

Carole Goble University of Manchester, UK / ELIXIR-UK Johan Gustafsson Australian BioCommons, University of Melbourne, Australia

WCI Webinar, 16 July 2025

Where can I find workflows?

Platforms / community repositories

Galaxy PROJECT

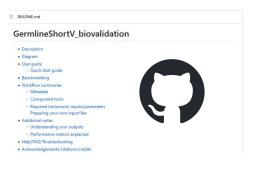
IWC -Intergalactic Workflow Commission



A global community effort to collect a curated set of open-source analysis pipelines built using Nextflow.



GitHub



Search engines

Publications

Murigneux, V., Roberts, L.W., Forde, B.M. *et al.* MicroPIPE: validating an end-to-end workflow for high-quality complete bacterial genome construction. *BMC Genomics* 22, 474 (2021). https://doi.org/10.1186/s12864-021-07767-z

Lott, M. J., Wright, B. R., Neaves, L. E., Frankham, G. J., Dennison, S., Eldridge, M. D. B., Potter, S., Alquezar-Planas, D. E., Hogg, C. J., Belov, K., & Johnson, R. N. (2022). Future-proofing the koala: Synergising genomic and environmental data for effective species management. Molecular Ecology, 31, 3035–3055. https://doi.org/10.1111/mec.16446

Data Repositories



Overcome a distributed, fragmented and variable world...

Use a registry



http://workflowhub.eu http://workflowhub.org

Central Integrated Searchable Standardised Citable Interoperable Rich metadata

WorkflowHub: a registry for computational workflows

Gustafsson, O.J.R., Wilkinson, S.R., Bacall, F. *et al.* WorkflowHub: a registry for computational workflows. *Sci Data* 12, 837 (2025). <u>https://doi.org/10.1038/s41597-025-04786-3</u>

scientific data

Check for updates

OPEN WorkflowHub: a registry for ARTICLE computational workflows

Ove Johan Ragnar Gustafsson¹, Sean R. Wilkinson¹², Finn Bacall³, Stian Soiland-Reyes^{3,4}, Simone Leo⁵, Luca Pireddu⁵, Stuart Owen³, Nick Juty³, José M. Fernández^{6,7}, Tom Brown⁸, Hervé Ménager^{9,10}, Björn Grüning¹¹, Salvador Capella-Gutierrez^{6,7}, Frederik Coppens¹² & Carole Goble³ ³

The rising popularity of computational workflows is driven by the need for repetitive and scalable data processing, sharing of processing know-how, and transparent methods. As both combined records of analysis and descriptions of processing steps, workflows should be reproducible, reusable, adaptable, and available. Workflow sharing presents opportunities to reduce unnecessary reinvention, promote reuse, increase access to best practice analyses for non-experts, and increase productivity. In reality, workflows are scattered and difficult to find, in part due to the diversity of available workflow engines and ecosystems, and because workflow sharing is not yet part of research practice. WorkflowHub provides a unified registry for all computational workflows that links to community repositories, and supports both the workflow lifecycle and making workflows findable, accessible, interoperable, and reusable (FAIR). By interoperating with diverse platforms, services, and external registries, WorkflowHub adds value by supporting workflow sharing, explicitly assigning credit, enhancing FAIRness, and promoting workflows as scholarly artefacts. The registry has a global reach, with hundreds of research organisations involved, and more than 800 workflows registered.

A first step for making workflows FAIR

Wilkinson, S.R., Aloqalaa, M., Belhajjame, K. et al. Applying the FAIR Principles to computational workflows. Sci Data 12, 328 (2025). <u>https://doi.org/10.1038/s41597-025-04451-9</u>

scientific data

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<u>nature</u> > <u>scientific data</u> > <u>comment</u> > article

Comment Open access Published: 24 February 2025
Applying the FAIR Principles to computational
workflows

Sean R. Wilkinson ☑, Meznah Alogalaa, Khalid Belhajjame, Michael R. Crusoe, Bruno de Paula Kinoshita, Luiz Gadelha, Daniel Garijo, Ove Johan Ragnar Gustafsson, Nick Juty, Sehrish Kanwal, Farah Zaib Khan, Johannes Köster, Karsten Peters-von Gehlen, Line Pouchard, Randy K. Rannow, Stian Soiland-Reyes, Nicola Soranzo, Shoaib Sufi, Ziheng Sun, Baiba Vilne, Merridee A. Wouters, Denis Yuen & Carole Goble

