

MS3: Initial EuroScienceGateway workflows registered



<https://eurosciencegateway.eu/>

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Milestone 3

Initial EuroScienceGateway workflows registered

Work Package 2

2024-02-29

Technical References

<i>Project Acronym</i>	<i>ESG</i>
<i>Project Title</i>	<i>EuroScienceGateway</i>
<i>Project Coordinator</i>	<i>Albert Ludwig University</i>
<i>Project Duration</i>	<i>September 2022 / August 2025</i>

<i>Document</i>	<i>MS3: Initial EuroScienceGateway workflows registered</i>
<i>Work Package</i>	<i>2</i>
<i>Task</i>	
<i>Dissemination Level*</i>	<i>PU (Public)</i>
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<i>Contributing Beneficiary/les</i>	<i>All partners</i>



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<i>Actual Submission Date</i>	

PU = Public

PP = Restricted to other programme participants (including the Commission Services)

RE = Restricted to a group specified by the consortium (including the Commission Services)

CO = Confidential, only for members of the consortium (including the Commission Services)

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#3				



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EuroScienceGateway MS3: Initial EuroScienceGateway workflows registered.

Zenodo

<https://doi.org/10.5281/zenodo.10728922>

Executive Summary

[WorkflowHub](#) is a registry of computational workflows, provided as a EOSC Service by ELIXIR-UK, and used by over 200 different research projects, institutions and virtual collaborations. For this milestone of EuroScienceGateway (ESG), the project has developed an onboarding guide for WorkflowHub and registered in WorkflowHub the initial ESG workflows that have been developed and maintained by the project.



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ESG onboarding guide for WorkflowHub

[EuroScienceGateway](#) (ESG) has developed a project-specific onboarding guide for WorkflowHub [[Soiland-Reyes 2024](#)]. The guide gives an overview of the structure used in WorkflowHub and pointers to general WorkflowHub onboarding.

The guide is managed as a living document in Google Doc, and registered as a Standard Operating Procedure in WorkflowHub <https://doi.org/10.48546/workflowhub.sop.8.1> - with versioned snapshots following.

Guide content include:

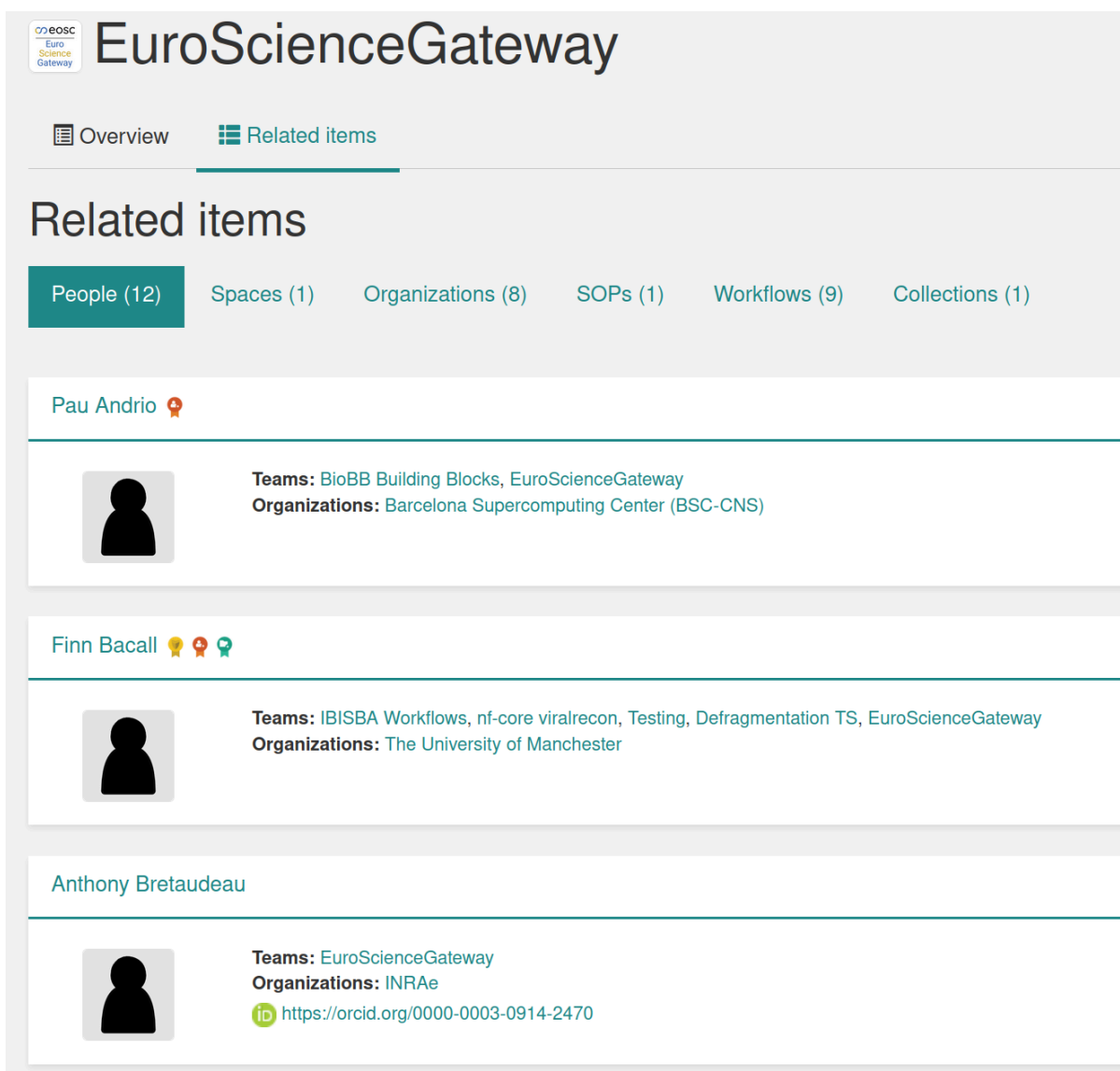
1. EuroScienceGateway workflow organisation in WorkflowHub
2. Registering EuroScienceGateway workflows in WorkflowHub
3. Linking your workflow GitHub repository with WorkflowHub
4. Keeping workflows up-to-date
5. Linking workflows with other workflows
6. Publishing workflows
7. Adding new teams and collections

