



Reproducible Research with Data Provenance

Responding to 6W and 1H Questions of Data Provenance

Sheeba Samuel

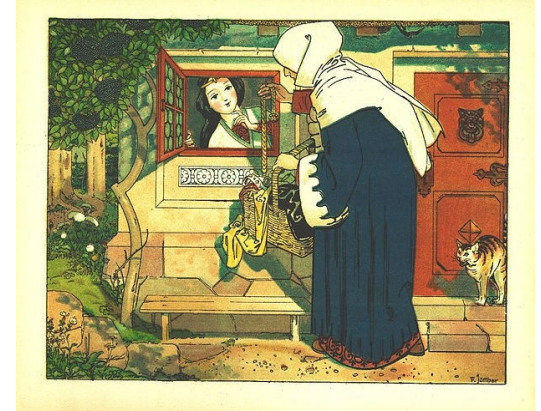
Chemnitz University of Technology, Chemnitz, Germany

Outline

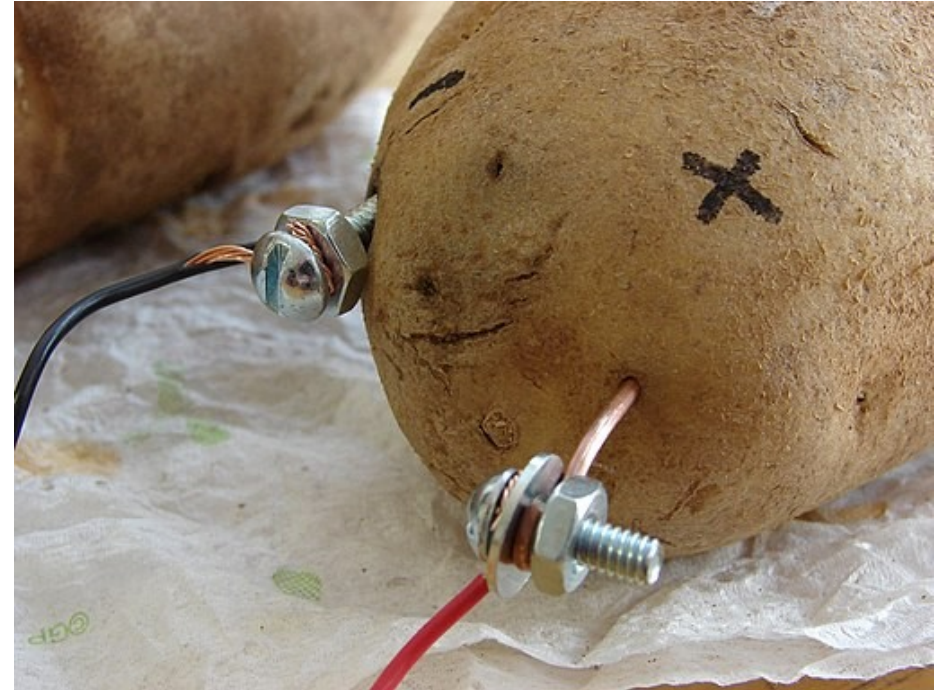


- Introduction
- Definitions: Reproducibility & Repeatability
- Reproducible Research
- Data Provenance and its Semantics
- Solutions to 6W and 1H questions of Data Provenance