Scientific Data 12, Article number: 328 (2025) Cite this article

8290 Accesses | 5 Citations | 22 Altmetric | Metrics

Recent trends within computational and data sciences show an increasing recognition and adoption of computational workflows as tools for productivity and reproducibility that also democratize access to platforms and processing know-how. As digital objects to be shared, discovered, and reused, computational workflows benefit from the FAIR

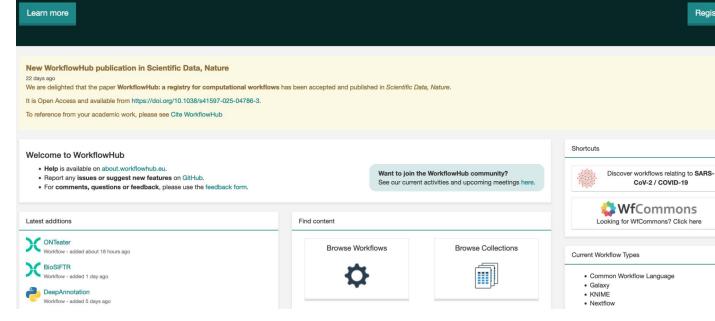
WorkflowHub

Search here ...

A registry for describing, sharing and publishing scientific computational workflows

WorkflowHub aims to facilitate discovery and re-use of workflows in an accessible and interoperable way. This is achieved through extensive use of open standards and tools, including CWL, RO-Crate, Bioschemas and GA4GH's TRS API, in accordance with the FAIR principles.

WorkflowHub supports workflows of any type in its native repository.



1,337 Workflows

26 System types

1,117 Users 355 Teams

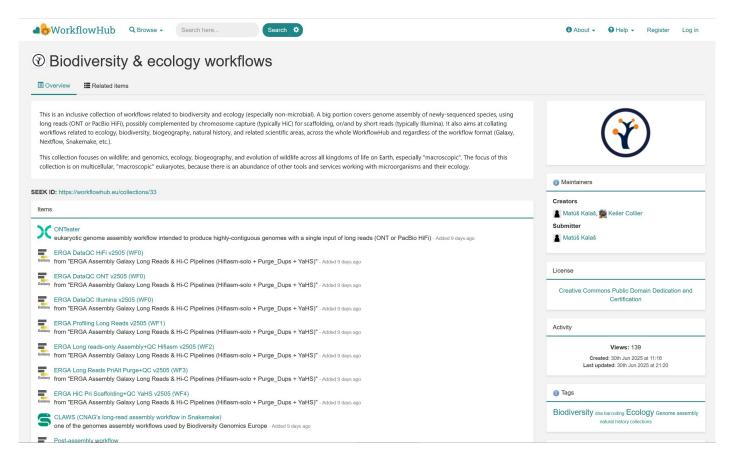
Register

33 Collections

3.669.916 Views

728,597 Downloads

Any discipline, any language, any maturity

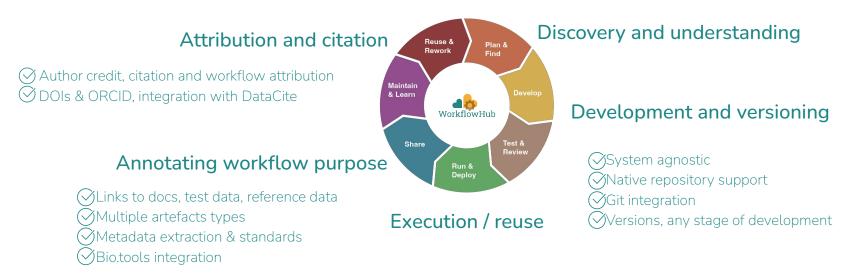


WorkflowHub acts as a Hub for workflows

How?

Supporting the workflow life cycle

Ease of access Welcoming all workflows



Using global and community standards

EDAM

Common metadata about the

workflow, tools & parameters

https://bioschemas.org/ https://edamontology.org/

https://citation-file-format.github.io/

CITATION.cff

Bioschemas

Standardised machine processable metadata For reproducibility, metadata matters!

