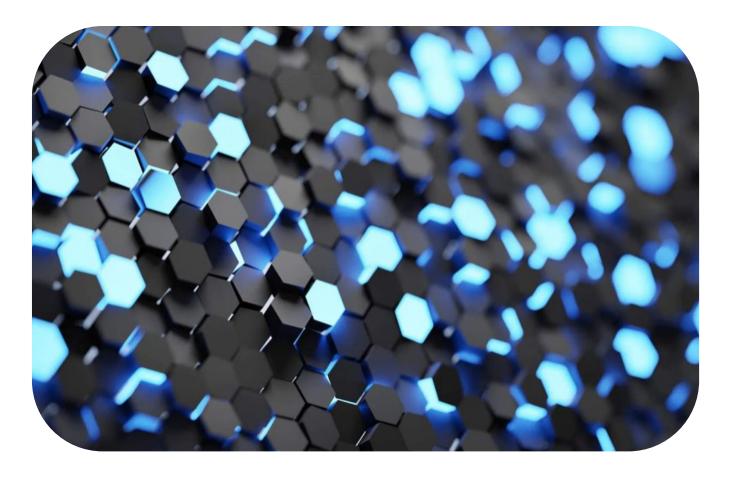






### Services for Research

Our large-scale computing and data analytics services are helping scientists to accelerate their research.



Our internal services provide tools for coordination of the EGI Federation, improving how we work together.

### Services for Federation



### **Services for Business**

We help companies to exploit and provide services and resources for compute- and data-intensive research and innovation.





# Access policies

# Wide access

Users can freely access scientific data and digital services provided by EGI resource providers

## **Policy-based**

Users are granted access based on policies defined by the EGI resource providers or by the EGI Foundation

#### Example:

- EGI Notebooks open instance
- EGI Cloud pool for application piloting

Example:

• Biomed HTC VO pool for life sciences • INFN-Bari (IT), IN2P3-IRES (FR), ULAKBIM (TR) provide Clouds for the National **Bioinformatics Infrastructure of Sweden** 

# Market-driven

Users can negotiate a fee to access services either directly with EGI resource providers or indirectly with the EGI Foundation

Example:

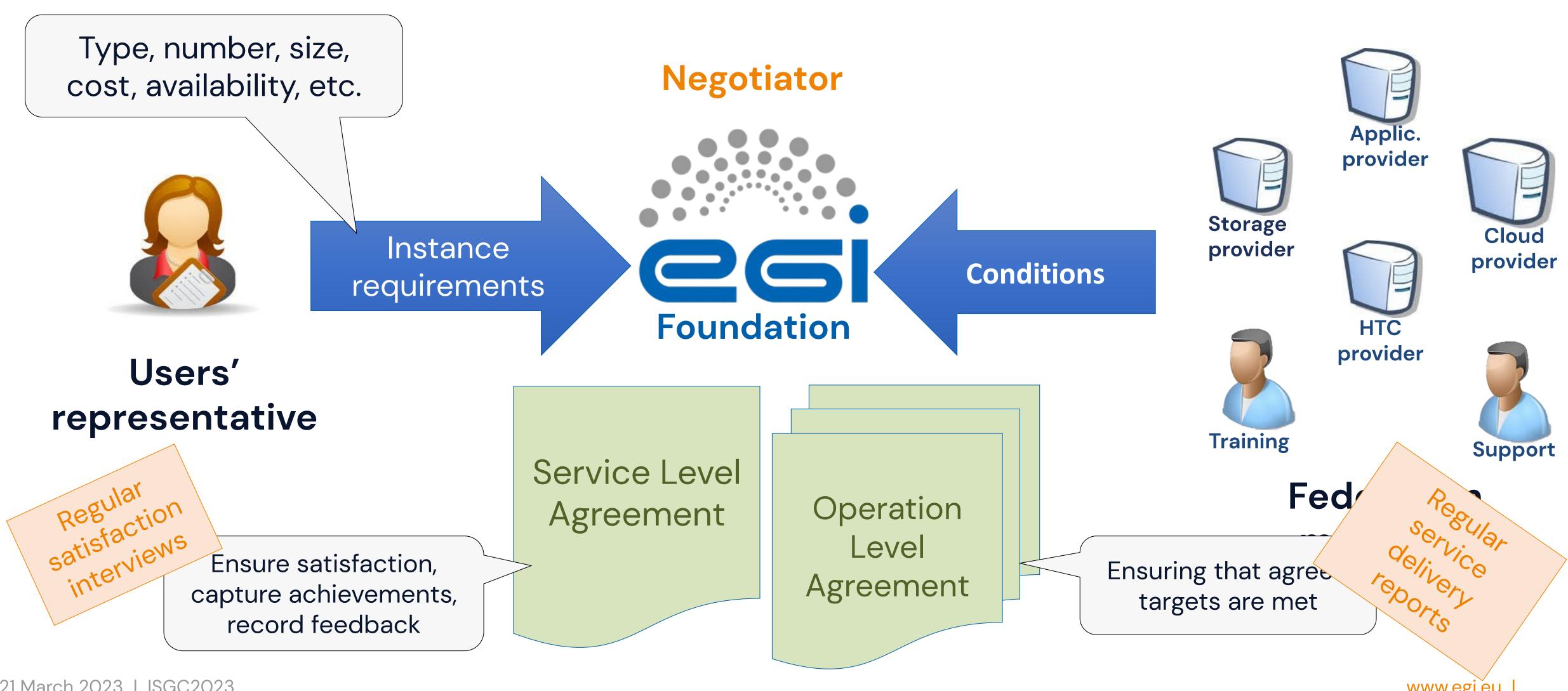
- FitSM training by EGI Foundation
- 4 EGI Cloud providers deliver to Exprivia







# Allocating services and resources



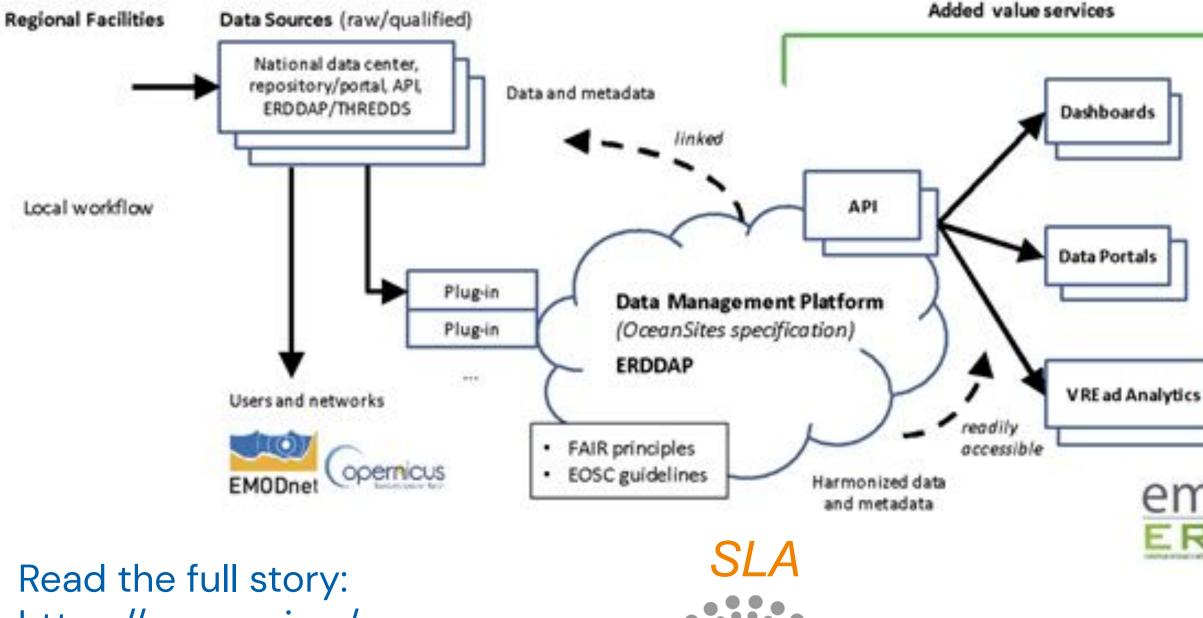
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# An SLA example





Centro de Supercomputación de Galicia

OLA-1 OLA-2

CESGA INFN

Istituto Nazionale

di Fisica Nucleare

Sezione di Bar

Read the full story: <u>https://www.egi.eu/cas</u> <u>e-study/emso-eric/</u>

Check the SLA-OLA documents and reports: <u>https://documents.e</u> <u>gi.eu/document/353</u> <u>g1March 2023 | ISGC2023</u>





The Services are defined by the following properties:

#### Cloud Compute (category: Compute)

Description: https://www.egi.eu/services/cloud-compute/



- Cloud Compute
  - Number of virtual CPU cores: 192
  - Memory per core (GB): 2.5GB. A total of 512GB is provided
  - Local disk (GB): 50
  - Public IP addresses:
  - Allocation type: Pledged
  - Payment mode offer: Sponsored
  - Other technical requirements:
  - Duration: 01/12/2019 30/06/2023
  - Supported VOs: vo.emso-eric.eu
- VO ID card: <u>https://operations-portal.in2p3.fr/vo/view/voname/vo.emso-eric.eu</u>
- VO-wide list: <u>https://vmcaster.appdb.egi.eu/store/vo/vo.emso-eric.eu/image.list</u>

#### Resource Centre: RECAS-BARI (Country: Italy)

- Cloud Compute
  - Number of virtual CPU cores: 300
  - Memory per core (GB): A total of 1.2TB is provided
  - Local disk (GB):
  - Public IP addresses:
  - Allocation type: Pledged
  - Payment mode offer: Sponsored
  - Other technical requirements:
  - Duration: 01/12/2019 30/06/2023
  - Supported VOs: vo.emso-eric.eu
- o VO ID card: https://operations-portal.in2p3.fr/vo/view/voname/vo.emso-eric.eu
- o VO-wide list: https://vmcaster.appdb.egi.eu/store/vo/vo.emso-eric.eu/image.list

#### Online Storage (category: Storage)

Description: https://www.egi.eu/services/online-storage/

- Resource Centre: CESGA (Country: Spain)
  - Online Storage
    - Guaranteed storage capacity [TB]: 0.6
    - Opportunistic storage capacity [TB]:



5



#### EGI VO

#### **VICE LEVEL AGREEMENT**

#### 2 Service hours and exceptions

The Services operate during the following hours: twenty-four (24) hours a day, seven (7) days a week, three hundred sixty-five (365) days a year.

The following exceptions apply:

<sup>2</sup> CDMI, POSIX, SWIFT, etc.
 <sup>3</sup> DPM, dCache, STORM, etc.
 <sup>4</sup> CDMI, POSIX, SWIFT, etc.
 <sup>5</sup> DPM, dCache, STORM, etc.
 <sup>6</sup> <u>http://accounting.egi.eu/</u>
 <sup>7</sup> <u>http://argo.egi.eu/</u>

esi

 Planned maintenance windows or service interruptions ("scheduled downtimes"<sup>8</sup>) will be notified via email in a timely manner i.e. 24 hours before the start of the outage<sup>9</sup>.

Downtime periods exceeding 24 hours need justification.

#### **3** Support

Support is provided via EGI Service Desk<sup>10</sup>. Access requires a valid X.509 or the login via a EGI SSO account<sup>11</sup>. Support is available between:

- Monday to Friday.
- From 9:00 to 17:00 in the time zone of the relevant Resource Centres.

Service times always apply with the exception of public holidays in the country of the supporting Resource Centres.

#### 3.1 Incident handling

Incidents will be handled according to the Quality of Support level that is estimated according to the impact of the outage or service quality degradation.

The Quality of Support in this Agreement has level: Medium<sup>12</sup>

Incident priority	Response time
Less urgent	5 working days







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# EGI allocations for the Asian Pacific (AP)

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# EGI resource pool for Asia Pacific

- With a community specific Notebooks installation
- With a community specific Replay installation
- Purposes:

  - o To enable sharing of cloud resources from the region
  - o To facilitate application sharing from the region

A Virtual Organisation (alias resource pool) in the EGI cloud federation

o To facilitate open science in the region  $\rightarrow$  IN THE SCOPE OF THE TUTORIAL TODAY o To facilitate data sharing related to environmental sciences from the region





## Documentation

### https://docs.egi.eu/users/getting-started/communities/dmcc/

<b>Q</b> Search	For Users / Getting St
For Users	
<ul> <li>Getting Started</li> </ul>	Disaster I
Architecture	EGI infrastructure f
OpenStack Providers	This is the documentat
Command Line	Asian Pacific region.
<ul> <li>Communities</li> </ul>	
Disaster Mitigation and	About the c
Agriculture ▶ Tutorials	Hazard risk estimation studies and applicatior
<ul> <li>Authentication &amp; Authorization</li> </ul>	the mechanisms of the to reproduce the proce open science platform
Compute	facilities are sharable,
▶ Data	This knowledge base is
Security	This knowledge base is that are contributed to
<ul> <li>Development</li> <li>Environments</li> <li>Tracining Infractory et une</li> </ul>	<ul> <li>Academia Sinica, Centre (ASGC))</li> </ul>
Training Infrastructure	<ul><li>Institute of Earth</li><li>Research Centre</li></ul>

tarted / Communities / Disaster Mitigation and Agriculture

### **Mitigation and Agriculture**

for the Disaster Mitigation and Agriculture community

tion to support the Disaster Mitigation and Agriculture community in the

#### community

and prediction by numerical simulation is crucial to disaster mitigation ns. The Disaster Mitigation and Agriculture community investigates in-depth e selected disaster events and develops the appropriate simulation models esses by case studies. The collaboration framework aims at becoming an of disaster mitigation so that all the tools, data, resources and simulation and the simulations are reproducible.

s enriched by the simulation models, portals, data and visualisation facilities by the members:

, Taiwan (Leading Partner, represented by Academia Sinica Grid Computing

n Science, Academia Sinica, Taiwan of Environmental Changes, Academia Sinica, Taiwan





# Demo: How to use the EGI Cloud resources pool for Asia Pacific

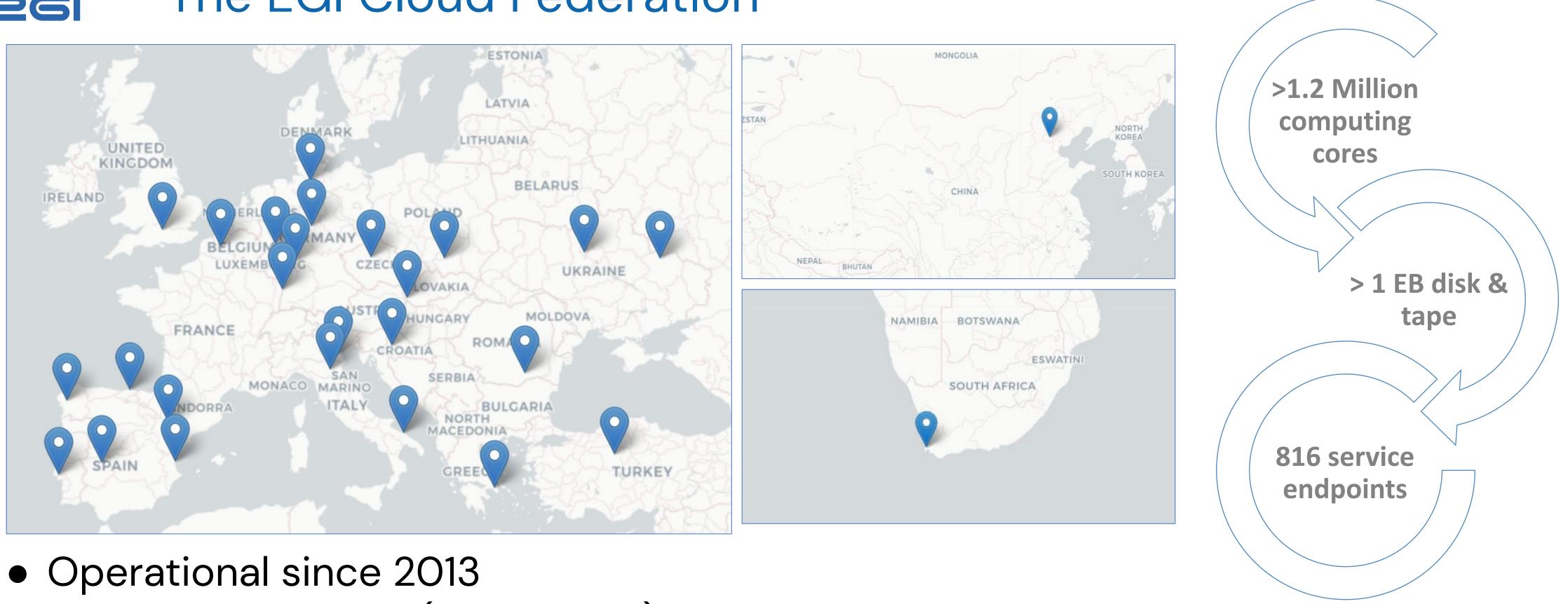
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# The EGI Cloud Federation



