

Computational method preservation: workflows and models matter

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ISBE & FAIRDOM

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Computer Engineering and Service Perspective

Astronomy

Digital
Preservation

Helio
Physics

Social
Science

Public Health
Epidemiology

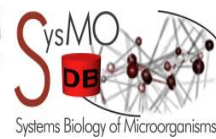
Systems Biology

Synthetic Biology

Pharmacology

Genomics

Biodiversity



Software and data

- Cultural and technical trends in software development are in our favour
 - Better dependency management for software
 - Better testing and integration
 - Better version control
 - More collaborative open development
 - Developers hate the 'it worked on my machine' bugs
- Computational cloud culture
 - Cheaper for research groups
 - Better for collaborative projects
 - Better for scaling to large data sets
 - Requires running code in different environments
 - Local, single machine, multi-machine
- Virtual machines and related technology work
 - Fit researcher workflow
 - Make it easier to develop and debug
 - Must manage dependencies for commercial environments
- Virtual machines let you bring computation to data
 - Data is too big to download
 - Data protection, licensing issues get in the way, too
- How can virtual machines last?
 - Is there a Universal Virtual Machine?
 - Is there a virtual machine designed for the longer term?
 - Can virtual machines be part of the scholarly record?

[Adam Farquhar,
14 March 2016]

Morin et al Shining Light into Black Boxes
Science 13 April 2012: 336(6078) 159-160

Ince et al The case for open computer programs
Nature 482, 2012

The Research community produces software

- 91% scientific software is important for their own research
- 84% developing scientific software is important for their own research
- 53% claimed to spend more time developing scientific software than they did 10 years ago
- 38% spend at least one fifth of their time developing software



USAP/GETTY

Computer systems have been prone to error since the early days.

REPRODUCIBILITY

Journal buoys code-review push

Nature Biotechnology asks peer reviewers to assess accessibility of software used in computation

BY ERIKA CHECK HAYDEN

The finding seemed counterintuitive: warming in North America was driving plant species to lower elevations — not towards higher, cooler climes, as ecologists had long predicted. But the research published in *Global Change Biology* indeed turned out to be wrong. In February, the journal retracted the paper after its intriguing conclusion was found to be the result of errant software code¹.

Worried about a rising tide of results that fail to measure up, journals are starting to take action. In the latest such move, *Nature*

Biotechnology anno to prevent such emb pages (*Nature Biote* peer reviewers will n availability of docum used in computatioi description of the v exploring whether pe plex code using servi of software that allow a shareable represent environment.

Researchers say th needed. They note t

"An article about **computational science** in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the **complete software development environment**, [the complete data] and the complete set of instructions which generated the figures."

David Donoho, "Wavelab and Reproducible Research," 1995

WORLD VIEW A personal take on events



WELLCOME LIBRARY/LONDON

Funders must encourage scientists to share

To realize the full potential of large data sets, researchers must agree on better ways to pass data around, says Martin Bobrow.

How can we make best use of the vast amounts of data on genomics, epidemiology and population-level health being collected by researchers? Maximizing the benefits depends

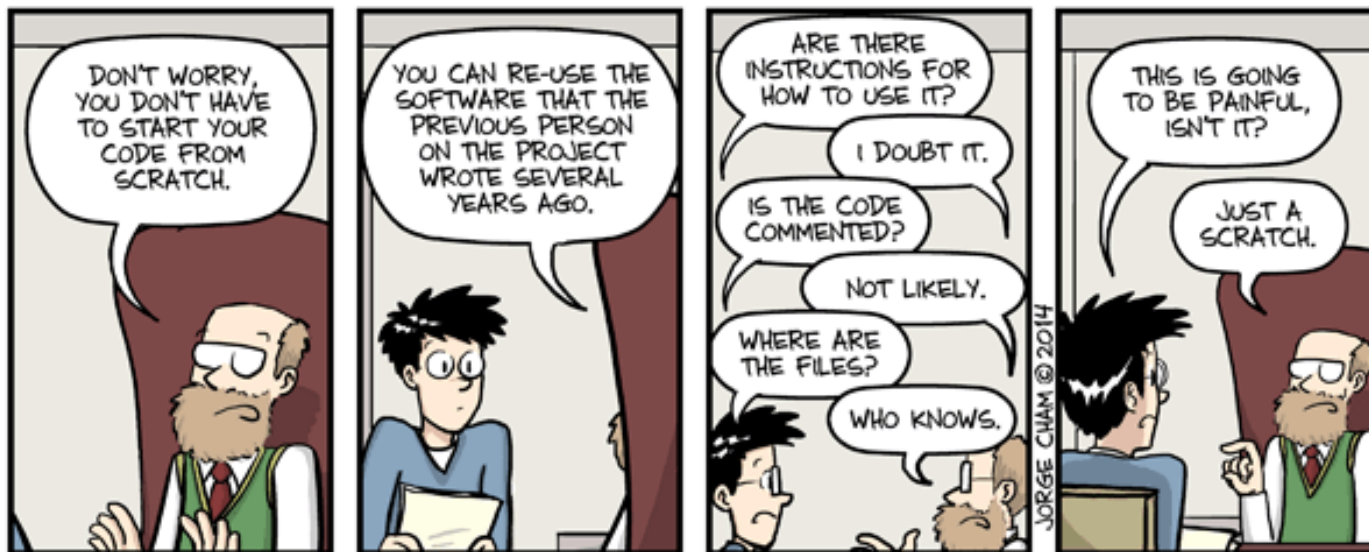
and the undertakings they ask of potential data users, are usually similar across studies. Where possible, funders should encourage the streamlining and standardization of this process, while allowing for the fact

Preservation of Method

method isn't described here b/c this High Impact Report is 200 words. see Supplement Appendix L for vague description
[#overlyhonestmethods](#)

You can download our code from the URL supplied.
Good luck downloading the only postdoc who can get it to run, though [#overlyhonestmethods](#)

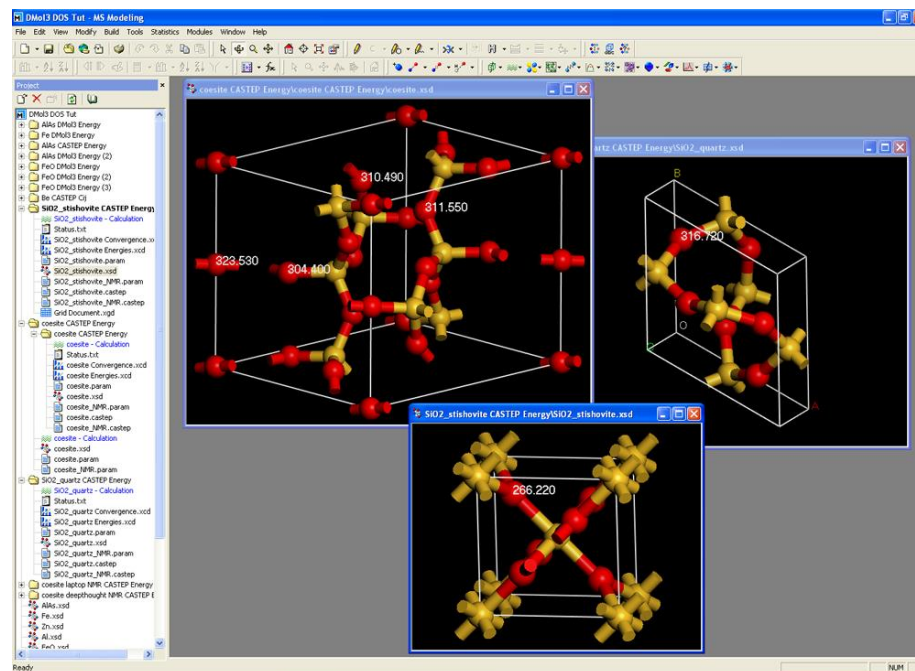
4:52 PM - 8 Jan 2013



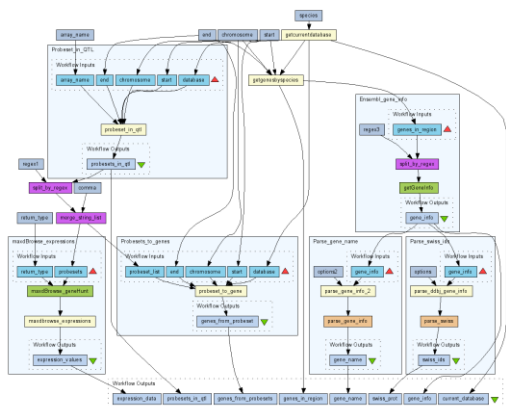
WWW.PHDCOMICS.COM

Transitory

Long Lived
Computational
Chemistry – CASTEP
Since 1990s



Sharing, publishing and preserving pieces of process



<http://www.mygrid.org.uk/tools/taverna/>

computational workflows software

Monitor the formation of an aromatic imine by HMR and CMR in CDCl₃

1. Make up separate 1 mL of 1M solutions of piperonal and 5-methylfurfurylamine in CDCl₃.
2. Take HMRs and CMRs of the aldehyde and amine. Use 5 sec relaxation time and acquire for about 15 mins for the CMR. This should be good enough based on [James' results](#) at 1M in methanol.
3. Combine the two solutions into a 1 dram vial and shake vigorously then transfer to an NMR tube.
4. Take HMR at 5, 10 and 20 minutes after mixing.
5. Take CMR at 25 min after mixing.
6. Take HMR at 40 min after mixing.
7. Take CMR at 45 min after mixing.
8. Take HMR at 80 mins after mixing.
9. Take CMR at 85 mins after mixing.
10. Continue to take NMRs after interval doubling until no more change is observed.

SOPS

<http://openwetware.org>

<http://usefulchem.wikispaces.com/page/code/EXPLAN001>

JAK2/STAT5 model - JWS Online Model Simulation

compartments

Gravity* 0.3

Repulsion* 1000

Off On

Pool threshold* 4

Species: Pin Unpin

Reactions: Pin Unpin

Reset schema Save schema

Middle-click: pin/unpin nodes
Shift-click: pool/unpool species
Right-click: context menu

models



The University of Manchester

Sharing, publishing and preserving pieces of process

- Monitor the formation of an aromatic imine by HMR and CMR in CDCl₃
1. Make up separate 1 mL of 1M solutions of piperonal and 5-methylfurfurylamine in CDCl₃.
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SOPS



vetware.org

<http://usefulchem.v>

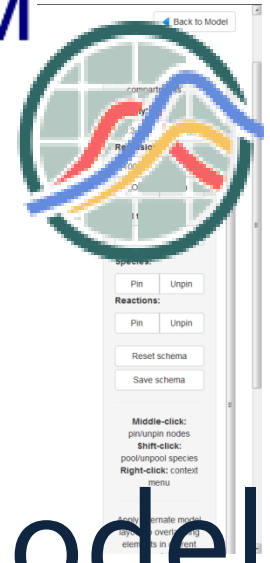
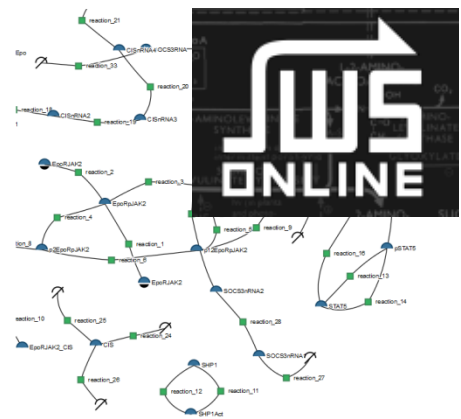
:/EXPLAN001

FAIRDOM

my experiment

JAK2/STAT5 model - JW:
Model Simulation

- Reactions
- Parameters
- Fixed species
- Initial values
- Functions and Rules
- Events
- Constraints