EDAM Reuse & Plan & Rework Find Maintain & Learn GA4GH-APIS Bioschemas WorkflowHub Test & Share Review Run & ^rAlRsignposting Deploy CWL COMMON

Workflow Run {ﷺ RO-Crate

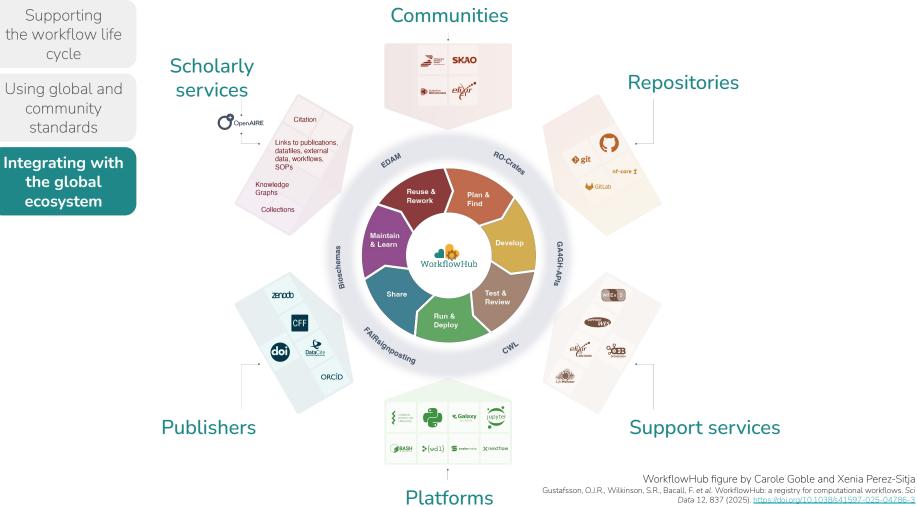
FAIR Digital Object format packaging workflows, metadata, companion data objects, logs

https://www.researchobject.org/ro-crate/ https://github.com/ResearchObject/workflow-run-crate



Common workflow description independent of platform <u>https://www.commonwl.org</u> Abstract CWL

WorkflowHub figure by Carole Goble and Xenia Perez-Sitja Gustafsson, O.J.R., Wilkinson, S.R., Bacall, F. et al. WorkflowHub: a registry for computational workflows. *Sci Data* 12, 837 (2025). https://doi.org/10.1038/s41597-025-04786-3



Data 12, 837 (2025). https://doi.org/10.1038/s41597-025-04786-3

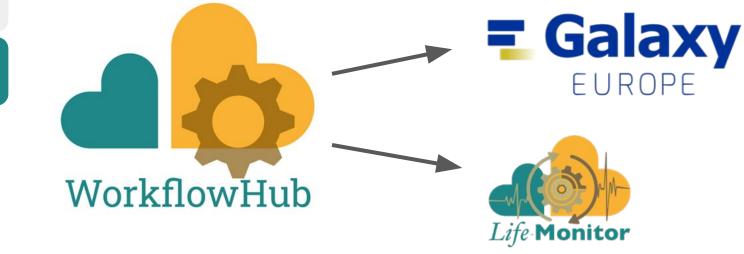
Ecosystem execution & monitoring

Using global and community standards

Supporting

the workflow life cycle

Integrating with the global ecosystem



TRS API



Collaborate. Innovate. Accelerate.



"Webby" FAIR Digital Object format

Using global and community standards

Integrating with the global ecosystem

Scholarly publication

A) *n* CIENCE Sector Consistent with its immense significance. The software should be cited in the references and include the version (if unknown the date of access should be used) and identifier (a persistent identifier like a DOI or a URL to where the software exists). Computational workflows should also be registered in workflowhub.eu and the DOIs cited in the relevant places in the manuscript. If an article exists that describes the software, it should be cited as an additional reference, as well as citing the software itself.

Knowledge Graph



Scrape



Use WorkflowHub's API to download the archive of RO-

Crates. Store them



snakemake

Check RO Crates

Ensure the downloaded ROcrates pass basic sanity checks



Read the JSON-LD from each RO-Create and merge into a single RDF graph

Combine RO-Crates

Merge



Query the graph and use the results to call out to external services. Insert the acquired data into the graph