- 28 Cloud Providers (OpenStack)
- Providing different functionalities and more dynamic platforms for scientists
- 69,863,034 Cloud CPU/h consumed in 2022
- 105 Virtual Organisations supported (Virtual Organisation = Resource pool)
- Access via GUI, CLI, OpenStack native and libcloud APIs, Terraform





# Kubernetes (Containers) in the EGI Cloud

### **Self-deployed by users**

OpenStack)

Automated deployment with Infrastructure Manager (IM)

Select site, size of VMs and go

**Rancher-based access to managed clusters (under development)** 

- Rancher integrated with EGI Check-in
- Access to pre-configured clusters managed by expert operators

• Spin up some VMs and deploy kubernetes (works with existing tooling targeting)





## Federation services for Cloud

Infrastructure Manager orchestrates deployment of Virtual Infrastructures Multi-cloud following Infrastructure as a Code (IaC) paradigm Rely on Ansible and Helm to manage definition of complex infrastructure Manages whole life-cycle: deployment, monitoring, reconfiguration (such as 

- scaling-up or down) and removal.
- Support for TOSCA

Start a virtual machine with	IM Dashboard Infrastructures Advanced - External Links -
extra HD	
	Launch a Kubernetes Virtual Cluster
	<b>Description:</b> TOSCA template for launching a Kubernetes Virtual Cluster with an extra HD for Dask, JupyterHub and Elasticity extras available.
SLURM virtual cluster	Infrastructure Name
	description
slurm workload manager	HW Data Kubernetes Data Cloud Provider Selection
	Number of WNs in the cluster
Launch a Storm Virtual	1
Cluster	Number of CPUs for the front-end node
	2
	Amount of Memory for the front-end node
	8 GB
	Flavor name of the front-end node. Only required in case of special flavors (i.e. with GPUs)