<http://www.mygrid.org.uk/tools/taverna/>
computational workflows

models

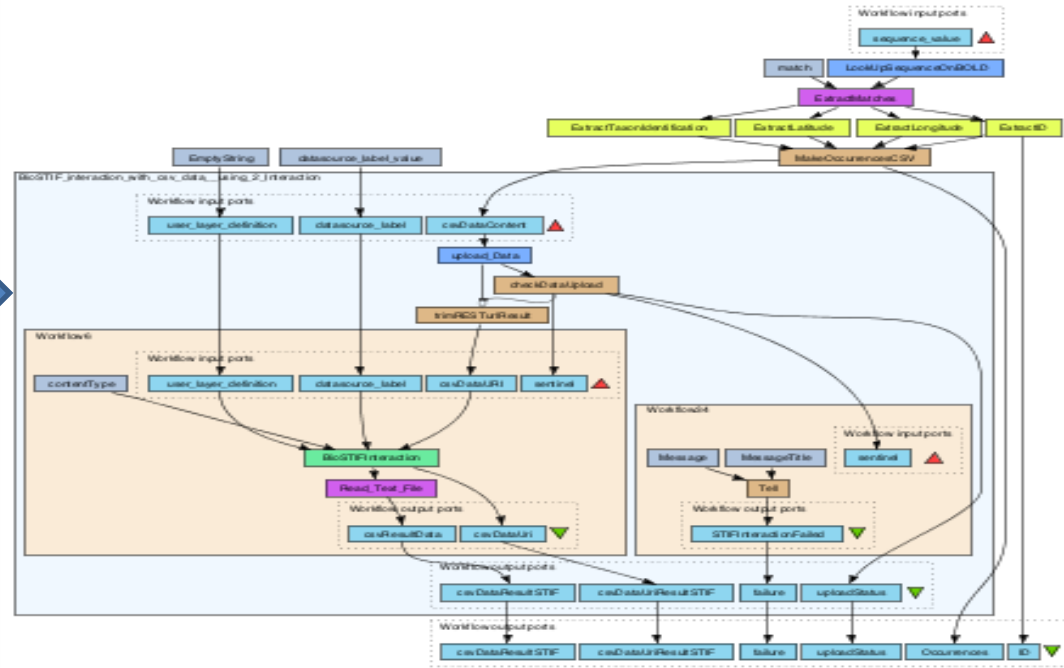
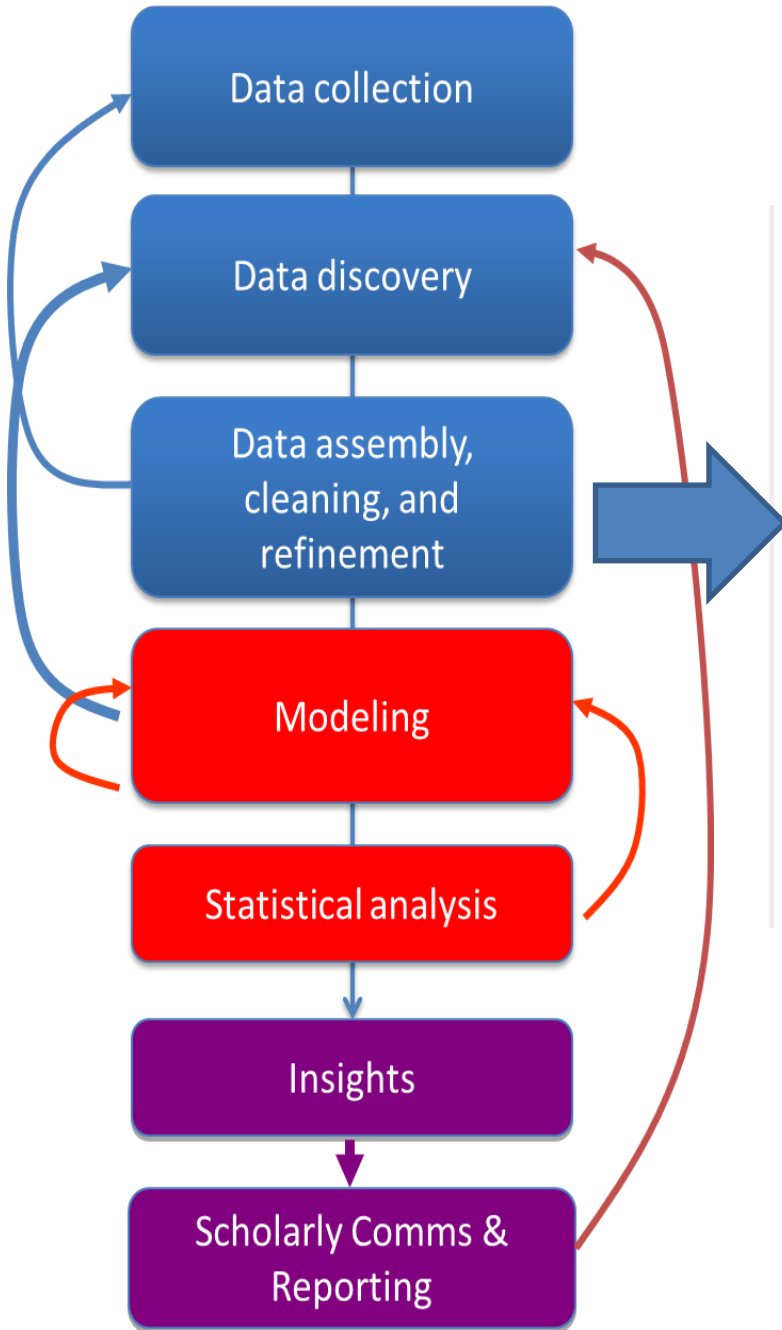
software

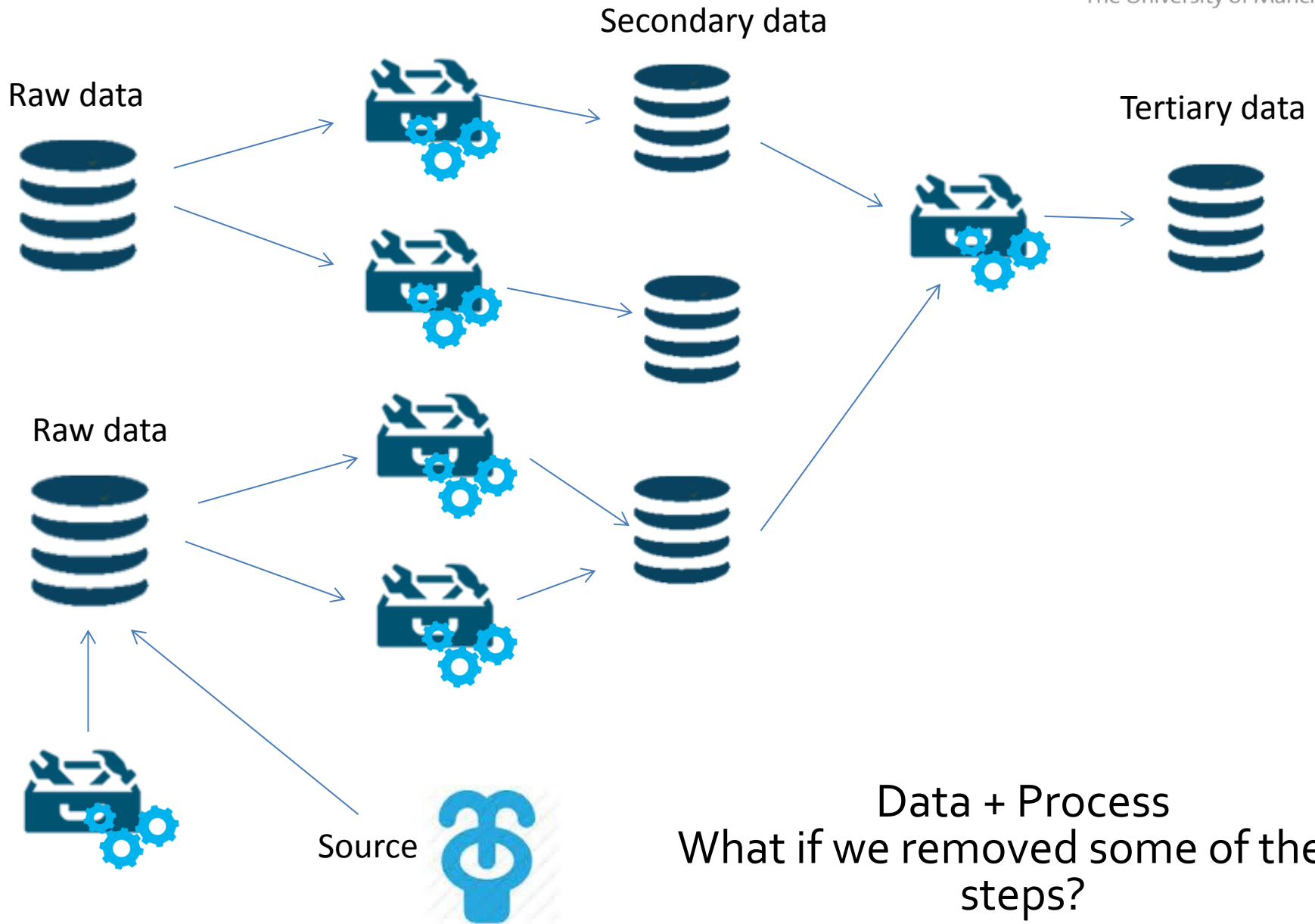


Olive Executable Archive



Complex Assemblies





Workflow + History Publishing

(GIGA)ⁿ DB

Revolutionizing data dissemination, organization, and use

☆ ▼ ↻  scholar

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Data released on December 30, 2013

GigaGalaxy workflows and histories from “Galaxy tools to study genome diversity”

Bedoya-Reina, OC; Ratan, A; Burhans, R; Kim, HL; Giardine, B; Riemer, C; Li, Q; Olson, TL; Loughran Jr, TP; vonHoldt, BM; Perry, GH; Schuster, SC; Miller, W (2013): GigaGalaxy workflows and histories from “Galaxy tools to study genome diversity” GigaScience Database. <http://dx.doi.org/10.5524/100069>

Intra-species genetic variation can be used to investigate population structure, selection, and gene flow in non-model vertebrates; and due to the plummeting costs for genome sequencing, it is now possible for small labs to obtain full-genome variation data from their species of interest. However, those labs may not have easy access to, and familiarity with, computational tools to analyze those data.

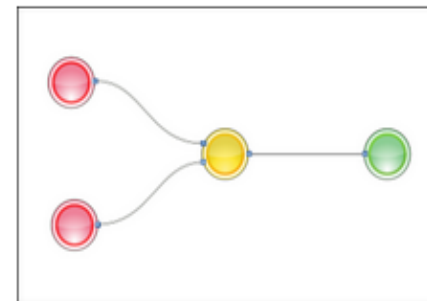
A suite of tools for the Galaxy web server have been created aimed at handling nucleotide and amino-acid polymorphisms discovered by full-genome sequencing of several individuals of the same species, or using a SNP genotyping microarray.

In addition to providing user-friendly tools, a main goal is to make published analyses reproducible. These tools are presented in a GigaScience publication (doi: [10.1186/2047-217X-2-17](https://doi.org/10.1186/2047-217X-2-17)), and in order to facilitate readers to repeat and recreate the examples given in the paper, we present here the pipelines and histories, both accessible from our [GigaGalaxy](#) server, and as Galaxy XML files available to download. The five workflows included relate to examples in the paper dealing with nuclear-genome diversity in non-human vertebrates, and also illustrate the application of the tools to fungal genomes, human biomedical data, and mitochondrial sequences.

Related manuscripts:

doi:[10.1186/2047-217X-2-17](https://doi.org/10.1186/2047-217X-2-17)

Workflow, Software



[Scott Edmunds]

"Mapping present and future predicted distribution patterns for a meso-grazer guild in the Baltic Sea" Sonja Leidenberger et al



Workflow Commons interface showing the 'Biodiversity workflow' details. The workflow is titled 'Biodiversity workflow' and was created on 2013-09-02. It includes a description, a preview of the workflow diagram, and a list of metadata including workflow type (Taverna 2), uploader (Renato De Giovanni), license (CC BY), credits, and tags. The workflow is shared with groups 'BioVeL' and 'BioVeL manual' and is featured in the 'Ecological niche modelling workflow' pack.

WORMS (World Register of Marine Species) interface showing taxon details for *Gasterosteus aculeatus* Linnæus, 1758. The interface lists relationships between species, such as *Idotea chelipes* preying on *Fucus* algae, and *Fucus vesiculosus* being eaten by *Idotea*. A list of relationships is provided at the bottom, detailing the flow of data between different models and workflows.