As part of the EuroScienceGateway project is about maturing the WorkflowHub EOSC service, similar project-specific guides have now been developed for the Biodiversity Genomics Europe ([BGE](#)) project, Beyond COVID-19 ([BY-COVID](#)), BioDiversity Digital Twin ([BioDT](#)). As these projects are larger and combine existing collaboration networks and e-Infrastructures, their organisation in WorkflowHub are more complex than ESG.

Registering ESG workflows in WorkflowHub

Within the WorkflowHub, a [EuroScienceGateway team](#) groups the contributors, organisations and workflows developed by the ESG project. Each contributor can register for a separate account, and their workflows can be given shared attribution.





eosc Euro Science Gateway

EuroScienceGateway

Overview Related items

Related items

People (12) Spaces (1) Organizations (8) SOPs (1) Workflows (9) Collections (1)

Pau Andrio 🏆

Teams: BioBB Building Blocks, EuroScienceGateway
Organizations: Barcelona Supercomputing Center (BSC-CNS)

Finn Bacall 🏆 🏆 🏆

Teams: IBISBA Workflows, nf-core viralrecon, Testing, Defragmentation TS, EuroScienceGateway
Organizations: The University of Manchester

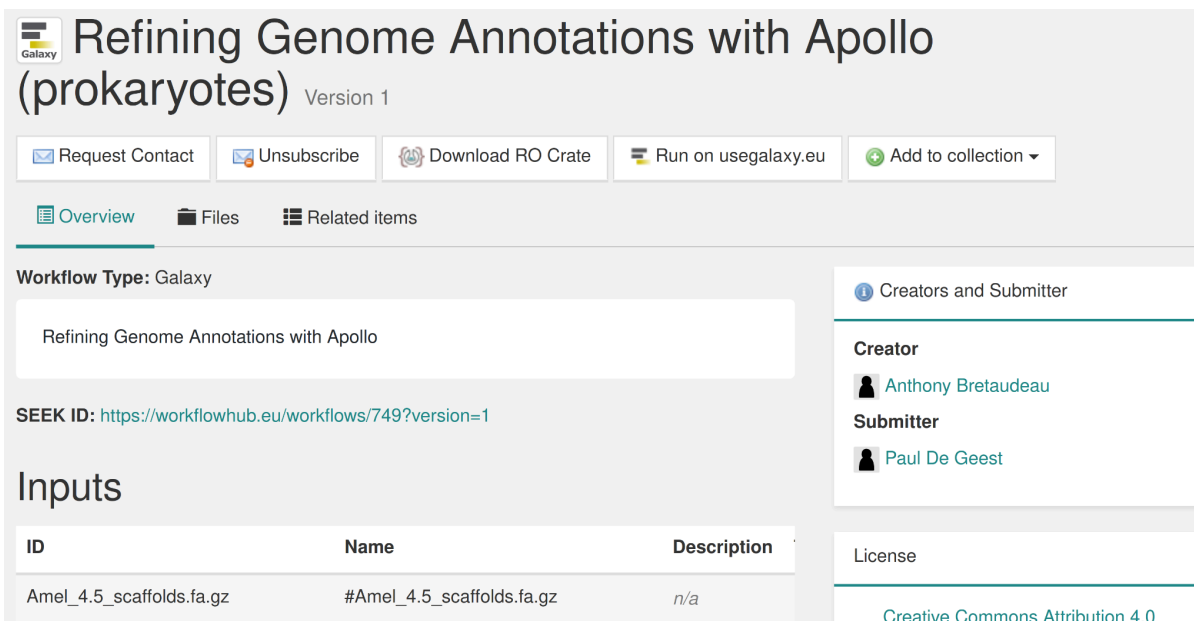
Anthony Bretaudeau

Teams: EuroScienceGateway
Organizations: INRAe
id <https://orcid.org/0000-0003-0914-2470>

Figure 1: The WorkflowHub team <https://workflowhub.eu/projects/166> shows registered people, organisations, standard operating procedures, workflows and collections.

Workflows are registered as [Workflow RO-Crates](#), capturing the workflow definition and its metadata as a FAIR Digital Object [Soiland-Reyes 2022]. [RO-Crate](#) is a general-purpose FAIR packaging mechanism for data, metadata and software.





Refining Genome Annotations with Apollo (prokaryotes) Version 1

Request Contact | Unsubscribe | Download RO Crate | Run on usegalaxy.eu | Add to collection