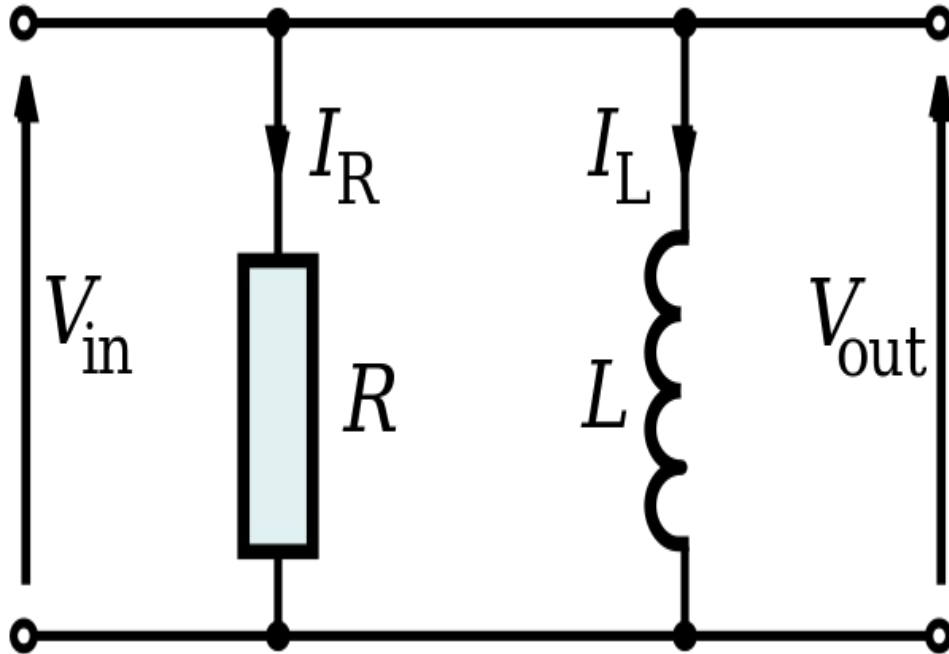
Story



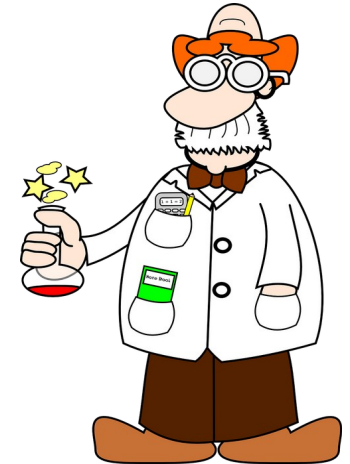
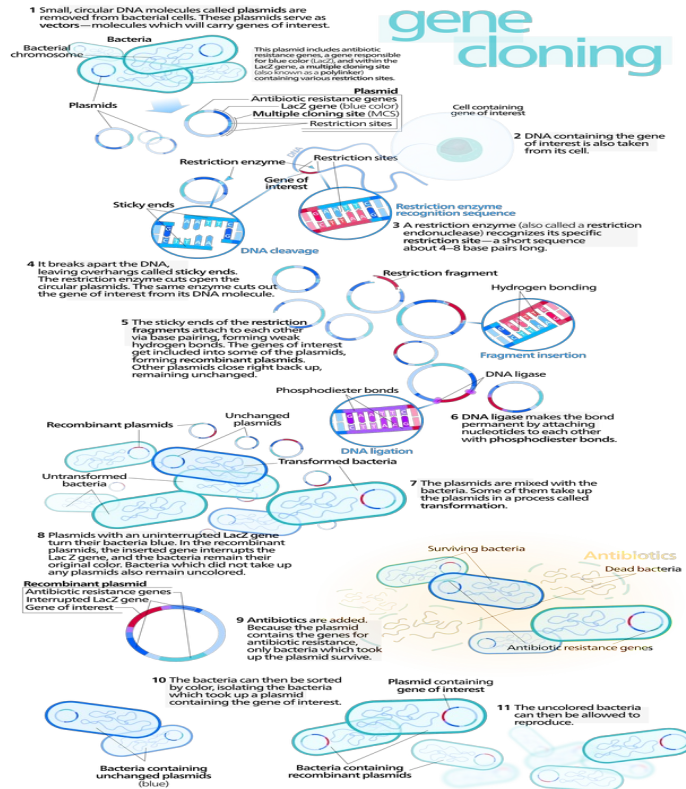
Story of an Experiment