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```
www.egi.eu
```



puts





Common registry for Virtual Appliances (VA) • VM image + metadata

Available for running at the EGI cloud or on any hypervisor

**Community-level management of VAs** 

Automatic distribution to providers

🔴 🔍 🧶 🧱 Cloud Marketplace	× +		
	appdb.egi.eu/?p=eyJ1cmwiOilvYXBwcy	vlsInF1ZXJ5Ijp7ImZsdCl6lisqJmFwcGxpY2I	F0aW   🦁 🔺 🛛 🗛
Register New 🗸 🛛 My Items 🗸	Administrative v About v Contact v	© ▼ Se	earch 🔍 🗬 o 🤷 v Hel
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Home > Cloud Marketplace			go to the VMOps dashboard
Cloud Marketplace	Search virtual appliances	Q (0)	Date Added 🔹 Descending 🗸 💷
Top Rated Newest Most Visited	Filters: refine your search   ▼	1 2 4 5 6 7 8	116 matches in 0.39
Recently Updated All vAppliances Application Development Application Servers Application Stacks Big Data Business Apps Collaboration Content Apps Data Storage	Cassandra The Apache Cassandra database is the right choice when you need scalability and Download	Image: Sector of the sector	Image with SEBAI requirements installed
Databases & Caching Enterprise Apps IT Administration Information & Data Mgnt Infrastructure Apps To Software Appliances	CODE-RADE client VM Wirtual appliance configured to mount the CODE-RADE CVMFS	PDAS-Ophidia This Virtual Appliance relates to the PDAS- Ophidia big data analytics framework	esc-engine e-science engine image which will connect to the upv server upon instantiation
Virtual Organizations Sites / Resource Providers Browse graphically	102 visits 2 votes	400 Lit.	16 visits CentOS-6-x86_64
by Category by Discipline	ጥረል This image contains an Apache Hadoop node	EGI built CentOS 7	CentOS 6 image for clouds (qcow2)
Uiew your profile	Download	Download 20 sites	Download





# EGI Notebooks in the Asia Pacific VO

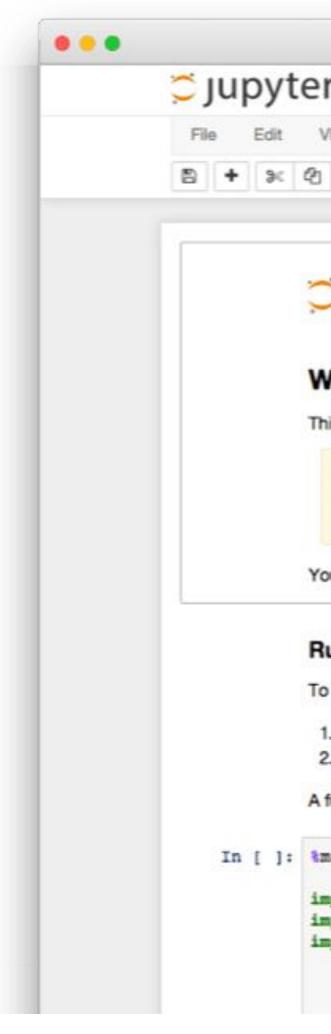
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The Jupyter Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and narrative text.

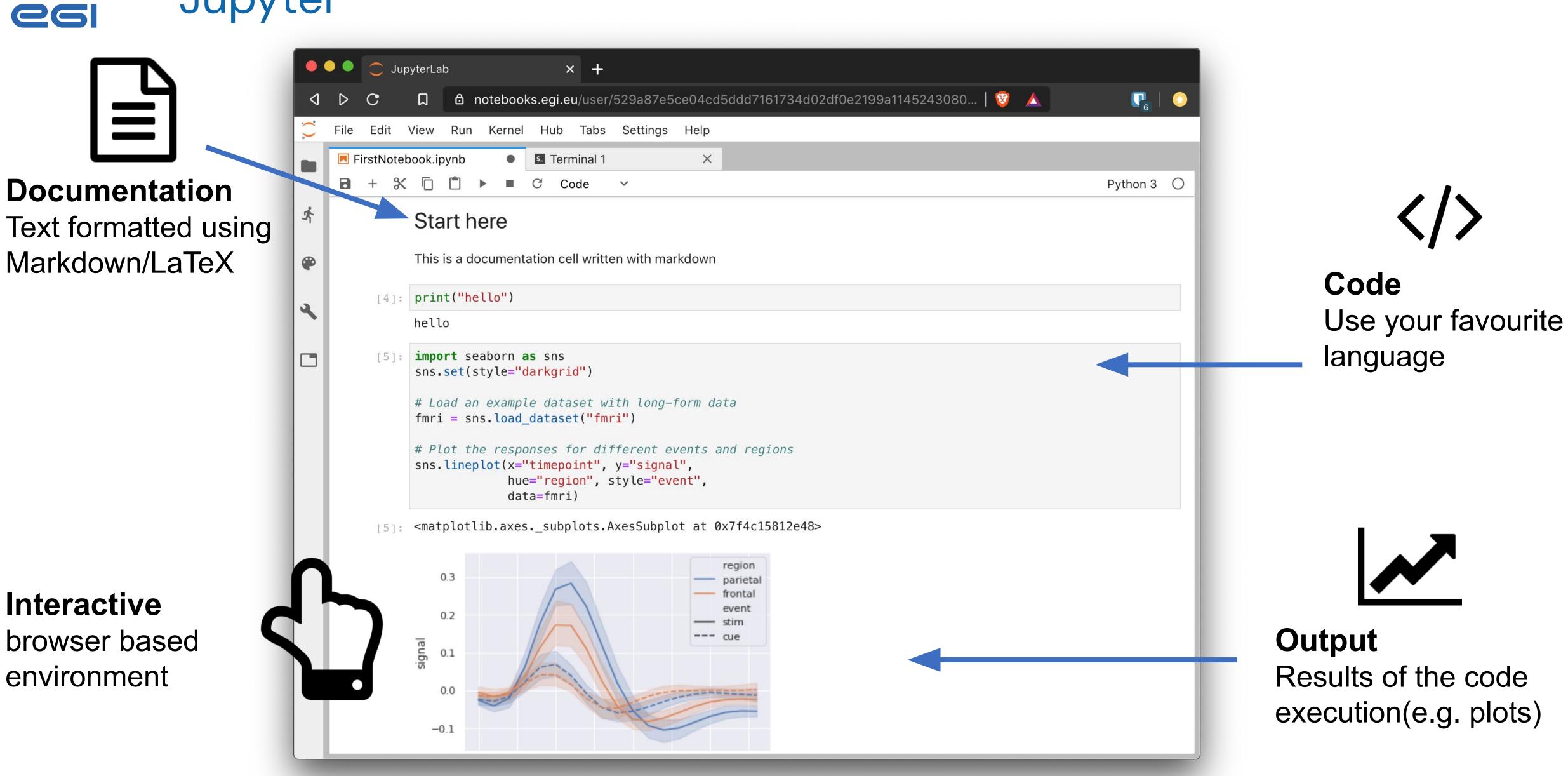


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## Jupyter





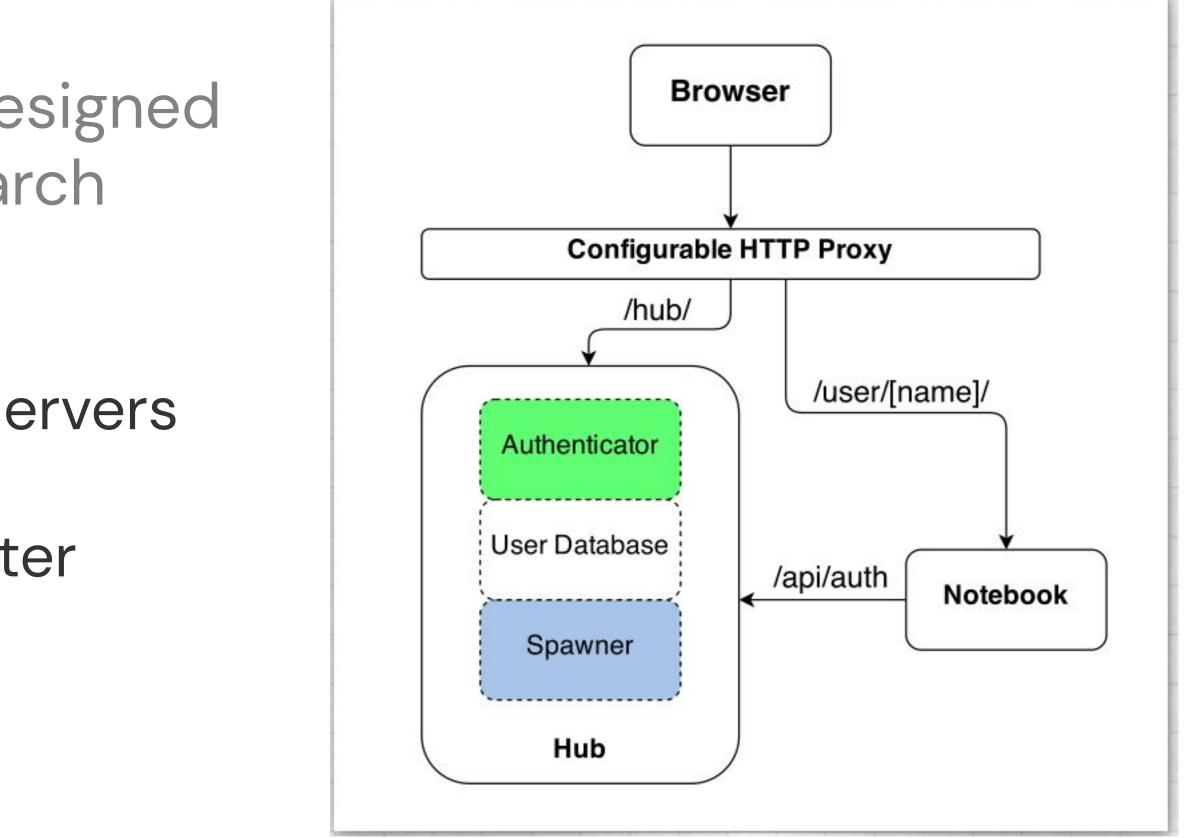
JupyterHub

### Jupyter is single user by design

JupyterHub is a multi-user version designed for companies, classrooms and research labs:

- Manages Authentication
- Spawns single-users notebooks servers on-demand
- Gives each user a complete Jupyter server









### EGI Notebooks



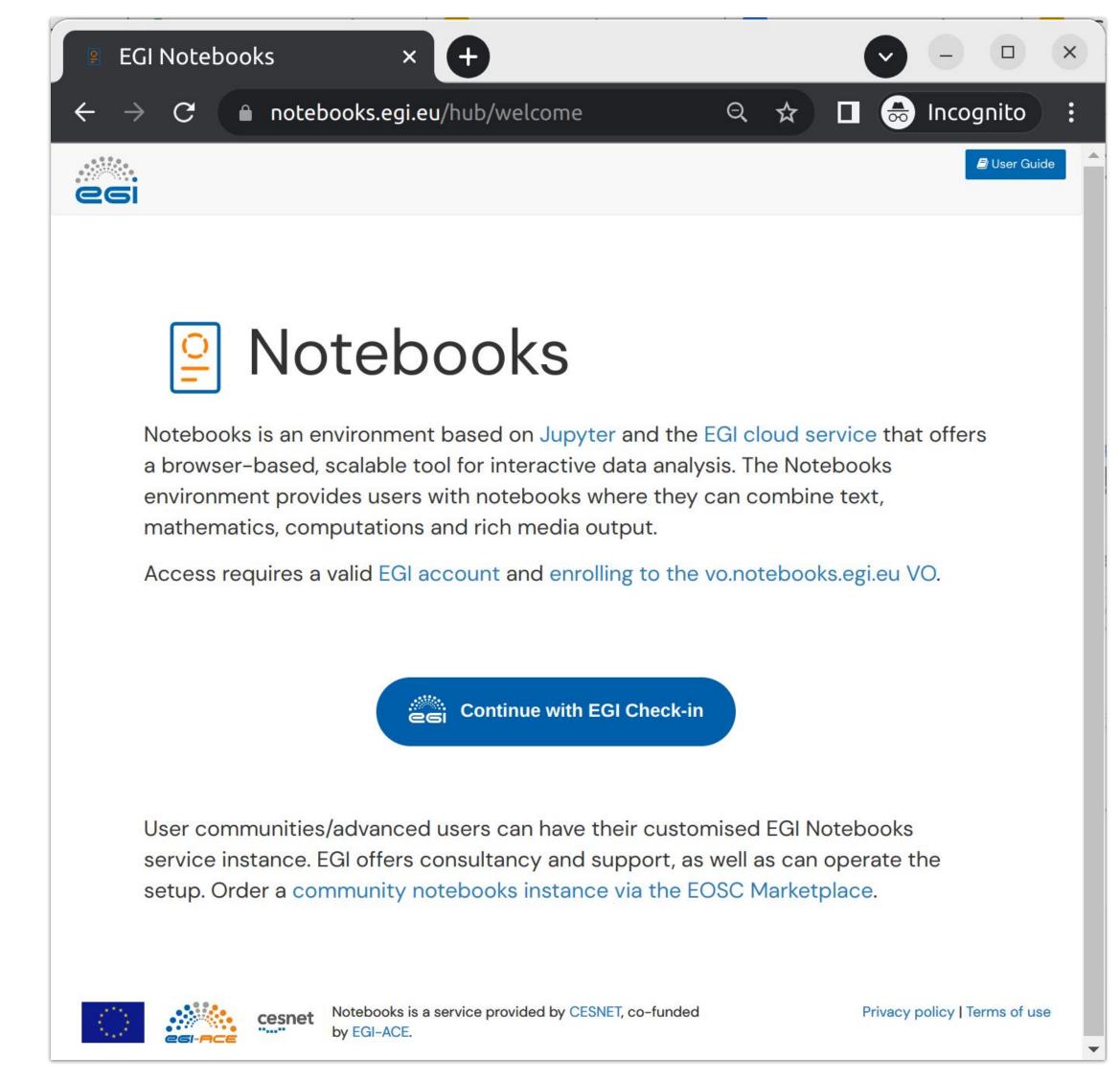
### JupyterHub hosted in the EGI Cloud

- Offers Jupyter notebooks 'as Service'
- One-click solution: login and start using

### Main Features:

- Easy access: Login with the EGI AAI Check-In service
- Persistent storage for notebooks
- Use EGI computing and storage resources from your notebooks

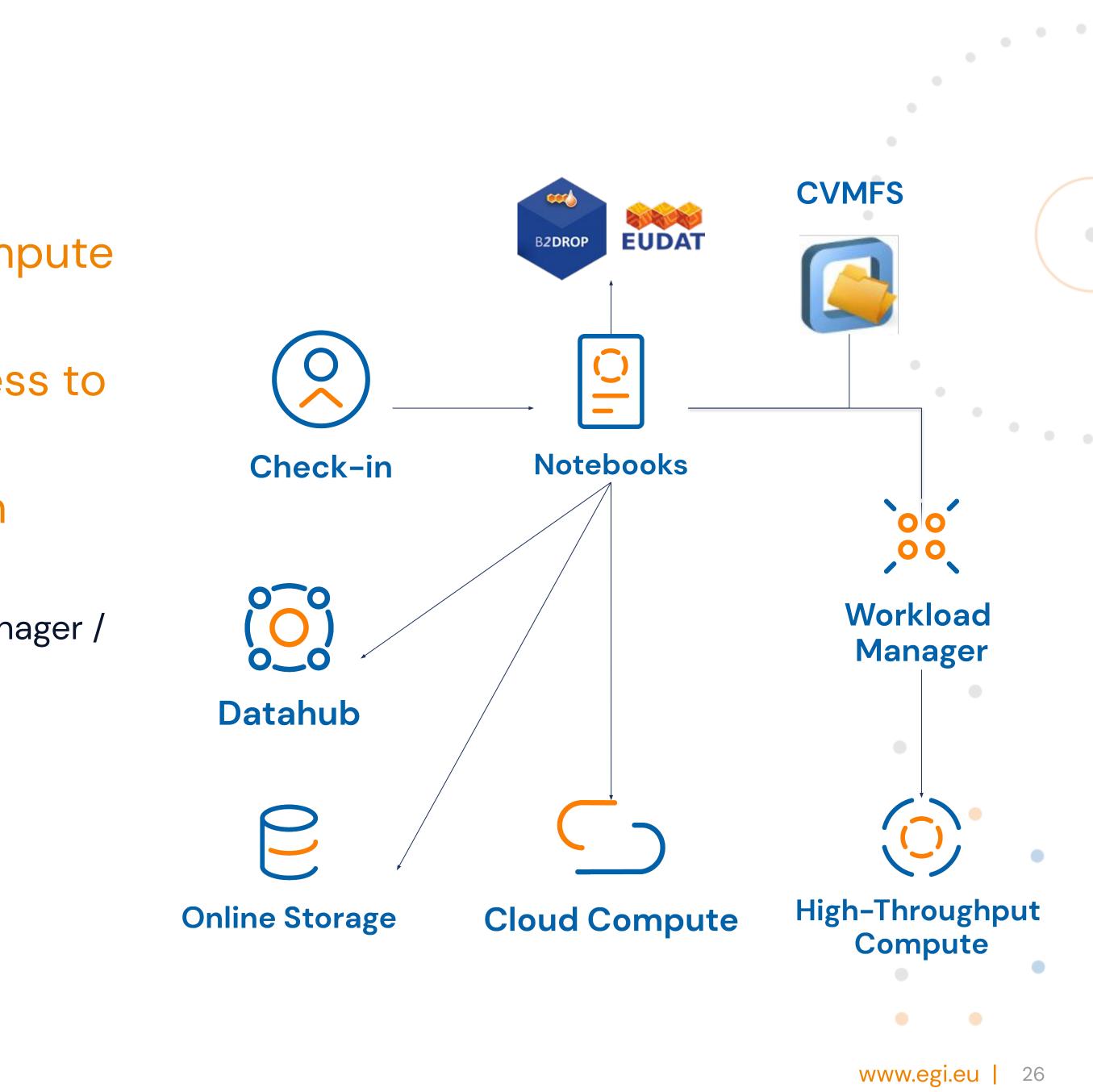
## https//notebooks.egi.eu





# EGI Notebooks integrations

- 1. Runs on EGI Cloud providers (Cloud Compute / Online Storage)
- 2. Uses Check-in for authentication + access to other services
- 3. Makes user-level software available from **CVMFS** 
  - DIRAC client for submission of jobs to Workload Manager / High Throughput Compute
  - Fedcloudclient for interaction with Cloud Compute
- 4. Transparent access to Datahub spaces
- 5. Access to 3rd party services: B2DROP





EGI Notebooks offers different computing environments:

- Default: Python, R, Julia, Octave and a wide range of data science libraries
- MATLAB (Basic/Full): Run MATLAB on EGI resources (requires a license!)

#### Server Options

#### Default EGI environment – 6 GB RAM / 2 core

The Default notebook environment includes Python, R, Julia and Octave kernels

MATLAB Environment (Basic) – 4GB RAM / 4 cores

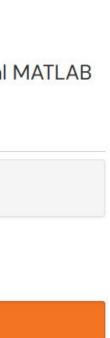
The MATLAB environment (requires a valid license), includes Python and MATLAB kernels

#### MATLAB Environment (Full) – 4GB RAM / 4 cores

The MATLAB environment (requires a valid license), includes Python, MATLAB kernels and additional MATLAB packages

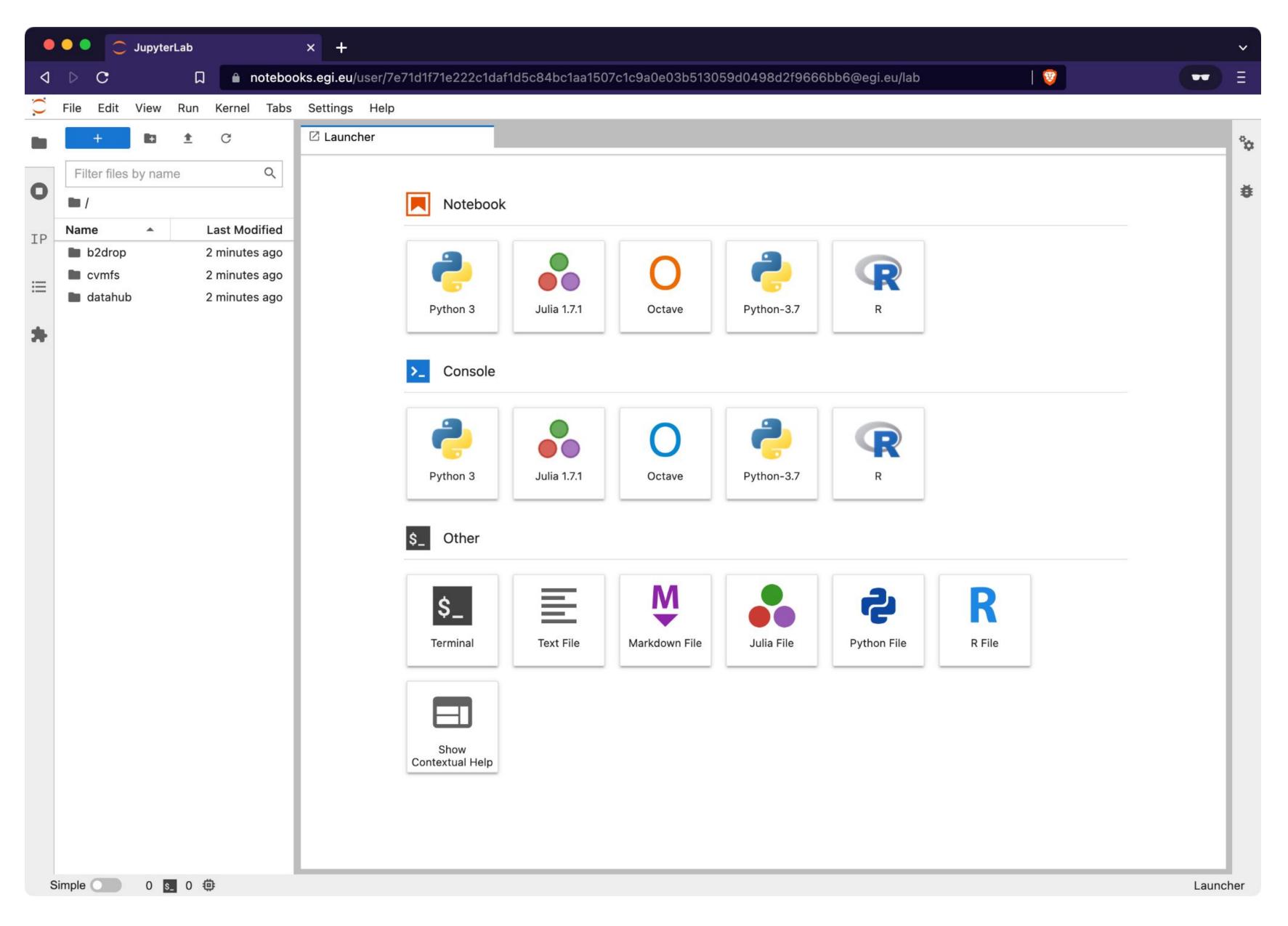
**B2DROP** connection

Start





# JupyterLab interface

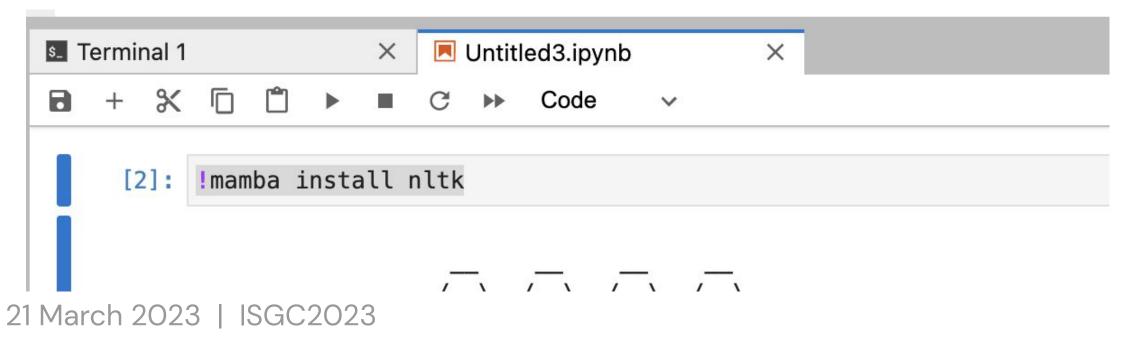






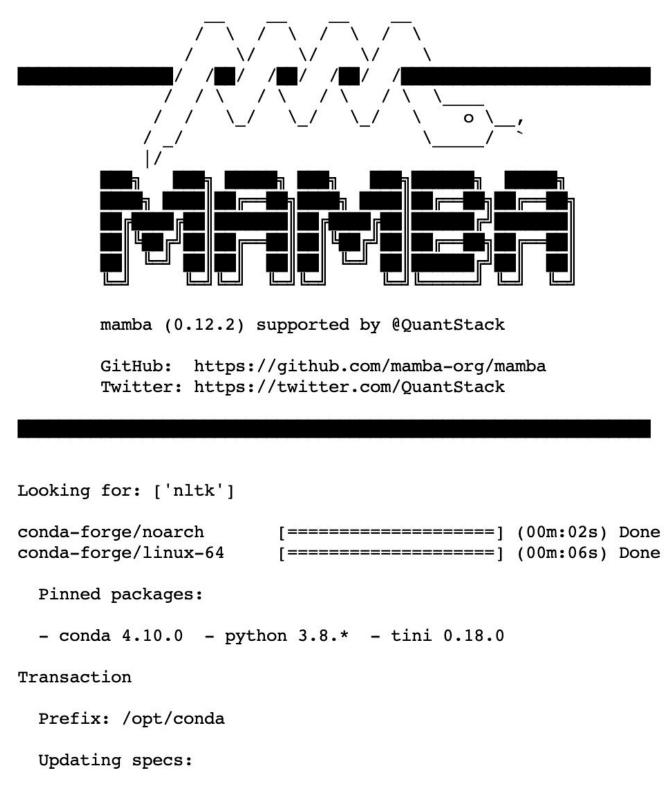
Installing Software

- (Most) software in the environment is managed with conda (mamba)
- Adding packages can be done at any time with mamba or pip
- This is installed in /opt/conda which is wiped out for every new server session!
  - Include a installation cell on your notebooks to avoid not having the needed libraries
  - Ask us for adding them to the environment!



#### Iterminal 1

jovyan@jupyter-529a87e5ce04cd5ddd7161734d02df0e2199a11452430803e714cb1:~\$ mamba install nltk



X

- nltk



# Accessing your data and code

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#### Persistent home

- Can be used to store data (10GB limit)
- Files will be kept even if the notebook server dies

#### nbgitpuller

- Get code from any git repository from a single URL
- https://hub.jupyter.org/nbgitpuller/link.html

#### CMVFS

- Selected CVMFS repositories available
- Easy to add community specific ones

#### DataHub

- Access to your accessible spaces in datahub
- Share data and assign PIDs to shared spaces

#### B2DROP

- Access data stored in EUDAT's B2DROP service
- External web server

•





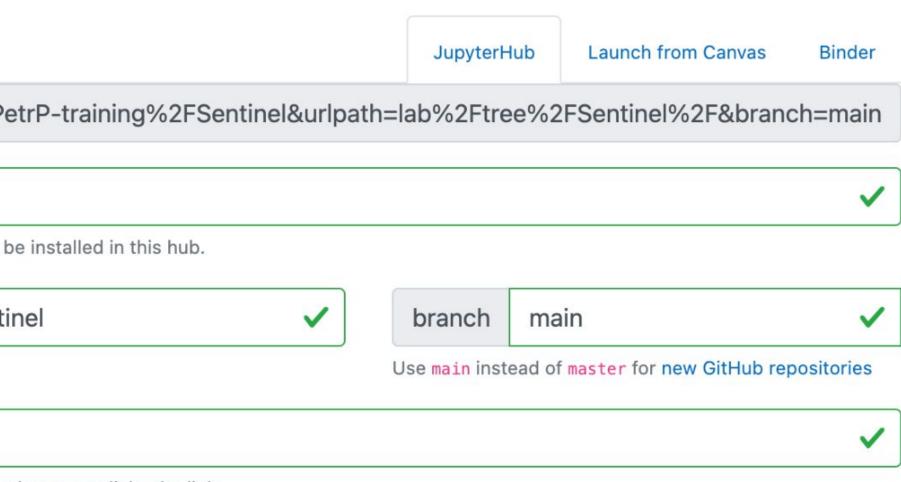
nbgitpuller

https://hub.jupyter.org/nbgitpuller/link.html

### Easily clone GitHub repositories into your home with a shareable link.

# Try it: https://go.egi.eu/x8oui

ser-redirect/git-pull?	repo=https%3A%2F%2Fgithub.com%2FPe
JupyterHub URL	https://notebooks.egi.eu/
	The JupyterHub to send users to. nbgitpuller must be
Git Repository URL	https://github.com/PetrP-training/Sentir
File to open	index.ipynb
	This file or directory from within the repo will open w
Application to Open	O Classic Jupyter Notebook
	○ RetroLab
	JupyterLab
	○ RStudio
	○ Shiny
	○ Custom URL
	Relative URL to redirect user to



when user clicks the link.





#### CernVM-FS

- CernVM-FS (CVMFS) is implemented as a POSIX read-only file system in user space (a FUSE module).
- Files and directories are hosted on standard web servers and mounted in the universal namespace /cvmfs.

### Main features

- Allows centrally managed software distribution across federated environments.
- Allows to make content available as a read-only file system that efficiently downloads and caches files on demand

### **Documentation**

https://docs.egi.eu/users/compute/software-distribution/

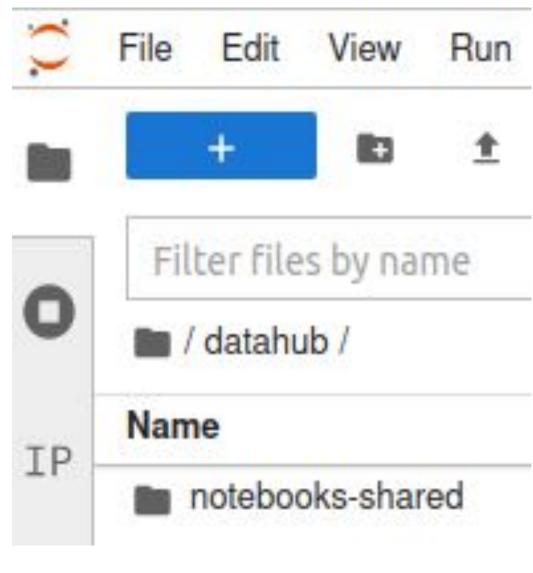




### EGI DataHub

Service based on **Onedata** technology

- It allows transparent data access under a common namespace regardless of the location open access
- Access restricted to members of a Virtual Organization (VO)
- Data can be accessed via a GUI or APIs
- Allows replication of data from data providers for resiliency and availability purposes. Replication may take place either on demand or automatically.
- Easy integration with other EGI components thanks to integration with EGI **Check-in** service, the EGI Authentication and Authorization Infrastructure (AAI)



# $\mathbf{UN} = \mathbf{JA} \mathbf{IA}$

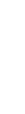
www.egi.eu



































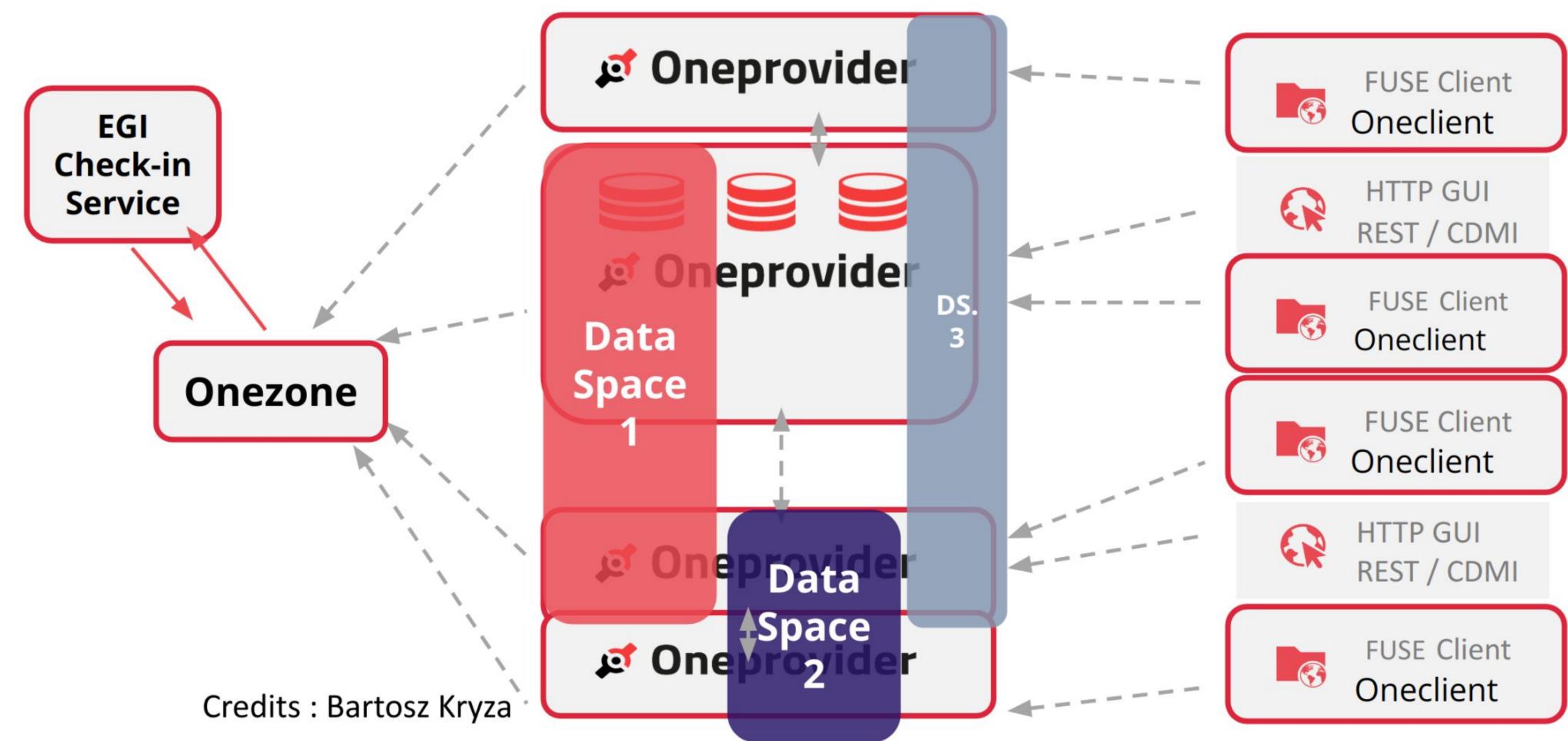














#### B2DROP

## **B2DROP is EUDAT Sync & Share solution**

- Based on NextCloud
- WebDav interface that can be accessed remotely

If you want to access your space from the EGI Notebooks:

- Go to <u>B2DROP security configuration</u>
- Create an app password
- Copy credentials into the EGI Notebooks
- Tick the "Remember B2DROP credentials" box to not keep these credentials in your settings

#### Server Options

#### Default EGI environment – 6 GB RAM / 2 core

The Default notebook environment includes Python, R, Julia and Octave kernels

#### • MATLAB Environment (Basic) – 4GB RAM / 4 cores

The MATLAB environment (requires a valid license), includes Python and MATLAB kernels

#### MATLAB Environment (Full) – 4GB RAM / 4 cores

The MATLAB environment (requires a valid license), includes Python, MATLAB kernels and additional MATLAB packages

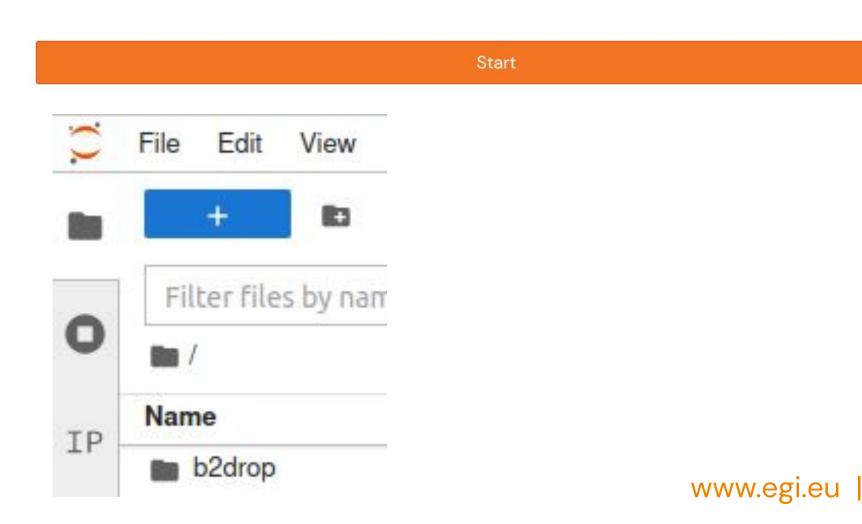
B2DROP connection

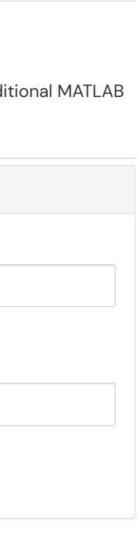
B2DROP app Username

Create new app password at B2DROP security configuration

B2DROP app Password

Remember B2DROP credentials







# Getting access with the EGI Notebooks in the Asia Pacific VO

TLP: GREEN Limited disclosure

ISGC 2023



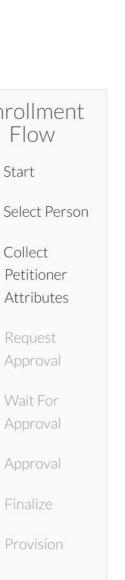


## Sign-up and join the VO for the AP region

## **1. Sign-up** (<u>https://aai.egi.eu/signup</u>) for an EGI Check-In account The subscription requires approval from the VO Manager.

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Sroups <	Join vo.environmental.egi.eu VO		Agree to Acceptable Use Policy and Conditions of Use (AUP) You must review and agree to the following AUP before continuing.	
Kr Collaborations	Thank you for your interest in participating in vo.environmental.egi.eu. Please, note that you will not be able to use your EGI ID to access EGI resources until your request to join the community has been approved by an administrator.  BEGIN  BEGIN		vo.environmental.egi.eu          I Agree	

2. Subscribe the vo.environmental.egi.eu Virtual Organisation (VO) by visiting the enrollment URL (https://go.egi.eu/8Hspz) with your EGI Check-In account.



ncognito





# Hands-on: Running your first notebooks

**TLP: GREEN Limited disclosure** 

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## A very simple notebook

#### Your first notebook

This is a markdown cell, you can format text using Markdown.

In [1]: a = 5

b = 6a + b

Out[1]: 11

#### Variables

The variables defined in previous cells are available in following cells