Perform enrichment

Enrich

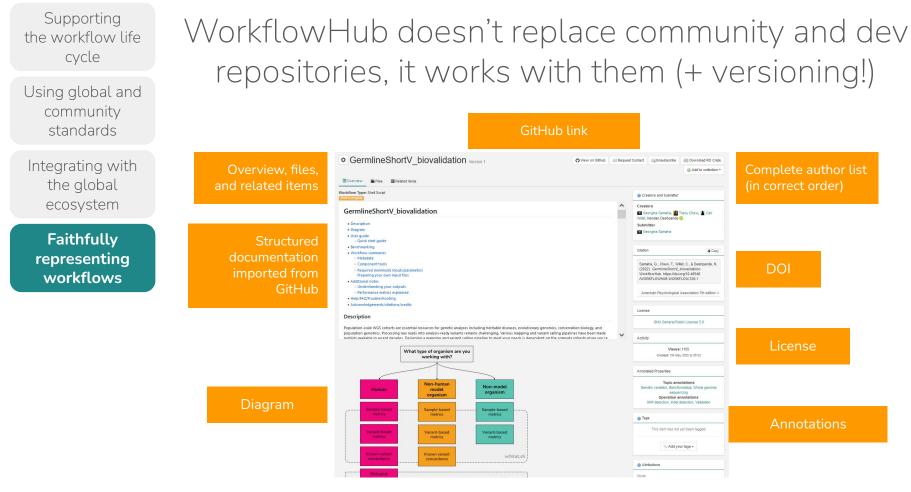


Publish

Share

Publish the finished graph to Zenodo





Samaha, G., Chew, T., Willet, C., & Deshpande, N. (2022). GermlineShortV_biovalidation. WorkflowHub. https://doi.org/10.48546/WORKFLOWHUB.WORKFLOW.339.1

Using global and community standards

Integrating with the global ecosystem

> Faithfully representing workflows

Streamlined processes

1. Register yourself on WorkflowHub

Username Username The username should contain a minimum of 3 characters. Email address Email address Password Password Password should contain a minimum of 10 characters. Confirm Password Password □ I have read and agree to the Terms and Conditions and the Data Policy Alternatively... • Log in using LS Login Already registered? - goto Login elixir LOGIN

Register

Register an account for WorkflowHub

Log in using GitHub ()

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Faithfully representing workflows

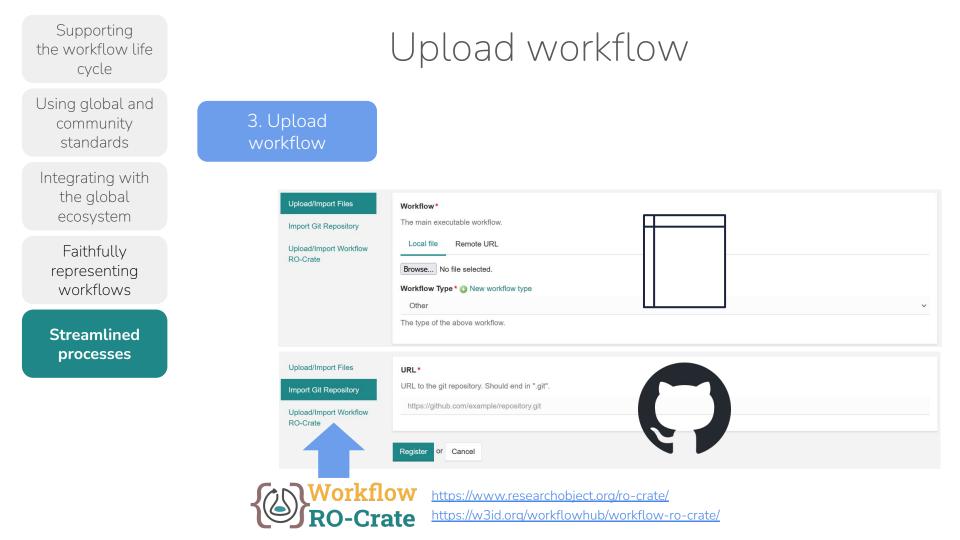
Streamlined processes

Create a team, or join an existing team

	() Space	Space
	Select the Space you wish to associate the new Team with, out of the following list that you administer.	
	Australian BioCommons	v
	Alternatively you can choose to create a new Space, which your new Team will be associated with.	
	□ Create a new Space?	
	Team	—
	Please provide some basic details about the Team that will be created. You will be able to update and add additional informa Title *	Team
	Description	
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oin an	age	
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2. Create a team, or

existing team



Supporting the workflow life cycle	Complete metadata				
Using global and community standards	3. Upload4. Completeworkflowmetadata				
Integrating with the global ecosystem	New Workflow Westflow Type * 0 Mere water Galaxy Time*	Add license (auto if license in GitHub)			
Faithfully representing workflows	Pedde Hifl genome assembly visual httaan v2.1 Description B I H H H H H H H H H H H H H H H H H H	Acade Software Lones 20 For more information on this Lones, please well Map. Rightmensures origitionses/Acadre-20			
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	Select a team.	•			