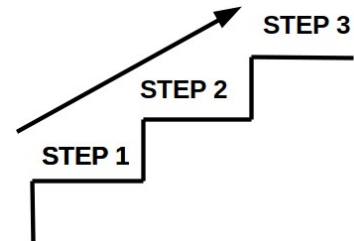
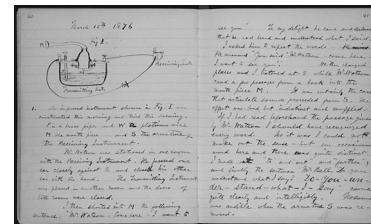
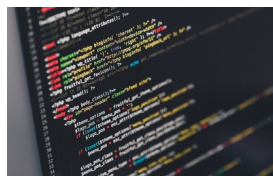
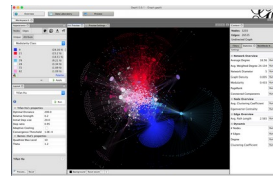
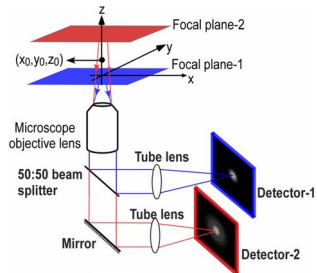
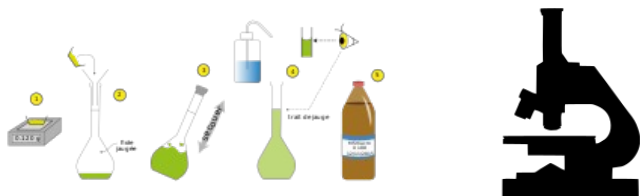
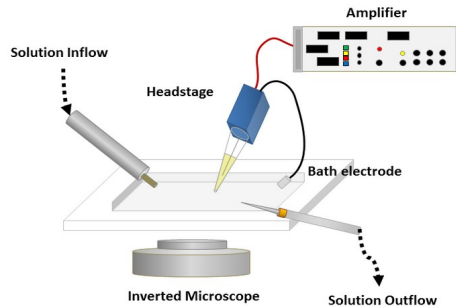
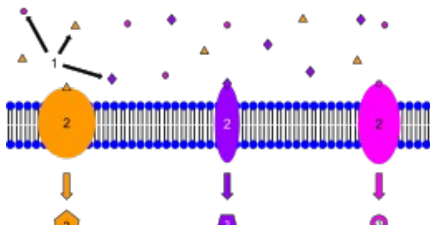
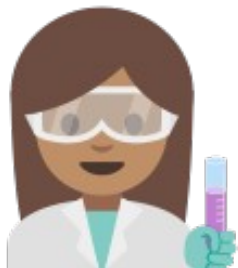
Story of an Experiment



Story of an Experiment



Scientific Experiments

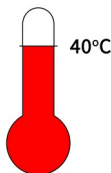


STEP 3 Patch-Clamp Fluorometry: Electrophysiology meets Fluorescence

Jana Kusch¹ and Giovanni Ziletti²
¹University of Jena, Institute for Physiology 1, Jena, Germany and ²University of Jena, Institute for Physiology 1, Jena, Germany

Abstract: Ion channels and transporters are membrane proteins whose function is altered by conformational changes. Classical biophysical techniques provide insight into either the structure or the function of these proteins, but a full understanding of their biophysics requires a combination of these approaches. Here, patch-clamp and optical techniques combine spatial, temporal and molecular information to simultaneously detect conformational changes and ionic currents across the membrane. Since its introduction, patch-clamp fluorometry has been responsible for multiple advances in our knowledge of ion channel biophysics. Over the years, the technique has been applied to many different ion channel families to address several biophysical questions with a variety of spectroscopic approaches and electrophysiological configurations. This review illustrates the strength and the flexibility of patch-clamp fluorometry, demonstrating its potential as a tool for future research.

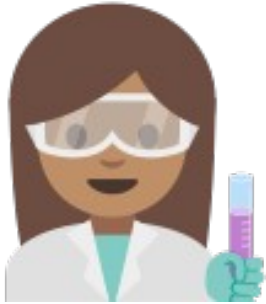
INTRODUCTION
Ion channels are pore-forming membrane proteins, which allow ions to permeate across the membrane. They are involved in many physiological processes such as the control of resting and action potentials, water homeostasis, excitation, and muscle contraction. Their activity is regulated by specific stimuli, including voltage, ligand binding, temperature, or mechanical stress. These stimuli cause conformational rearrangements that result in various gating



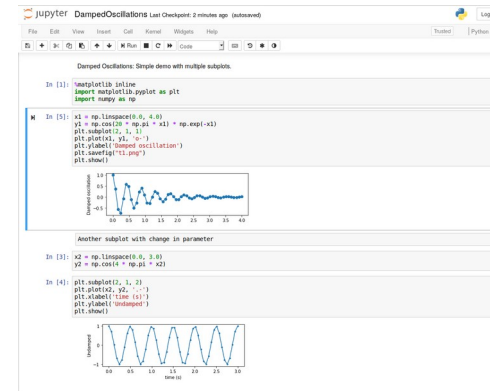
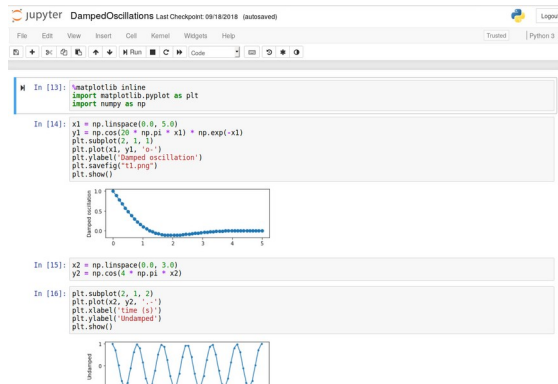
Computational Experiments