```
In [2]:
         a = a + 1
         print(b)
```

Out[2]: 6

#### Plotting

Output of cells can be more than just text

Code taken from Matplotlib tutorial subplot example

```
In [3]:
         %matplotlib inline
         import matplotlib.pyplot as plt
         import numpy as np
         np.random.seed(19680801)
         data = np.random.randn(2, 100)
         fig, axs = plt.subplots(2, 2, figsize=(5, 5))
         axs[0, 0].hist(data[0])
         axs[1, 0].scatter(data[0], data[1])
         axs[0, 1].plot(data[0], data[1])
         axs[1, 1].hist2d(data[0], data[1])
         plt.show()
```

#### 21 March 2023 | ISGC2023

To launch the notebook  $\Rightarrow$  go.egi.eu/xABiu

**OO-first-notebook.ipynb**  GitHub repo for this notebook Notebook fetched with the <u>nbgitpuller</u>



www.egi.eu |





## Climate Change Knowledge Portal (CCKP)

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### To launch the notebook ⇒ <u>https://go.egi.eu/KWIsA</u>

See: <u>"How to make datasets and application in CVMFS"</u>



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# Datasets are stored in CVMFS

1961-1999.

cckp\_historical\_rainfall.ipynb

by country for the period

Values are in millimeters (mm).

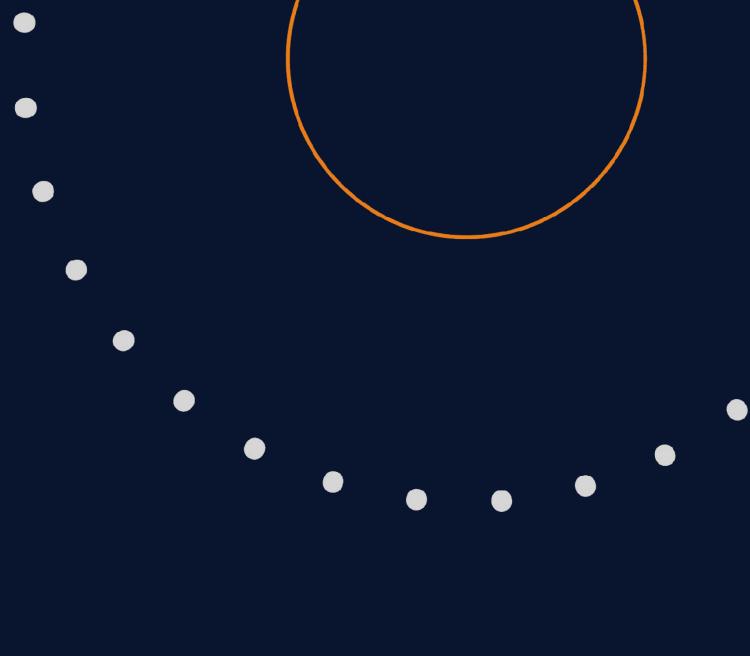






# Coffee break





ISGC 2023



EGI Check-in

Check-in provides authentication, authorization and user management for the EOSC Compute Platform

### **Standards based:**

SAML 2.0 / OpenID Connect 1.0 / OAuth 2.0 / LDAP

#### **Interoperable:**

- AARC and EOSC AAI compliant
- Support for legacy X.509 services via MasterPortal

### **Community management:**

- Comanage and Perun supported
- Other Community AAIs pluggable



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# Where to found the token in the EGI Notebooks

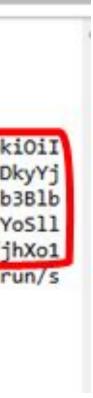
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egi.eu \$ ls

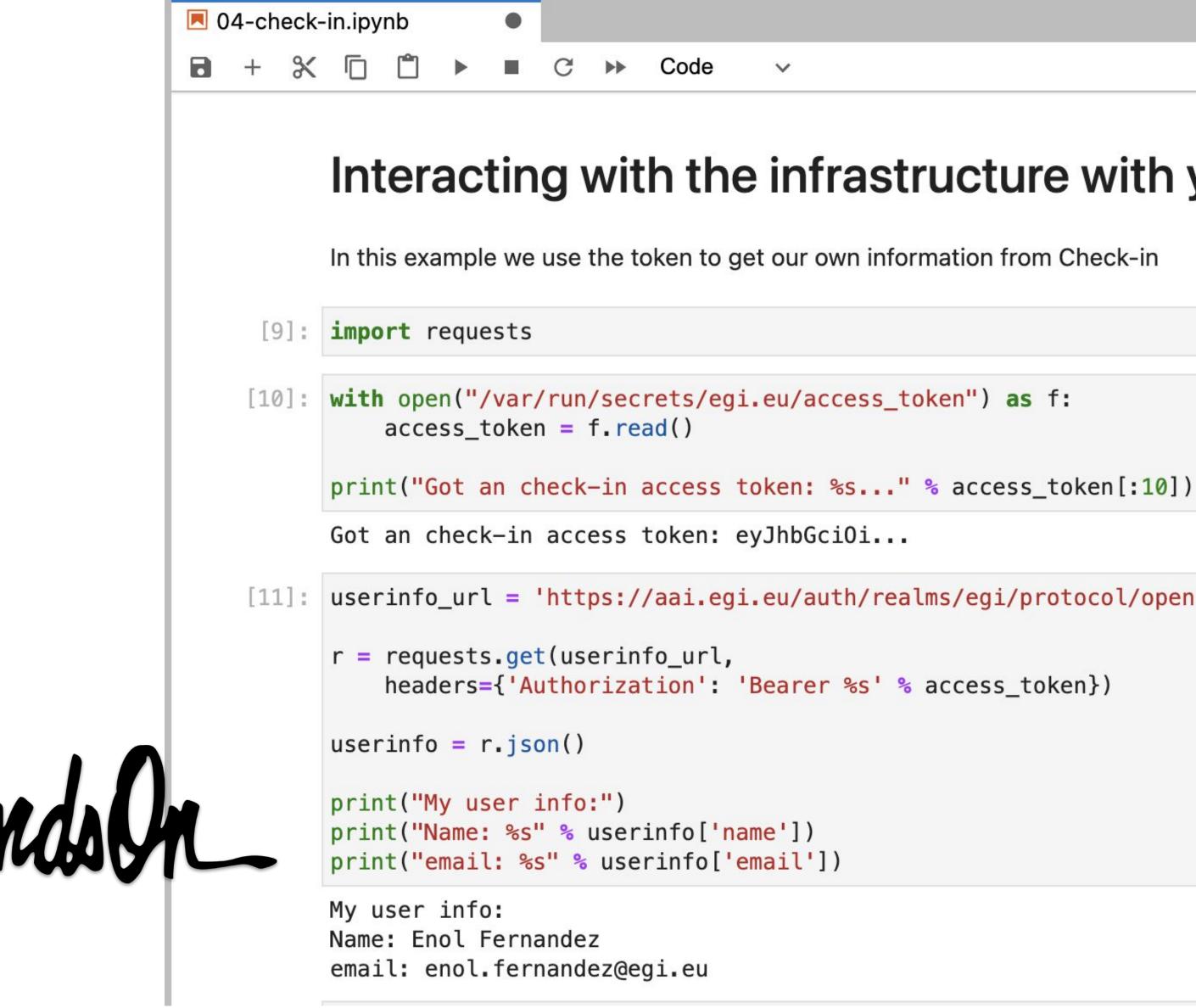
#### \$ cat access token

nhaZGFFajByamJVIn0.eyJleHAiOjE2NjM4NjM1NTEsImlhdCI6MTY2Mzg1OTk1MSwiYXV0aF90aW1lIjoxNjYzODU5MzE4LCJqdGkiOiI ZWFsbXMvZWdpIiwic3ViIjoiYjEwZDAzMjY0OGQwM2I3NWEyNGE3Nzk1MzMzNzZlMjM3NmY5ZGU2MTUwODUyMmJjZTA4M2VkODUwNDkyYj iLCJzZXNzaW9uX3N0YXRlIjoiZWVmMjFhZmEtM2U4OS00ZWI1LTlkMmEtNjdhOGVlYTAyMjkwIiwiYWNyIjoiMCIsInNjb3BlIjoib3Blb RfYWZmaWxpYXRpb24iLCJzaWQiOiJlZWYyMWFmYS0zZTg5LTRlYjUtOWQyYS02N2E4ZWVhMDIyOTAifQ.liN2-tMM4f-t5CYsBs3TYoSll rtlAU6kCrZ3B-PQE37Aqnvt2s20gBDNf9MksHyxyT6pbbaCRatiAYEXy6mDrD9tBjciZxIgS917leG-lF1hFfVl8iVzCOek\_nUL6fjhXo1 /guWy8ZGyW0m6Zx19cRus54egjovyan@jupyter-b10d032648d03b75a24a779533376e2376f9de61508522bce083ed8:/var/run/s





## Get info about yourself



#### Interacting with the infrastructure with your own credentials

[11]: userinfo\_url = 'https://aai.egi.eu/auth/realms/egi/protocol/openid-connect/userinfo'



## Sentinel image processing and analysis

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api/data/" + dataset, headers={"authorization": "Bearer {}".format(access_token)}, stream=True)	





# Approach to reproducible Open Science with EGI and EOSC

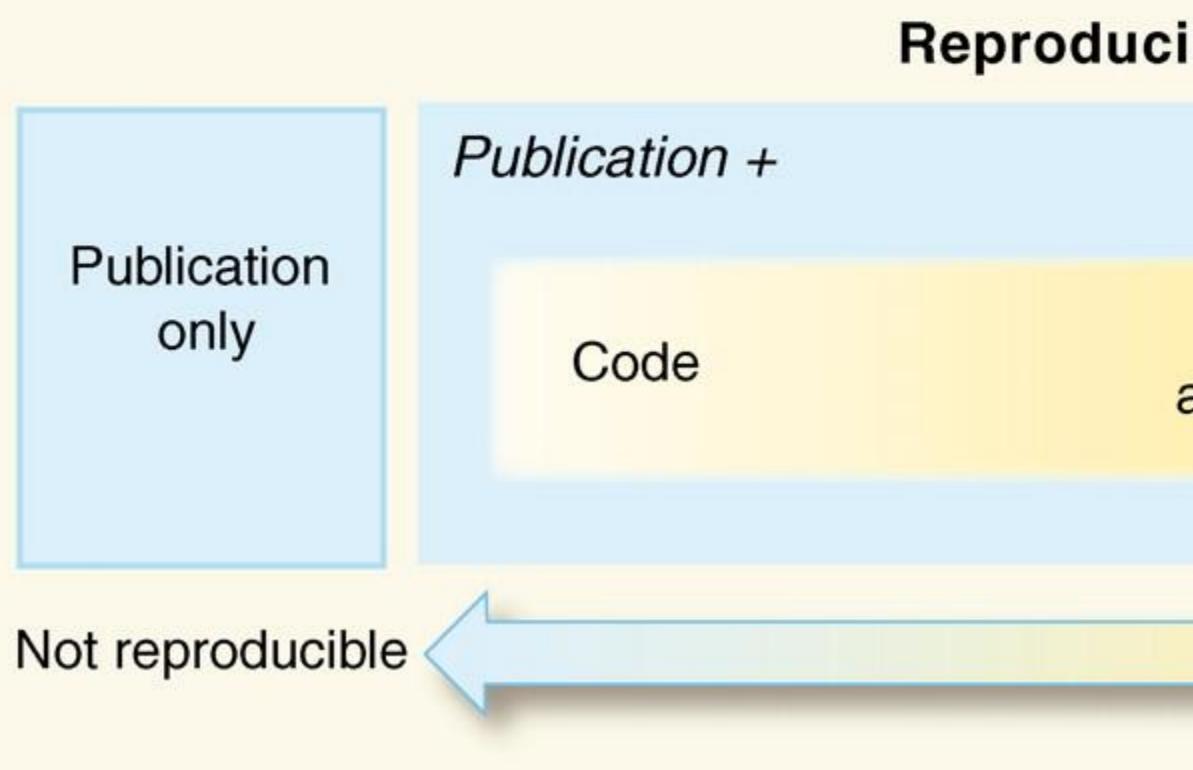
TLP: GREEN Limited disclosure

ISGC 2023





### Reproducibility: beyond sharing code and data



Peng, Science, 2011

21 March 2023 | ISGC2023

#### **Reproducibility Spectrum**

Code and data Linked and executable code and data Full replication

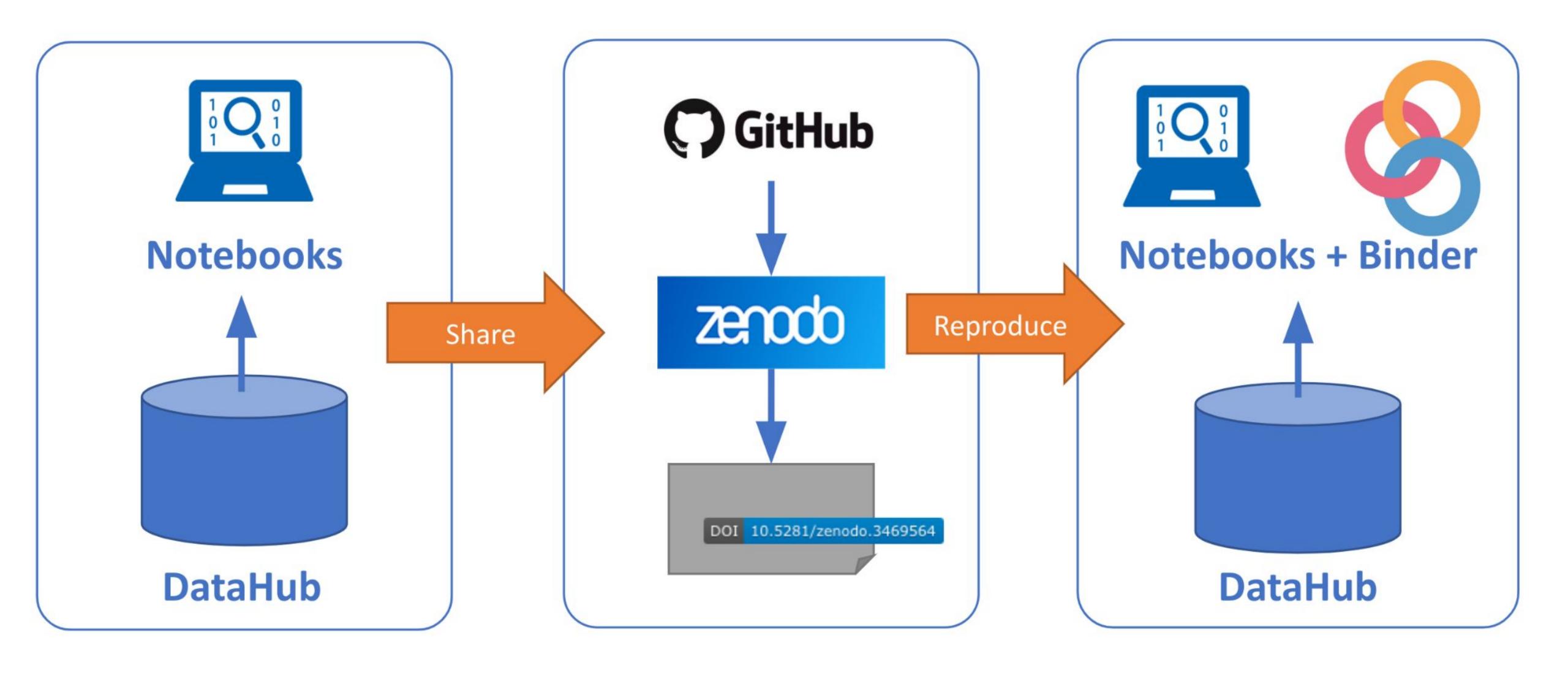
Gold standard

www.egi.eu | 47





### Reproducible Open Science in EGI/EOSC



21 March 2023 | ISGC2023

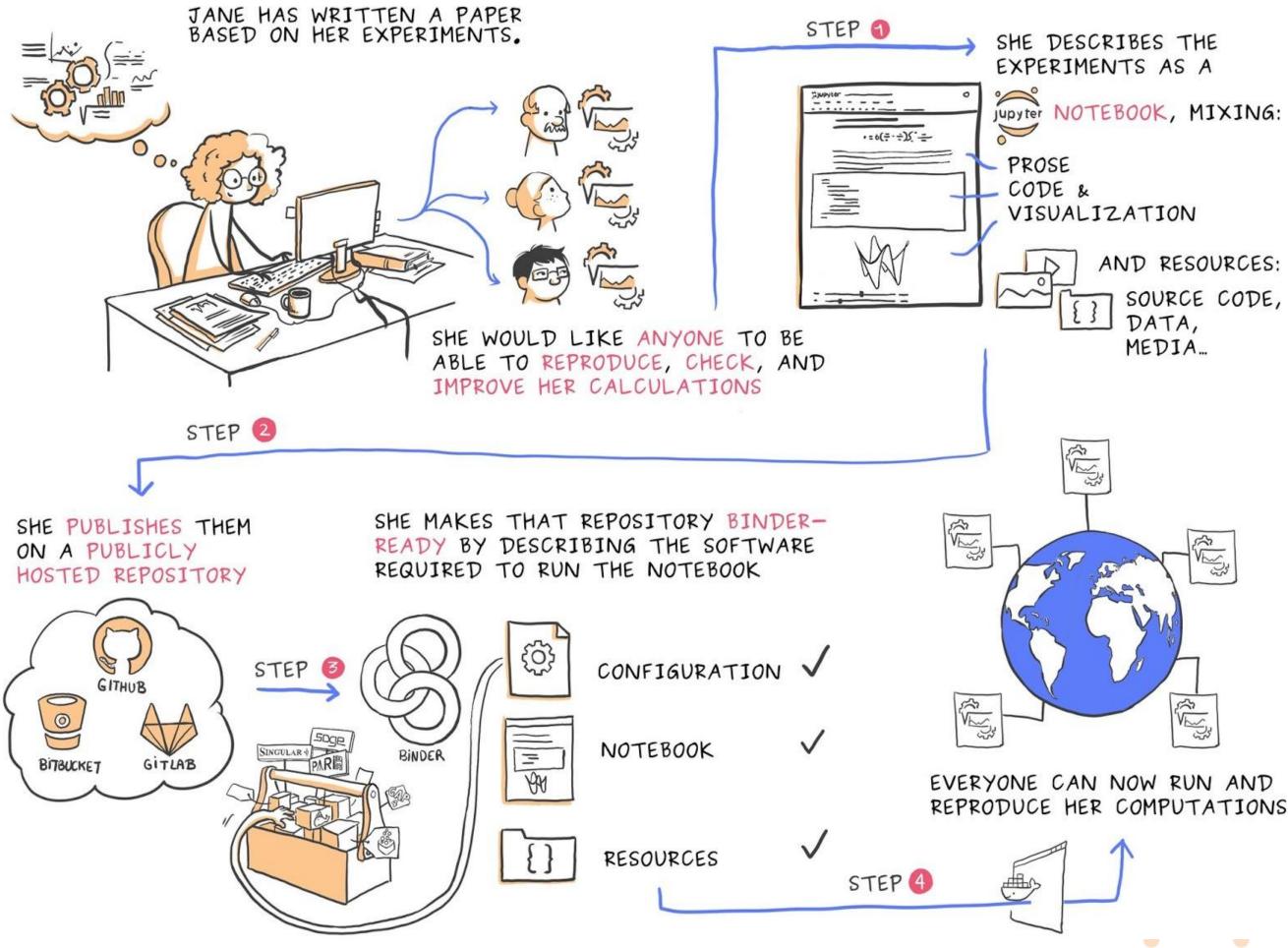


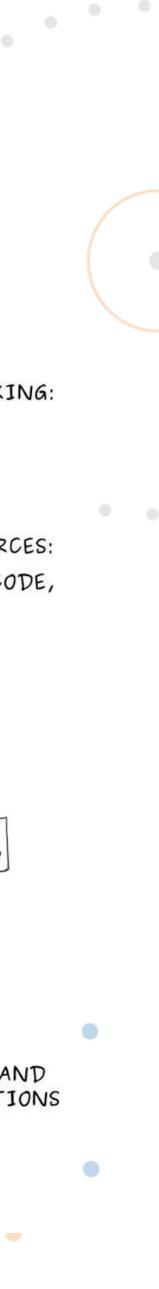


Binder: reproducing execution environments

An open-source web application to turn repositories in interactive notebooks

It uses modern technology in cloud orchestration (Kubernetes), interactive computing (Jupyter), scientific computing (the open-science ecosystem)









#### **BinderHub hosted by EGI**

- Offered 'as Service'
- Same access conditions as EGI Notebooks

#### Main Features:

- Use any binder-compatible repository
- Reproduce your notebooks with access to EGI resources (e.g. DataHub)
- No hard limits on sessions duration, customisable resource limits for users/communities

(+)EGI Replay × 🔲 🚓 Incognito replay.notebooks.egi.eu/hub/hub/login?next=... Q egi

# Replay

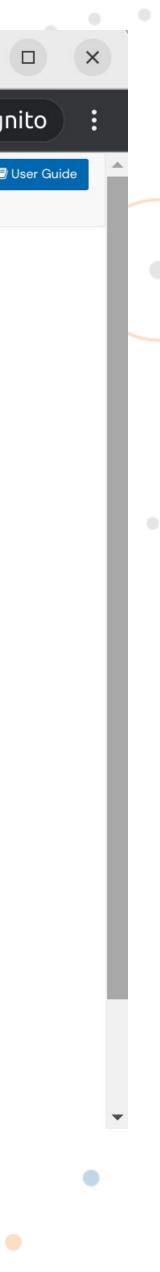
Replay offers an easy place to reproduce and share notebooks. It allows users to replay complex calculations, simulations, and visualisations scenarios by importing Notebooks and their runtime environment and share them with a single link. Replay works well with EGI Notebooks: use-cases include workshops, scientific workflows and streamline sharing among teams.

Access requires a valid EGI account and enrolling to the vo.notebooks.egi.eu VO.

Continue with EGI Check-in

Replay is based on Jupyter Binder and runs on the EGI cloud service. You can learn more at our documentation.