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> Faithfully representing workflows

Streamlined processes

Add context: SOPs, data, tools, workflows

	mplete adata	5. ,	Add context	
Attributions			Documents 🔺	
f this Workflow is based on any existing Workflows, please list them below So far you have specified the following attributions: No attributions	Other workflows		The following Documents are associated with this workflow:	Documents
Please type titles of Workflows into the box below - suggestions will be display Search		Wé	Select Document	
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Select Publication				
Associate Publications from other projects?			Associate Data files	
Presentations A	Durantation		() Tools 🔺	T
he following Presentations are associated with this workflow:	Presentations		The following Tools are associated with this Workflow:	Tools
No presentations			No Tools	
Select Presentation			SAssociate	bio.tools

Using global and community standards

Integrating with the global ecosystem

> Faithfully representing workflows

Streamlined processes

Review entry

							6. Review entry
Workflo	ow was successfully uploade	d and saved.					
	Version 1		ssembly using hifiasm	0	View on GitHub	Subscribe 🛛 🖗	⊚ Download RO Crate
	w Type: Galaxy bly, visualisation and qualit	y control workflow for	high fidelity reads built from circular consensus sequen	ice (PacBio HiFi) data	6		O Creators and Submitter Creators Gareth Price, Katherine Farquharson (D)
EEK ID: I	https://dev.workflowhub.eu/w	vorkflows/584?version=	1				Submitter
ID	Name	Description				Туре	Citation
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Step	S						Your Workflow is published and eligible for a DOI.
ID Na	ame		Description				👶 Generate a DOI
1 Hi	iFi Adapter Filter		toolshed.g2.bx.psu.edu/repos/galaxy-australia/hifiadapter	filt/hifiadapterfilt/2.0.0	+galaxy0		
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3 Haplotype resolved Bandage info toolshed.g2.bx.psu.edu/repos/iuc/bandage/bandage_info/0.8.1+galaxy1					License		
4 Ha	aplotype resolved Bandage in	age	toolshed.g2.bx.psu.edu/repos/iuc/bandage/bandage_imag	/e/0.8.1+galaxy3			Apache Software License 2.0

Using global and community standards

Integrating with the global ecosystem

Faithfully representing workflows

Streamlined processes

Fit-for-purpose data model

A data model that reflects the real-world collaborations that create workflows



Using global and community standards

Integrating with the global ecosystem

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> Streamlined processes

Fit-for-purpose data model

A data model that reflects the real-world collaborations that create workflows

	Australian BioCommons
	🚧 🚺 Australian BioCommons
	- 🗾 QCIF Bioinformatics
Space	MicroPIPE: validating an end-to-end workflow for high-quality complete bacterial genome construction.
	- 🔽 16S Microbial Analysis with mother - howto
🚨 Australian BioCommons	microPIPE: a pipeline for high-quality bacterial genome construction using ONT and Illumina sequencing
Overview Related items	16S_biodiversity_for_overlap_paired_end
The Australian BioCommons enhances digital life science research through world class collaborative -	16S_biodiversity_for_nonoverlap_paired_end
remains globally competitive, through sustained strategic leadership, research community engageme	scRNAseq Single Sample Processing STARSolo
Web page: https://www.biocommons.org.au/ Funding details:	
Core funding for the Australian BioCommons comes from the National Collaborative Research Infrastr University of Melbourne as the lead agent. This core funding is amplified through coinvestment from B	
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QCIF Bioinformatics	Workflow 1: Further Quality Control [16S Microbial Analysis With Mothur]
Gen Bioinformatios	Workflow 2: Data Cleaning And Chimera Removal [16S Microbial Analysis With Mothur]
Overview Related items	Workflow 3: Classification [Galaxy Training: 16S Microbial Analysis With Mothur]
Related items	Workflow 5: OTU Clustering [16S Microbial Analysis With Mothur]
	Workflow 6: Alpha Diversity [16S Microbial Analysis With Mothur]
People (5) Spaces (1) Organizations (1) Publications (1)	Workflow 7 : Beta Diversity [16S Microbial Analysis With Mothur]
	Taxonomy classification using Kraken2 and Bracken
	ONTVISC (ONT-based Viral Screening for Biosecurity)
	- 🗐 scRNAseq processing in galaxy
	🔄 🏢 16S Microbial Analysis with mothur (on Galaxy Australia)