➤ Repeatability



➤ Reproducibility





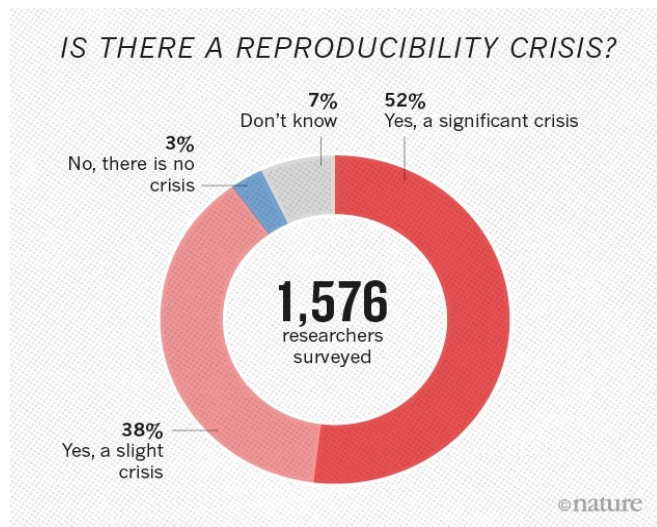
Definition of a Confused Terminology

	ACM Definition (August 24, 2020)	ACM Definition Revised (November 4, 2021)
Repeatability	Same team, same experimental setup	Same team, same experimental setup
Reproducibility	Different team, same experimental setup	Different team, different experimental setup
Replicability	Different team, different experimental setup	Different team, same experimental setup