1. *Fucus vesiculosus* 2050 distribution is an output from Ecological niche modelling workflow...
2. *Fucus vesiculosus* 2050 distribution is an input to BioVeL ESW DIFF Basic.
3. *Fucus vesiculosus* current distribution is an input to BioVeL ESW DIFF Basic.
4. *Fucus vesiculosus* current distribution is an output from Ecological niche modelling workflow.
5. *Fucus vesiculosus* current and 2050 difference is an output from BioVeL ESW DIFF Basic.



fair-dom.org

Sustainable Infrastructure
for Systems Biology

Sys Bio Commons data+ models + ops



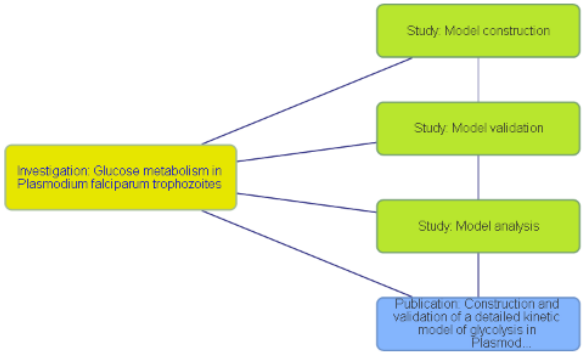
Home / Investigations Index / Glucose metabolism in Plasmodium falciparum trophozoites

Glucose metabolism in Plasmodium falciparum trophozoites

The investigation entails the construction and validation of a detailed mathematical model for glycolysis of the malaria parasite Plasmodium falciparum in the blood stage trophozoite form.

ID:56
Projects: Whole body modelling of glucose metabolism in malaria patients

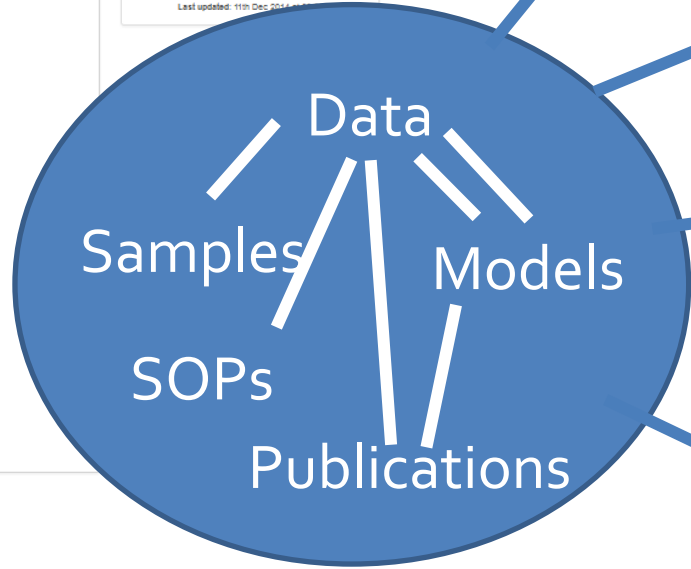
Selected item: Investigation: Glucose metabolism in Plasmodium falciparum trophozoites



Contributors

Activity

Views: 1135
Created: 3th Aug 2014 at 15:16
Last updated: 11th Dec 2014 at 15:16



Related Items

People (1) Projects (1) Studies (3) Assays (24) Data files (18) Models (19) SOPs (13) Publications (1)

David Van Niekerk

Projects: SysMO DB, Whole body modelling of glucose metabolism in malaria patients
Institutions: University of Stellenbosch

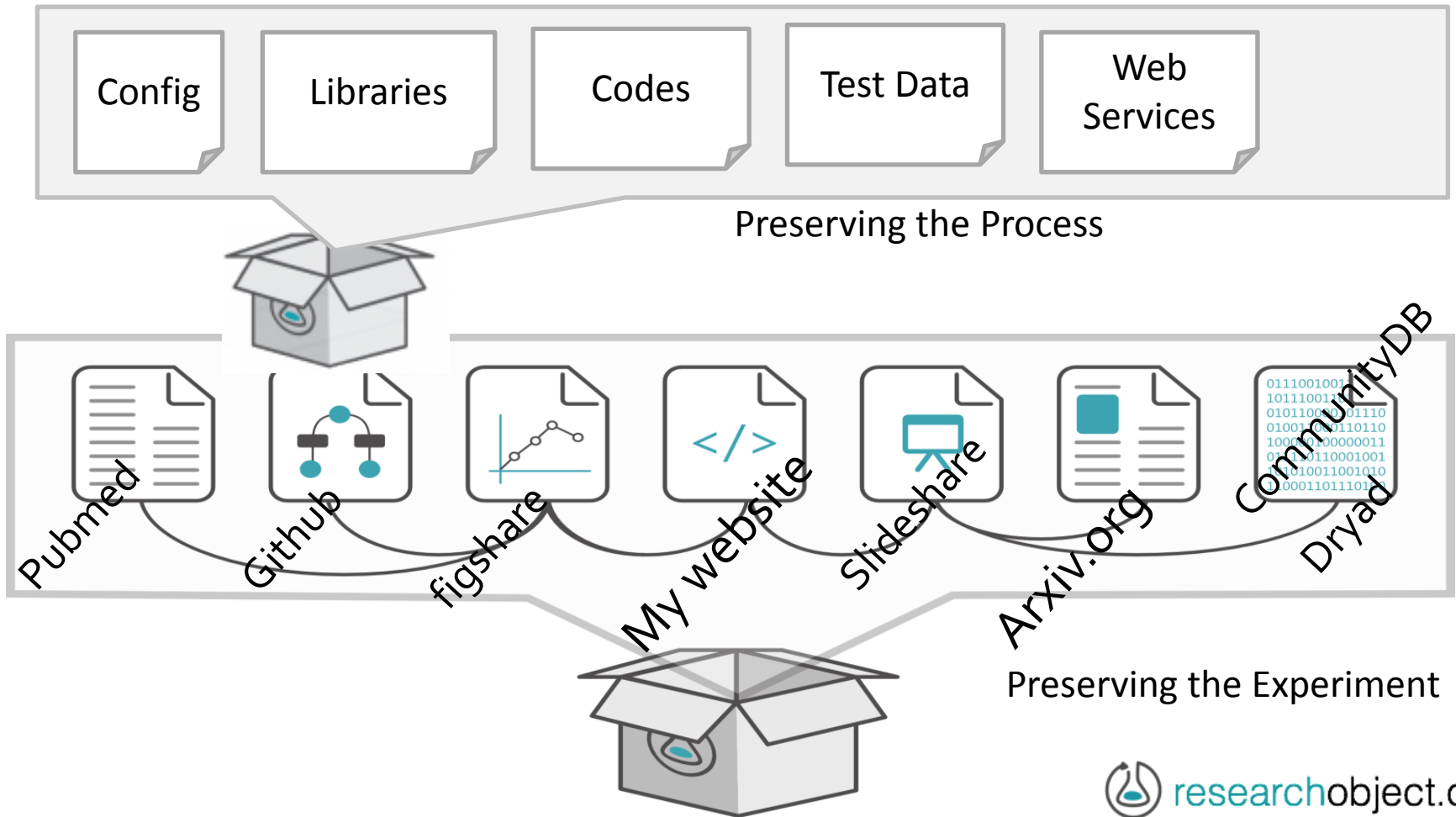
Disciplines: Moeeliler
Roles: Just one role

<https://doi.org/10.15490/seek.1.investigation.56>

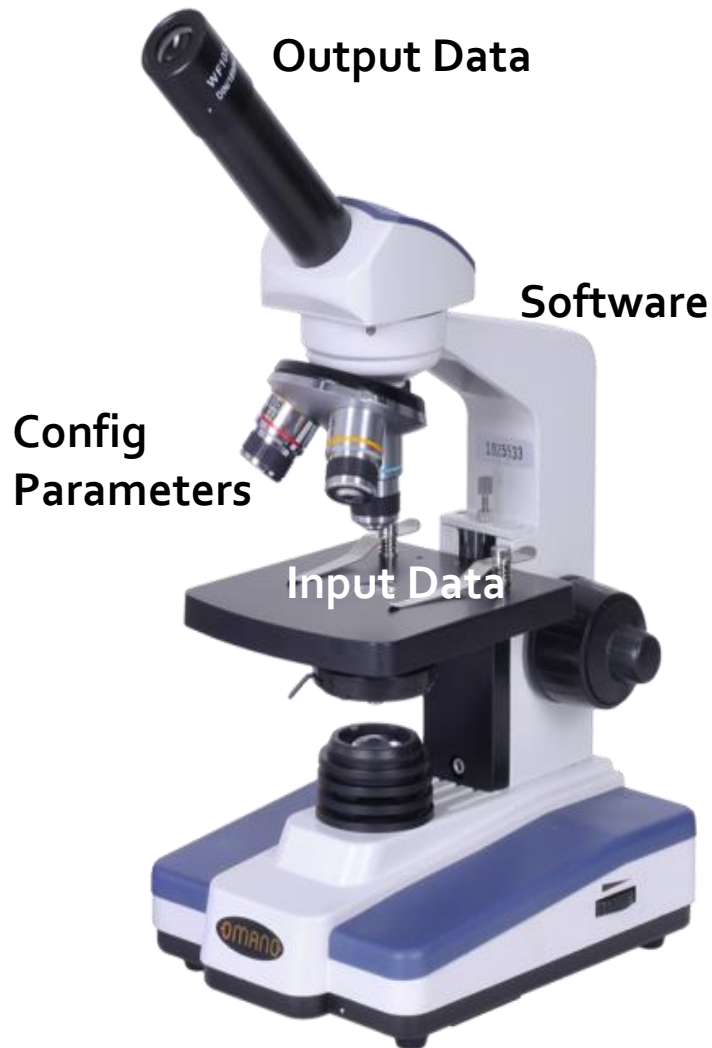
Scholarly Record: Crossing Silos, Compound Object

Datasets, Data collections
Standard operating procedures
Software, algorithms
Configurations,
Tools and apps, services

Codes, code libraries
Workflows, scripts
System software
Infrastructure
Compilers, hardware



Computational “Datascop” Instruments



Experiment

Materials

datasets, parameters,
algorithm seeds

Methods

techniques, algorithms,
spec. of the steps

Setup

Instruments

codes, services, scripts,
underlying libraries

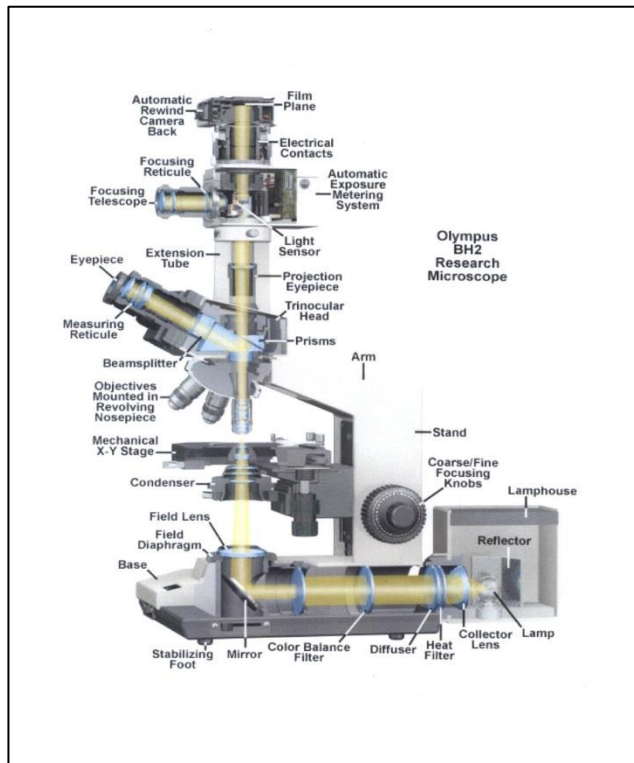
Laboratory

sw and hw infrastructure,
systems software,
integrative platforms

Computational Instrument Preservation

preserve or sustain? form or function? prepare to repair!