Using global and community standards

Integrating with the global ecosystem

> Faithfully representing workflows

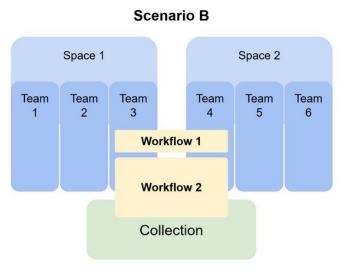
Streamlined processes

Fit-for-purpose data model

Note: these structures are flexible

Scenario A Space 1 Space 2 Team Team Team Team Team Team 2 3 4 5 6 1 Workflow 1 Workflow 2 Collection

- 3 *Teams* from space one, and 3 *Teams* from space two have created a *workflow* each
- These are both part of the same collection
- Spaces are not sharing a workflow, but do contribute to the same Collection



- Team #3 from space one, and team #4 from space two have collaborated to create 2x workflows
- Workflow 2 is contributed to a collection
- Spaces are sharing workflows via their component Teams, but do not directly share the workflows

Using global and community standards

Integrating with the global ecosystem

Faithfully representing workflows

Streamlined processes

Fit-for-purpose data model

User support

Wizards and streamlined processes

Select the Space you with to associate the new Taxa with, and of the following Anartishe BioCommon Anartishe Space motions to breats new Space, which your new Taxa with Cl Create a new Space? Taxa Passe provide some basic details about the Taxa that will be created. You with Table Description	legiter an account for WondhowHub sercame Username Username Username Username about contain a minimum of 3 characters. Imail address Seasord Passeord add contain a minimum of 10 characters. Seasord Contain Assessed Passeord Pas	Upload/Import Files Import Git Repository Upload/Import Workflow RO-Crate	Workflow* The main executable workflow. Local file Remote URL Browse No file selected. Workflow Type* New workflow type Other The type of the above workflow.	New Workflow type Data Tate Pactor kiff percent assertidy using Milliam V2.1 Description B / H is 4 = 1 is is is in a control workflow for high fidely reads built from circular consensus sequence (Pactio MFI) data. Assertidy, visualization and quality control workflow for high fidely reads built from circular consensus sequence (Pactio MFI) data.
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Using global and community standards

Integrating with the global ecosystem

> Faithfully representing workflows

> Streamlined processes

Fit-for-purpose data model

User support

User engagement, and training

WorkflowHub Club

WorkflowHub Club coordination call

This is the rolling minutes from the <u>WorkSouthub</u> takons. Feel free to join the <u>mailing bir</u>, suggest changes to the agends or to help softles the minutes of the call! Regular schedule is every other <u>Workssay</u> 10:00 uncert LUK time zone / 11:00 uncert European Time zone. When the clack scheme we will adds to the 10:00/11:00 resurtless. So winter it's WORK/CFF and unmmer it's WORK/CFF.



https://s.apache.org/workflowhub __minutes

Webinars / Workshops

Tools Platform and Single Cell Omics "bring your workflow" to WorkflowHub

🏥 Tue 13 May 2025 - 9:30 to 11:00 BST

We are exclude to induce you to an online event focused on exaling comparison latent works the practices with the use of Workflowk. All we will make use of energines workflows for the Single Cali Omics commently to present and epidere corcepts and fractisms that are to maily applicable to computational workflows.

Event Highlights:

Gain insights from experts on the importance of FAIR principles in computational workflows and how they can enhance reproducibility, collaboration, and findability.

Watch a live demonstration of workflow registration in WorkflowHub. Using computational workflows for handling and processing Single Cell data as examples, you will see how workflows can be easily registered, discovered, and shared within the scientific community.

51

Participate in an interactive session where you can bring your own workflows and learn how to register and manage them in WorkflowHub.