Reproducibility Crisis

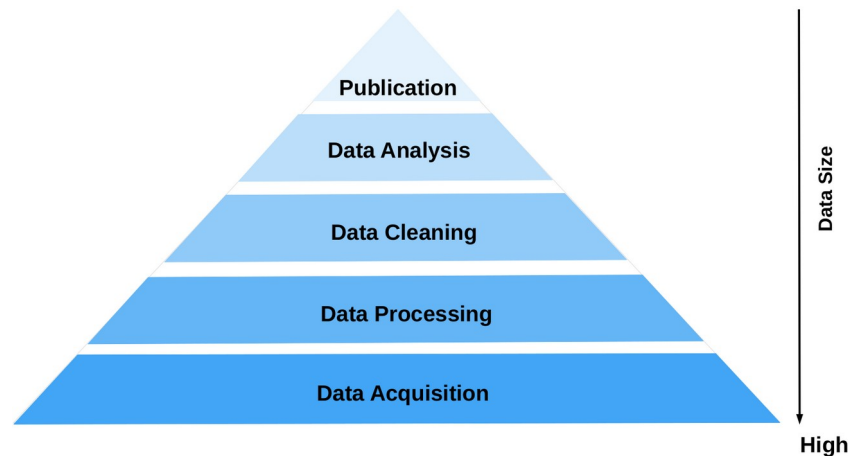
Reproducibility Crisis*



Source: 1,500 scientists lift the lid on reproducibility

Reproducibility Measures

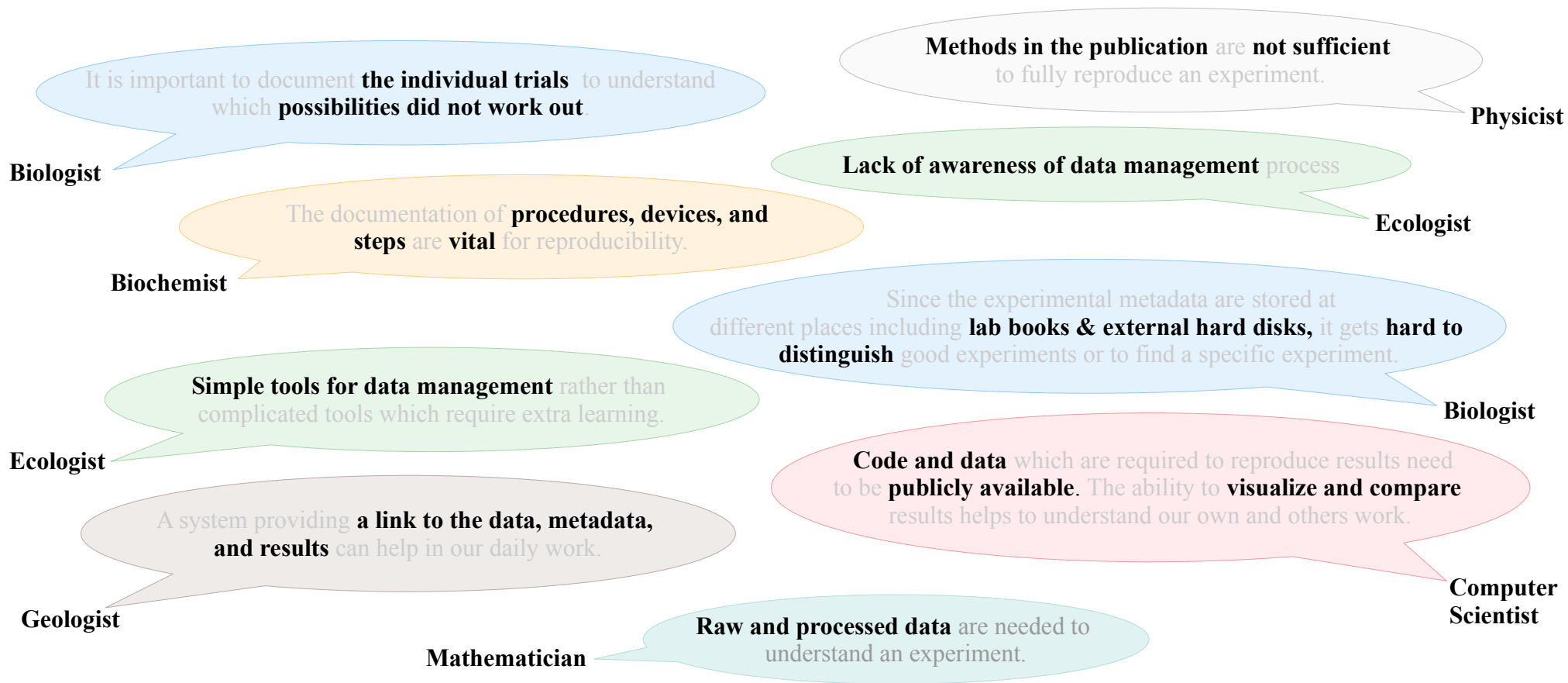
“Authors are required to make materials, data, code, and associated protocols promptly available to readers without undue qualifications.” - **nature**research



* [Kaiser 2015, Peng 2015, Begley and Ioannidis 2015, Baker 2016, Hutson 2018]



Insights from Interviews



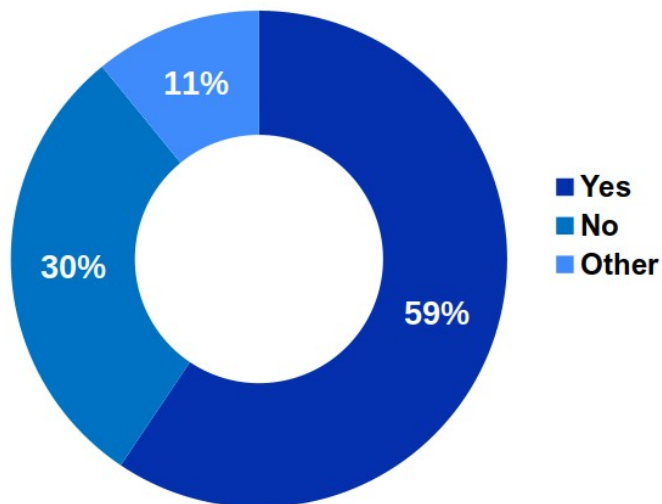
Survey on experiments and research practices for reproducibility