This Replay instance is operated by and uses resources from CESNET. User communities/advanced users can have their customised Binder instance. EGI offers consultancy and support, as well as can operate the setup. Email support \_at\_ egi.eu to request a community instance.







## Example: Number of Summer Days in Taipei with EGI Replay

#### From <a href="https://github.com/enolfc/isgc-2023-enes">https://github.com/enolfc/isgc-2023-enes</a>

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S	Sgc-2023-enes	o use EGI Replay	
	Sample binder repository using ENES data	o use EGI Replay	

### See: "How to make your datasets available in DataHub"



### QuickStart\_GeoPy

- Calculate the number of summer days in the specific location
- From the ENES Data Spaces
- Datasets are stored in DataHub







# How to make notebooks Reproducible and Shareable

**TLP: GREEN Limited disclosure** 

ISGC 2023

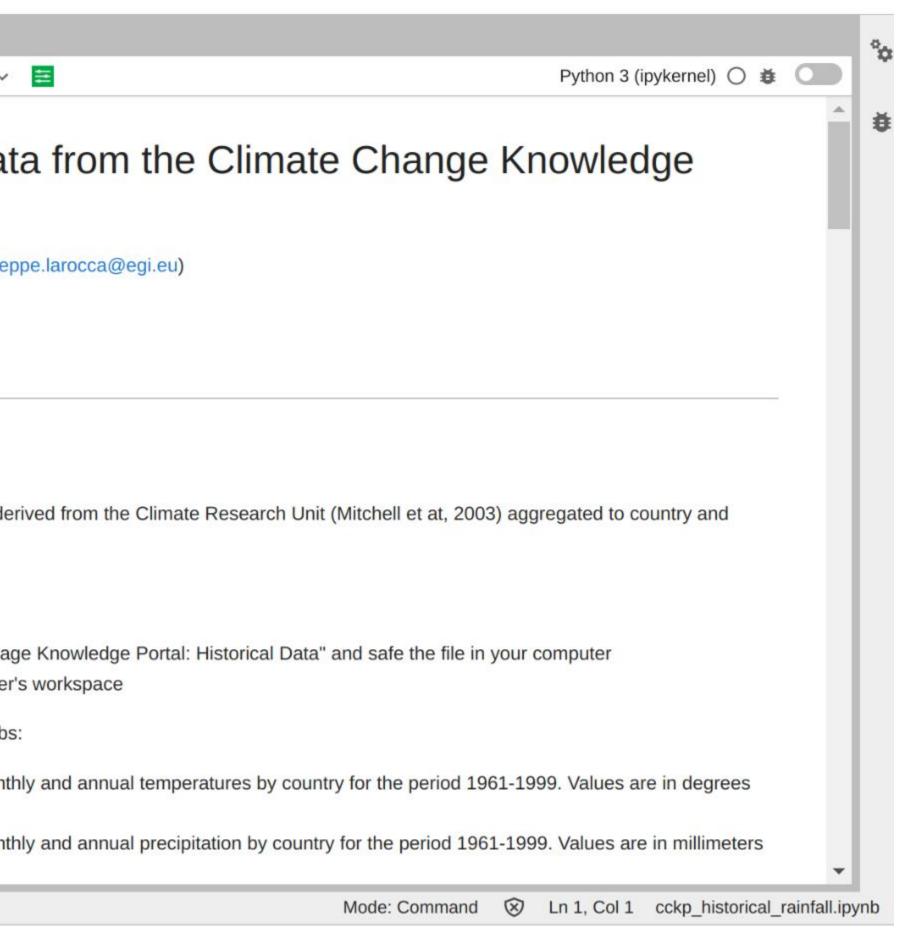




## 1. Create your first sharable notebook

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Rename Notebook						Calc	ulate	the h	istor	rical p	precip	pitation data d
Download						basir	n leve	ls.				
							Visit t	he W	/orld	Data	Cata	alogue
Expert Netebook As	E.											sources" tab
Save Current Workspace As						•	Down	load	a co	py of	f the '	"Climate Chna
Save Current Workspace						•	Uploa	d the	e .xlx	spre	adsh	neet in the use
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Log Out							Celsi					_
						•	Coun	try_p	reci	oitatio	onCR	<u>U</u> : mean mor
							(mm)					

#### Download your first notebook in your laptop (\*.ipynb)







### 2. Getting a GitHub account

 $\mathbf{O}$ 

Product V Solutions V Open Source V Pricing



GitHub Galaxy: A global enterprise event Register now to join us virtually from March 28–31.

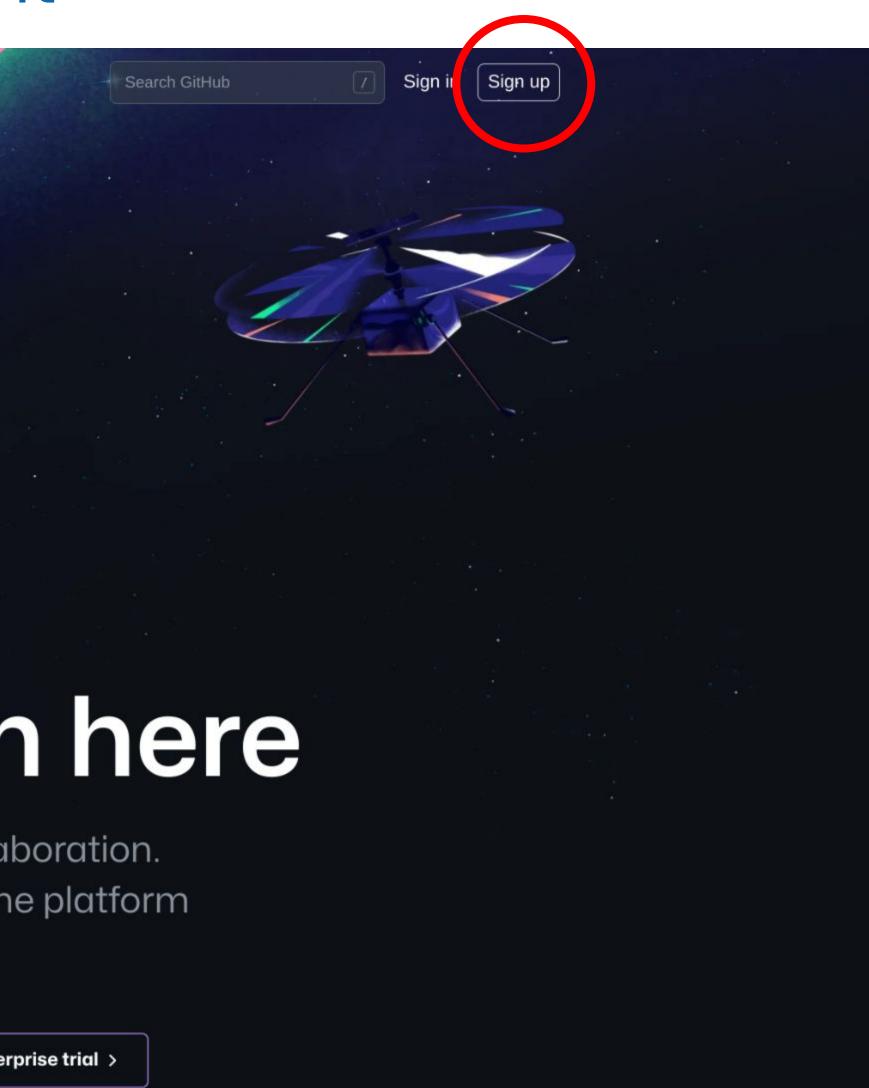
# Let's build from here

Harnessed for productivity. Designed for collaboration. Celebrated for built-in security. Welcome to the platform developers love.

Email address

Sign up for GitHub

Start a free enterprise trial >



Sign-up if you don't have an account already

www.egi.eu |







## 3. Creating a new GitHub repository

Search or jump to	Crea
	A repos
🚇 glarocca 🗸	Import
Top Repositories	Repos
Find a repository	Start you
EGI-Federation/python-appdb-info	No t
EGI-ILM/terraform-doc-internal	
EGI-Federation/fedcloud-vm-monitoring	
glarocca/pyEGI-AAI-CheckIn	Owner
larocca/ExPaNDS	
🗜 glarocca/panosc	
EGI-Federation/impact-report	Great r
how more	
	Descri
	$\circ \Box$
	Initializ
	Skip th
	🗹 Ado
	This

#### Create a new repository

A repository contains all project files, including the revision Import a repository.

#### **Repository template**

Start your repository with a template repository's contents.

No template -

**Owner** \*

Repository name \*

isgc2013\_rainfall

Great repository names isgc2013\_rainfall is available. leed in

#### **Description** (optional)

👭 glarocca 🗸

Public

Anyone on the internet can see this repository. You choose

#### Private

You choose who can see and commit to this repository.

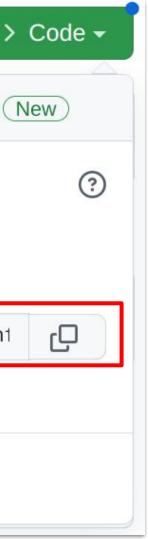
#### Initialize this repository with:

Skip this step if you're importing an existing repository.

#### Add a README file

This is where you can write a long description for your project. Lo

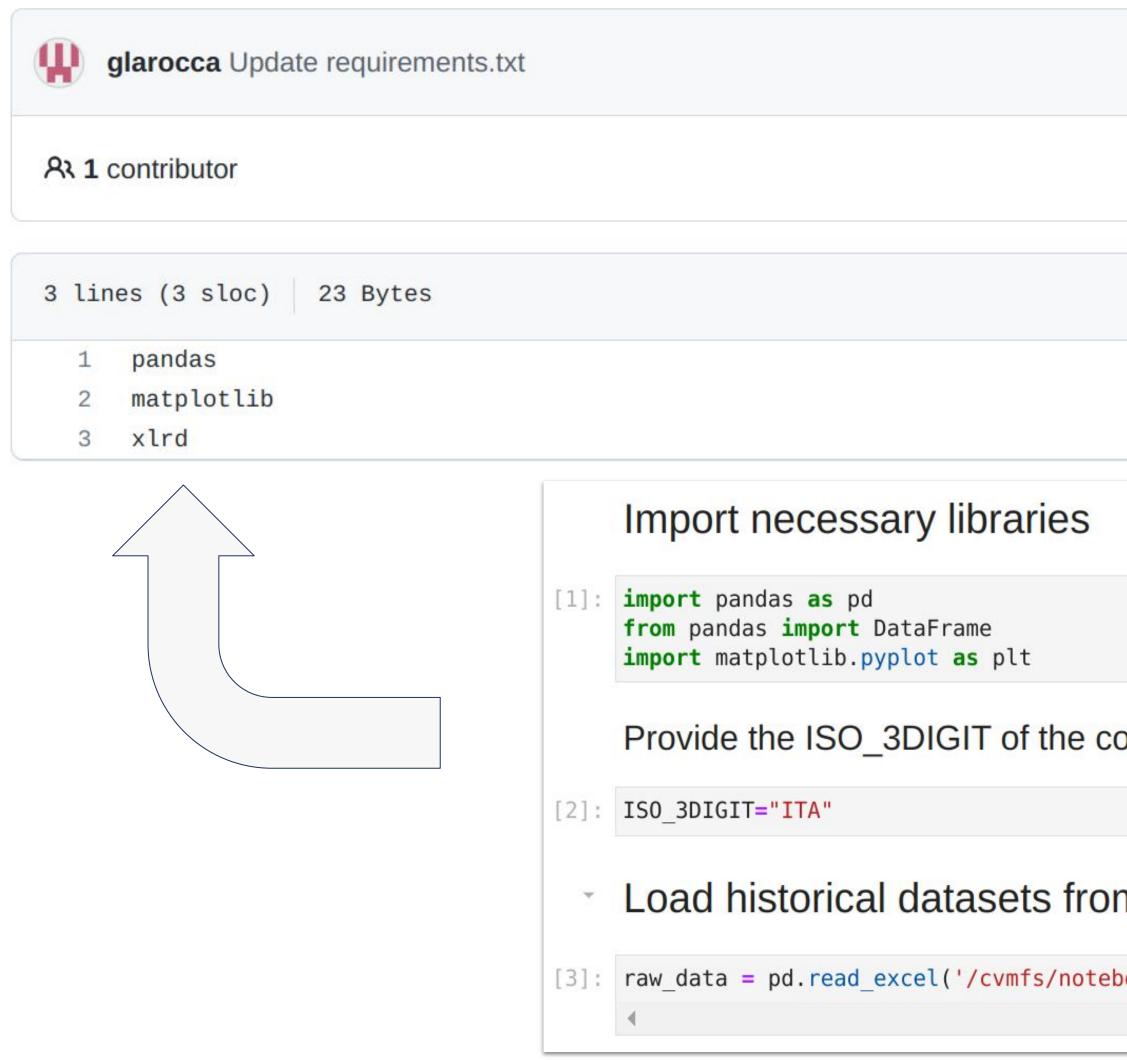
			2.		
history. Already have a project repository elsewhere?		Go to fi	ile	dd file 🗸	<
	Lo	ocal		Codespace	es
	▶ Clone				
			tHub CLI	1.	
	Use Git or che			/isgc2013_r e web URL.	aın
	Downloa	ad ZIP			
e who can commit.					
earn more.					





## 4. Adding dependencies

#### Create the 'requirements.txt' file in your repo



	Latest commit 7b83032 yesterday	Юн
	Raw Blame	•
ountry you are interested to analyse		
n local and create a DataFrame objec	t	
oooks.egi.eu/isgc-2023/cckp/cckp_historical_data_0.x	<pre>ls', sheet_name='Country_precipitat</pre>	tionC

www.egi.eu |





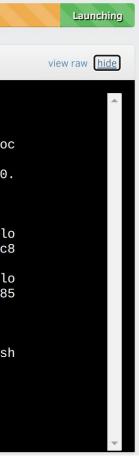


### 5. Executing Notebooks in Replay https://replay.notebooks.egi.eu/

#### Build and launch a repository

GitHub repository name or URL					
GitHub - https://github.com/g	larocca/isgc2013_rainfall.git				
Git ref (branch, tag, or commit)	Path to a notebook file (optional)				
HEAD	Path to a notebook file (optional)				
Copy the URL below and share you	ur Binder with others:				
https://replay.notebooks.egi.eu/v2/gh/glarocca/isgc2013_rainfall.git/HEAD					
Expand to see the text below, past	te it into your README to show a binder badge: 🔇 launch bind				
<pre>m [![Binder](https://rep </pre>	lay.notebooks.egi.eu/badge_logo.svg)](https://rep				
	lay.notebooks.egi.eu/badge_logo.svg ay.notebooks.egi.eu/v2/gh/glarocca/isgc2013_rainf				

	Already built!
	Build logs