Programme:

Welcome and Introduction
 Make your computational workflows findable and citable
 Discussion and questions

Gustafsson, O. J. R. (2025, June 4). Make your computational workflows findable and citable: WorkflowHub BYOW workshop. Zenodo. https://doi.org/10.5281/zenodo.15588745

FAIR workflows (WCI)

FAIR Computational Workflows WORKING COOLIPS - CAR COMPLITATIONAL WORKELOW The FAIR principles have laid a foundation for sharing and publishing digital assets and, in particular, data The FAIR principles emphasize machine accessibility and that all digital assets should be Findable, Arcessible Intermerable and Beusable Workflows encode the methods by which the scientific noncess 😫 15 members is conducted and via which data are created. It is thus important that workflows both support the creation O Active of FAIR data and themselves adhere to the FAIR minciples Subsections Members Bast martines for FAIR workflows Carola Goble Training material for EAID undefine Carola Cocca · Repositories, standards, projects for FAIR workflows Sean R. Wilkinson Events related to EAID workflow Michael R. Crusce Rosa Figueira Bibliography and references about FAIR workflows Luiz Gadelha Daniel Garijo Sandra Gesing Goals Johan Gustalss Bruno de Paula Kinos Farah Zaib Khan The working group is seeking workflow developers and users to directly inform the standards, p Karsten Peters-von Gehler and recommendations that make computational workflows FAIR. Randy K Rannow In this working group, we aim to Ziheng Sun Define FAIR principles for computational workflows that consider the complex lifecycle from specification to execution and data product Define metrics to measure the FAIBness of a workflow · Define recommendations for FAIR workflow developers and system

· Define processes to automate FAIRness in workflows by recording necessary provenance data

Wilkinson, S.R., Aloqalaa, M., Belhajjame, K. et al. Applying the FAIR Principles to computational workflows. Sci Data 12, 328 (2025). <u>https://doi.org/10.1038/s41597-025-0</u> <u>4451-9</u>



https://workflowhub.eu/projects/12



EUROPEAN REFERENCE GENOME ATLAS https://workflowhub.eu/programmes/33

nf-core 宜

A global community effort to collect a curated set of open-source analysis pipelines built using Nextflow. https://workflowhub.eu/projects/15















Cite workflows in methods section of genome reports/papers, credit workflow developers

GENOME REPORT

ERGA-BGE Reference Genome of the Striped Field Mouse (*Apodemus agrarius*), a Widespread and Abundant Species in Central and Eastern Europe

Franc Janžekovič^{1,}, Elena Buzan^{2,3}, Aja Bončina³, Nuria Escudero⁴, Rosa Fernández⁴, Astrid Böhne⁵, Rita Monteiro⁵, Laura Aguilera^{6,7}, Marta Gut^{6,7}, Francisco Câmara Ferreira^{6,7}, Fernando Cruz^{6,7}, Jèssica Gómez-Garrido^{6,7}, Tyler S. Alioto^{6,7}, Leanne Haggerty⁸, Fergal Martin⁸, Diego De Panis^{9,10*}

The genome was assembled using the CNAG CLAWS pipeline (Gomez-Garrido, 2024). Briefly, reads were preprocessed for quality and length using Trim Galore v0.6.7 and Filtlong v0.2.1, and initial contigs were assembled using NextDenovo v2.5.0, followed by polishing of

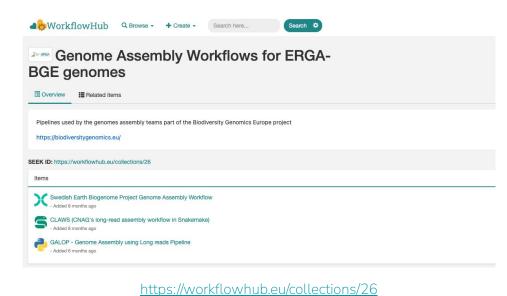
Summary analysis of the released assembly was performed using the ERGA-BGE Genome Report ASM Galaxy workflow (De Panis, 2024b), incorporating tools such as BUSCO v5.5, Merqury v1.3, and others (see reference for the full list of tools).

De Panis, D. (2024a). ERGA-BGE Genome Report ANNOT analyses. WorkflowHub.

https://doi.org/10.48546/WORKFLOWHUB.WORKFLOW.1096.1

- De Panis, D. (2024b). ERGA-BGE Genome Report ASM analyses (one-asm WGS Illumina PE + HiC). WorkflowHub. https://doi.org/10.48546/WORKFLOWHUB.WORKFLOW.1103.2
- Gomez-Garrido, J. (2024). CLAWS (CNAG's long-read assembly workflow in Snakemake).