Document



Preserve by Reporting
Archived Record

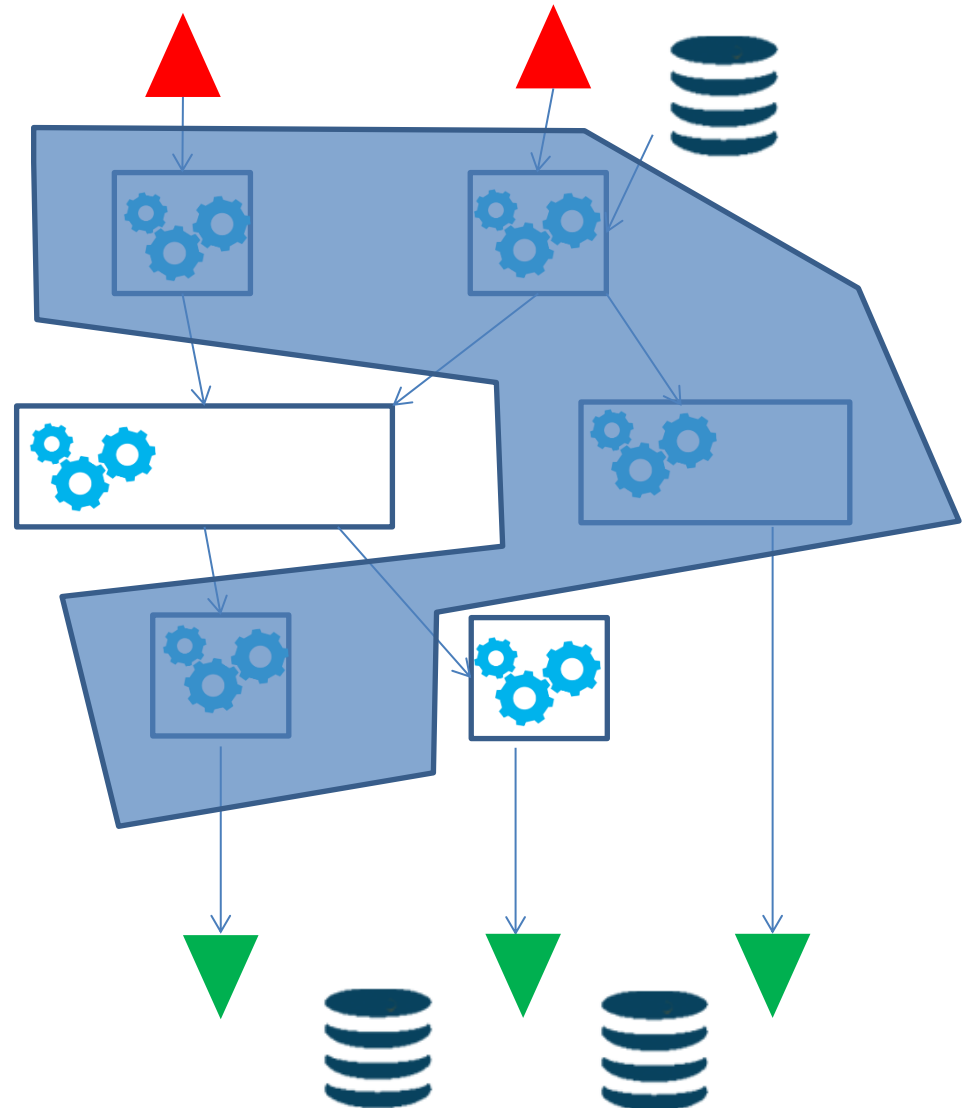
Preserve/Conserve/Reconstruct



Preserve by Maintaining
Active Instrument

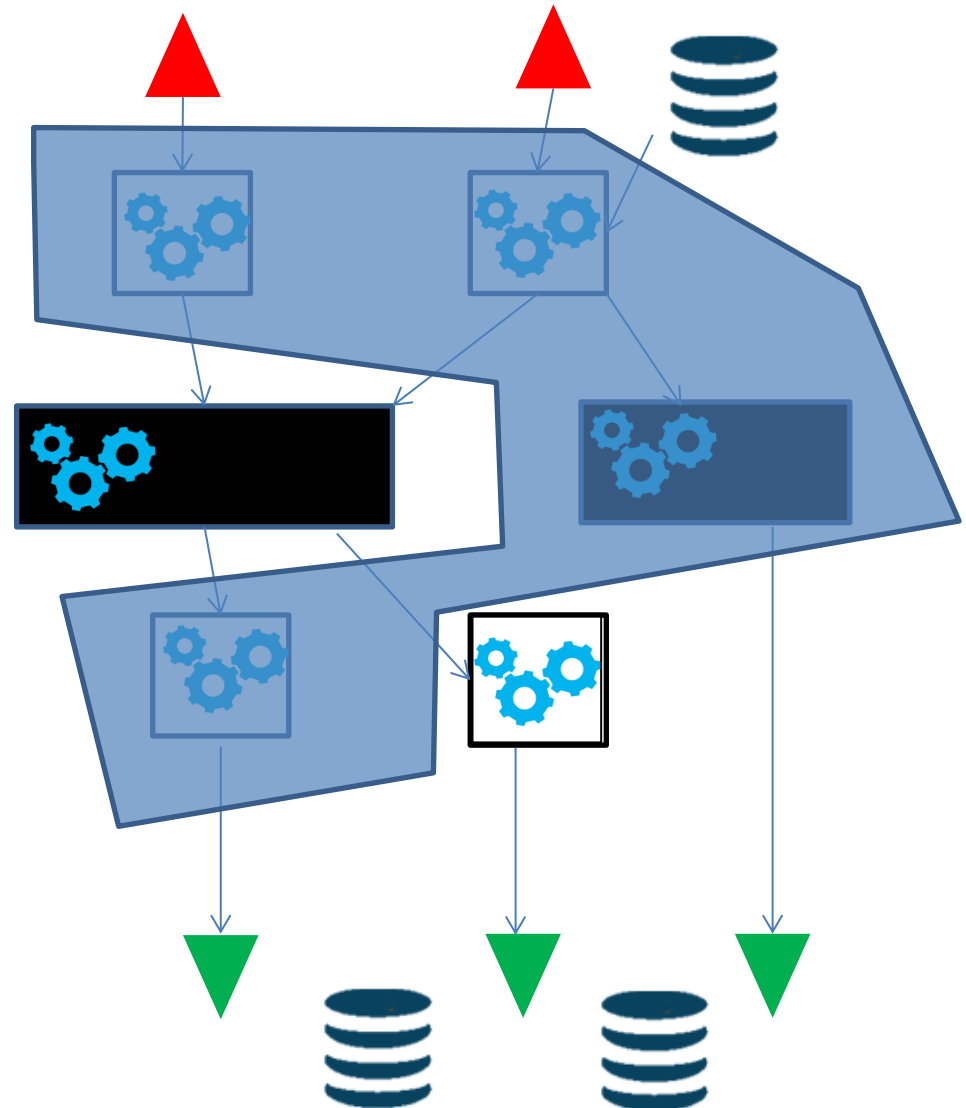
Method Preservation and Access

- Encapsulation
- Black Box
- Change



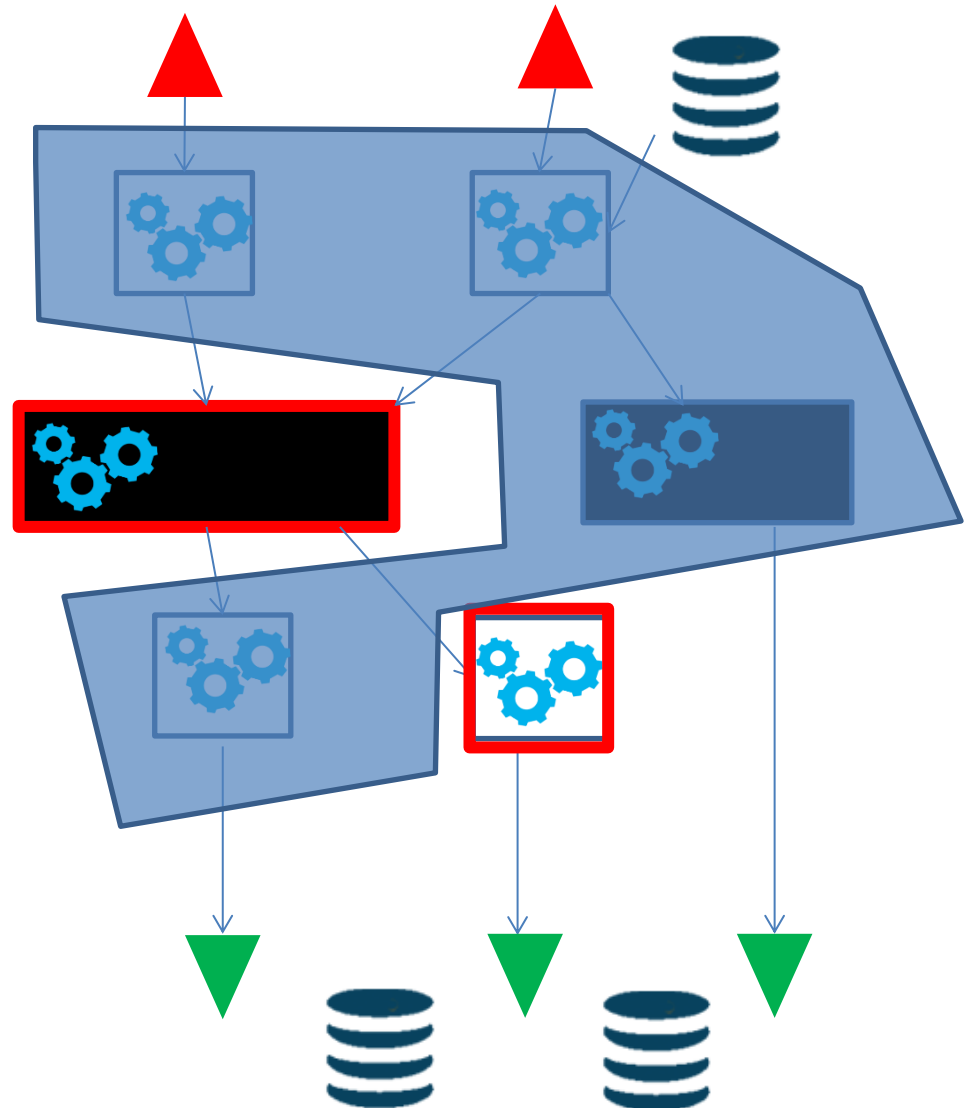
Method Preservation and Access

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- Black Box
- Change

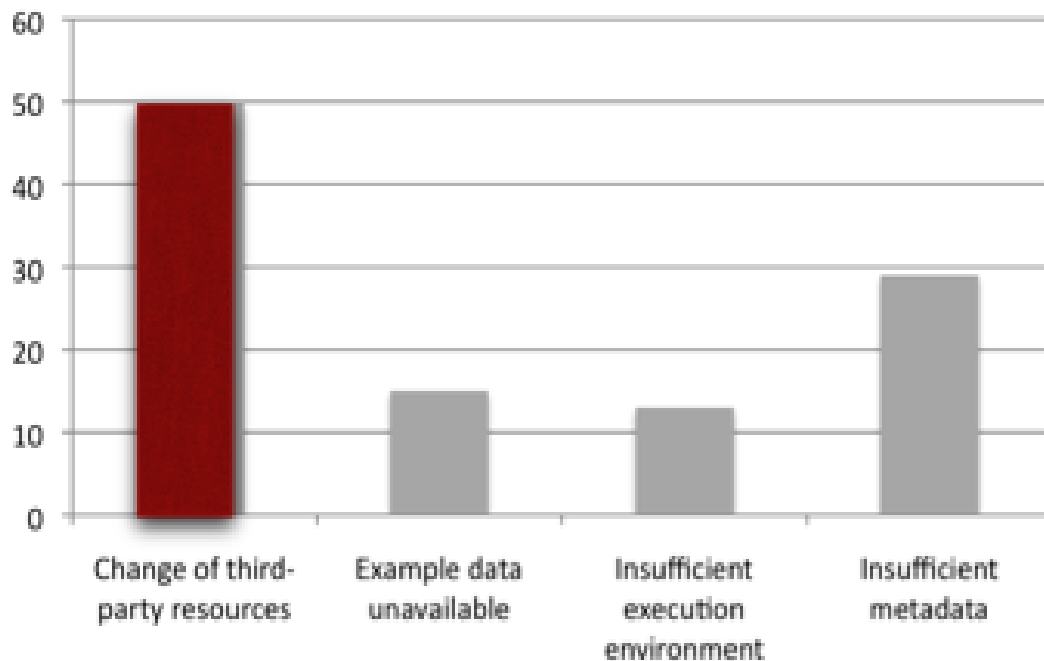


Method Preservation and Access

- Encapsulation
- Black Box
- Change



Instrument Entropy



Mitigate
Migrate
Adapt
Die

Detect, Repair, Preserve
Partial replication
Approximate reproduction
Verification, Benchmarks

