

FAIR Workflows and WorkflowHub

Policy for Findable, Accessible, Interoperable,
Reusable Workflows

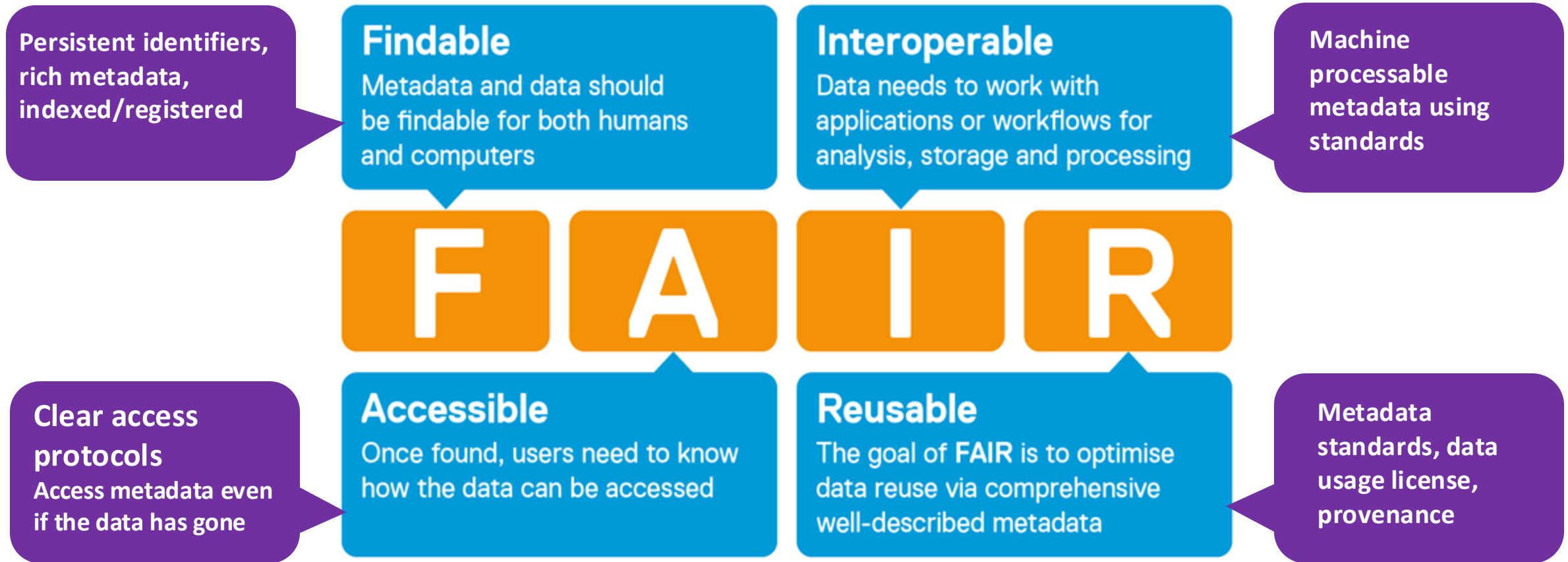
Professor Carole Goble
The University of Manchester, UK
ELIXIR UK

FAIR Principles

Objects discoverable, reusable using standards

Guidelines to set expectations between creators, providers and users

What



How

Why FAIR Computational Workflows?

How can I find already existing workflows?

Can I access them? Public or private? Git repository?

What language is it written in?

Can I rework it to use my tool?

Is it well enough described so I can understand it?

Can I use it? Adapt it?

Can I reuse it in our infrastructure?

Does it make FAIR data?

Can I establish a claim for it when I publish?



Will I get credit?

Can I track that credit?

Why FAIR Computational Workflows?

What workflow systems are used?

What is the impact of a workflow?

What workflows can be reused/exchanged?

Can we reproduce a publication result?

What is the workflow provenance for a result?

Can I build citation graphs for workflows?

What is the DOI for a workflow?