WorkflowHub. https://doi.org/10.48546/WORKFLOWHUB.WORKFLOW.567.2



Slide credit Tom Brown







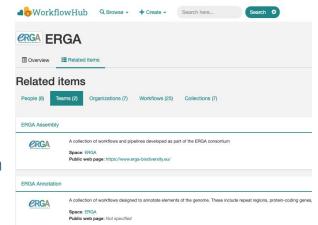
Collect workflows and best practices from the Reference Genome Community of Practice

<image>

WM Language-agnostic pipelines for generation of high-quality genome assemblies and annotations

Collected from and developed with the community of researchers developing and implementing workflows for assembly and annotation of reference genomes

Training and capacity building



ERGA space in WorkflowHub

Slide credit Tom Brown



SEEK ID: https://workflowhub.eu/collections/27

Items
ERGA DataQC HIFI v2409 (WF0)

ERGA DataQC Ilumina v2409 (WF0)

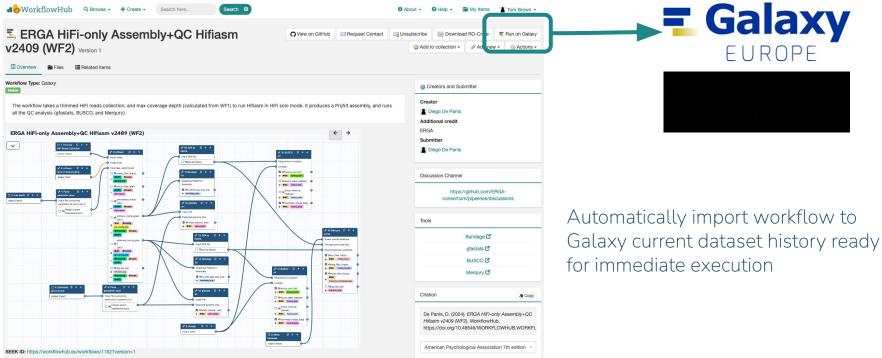
- ERGA Profiling HFI v2409 (WF1)
- Genoxy Added 8 months ago
- ERGA HIFI-only Assembly+QC Hiflasm v2409 (WF2) - Added 8 months ago
- ERGA HIFI PriAlt Purge+QC v2409 (WF3)
- ERGA HIC Pri Scaffolding+QC YaHS v2501 (WF4)







Reuse existing datasets, curated workflows and the Galaxy workflow infrastructure: launch automatically via WorkflowHub, collect metrics



DOI: 10.48546/workflowhub.workflow.1162.1

Slide credit Tom Brown

Some challenges and observations

Registration - getting it! Even for projects funded to do so

Automate from GitHub, nurture community champions, BYOW sessions

Metadata - getting it!

Automate from GitHub practices, partnerships with WfMS developers

Range of Workflow forms

From HPC where the machine matters, simulations where the run set up matters, to R and Python scripts

Registry / Repository

A record of active software held elsewhere vs file and forget archive

Bot Battering

Open comes with a down side - AI bot attacks

Some plans and prospects



Sustainability

Service for National and International Infrastructures: European (ELIXIR, Eurobioimaging..), European Open Science Cloud, Australian BioCommons...

Integrations and Discipline widening

Crosswalks with other registries (Lifewatch, MethodsHub, DockStore...)

More added-value features using the power of AI

Full fat FAIR workflow support, metadata acquisition and curation, workflow similarity tracking ... Smoothing support

Embedded into Journal, Funder and Policy maker FAIR practice

FAIR Workflow management planning

Community champions network

Some Acknowledgements

The University of Manchester, UK





Bacall





Frederik Coppens VIB, Belgium





Sean Wilkinson Oak Ridge National Labs, USA

Biodiversity Genomics

2RGP

Europe





Nick

Juty

Simone Leo CR4S. Sardinia



Stian Soiland-Reves

Fli Chadwick

PROJECT

Björn Grüning, Freiburg University, Germanv

= Galaxy





Phil Ewels, Segera

Tim Booth, U of Edinburgh, UK



COMMON WORKELOW LANGUAGE



Tom Brown. Leibniz Institute for Zoo and Wildlife Research. Berlin. Germany

Michael Crusoe, CWL



Alan Williams

The University of Manchester, UK



Some Acknowledgements

https://workflowhub.org