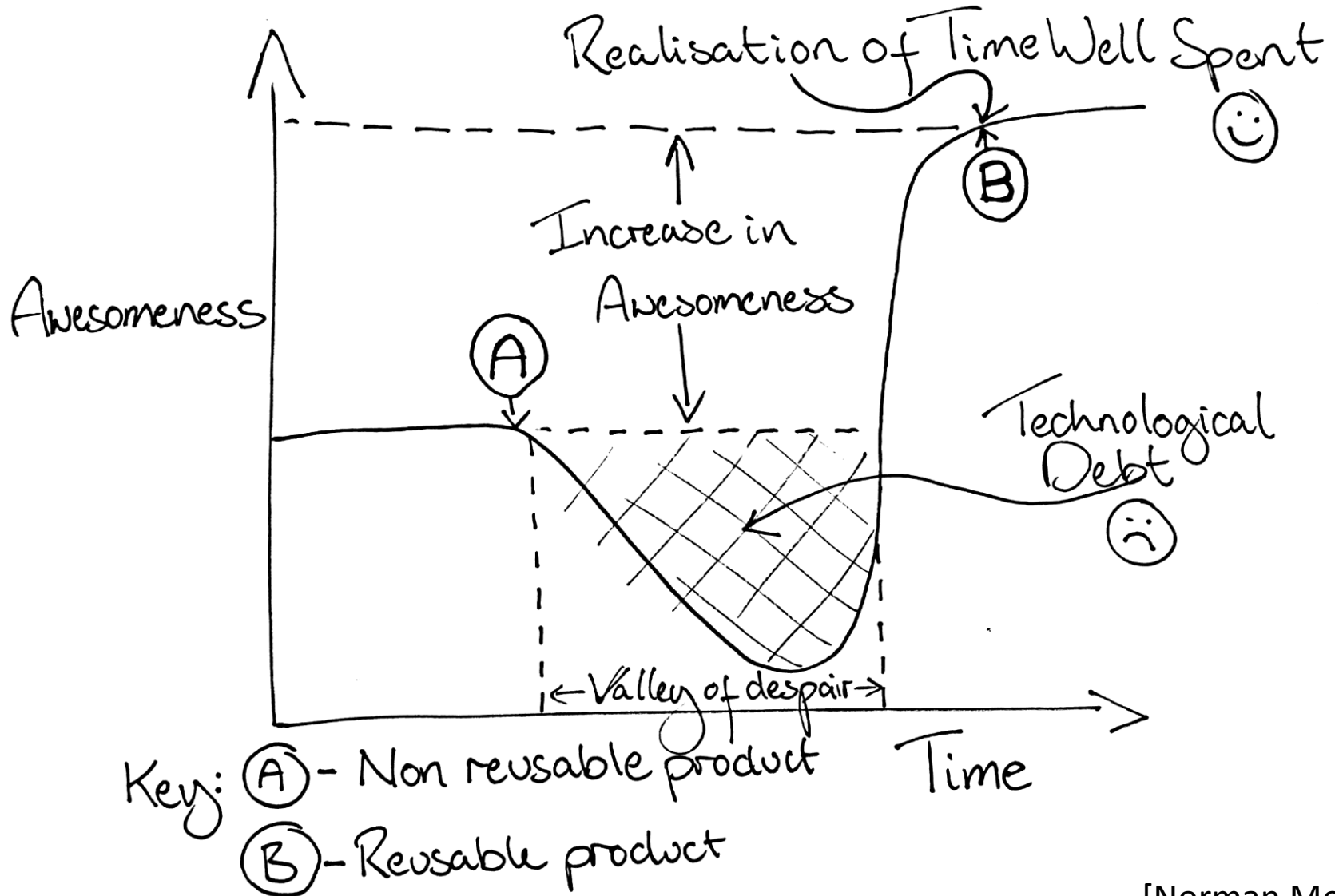
Zhao, et al. 2012
Why workflows break -
Understanding and combating
decay in Taverna workflows,
8th Intl Conf e-Science 2012



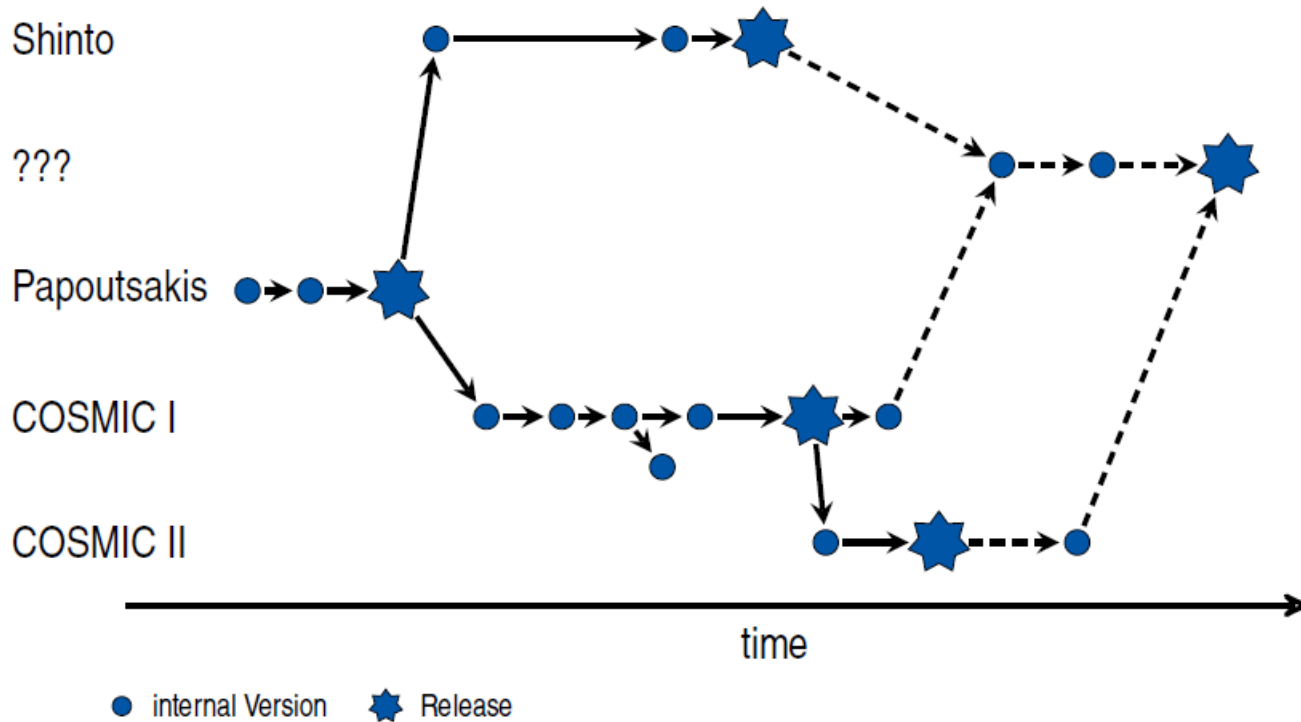
Target [Pack374](#) does not satisfy checklist for ready-to-release.

- ✗ Experiment hypothesis is not present
- ✗ Workflow design sketch is not present
- ✓ All workflow definitions are accessible
- ✗ One or more web services used by one of the workflows are inaccessible, including [btit](#)
- ✗ Input data is not present
- ✗ Experiment conclusions are not present

Instrument entropy



Instrument Evolution



- Fork.
- Merge.
- Version.
- Cite
- Snapshot.
- Live.

Dependency

multi-part and multi-sourced
availability & volatile activity of resources,
services, systems, components

Selective retention

sustained compared to preserved
what is “forever” clock cycle of software? of method?

Portability



Virtual Machines



Portable Packaging



Science as a Service



Integrative frameworks



Open Source

Workflows/Scripts

Models



Transparency

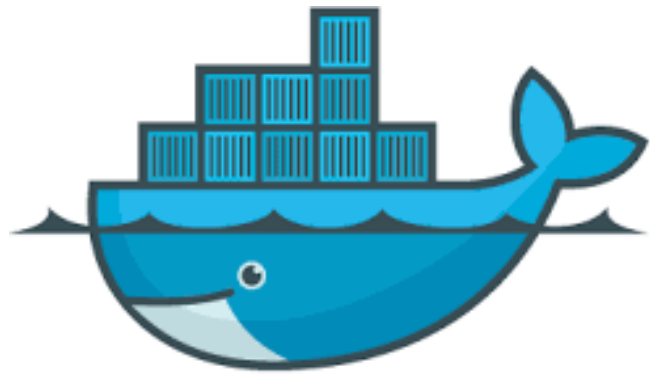




bio**boxes**

Bio Docker

Docker for Bioinformatics

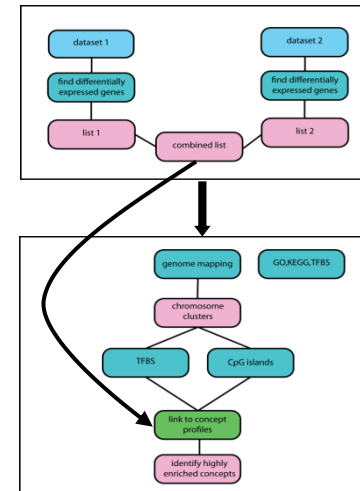


docker

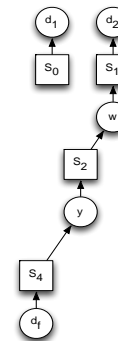
Pre-configured pre-packaged Docker containers

Method Preservation and Access

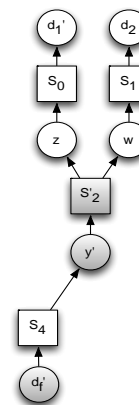
- Describing method apart from execution
- **Run provenance, Parameter provenance**
- Relating data and process



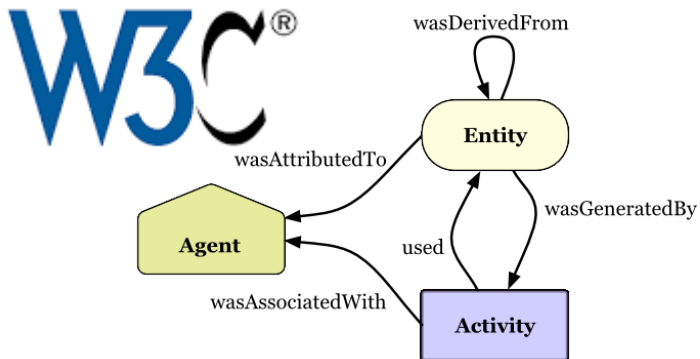
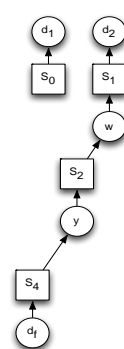
Run