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The FAIR Guiding Principles for scientific data management and stewardship

Workflows are Epistemic Artefacts



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Applying the FAIR Principles to computational workflows

<https://doi.org/10.1038/s41597-025-04451-9>

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Introducing the FAIR Principles for research software

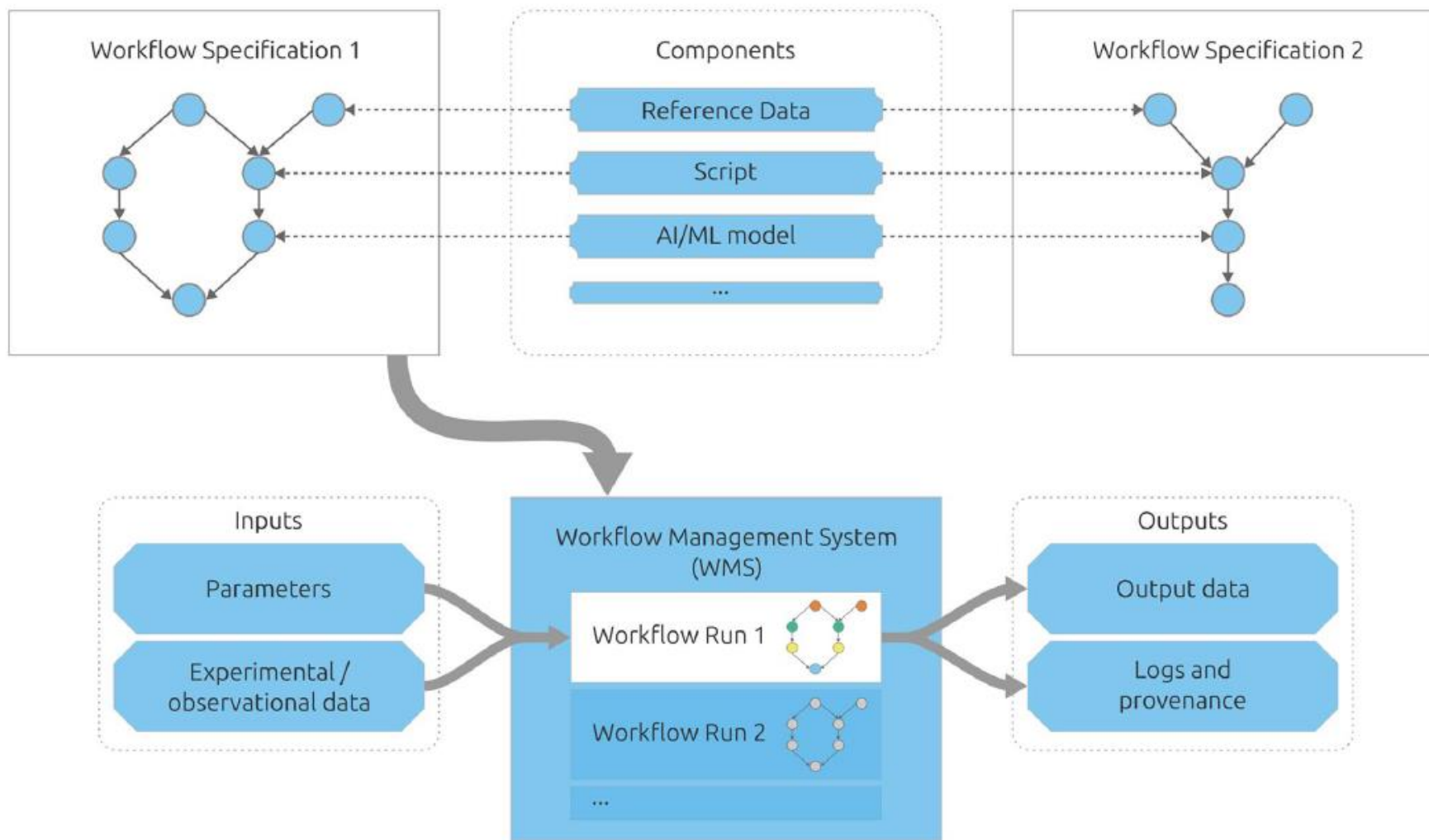
Workflows are Software



Applying the FAIR Principles to computational workflows

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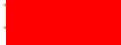