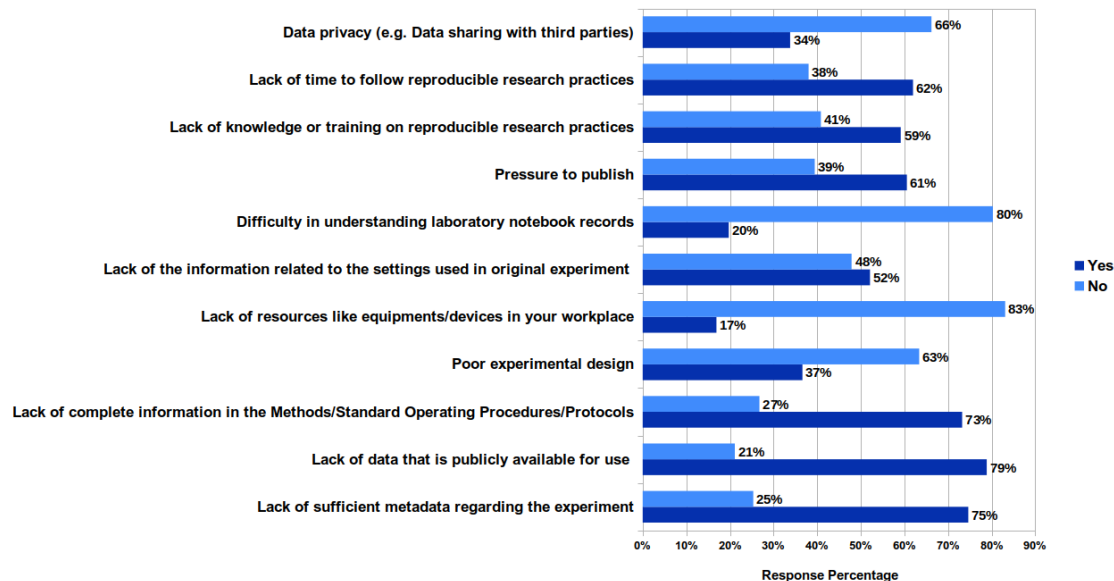
Findings

- More than half (59%) of the participants think that there is a reproducibility crisis
- 54% of the participants had trouble reproducing other's published results

Do you think there is a reproducibility crisis in your field of research?



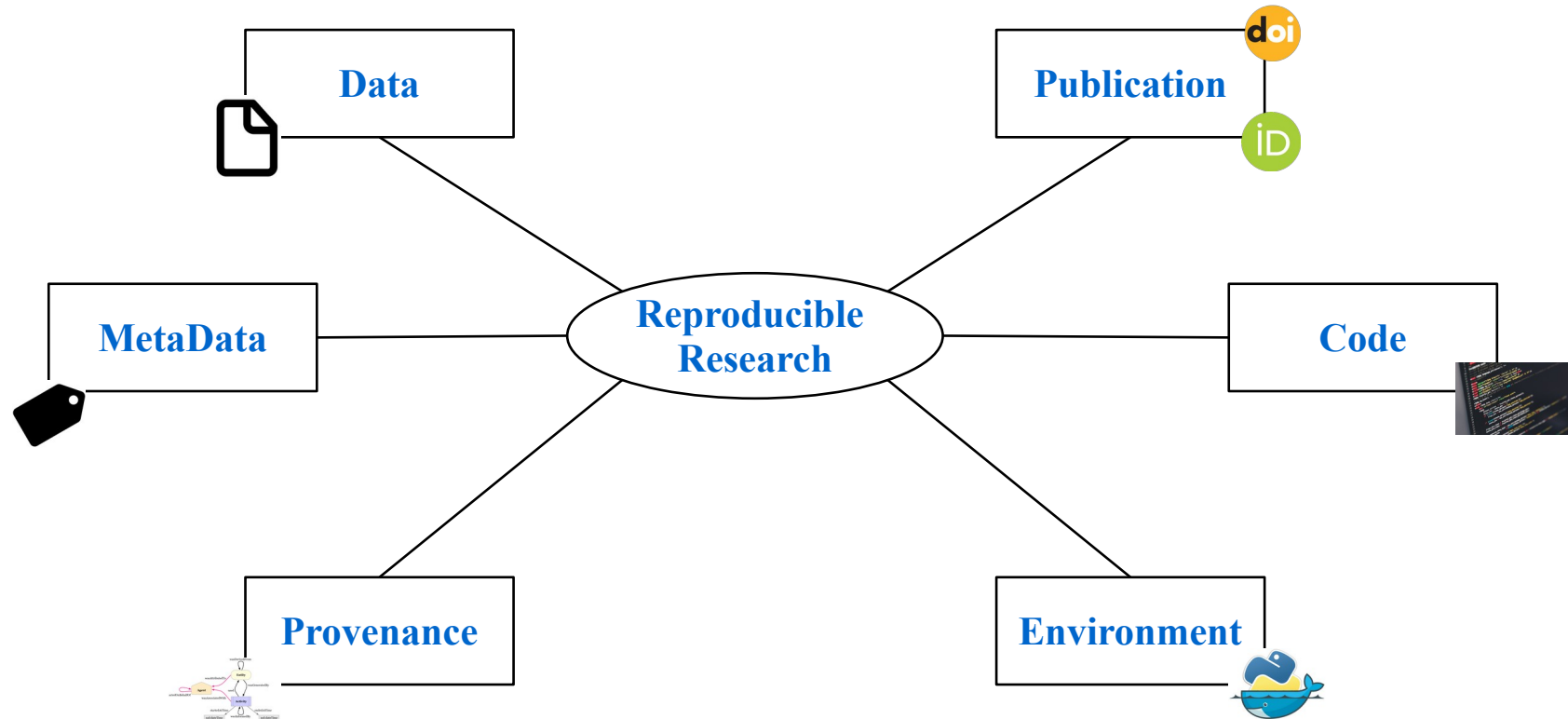
In your experience, what are the factors leading to poor reproducibility?