Run



Run



Preservation Potential of Provenance Untapped Big Data

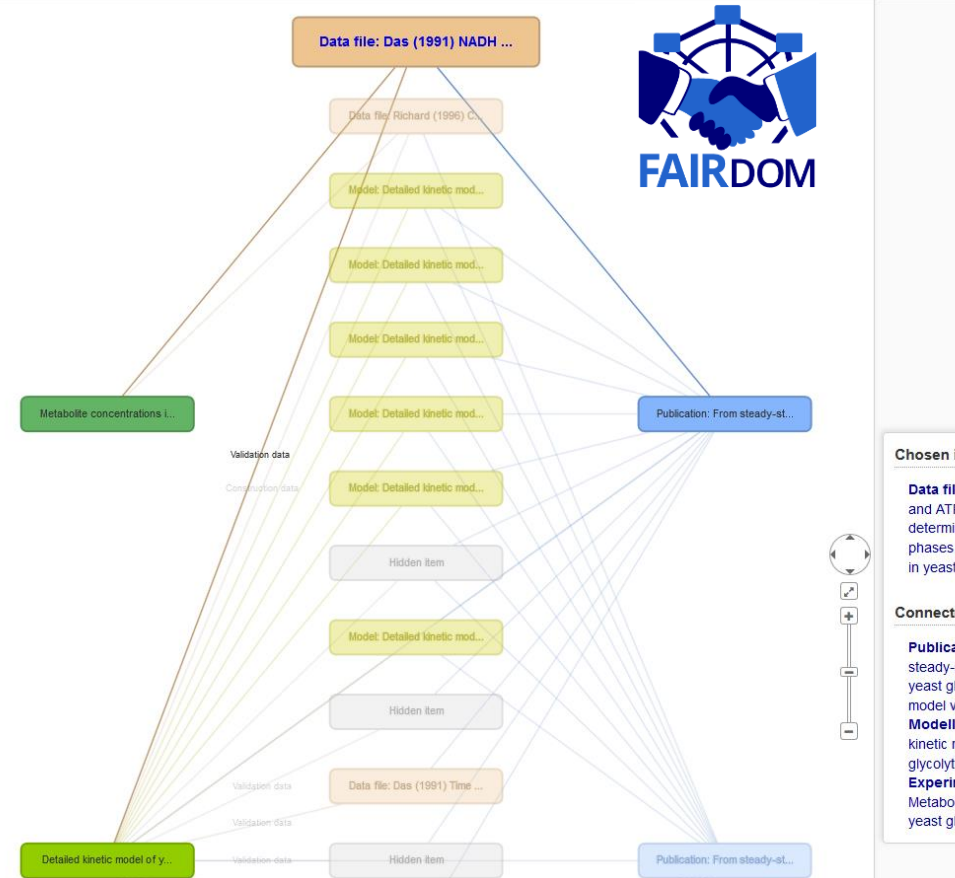
- Track versions
- Partially reproduce
- Reverse engineer
- Repair
- Alternates
- Black box recovery
- Calc data quality & trust
- Track contrib / credit
- What data to keep
- Track error propagation
- Optimisations

The screenshot displays the Galaxy web interface. At the top, there are navigation tabs: 'Analyze Data', 'Workflow', 'Shared Data', 'Visualization', 'Cloud', 'Help', and 'User'. Below the navigation, the page title is 'Galaxy History | aun1 | Galaxy vs MEGAN'. The main content area is titled 'Galaxy History ' Galaxy vs MEGAN'' and includes an annotation: 'Comparison of Galaxy vs. MEGAN pipeline.' The interface is divided into two columns. The left column, labeled 'Dataset', lists 14 datasets with their names and a magnifying glass icon. The right column, labeled 'Annotation', provides detailed descriptions for each dataset. The datasets listed are: 1: s1, 2: s234, 3: s1 max bit score, 4: s234 max bit score, 5: Join two Queries on data 3 and data 1, 6: Join two Queries on data 4 and data 2, 7: s1 within 5% of max, 8: s234 within 5% of max, 9: Fetch taxonomic representation on data 7, 10: Fetch taxonomic representation on data 8, 11: Find lowest diagnostic rank on data 9, 12: Find lowest diagnostic rank on data 10, 13: Draw phylogeny on data 11, and 14: Draw phylogeny on data 12.

Dataset	Annotation
1: s1	Results of comparison of Dataset 1 from Huson et al. 2007 against the nt database
2: s234	Results of comparison of Datasets 2, 3, and 4 from Huson et al. 2007 against the nt database
3: s1 max bit score	Results of comparison of Dataset 1 from Huson et al. 2007 against the nt database
4: s234 max bit score	Blast hits for Datasets 2, 3, and 4 grouped by maximum bitscore reported by megablast
5: Join two Queries on data 3 and data 1	Here blast results for dataset s1 are joined with maximum bitscore for each read
6: Join two Queries on data 4 and data 2	Here blast results for datasets s1, 2, and 3 are joined with maximum bitscore for each read
7: s1 within 5% of max	This dataset contains blast hits +/- 5% of the maximum bitscore
8: s234 within 5% of max	This dataset contains blast hits +/- 5% of the maximum bitscore
9: Fetch taxonomic representation on data 7	Taxonomic representation for retained Sample 1 reads
10: Fetch taxonomic representation on data 8	Taxonomic representation for retained Sample 2, 3, and 4 reads
11: Find lowest diagnostic rank on data 9	Identify reads from Sample 1 that are diagnostic below the Kingdom level
12: Find lowest diagnostic rank on data 10	Identify reads from Samples 2-4 that are diagnostic below the Kingdom level
13: Draw phylogeny on data 11	Render phylogenetic trees for Sample 1
14: Draw phylogeny on data 12	Render phylogenetic trees for Samples 2-4

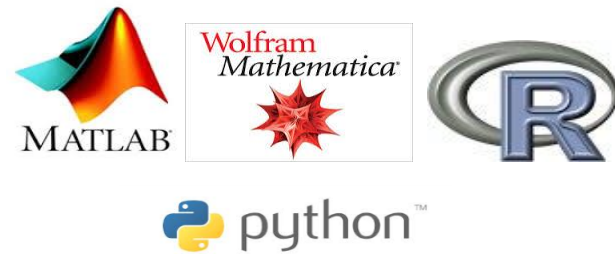
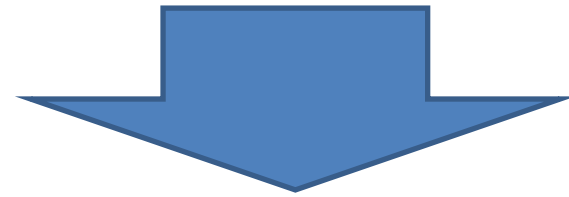
Method Preservation and Access

- Describing method apart from execution
- Run provenance, Parameter provenance
- Relating data and process
 - Validation
 - Construction
 - Predicted



Method Preservation and Access

- Describing method apart from execution
- Run provenance, Parameter provenance
- Relating data and process





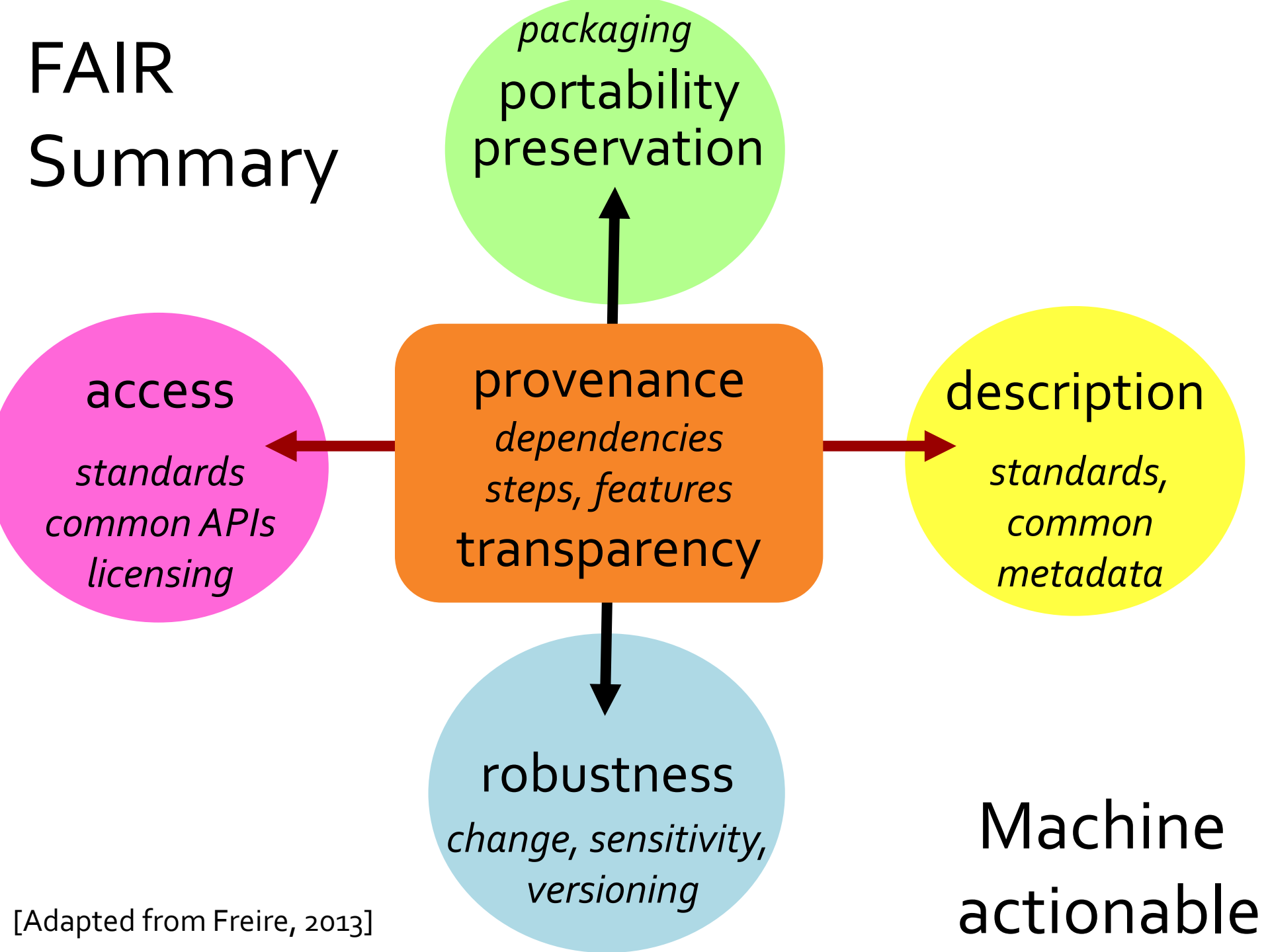
Common Workflow Language

workflow mark up

- Community grassroots effort
- Portability of data analysis workflows
- Describe analysis tools and workflows
- Builds on pre-existing technologies
 - [JSON-LD](#) and [Avro](#) for data modelling
 - [Docker](#) for portable runtime environments.



FAIR Summary





systematic way of dealing
with workflow
reproducibility, **preservation**,
portability, **repair**

Standards.

Graceful degradation.

Technology Independent.

Machine-processable.

Incremental.

Multi-platform.