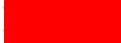



F

A

I

R

Guideline	Based on ¹
F1. A workflow is assigned a globally unique and persistent identifier.	 
F1.1. Components of the workflow representing levels of granularity are assigned distinct identifiers.	
F1.2. Different versions of the workflow are assigned distinct identifiers.	
F2. A workflow and its components are described with rich metadata.	 
F3. Metadata clearly and explicitly include the identifier of the workflow, and workflow versions, that they describe.	 
F4. Metadata and workflow are registered or indexed in a searchable FAIR resource.	 
A1. Workflow and its components are retrievable by their identifiers using a standardized communications protocol.	 
A1.1. The protocol is open, free, and universally implementable.	 
A1.2. The protocol allows for an authentication and authorization procedure, when necessary.	 
A2. Metadata are accessible, even when the workflow is no longer available.	 
I1. Workflow and its metadata (including workflow run provenance) use a formal, accessible, shared, transparent, and broadly applicable language for knowledge representation.	 
I2. Metadata and workflow use vocabularies that follow FAIR principles.	
I3. Workflow is specified in a way that allows its components to read, write, and exchange data (including intermediate data), in a way that meets domain-relevant standards.	 
I4. Workflow and its metadata (including workflow run provenance) include qualified references to other objects and the workflow's components.	 
R1. Workflow is described with a plurality of accurate and relevant attributes.	 
R1.1. Workflow is released with a clear and accessible license.	 
R1.2. Components of the workflow representing levels of granularity are given clear and accessible licenses.	 
R1.3. Workflow is associated with detailed provenance of the workflow and of the products of the workflow.	 
R2. Workflow includes qualified references to other workflows.	 
R3. Workflow meets domain-relevant community standards.	 

WorkflowHub

ERGA HiC Collapsed Scaffolding+QC YaHS v2311 (WF4) Version 1

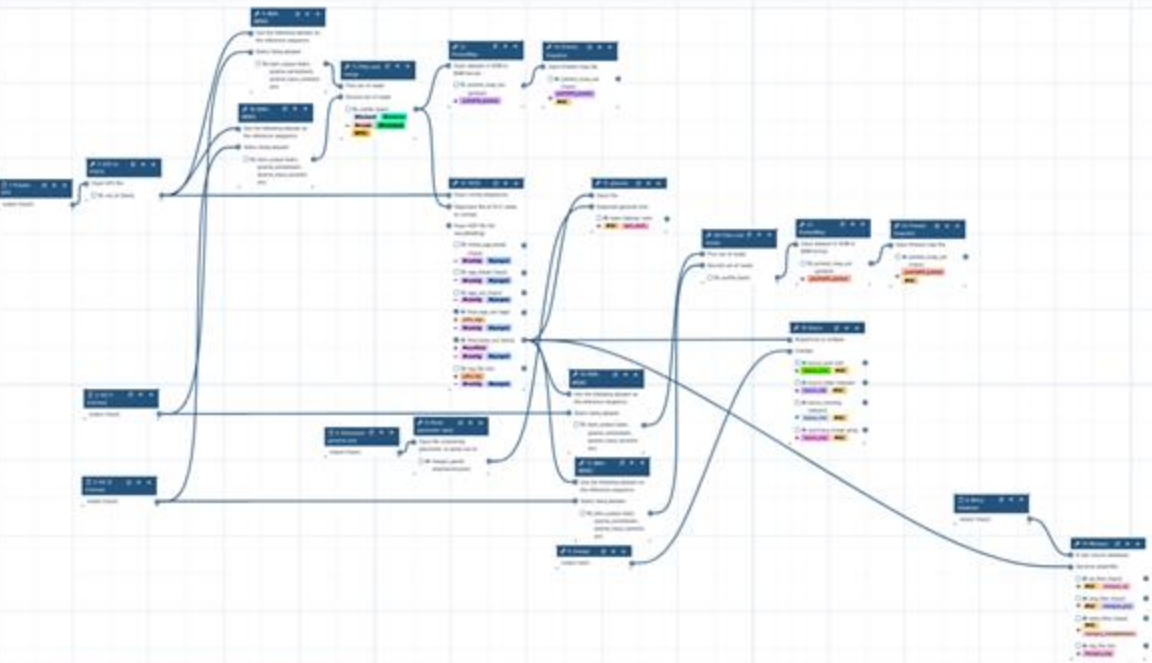
View on GitHub Download RO-Crate Run on Galaxy

Overview Files Related items

Workflow Type: Galaxy

The workflow takes trimmed HiC forward and reverse reads, and one assembly (e.g.: Hap1 or Pri or Collapsed) to produce a scaffolded assembly using YaHS. It also runs all the QC analyses (gfastats, BUSCO, and Merquy).