File -	<pre>Found built image, launching Launching server Server requested 2023-03-13T16:09:49.236416Z [Normal] Successfully assigned binder/jupyter-glaroo ca5 to k8s-w-ingress 2023-03-13T16:09:52Z [Normal] Container image "jupyterhub/k8s-network-tools:2.0. 0" already present on machine 2023-03-13T16:09:53Z [Normal] Created container block-cloud-metadata 2023-03-13T16:09:53Z [Normal] Started container block-cloud-metadata 2023-03-13T16:09:53Z [Normal] Pulling image "docker-notebooks.fedcloud-tf.fedcloud.eu/binder-glarocca-2disgc2013-5frainfall-674ed6:dc2b600eb072484850d231d2542c8 a0018cd410f" 2023-03-13T16:10:56Z [Normal] Successfully pulled image "docker-notebooks.fedcloud ud-tf.fedcloud.eu/binder-glarocca-2disgc2013-5frainfall-674ed6:dc2b600eb07248485 0d231d2542c8a0018cd410f" in 1m1.414306408s 2023-03-13T16:10:57Z [Normal] Created container notebook 2023-03-13T16:10:58Z [Normal] Container image "eginotebooks/oneclient-sidecar:sh a-8172f71" already present on machine 2023-03-13T16:10:59Z [Normal] Created container oneclient 2023-03-13T16:10:59Z [Normal] Created container oneclient 2023-03-13T16:10:59Z [Normal] Started container oneclient 2023-03-13T16:10:59Z [Normal] Created container oneclient 2023-03-13T16:10:59Z [Normal] Created container oneclient 2023-03-13T16:10:59Z [Normal] Created container oneclient 2023-03-13T16:10:59Z [Normal] Created container oneclient 2023-03-13T16:11:00Z [Normal] Started container oneclient</pre>
	Build logs Pushing image Pushing image Pushing image Pushing image Pushing image Pushing image
der <pre> play.notebooks.egi.eu/v2/gh/g </pre>	Pushing image Pushing image Pushing image Pushing image Pushing image Successfully pushed docker-notebooks.fedcloud-tf.fedcloud.eu/binder-glarocca-2d: ainfall-674ed6:dc2b600eb072484850d231d2542c8a0018cd410fBuilt image, launching Launching server Server requested 2023-03-13T16:09:49.236416Z [Normal] Successfully assigned binder/jupyter-glaroc w-ingress 2023-03-13T16:09:52Z [Normal] Container image "jupyterhub/k8s-network-tools:2.0 present on machine 2023-03-13T16:09:53Z [Normal] Created container block-cloud-metadata 2023-03-13T16:09:53Z [Normal] Started container block-cloud-metadata 2023-03-13T16:09:55Z [Normal] Pulling image "docker-notebooks.fedcloud-tf.fedcloud-
fall.git/HEAD	r-glarocca-2disgc2013-5frainfall-674ed6:dc2b600eb072484850d231d2542c8a0018cd410







### Unable to launch the server https://replay.notebooks.egi.eu/

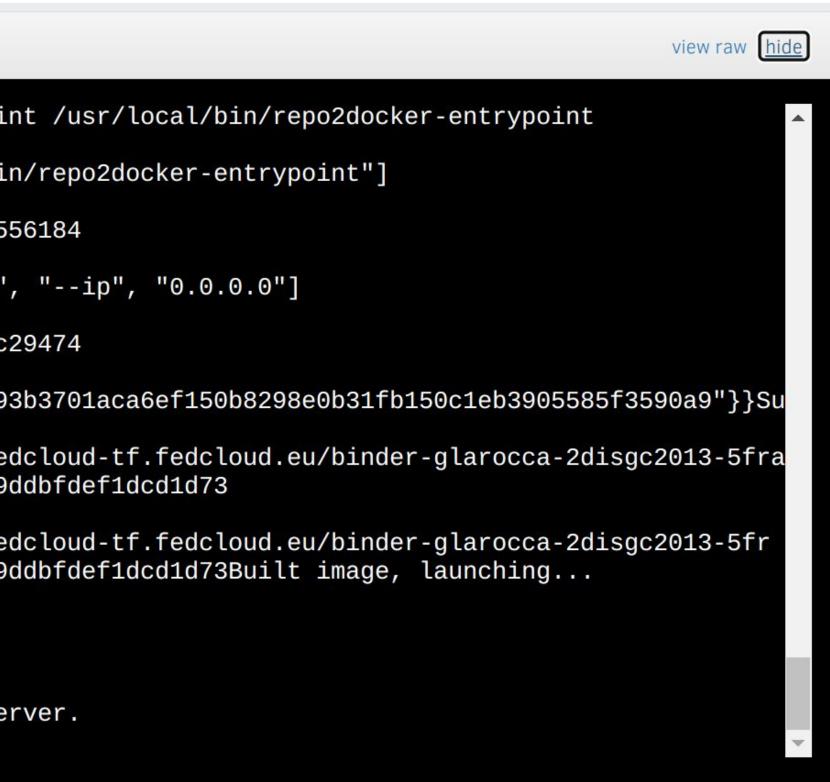
Build logs

Step 49/51 : COPY /repo2docker-entrypoi
> 3dda7421129e
<pre>Step 50/51 : ENTRYPOINT ["/usr/local/bi</pre>
> Running in 96ff2f556184
Removing intermediate container 96ff2f5
> b9b8b51524cc
<pre>Step 51/51 : CMD ["jupyter", "notebook"</pre>
> Running in 2be6bdc29474
Removing intermediate container 2be6bdc
> 46d5422a2fab
{"aux": {"ID": "sha256:46d5422a2fabb769
ccessfully built 46d5422a2fab
Successfully tagged docker-notebooks.fe
infall-674ed6:e842592725541fa91123f33e9
Pushing image
Successfully pushed docker-notebooks.fe
infall-674ed6:e842592725541fa91123f33e9
Launching server
Launch attempt 1 failed, retrying
Launch attempt 2 failed, retrying
Launch attempt 3 failed, retrying
User glarocca5 already has a running se
User glaroccas alleady has a fulliting se

Only 1 server per user is allowed! Stop server at: <a href="https://replay.notebooks.egi.eu/hub/hub/home">https://replay.notebooks.egi.eu/hub/hub/home</a>

Stop My Server My Server

21 March 2023 | ISGC2023







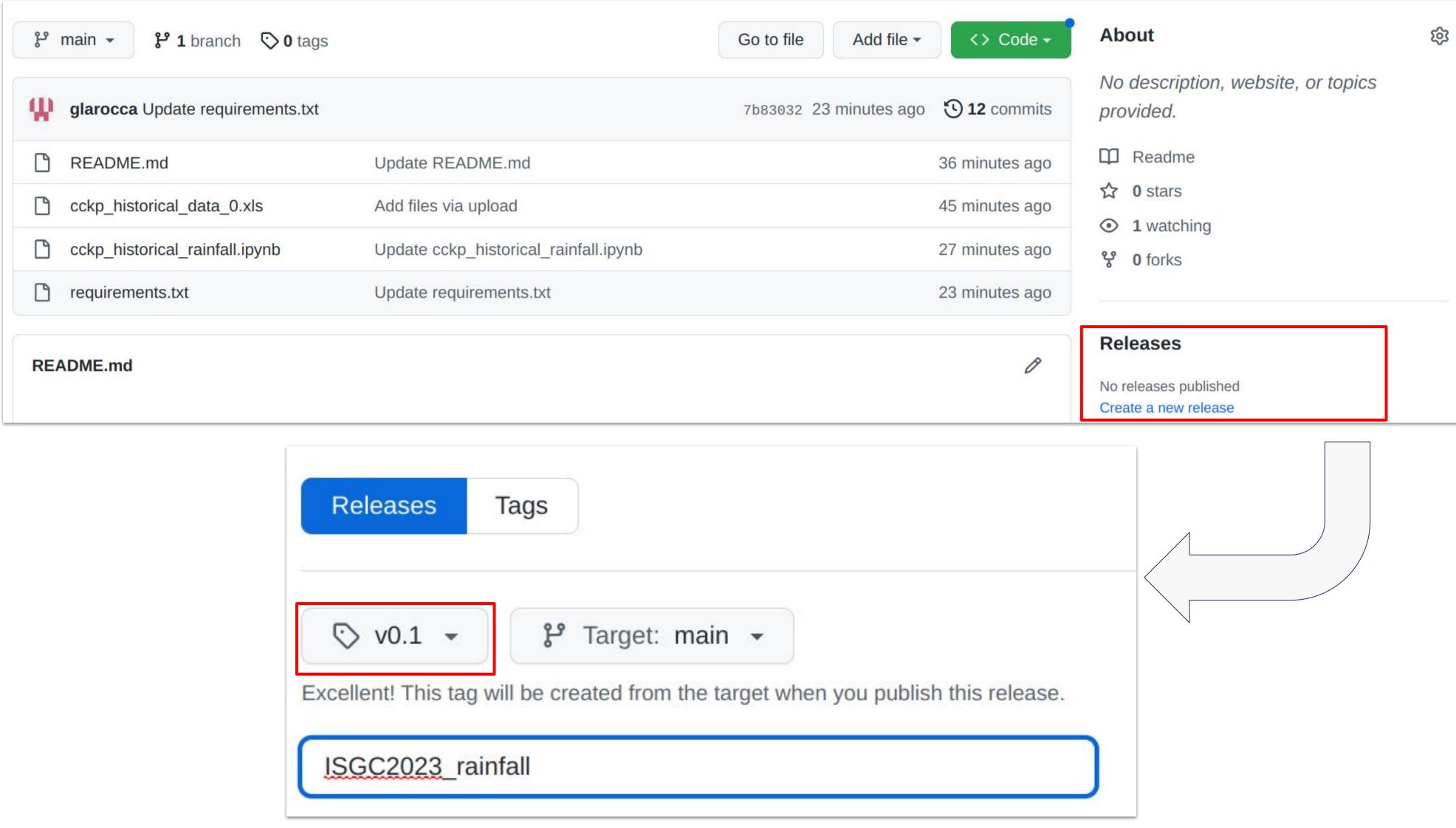
## 6. Adding Binder badge in the GitHub repository

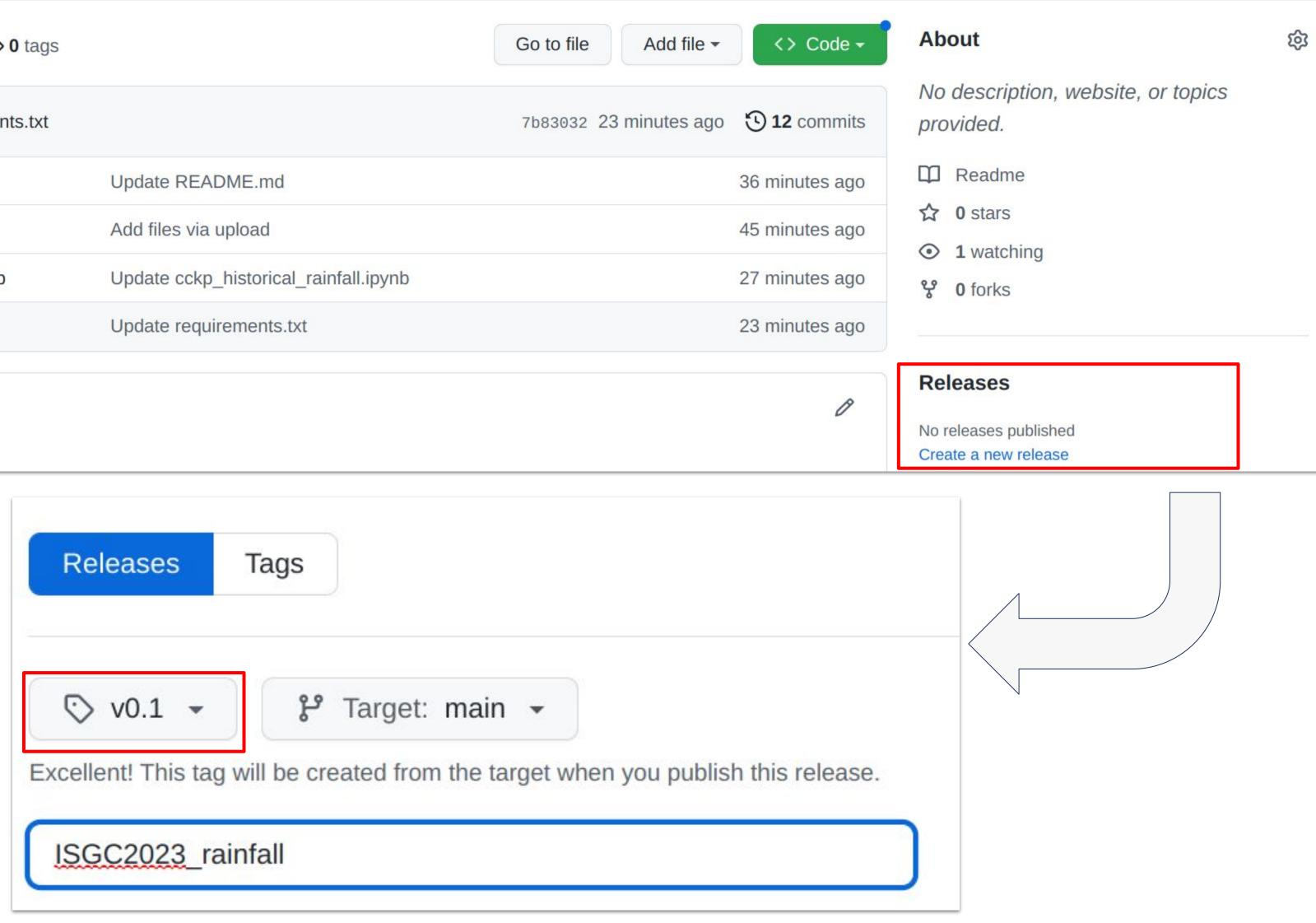
isgc2013_rain	fall / README.md in main			C	ancel cha	nges
<> Edit file	O Preview	Spaces \$	2	\$	Soft wrap	•
1 <b># isgc2</b> 2	013_rainfall					
3 This is	my first shared notebook					
4 5 <u>[![Bind</u> 6	<u>er](</u> https://replay.notebooks.egi.eu/badge_logo.svg) <u>](</u> https://replay.notebooks.egi.eu/v2/gh/glarocca/ISGC2023_rain	nfall.git/HE/	ND)			
7						





## 7. Create a new Release for the repository









### 8. Making repository citable https://zenodo.org/

zenodo	Search	Q Upload Communities
		Resear
		Citeable. Discoverable. Uploads get a Digital Object Identifier (DOI) to nand uniquely citeable. Communities Accept or reject uploads to your own communit EU projects, institutions or entire disciplines).

#### **Trusted Research Data Management**

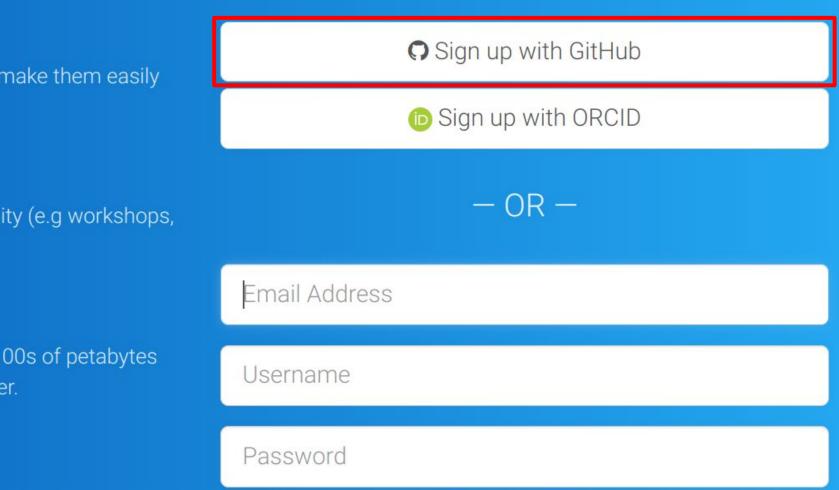
Built on top of CERN's expertise in managing 100s of petabytes of research data from the Large Hadron Collider.

Siuseppe.larocca@ct.infn.it

•

# Zendo

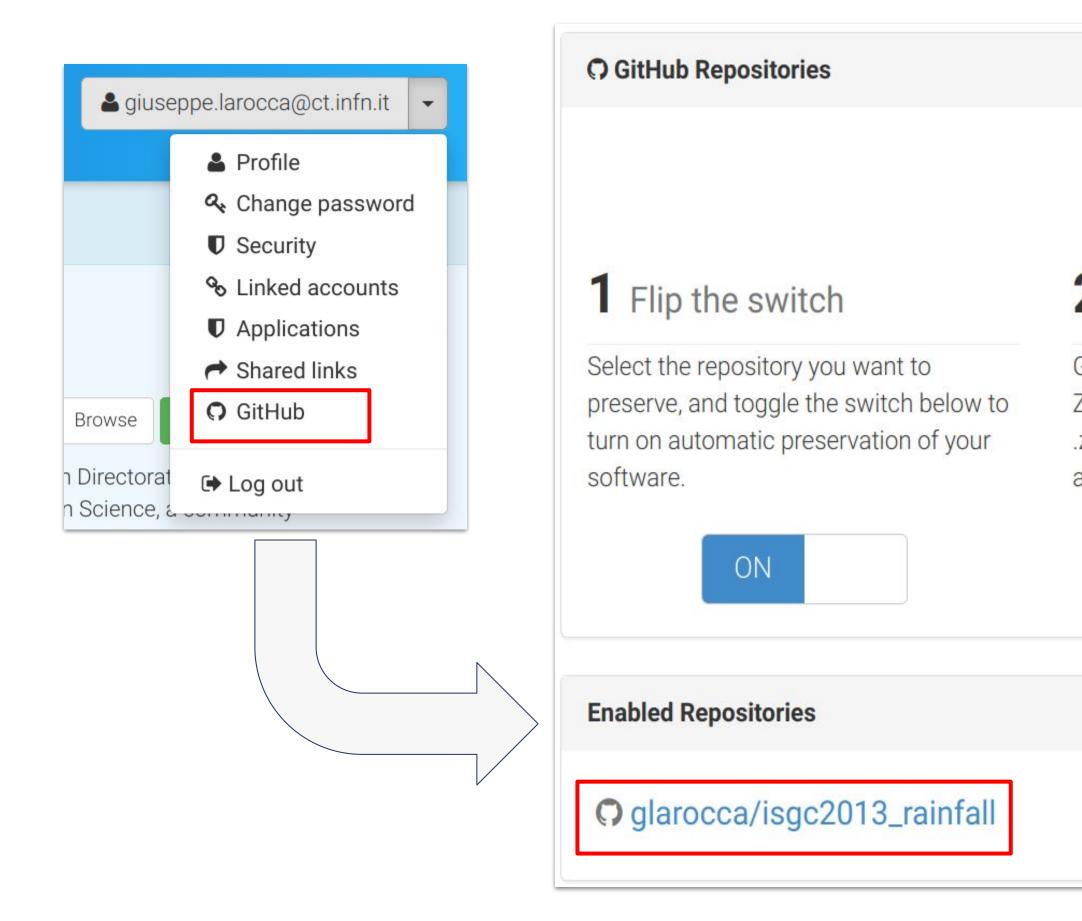
#### ch. Shared! Sign up today.

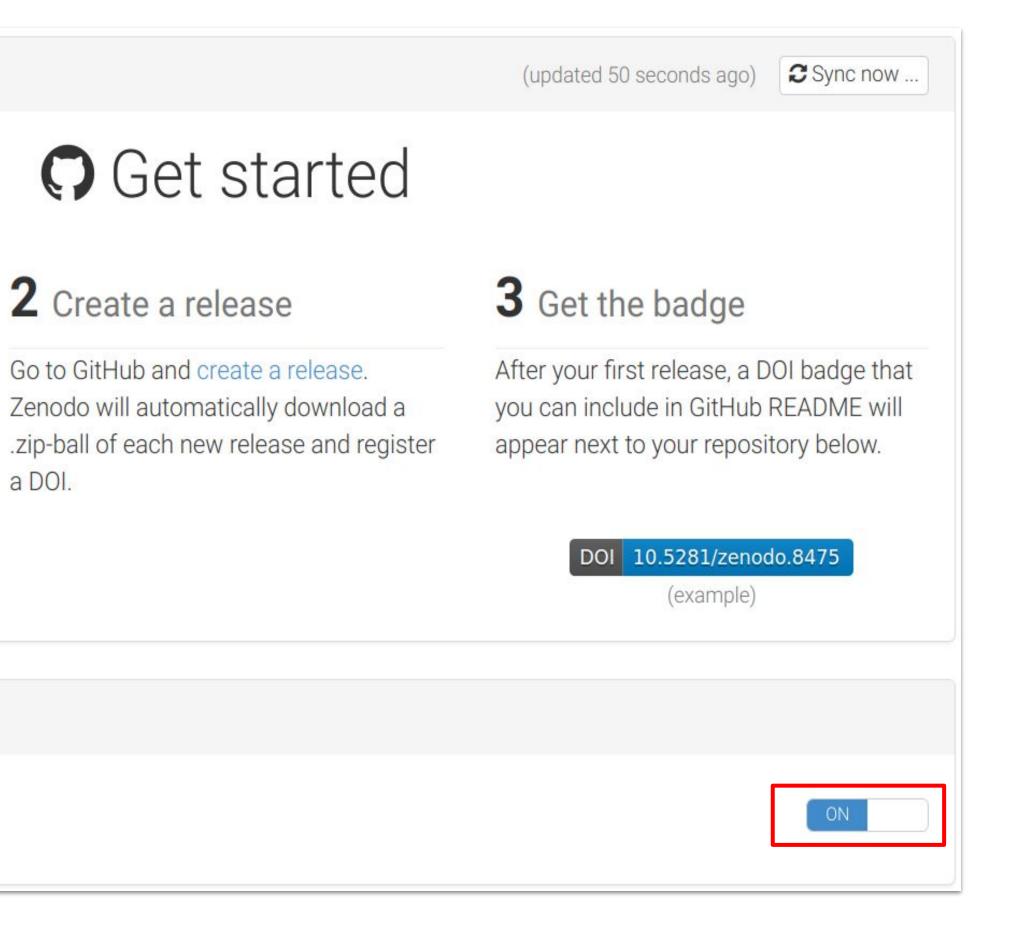
















### 10. Get Zenodo DOI

#### Click on the Enabled Repository



#### www.egi.eu |



## 11. Add Zenodo badge in repository

#### Click on the DOI icon to view details





ON
<b>O</b> Create release
shed
s ago

#### DOI Badge

This badge points to the latest released version of your repository. If you want a DOI badge for a specific release, please follow the DOI link for one of the specific releases and grab badge from the archived record.

Markdown

[![DOI](https://zenodo.org/badge/613453962.sv	vg)](https://zenodo.or
---	------------------------

reStructedText