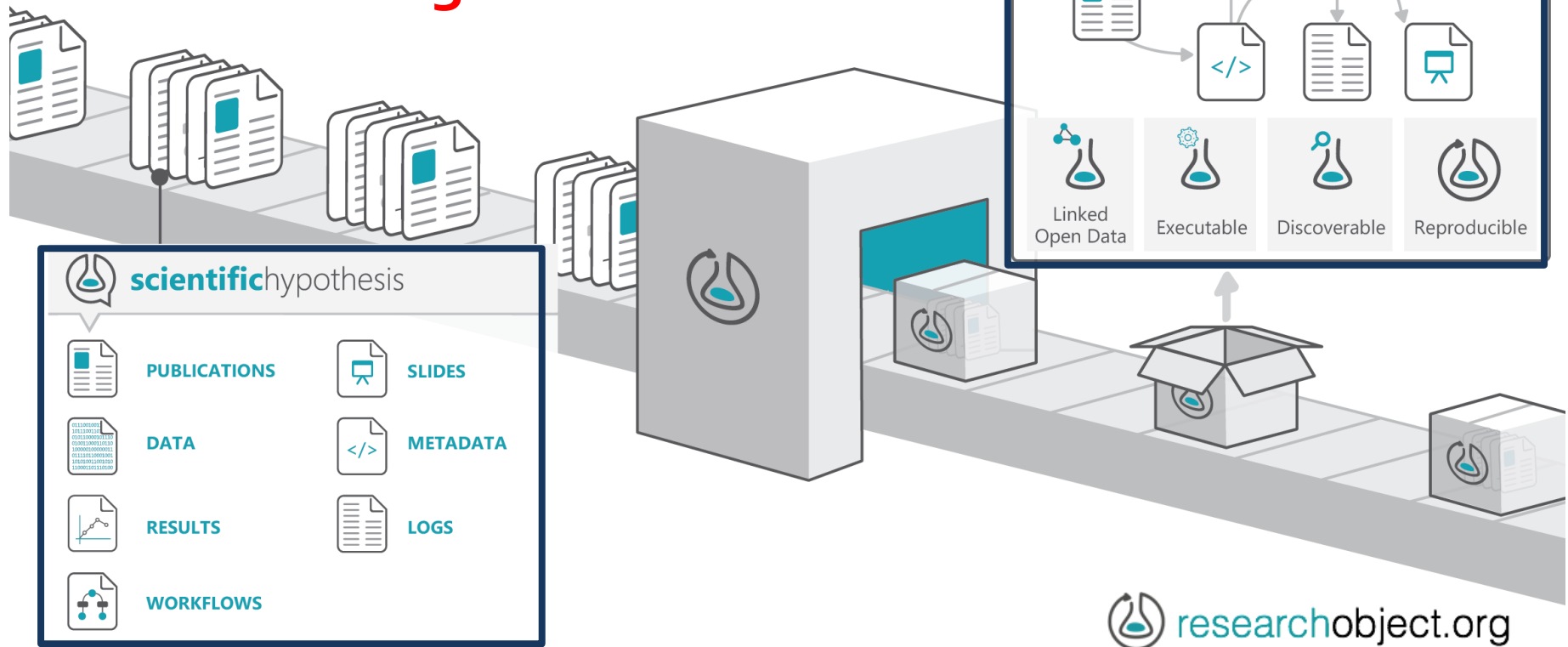
Commodity tooling.

The least possible.
The simplest feasible.
Low tech.

Framework to bundle, port and link local and referenced resources.

Metadata Objects that carry **Research Context** and honour externally hosted resources

Units of exchange.

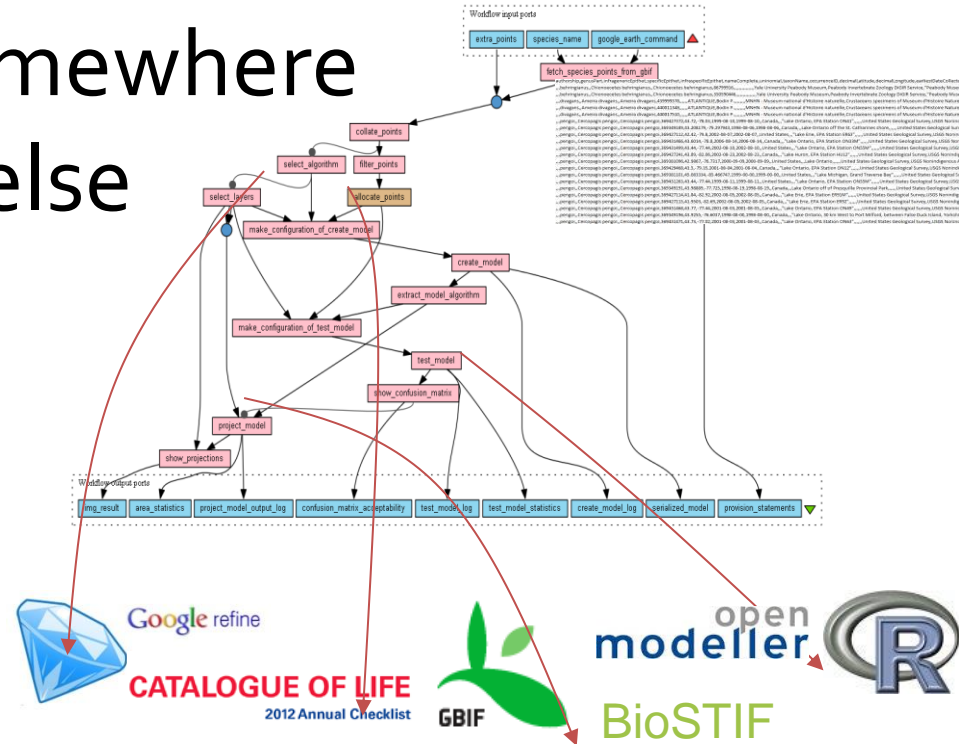


Multi-various products, platforms, resources.

First class citizens - id, manage, credit, track, profile, focus



Except the bits
are somewhere
else

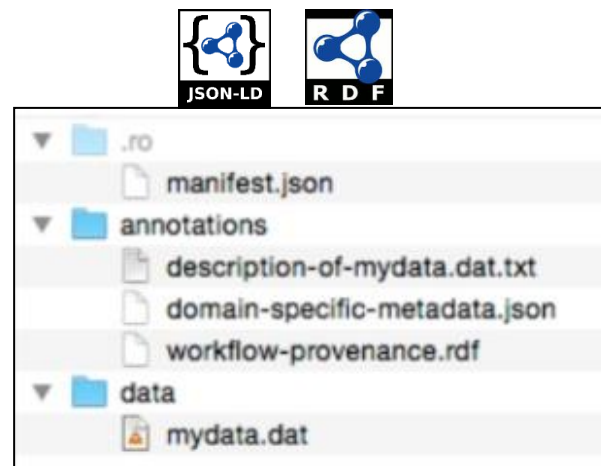


Metadata objects



Manifest

Metadata
Describes the aggregated resources, their annotations and their provenance



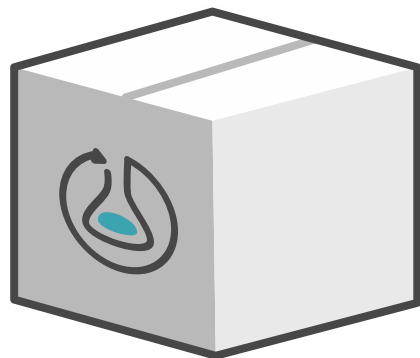
Container

Packaging content and links to content:

Zip files, Docker images, BagIt, ...

Catalogues & Commons Platforms:

FAIRDOM SEEK, STELAR eLab, ...



Metadata and Manifests



Manifest Construction

- **Identification** – id, title, creator, status.... *doi, epic, orcid, purl, RII, identifiers.org*
- **Aggregates** –to link things together.... *OAI-ORE*
- **Annotations** – about things & their relationships.... *W3C OADM*

<http://w3id.org/ro/>

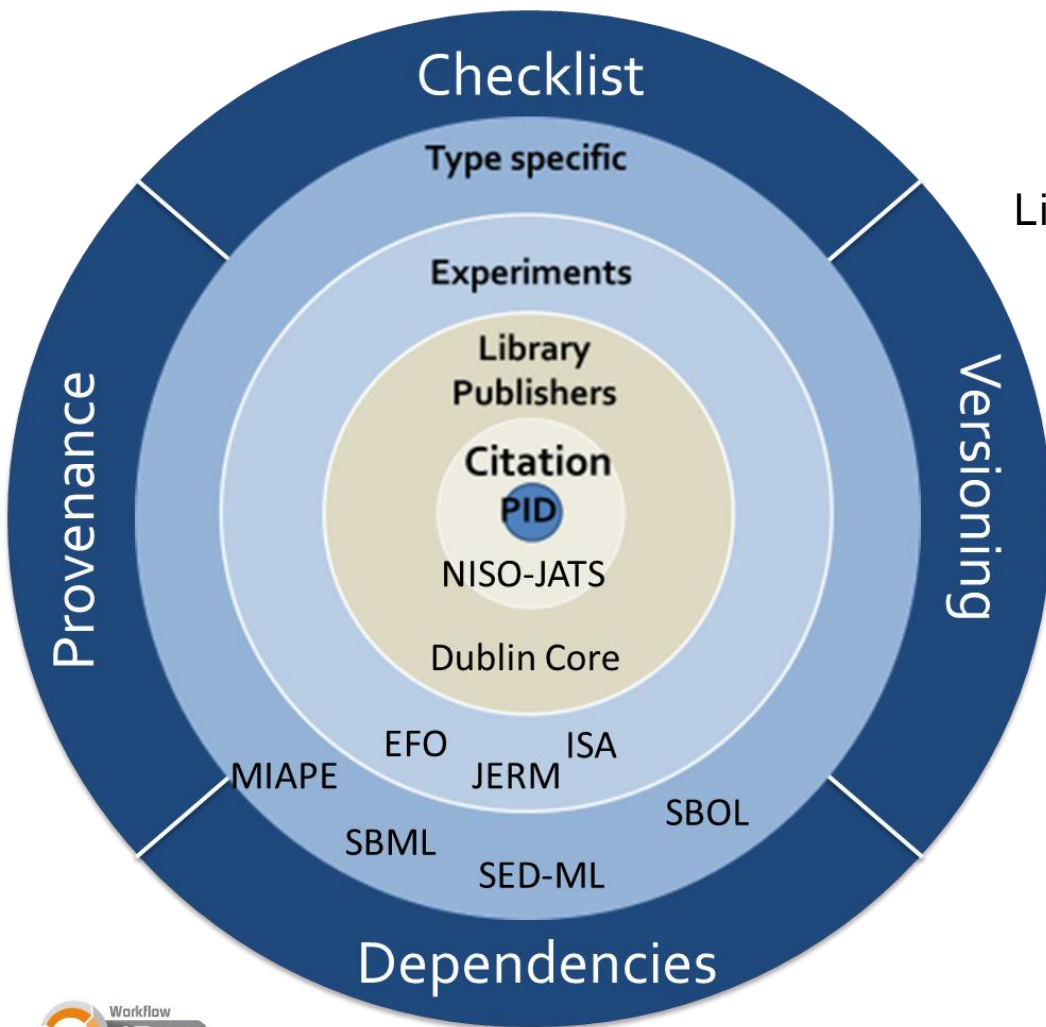


Manifest Description

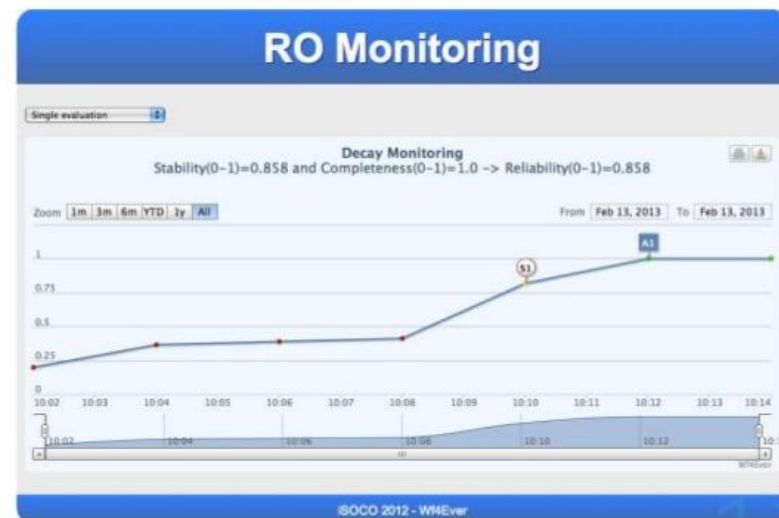
- **Checklists** – what should be there
- **Provenance** – where it came from
- **Versioning** – its evolution
- **Dependencies** – what else is needed

Manifest Content Profiles

Workflow RO, Sys Bio RO ...



Gamble et al (2012)
MIM: A Minimum Information Model
vocabulary and framework for Scientific
Linked Data [10.1109/eScience.2012.6404489](https://doi.org/10.1109/eScience.2012.6404489)



Construction and validation of a detailed kinetic model of glycolysis in *Phasmodium falciparum*
<https://dx.doi.org/10.1111/febs.13237>

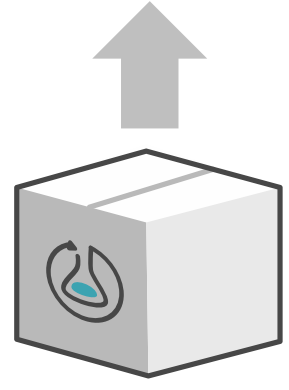
The abstract discusses the construction and validation of a detailed kinetic model of glycolysis in *Phasmodium falciparum*. The introduction describes the model's structure and its application to studying the parasite's metabolism.