ERGA HiC Collapsed Scaffolding+QC YaHS v2311 (WF4)



SEEK ID: <https://workflowhub.eu/workflows/702?version=1>

Creators and Submitter

Creator
Diego De Panis

Additional credit
ERGA

Submitter
Diego De Panis

Discussion Channel
<https://github.com/ERGA-consortium/pipelines/discussions>

License
MIT License

Activity
Views: 3633 Downloads: 361 Runs: 1
Created: 9th Jan 2024 at 11:00

Annotated Properties
Topic annotations
Whole genome sequencing
Operation annotations
Genome assembly, Scaffolding

Tags
ERGA HiC native ASSEMBLY+QC



<https://workflowhub.eu>

1200+ Workflows
332 Teams
26 Workflow languages/types

DOI
Versioning
Rich metadata (schema.org)
Git integration
WfMS integration

scientific **data**



OPEN ARTICLE WorkflowHub: a registry for computational workflows

Ove Johan Ragnar Gustafsson¹, Sean R. Wilkinson², 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✉

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.

<https://doi.org/10.1038/s41597-025-04786-3>

FAIR Metadata packaging and exchange



Workflow Run
 RO-Crate

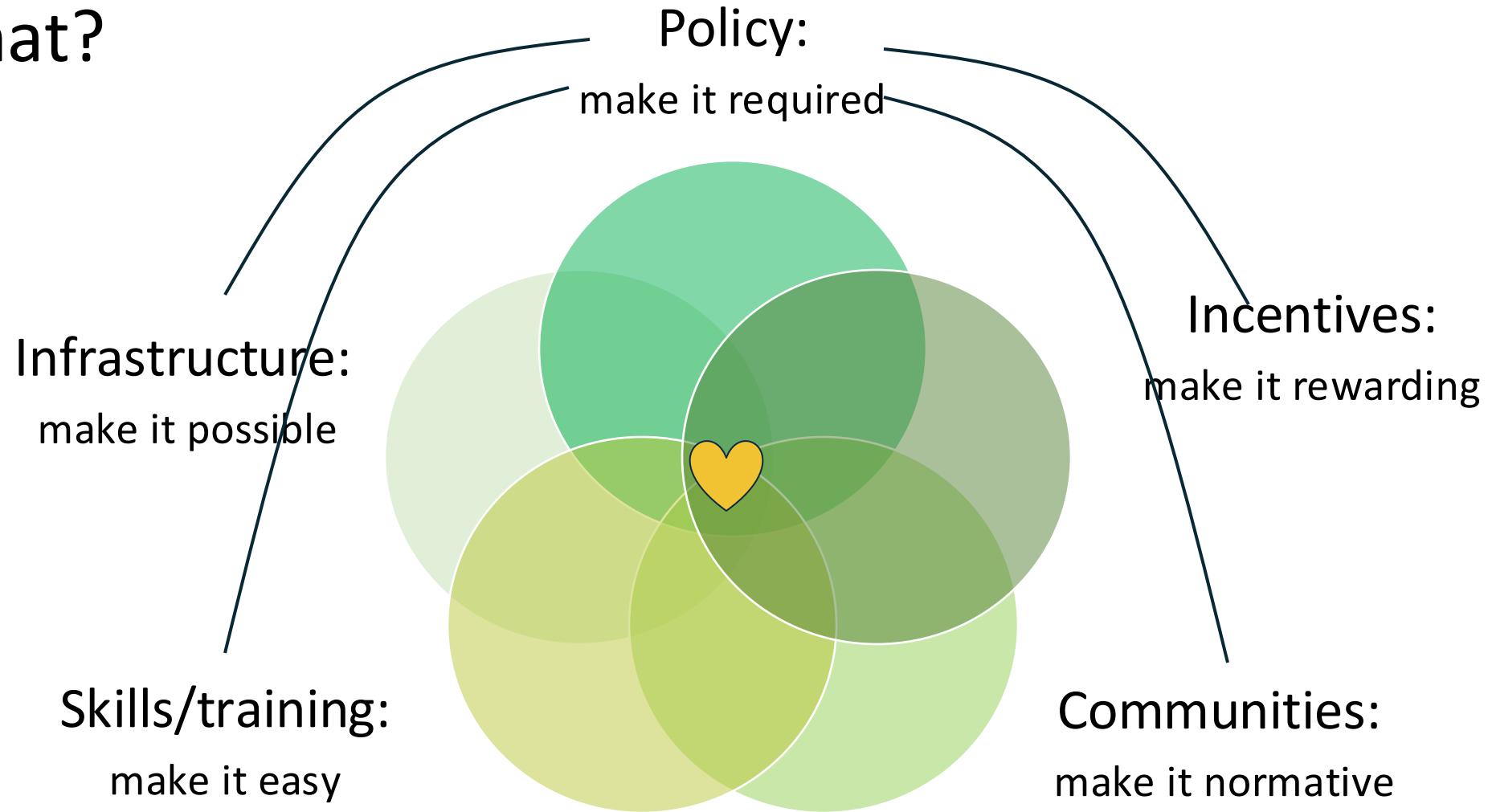
The logo for Workflow Run RO-Crate consists of a smaller version of the RO-Crate icon (a brown curly brace containing a circular arrow and a teal drop) followed by three small, overlapping squares in purple, light blue, and teal. To the right of these elements, the text "Workflow Run" is in a dark blue serif font, and "RO-Crate" is in a teal sans-serif font.