Overview | Files | Related items

Workflow Type: Galaxy

Refining Genome Annotations with Apollo

SEEK ID: <https://workflowhub.eu/workflows/749?version=1>

Inputs

ID	Name	Description
Amel_4.5_scaffolds.fa.gz	#Amel_4.5_scaffolds.fa.gz	n/a

Creators and Submitter

Creator
Anthony Bretaudeau

Submitter
Paul De Geest

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Figure 2: Workflow <https://workflowhub.eu/workflows/749?version=1> with options for **Download RO-Crate** and **Run on usegalaxy.eu**

Galaxy workflows registered this way can be launched from WorkflowHub (Figure 2) directly onto the usegalaxy.eu instance [Schaaf 2023]. This feature is also used by the GTN as part of a snippet (Figure 3) that enables such launching of workflows from a particular tutorial [Rasche 2023].

Workflows

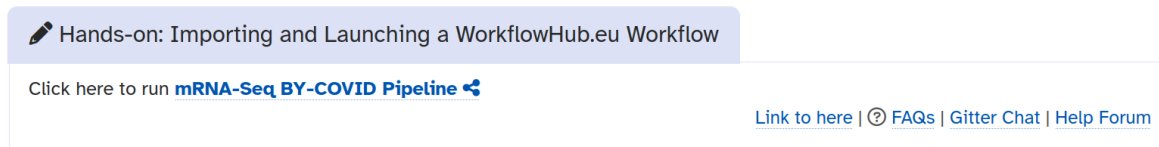
In some tutorials you aren't as interested in teaching users the individual steps for analysing data, but rather want to focus on some downstream aspects of analysis, or to showcase the best practice workflows that are already available for a user to use! In those cases it can be useful to have a nicer way of inviting the user to execute those steps.

WorkflowHub

You can use a dedicated snippet to invite users to run a WorkflowHub workflow:

```
{% snippet faqs/galaxy/workflows_run_wfh.md title="mRNA-Seq BY-COVID Pipeline" wfhub_id="685" %}
```

Rendered:



Hands-on: Importing and Launching a WorkflowHub.eu Workflow

Click here to run [mRNA-Seq BY-COVID Pipeline](#)

[Link to here](#) | [FAQs](#) | [Gitter Chat](#) | [Help Forum](#)

Note that it links to a specific workflow, on any Galaxy server. When this tutorial is opened from within the Tutorial Mode, that link will change to one on the current server, removing the intermediate step.

Figure 3: Galaxy Training Network [guide for embedding WorkflowHub](#) execution snippets in tutorials.