The screenshot shows the FAIRDOM website interface for the investigation 'Central Carbon Metabolism of Sulfolobus solfataricus'. It includes a search bar, navigation links, and a sidebar with 'Contributors', 'Activity', and 'Scales' sections.



<https://doi.org/10.15490/seek.1.investigation.56>

This screenshot shows the same FAIRDOM investigation page as above, but with a 'doi' logo overlaid on the left side. The page content remains the same, showing the investigation title and sidebar.



archive

The screenshot shows a file explorer window displaying the contents of an archive named 'investigation-6.ro.zip'. The files listed include folders for 'pro', 'data_files', 'investigations', 'models', 'sops', and 'mimetype', along with their sizes and modification dates.



zenodo

Living

Snapshot

Preserved
 Model
 SOPs
 Data files
 Links with data files
 Experimental context

The screenshot shows a terminal window with commands for extracting files from the 'investigation-6.ro.zip' archive. Below the terminal is a LibreOffice Calc spreadsheet with a table of data. The table has columns for 'Time (min)', 'IPG (mM)', 'FAP (mM)', 'DMAP (mM)', and 'GAP (mM)'. The data rows show values for these parameters at different time points.

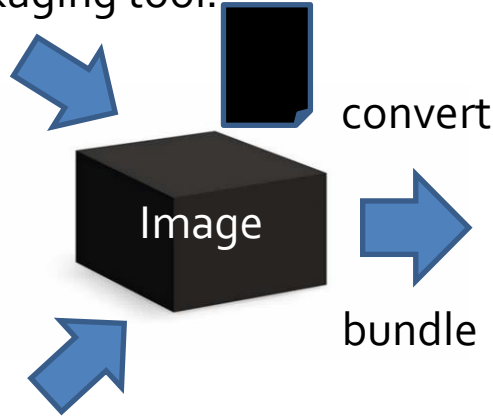
Time (min)	IPG (mM)	FAP (mM)	DMAP (mM)	GAP (mM)	
1	4.447704725	0.0004444	0.0002134	0.0005079	
2	20	0.411308449	0.22117384	0.1977619	
4	0.2971904762	0.394240525	0.20465782	0.19444444	
5	60	0.494264603	0.402884919	0.15001301	0.14325397

ATLAS Collider Data Analytics

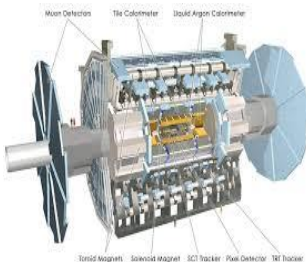
Vardeman, Da Huo
University of Notre Dame



Portable, lightweight
application runtime
and packaging tool.



All data and files
of the execution
+ Instructions



ATLAS and CMS detector data

Relate files
and layers
Add provenance
and annotations
Link in other
content

manifest



read



run



archive



zenodo

Preserved
Same data
Same code
Same run time
environment



Asthma Research

e-Lab



The Farr Institute of Health Informatics Research



NIH Big Data to Knowledge (BD2K)

Metagenomics

pipelines and **BD2K**

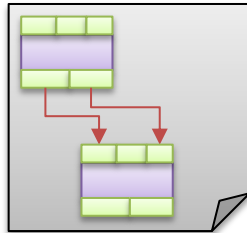
LARGE datasets

RO Workflow Run

Bundles



CWL



Standardised packing of Systems Biology models



Export RO from WebCAT



European Space Agency RO Library

Research Object Bundles for Data Releases As if they were software Dataset "build" tool



Principles & Conventions

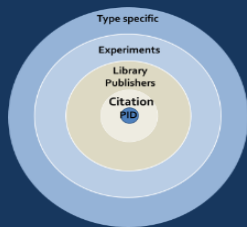
Multi-Owned

Policies
Tools
Repositories

Lifecycle
Steward
Ship

Training
Credit

Annotation
profiles
*progressive
extensions*



Metadata formats



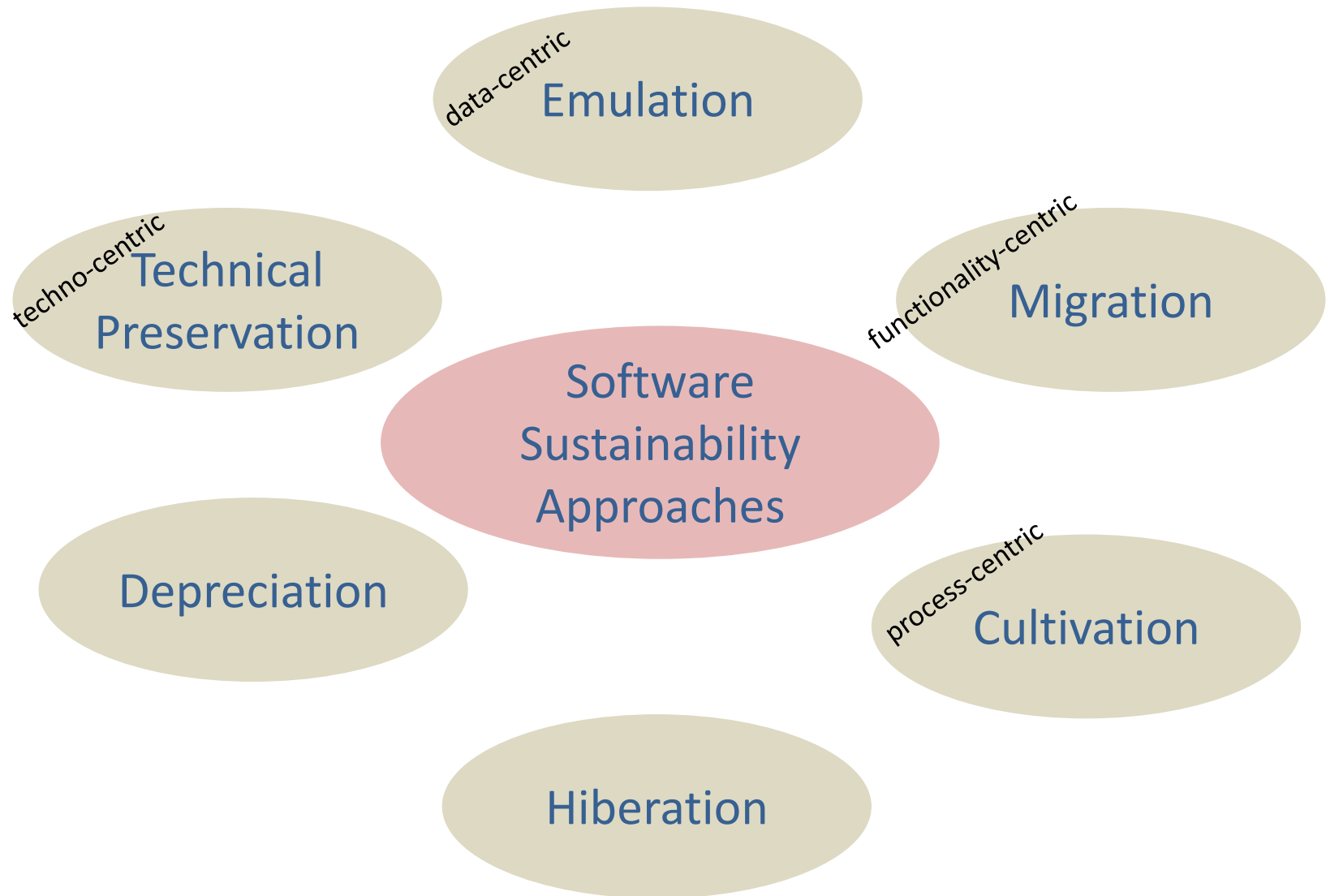
Manifest
Core model
using standards



API specification

Implementation
Profiles
*using legacy &
commodity
platforms*





Software Artisans

56%

Of UK researchers develop their own research software or scripts

73%

Of UK researchers have had no formal software engineering training



Software
Sustainability
Institute



DATA CARPENTRY

MAKING DATA SCIENCE MORE EFFICIENT



Software
Sustainability
Institute



Software Credit Workshop

The workshop (19 October 2015 at the National History Museum, London) explored what contribution software can and should make for academic reputational credit; i.e. how the production of software tools and applications contributes to career advancement in the academic research setting for both researchers who build software as part of their research and developers who build tools and support research.

The aim of the workshop focused on capturing the current credit needs of those who produce software as part of or in support of research. In addition we attempted to capture best practice currently being used to achieve credit for software and its impact on research.

The workshop and attendees will make progress on key topics that will explore how publishers, developers, libraries, funders and researchers can help give appropriate credit and recognition to those who produce software.

The workshop was aimed at researchers who produce software as part of their research, developers who work with researchers, those who are involved in applied research, those who are involved in citation for research, those who are involved in the altmetrics funders, public University departments



Page Tags

Software

Code as a Research Object

Mozilla Science Lab

Get credit for your code!

Archive your GitHub code repository to figshare and receive a citable DOI.



GitHub

Edit, share and improve your code



Mozilla Science Lab

Tools to get your research on the web.



figshare

Persistent, citable, long-term archiving for your research outputs.

Register us

GROUP MENU

- Group Home
- Members
- Links & Files
- Google Forum
- Calendar
- Subscribe to group

GROUP LEADER

Daniel S. Katz



GROUP LEADER

Arfon Smith



FORCE11 » Groups » Software Citation Working Group

SOFTWARE CITATION WORKING GROUP

MISSION STATEMENT

The software citation working group is a cross-team committee like existing initiatives working on software citation to produce a consistent policy for software citation. The working group will review existing efforts and make a set of recommendations to be put forward for endorsement by the organizations represented by their role in the community.

The group will produce a set of principles, illustrated with working examples. This group will not be producing detailed specifications or technical solutions.

Co-chairs: **Dan Katz** & **Arfon Smith**

TIMELINE

- April 2015: Working group established
- ...
- February 2016: Formal recommendations presented at Force11 2016



Search packages, authors, and topics

librosa

Python module for audio and music processing



Tags

- sound
- multimedia
- music
- audio
- sound/audio
- analysis

Key contributors

- Brian McFee
- Matt McVicar
- Colin Raffel

Downloads

1.5k 100 percentile

Software reuse

842 100 percentile

Citations

0 0 percentile

Engagement

321 300 percentile

People depend on
my software?!

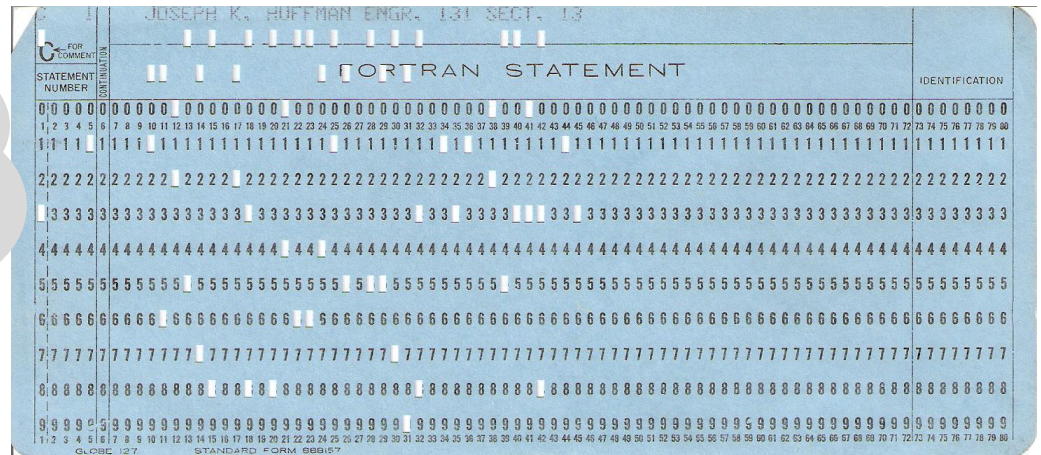
But I'm a researcher not a
service provider...



Software is free,
like free puppies.



The invisibility of
infrastructure.



Links

- <http://www.researchobject.org>
- <http://www.wf4ever-project.org>
- <http://www.fair-dom.org>
- <http://seek4science.org>
- <http://rightfield.org.uk>
- <http://www.software.ac.uk>