<https://www.researchobject.org/ro-crate/>

<https://www.researchobject.org/workflow-run-crate/>
<https://doi.org/10.1371/journal.pone.0309210>



What?



Who? Interlinked Policy Stakeholders

Policy Forums – OECD, ReSA, RDA, UNESCO, G7, CODATA...

Funders - National, European, Charities...

Publishers - Journals...

Institutions – Universities, National Labs...

Workflow Communities – nf-core, Galaxy, MGnify...

Research Communities/Societies – ELIXIR...

Enablers

Training Community Groups - Carpentries...

Infrastructure Providers – Galaxy, nextflow, WorkflowHub...

FAIR

Policy



Policy



FAIR Impl

Share workflows

Workflow authorship
recognised in career
development

Reuse workflows

Workflow used in
publication is reproducible

Register workflow

PIDs for workflows
and workflow
versions

PID, Metadata &
licensing

PID, Metadata &
provenance

Workflow registry
CodeMeta, schema.org

Workflow registry
Citation.cff

Infrastructure produce
PIDs & metadata export

Infrastructure produce
PIDs, metadata &
history export

Community level guidance and policy ...

Communities make workflow standards and registration:

- Normative
- Possible
- Required

CodeMeta
Citation.cff



Requirements

All nf-core pipelines *must* follow the following guidelines:

- Nextflow: Workflows must be built using Nextflow.
- Community owned: Pipelines are owned by the community.
- Identity and branding: Primary development must on the nf-core organisation.
- Workflow specificity: There should only be a single pipeline per data / analysis type.
- Workflow size: Not too big, not too small.
- Workflow name: Names should be lower case and without punctuation.
- Use the template: All nf-core pipelines must be built using the nf-core template.
- Software license: Pipelines must open source, released with the MIT license.
- Bundled documentation: Pipeline documentation must be hosted on the nf-core website.
- Docker support: Software must be bundled using Docker and versioned.
- Continuous integration testing: Pipelines must run CI tests.
- Semantic versioning: Pipelines must use stable release tags.
- Standardised parameters: Strive to have standardised usage.
- Single command: Pipelines should run in a single command.
- Keywords: Excellent documentation and GitHub repository keywords.

<https://nf-co.re/docs/guidelines/pipelines/overview>

Publishers...



scholarly ecosystem, 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](https://www.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.

IMPERIAL

Search

Scholarly Communication

Imperial Home / Research / Support for staff / Scholarly Communication /
Research data management / Sharing data / Making research software open and shareable

**Making research software
open and shareable**

Why share research software?

Persistent Identifier proliferation
Feed KG and citation engines
Do not disrupt publication process

Career credit
Institutional support

Institutions...

- Normative
- Possible
- Required
- Rewarding

Infrastructure Providers...



*Built in
PID minting, registration, metadata
collection ...*

What about the rest of the ecosystem?

- Easy
- Normative
- Possible
- Required
- Rewarding

Policy Partnerships

Leverage/infiltrate current software and data policy



Research Software Policy Forum <https://www.researchsoft.org/software-policies/>



Committee for Scientific and Technological Policies, Policy Toolkit

Open Research Funders Group



Toolkit

or create our own WCI Policy?

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