```
.. image:: https://zenodo.org/badge/613453962.svg
  :target: https://zenodo.org/badge/latestdoi/613453962
```

HTML

<a href="https://zenodo.org/badge/latestdoi/613453962"><img src="https:/

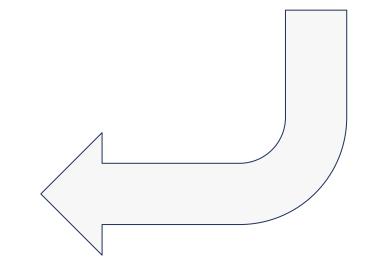
Image URL

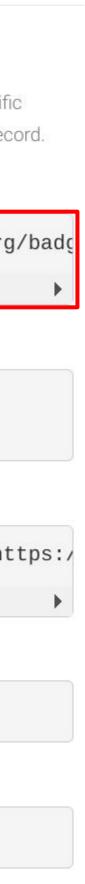
https://zenodo.org/badge/613453962.svg

Target URL

https://zenodo.org/badge/latestdoi/613453962

Spaces 🜲







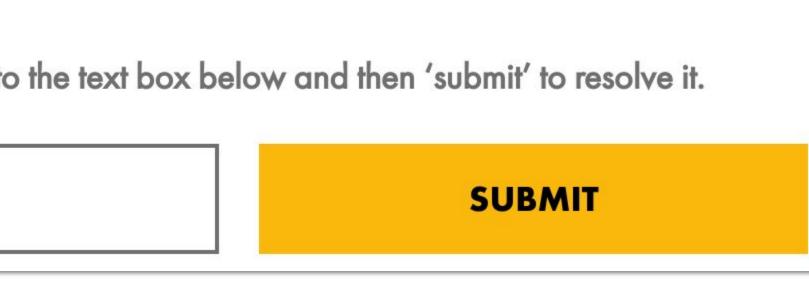
### 12. Check if the DOI is valid https://www.doi.org/

#### **TRY RESOLVING A DOI NAME**

Type or paste a known DOI name exactly—including its prefix and suffix—into the text box below and then 'submit' to resolve it.

10.5281/zenodo.7729979









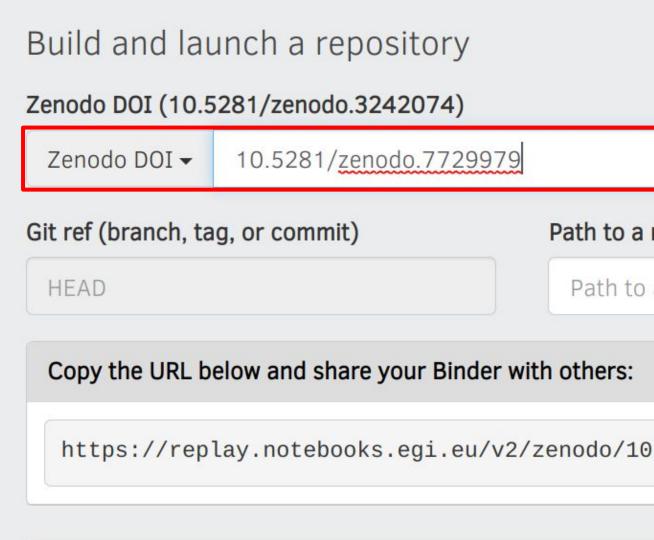
## 13. Use the DOI to reproduce the repository

https://replay.notebooks.egi.eu/



Turn a Git repo into a collection of interactive notebooks

New to Binder? Get started with a Zero-to-Binder tutorial in Julia, Python, or R.



21 March 2023 | ISGC2023

Expand to see the text below, paste it into your README

Have a repository full of Jupyter notebooks? With Binder, open those notebooks in an executable environment, making your code immediately reproducible by anyone, anywhere.

a notebook file (optional)		
o a notebook file (optional)	File 🗸	launch
0.5281/zenodo.7729979/		Ê
to show a binder badge: 🚱 launch binder		

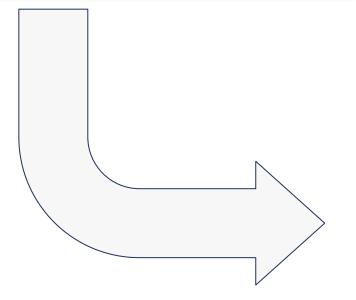




### 14. About CITATION files to your GitHub repository

#### Add a **CITATION.cff** file to the root of a repository

<> E	Edit new file  O Preview			
1	cff-version: 1.2.0			
2	message: "If you use this software, please cite it as below."			
3	authors:			
4	- family-names: "La Rocca"			
5	given-names: "Giuseppe"			
6	orcid: "https://orcid.org/0000-0002-8011-1450"			
7	title: "EGI Notebook example"			
8	version: 2.0.4			
9	doi: 0.5281/zenodo.7729979			
10	date-released: 2023-03-13			
11	url: "https://github.com/github/linguist"			



Go to file Add file - <> Code -	About
e842592 now 🕑 14 commits	No description, website, or topics provided.
now	Readme
12 minutes ago	Cite this repository -
Cite this repository If you use this software i using the following meta	n your work, please cite it data. <u>Learn more</u>
APA BibTeX	
La Rocca, G. (2023). EGI	Notebook example
View ci	tation file





# Future outlook: How to access and process data from the European Open Science Cloud

TLP: GREEN Limited disclosure

ISGC 2023





European Open Science Cloud https://eosc.eu/

The European Open Science Cloud (EOSC) is an environment for hosting and processing research data to support EU science.

The ambition of the European Open Science Cloud (EOSC) is to provide European researchers, innovators, companies and citizens with a federated and open multi-disciplinary environment where they can publish, find and re-use data, tools and services for research, innovation and educational purposes.

This environment will operate under well-defined conditions to ensure trust and safeguard the public interest.

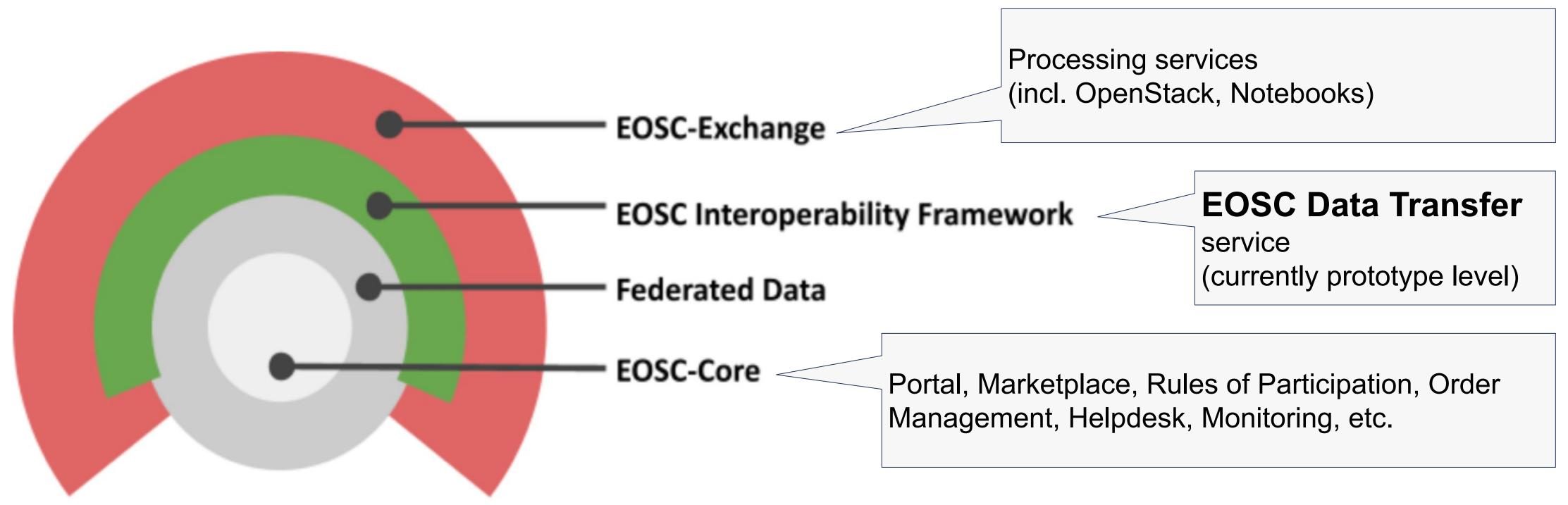
EOSC ultimately aims to develop a Web of FAIR Data and services for science in Europe upon which a wide range of value-added services can be built. These range from visualisation and analytics to long-term information preservation or the monitoring of the uptake of open science practices.







**EOSC** Architecture



EOSC Multi-Annual Roadmap 2023-2024 (May 2022)

21 March 2023 | ISGC2023





What we will see in this demo:

- 1.) Use the EOSC Marketplace to find a dataset
- 2.) Get the DOI of the dataset to be transferred
- 3.) Click on the dataset and open the EOSC Explore interface
- 4.) Select the settings for the data transfer (using the dev instance!)
- 5.) Initiate the data transfer
- 6.) Use the AWS CLI to check the files transferred to the destination





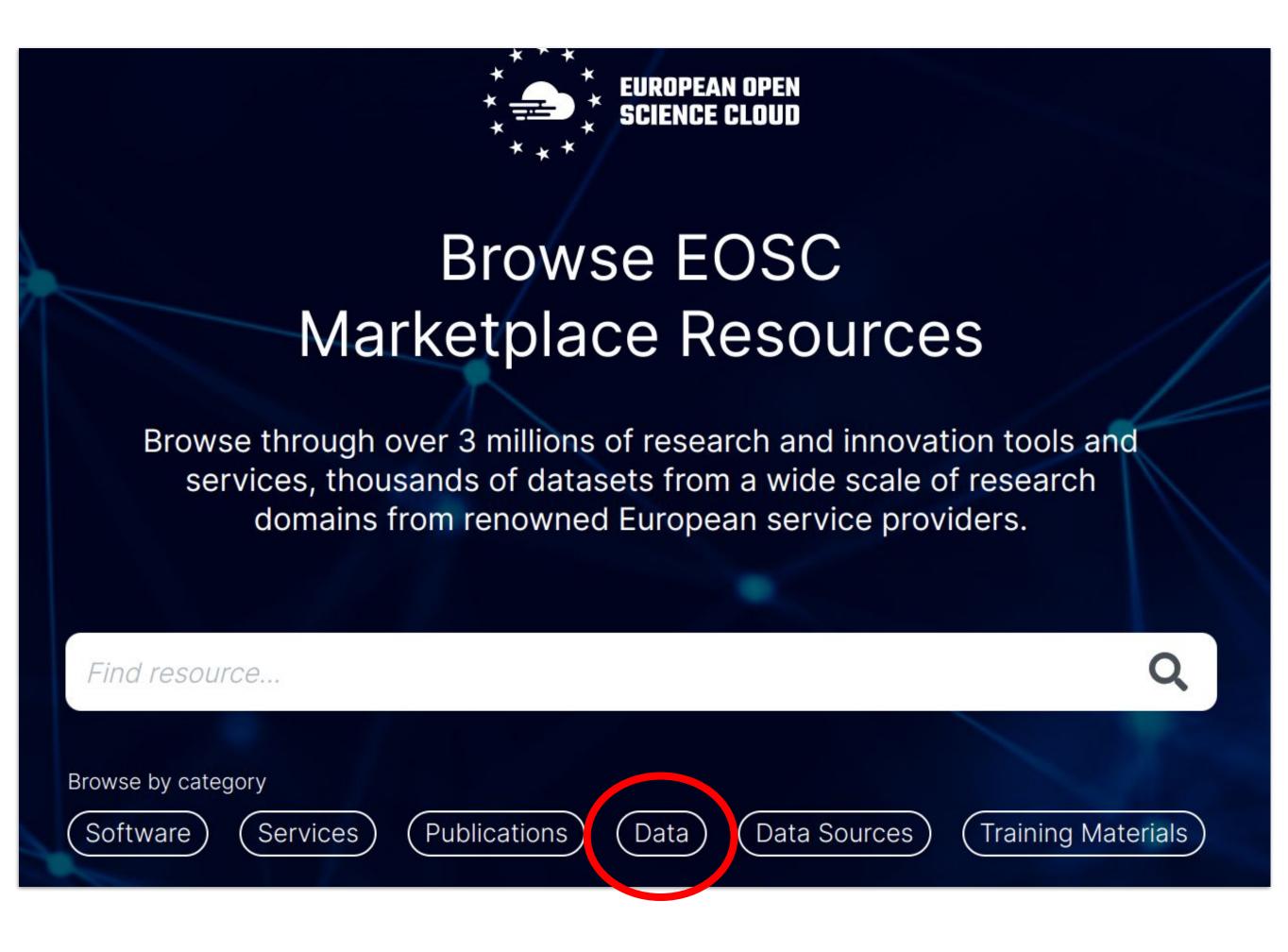


**EOSC Data Transfer** 

### 1.) Find the dataset in the EOSC Marketplace

- Access the EOSC Marketplace: <u>https://marketplace.eosc-portal.eu/</u>
- Select Data as "Category"





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### **EOSC Data Transfer**

### 2.) Get the dataset to be transferred (e.g.: Trialstreamer)

Filters		6 search results in Data			
Research step	clear all				
Discover Research (	Dutputs (6)	Dataset Open Access			
		Trialstreamer data			
Access right	clear all	Copen access			
Open access (6)		Author names: Marshall lain			
Restricted (0)		Storr Anna Thomas James			
Closed (0)		DOI: 10.5281/zenodo.5734			
Embargo (0)		Trialstreamer annotated			
		subsequent updates (daily			
Year range	clear all				

### DOI: 10.5281/zenodo.5734208

21 March 2023 | ISGC2023



#### s English

#### a

Type: dataset

n Nye Benjamin Kuiper Joël Marshall Rachel Soboczenski Frank Nenkova Ani Noel Wallace Byron

1208

collection of RCTs. This respository contains baseline files (large), and

ly for PubMed, weekly for ICTRP).





### EOSC Data Transfer

### 3.) Click on the dataset to access the file in the EOSC Explorer

	Research Data . Dataset . 2020 Trialstreamer data
	Marshall, Iain; Nye, Benjamin; Kuiper, Joël; Marshall, Rachel; Soboczenski, Frank; Nenkova, Ani; Noel Storr, Anna;
	OPEN ACCESS ENGLISH
	DOI: 10.5281/zenodo.5734208
	Published: 26 Apr 2020
	Publisher: Zenodo
ACTIONS	Summary       Related research (2)         Abstract       Trialstreamer annotated collection of RCTs. This respository contains baseline files (large), and subsequent updated and the second sec
"	2 Research Products, Page 1 of 1
ት «	Powered by OpenAIRE Research Graph . Last update of records in OpenAIRE: Feb 13, 2023
21 March 2023	



+2 Authors

# **WARNING**

- Datasets must be stored in Zenodo!

s (daily for PubMed, weekly for ICTRP).

- S3 support in EOSC Data **Transfer portal is not fully** working. It will be available in production in April 2023.









### **EOSC Data Transfer**

### 4.) Start the data transfer using the dev instance

#### EOSC Data Transfer [demo]

https://dx.doi.org/10.5281/zenodo.6669532

109 files found:

- thatstreamer-update-pubmed-2022-05-16.csv
- trialstreamer-update-pubmed-2022-05-23.csv
- trialstreamer-update-pubmed-2022-05-30.csv
- trialstreamer-update-pubmed-2022-06-06.csv
- trialstreamer-update-pubmed-2022-06-13.csv
- trialstreamer-update-pubmed-2022-06-20.csv

Transfer status: submitted.

### 5.) Click on "Transfer" to initiate the data transfer

21 March 2023 | ISGC2023



		×
s3	•	•
Destination system (e.g. hostname:8080):		
s3.cl2.du.cesnet.cz		
Provide authentication: Give access key	Give secret key	
ACMOVA5LBOL0JJ875C	•••••••••••••••••••••••••••••••••••••••	
Destination path (e.g. /folder1/folder2):		
/enolfc-test-bucket		
	×	
		-
	>> TRANSFER	





### **EOSC Data Transfer**

### 6.) Use the AWS client to check the files transferred in the S3 bucket

larocca@akt	tarus:~\$ a	aws s3end	dpoint-url https://s3.0
2023-03-10	11:36:02	1146	ENESDS_CMIP6.csv
2023-03-14	14:39:42	10280772	emojis.zip
2023-03-13	18:02:58	1152716971	<pre>tasmax_day_CMCC-ESM2_s</pre>
2023-03-13	18:07:42	1150771873	tasmax_day_CMCC-ESM2_s
2023-03-14	07:52:41	1148226564	<pre>tasmax_day_CMCC-ESM2_s</pre>
2023-03-14	07:55:09	504796434	tasmax_day_CMCC-ESM2_s
2023-03-16	11:03:27	179	trialstreamer-update-
2023-03-16	11:03:29	25688160	trialstreamer-update-p
2023-03-16	11:00:24	23538134	trialstreamer-update-p
2023-03-16	11:02:27	179	trialstreamer-update-p
2023-03-16	11:01:17	179	trialstreamer-update-
2023-03-16	11:03:35	154835212	trialstreamer-update-p
2023-03-16	11:00:22	37251724	trialstreamer-update-
2023-03-16	11:01:19	179	trialstreamer-update-p
2023-03-16	11:00:30	92992913	trialstreamer-update-
2023-03-16	11:00:21	46631156	trialstreamer-update-p
2023-03-16	10:58:11	16030071	trialstreamer-update-p
2023-03-14	14:39:42	20608411	trialstreamer.csv



#### cl2.du.cesnet.cz ls s3://enolfc-test-bucket