In addition, an [ESG Workflow Collection](#) has been created - the purpose of this is to also aggregate pre-existing and third-party workflows which have been helped or further developed by ESG, such as in the Galaxy Training Network ([GTN](#)) and Intergalactic Workflow Commission ([IWC](#)), both which are community-led initiatives with participants outside ESG.

Registered workflows

As of 2024-02-28, the WorkflowHub ESG collection contains the workflows shown in Table 1:

Title	Creators	License
Gravitational Wave source Cone Search (CWL)	Volodymyr Savchenko	Creative Commons Attribution 4.0
Example Multi-Wavelength Light-Curve Analysis (Galaxy)	Volodymyr Savchenko	Creative Commons Attribution 4.0
Refining Genome Annotations with Apollo (prokaryotes) (Galaxy)	Anthony Bretaudeau	Creative Commons Attribution 4.0
Visualizing NDVI time-series data with HoloViz (Galaxy)	Marie Jossé	Creative Commons Attribution 4.0
Calculating and visualizing OBIS marine biodiversity indicators (Galaxy)	Marie Josse	Creative Commons Attribution Share-Alike 4.0
Finding the Muon Stopping Site using PyMuonSuite (Galaxy)	Leandro Liborio , Muon Spectroscopy Computational Project	MIT License



Sentinel 5P volcanic data visualization (Galaxy)	Marie Jossé	Creative Commons Attribution 4.0
Functional protein annotation using EggNOG-mapper and InterProScan (Galaxy)	Anthony Bretaudeau	Apache Software License 2.0
Genome annotation with Funannotate (Galaxy)	Anthony Bretaudeau	Apache Software License 2.0
Masking repeats with RepeatMasker (Galaxy)	Anthony Bretaudeau	Apache Software License 2.0

Table 1: Workflows registered in <https://workflowhub.eu/collections/13>

As the [ESG use cases](#) are maturing, further workflows will be registered during the second phase of the project.

Additional [Galaxy Training Network](#) (GTN) workflows are being considered for WorkflowHub registration, however as some of these workflows are building blocks meant to be completed according to a particular tutorial, these will be better suited for a separate collection, as they may not be directly suitable for scientific use.

In contrast, the Intergalactic Workflow Commission ([IWC](#)) has developed mature, production-grade workflows for Galaxy. The separate [IWC team](#) in WorkflowHub has registered 47 workflows as of 2024-02-28. These are automatically registered by the WorkflowHub Bot, which scans the [IWC GitHub repositories](#) and registers the workflows according to their RO-Crate metadata. As many of these also have defined tests, WorkflowHub is able to show their test status via the [LifeMonitor](#) service, picked up from the [test definition](#) in their RO-Crate (Figure 4).



The screenshot shows a workflow page on WorkflowHub. At the top, the workflow name is 'baredsc/baredSC-1d-logNorm v0.2 (latest)'. Below the name are three tabs: 'Overview' (selected), 'Files', and 'Related items'. Under the 'Overview' tab, it says 'Workflow Type: Galaxy'. There is a 'Tests Passing' badge with a green checkmark. Below that, a description reads: 'Run baredSC in 1 dimension in logNorm for 1 to N gaussians and combine models.' At the bottom, the SEEK ID is provided as a link: 'https://workflowhub.eu/workflows/615?version=2'.

Figure 4: Workflow <https://workflowhub.eu/workflows/615?version=2> indicates **Tests Passing** and links to the [LifeMonitor test results](#).

References

[Rasche 2023] Helena Rasche (2023):

Tutorial Feature: Easier launching of WorkflowHub & Dockstore Workflows

Galaxy Training Network

<https://training.galaxyproject.org/training-material/news/2023/12/12/tutorial-run-wfh-ds.html>

[Schaaf 2023] Sebastian Schaaf (2023):

"Run on Galaxy" button in WorkflowHub.

Galaxy Community Hub

<https://galaxyproject.org/news/2023-11-13-run-in-galaxy-button-workflowhub/>

[Soiland-Reyes 2022] Stian Soiland-Reyes, Peter Sefton, Leyla Jael Castro, Frederik Coppens, Daniel Garijo, Simone Leo, Marc Portier, Paul Groth (2022):

Creating lightweight FAIR Digital Objects with RO-Crate.

Research Ideas and Outcomes **8**:e93937

<https://doi.org/10.3897/rio.8.e93937>

[Soiland-Reyes 2024] Stian Soiland-Reyes, Carole Goble, Finn Bacall (2024):

EuroScienceGateway Guide to using WorkflowHub. Version 2.

WorkflowHub

<https://doi.org/10.48546/workflowhub.sop.8.2>



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