```
_ssp585_r1i1p1f1_gn_20150101-20391231.nc
_ssp585_r1i1p1f1_gn_20400101-20641231.nc
_ssp585_r1i1p1f1_gn_20650101-20891231.nc
_ssp585_r1i1p1f1_gn_20900101-21001231.nc
-pubmed-2021-01-04.csv
-pubmed-2021-08-23.csv
-pubmed-2021-11-22.csv
-pubmed-2022-01-24.csv
-pubmed-2022-01-31.csv
-pubmed-2022-02-07.csv
-pubmed-2022-03-21.csv
-pubmed-2022-04-11.csv
-pubmed-2022-04-18.csv
-pubmed-2022-05-02.csv
-pubmed-2022-06-13.csv
```







TLP: GREEN Limited disclosure

# Take-away message and next steps

ISGC 2023





### Key messages

- EGI established a cloud + Notebooks + Replay services to facilitate big data science in the Asia Pacific region
  - Current provider: CESNET
- Use the EGI Notebooks and the EGI Replay services to facilitate applications sharing and reproducible
- Use the EGI DataHub, B2DROP, CVMFS services to store and share datasets
- Open to scientists to run simulations
- Open for application developers to share big data applications
- Open for data providers to share data
- Open for OpenStack providers to share compute/storage

Documentation: <u>https://docs.egi.eu/users/getting-started/communities/dmcc/</u>

www.egi.eu





## Upcoming EGI Conference

https://indico.egi.eu/event/6071/abstracts/



### Call for Contributions is open!

www.egi.eu | 79





# Thank you! Q & A

### Feedback form: https://survey.egi.eu/576676

#### www.egi.eu Y



This work is partially funded by the EU research and innovation programme

in