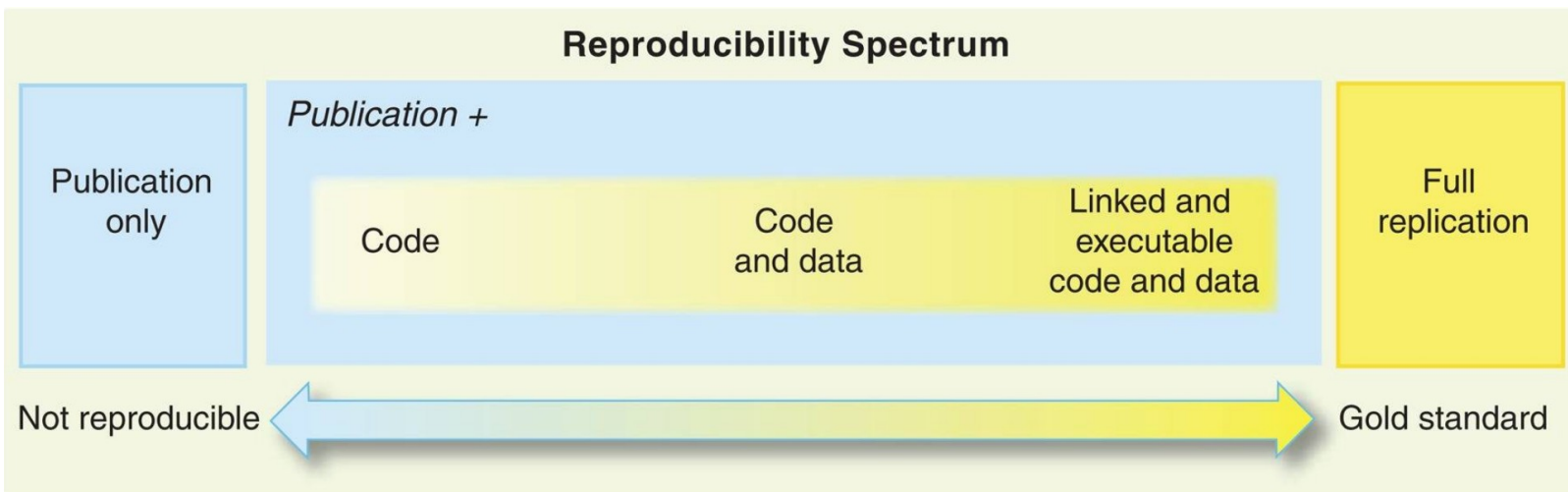
What is Reproducible Research?

- Reproducible Research refers to the idea that scientific results are documented and published in a way that others may verify the findings and build upon them.





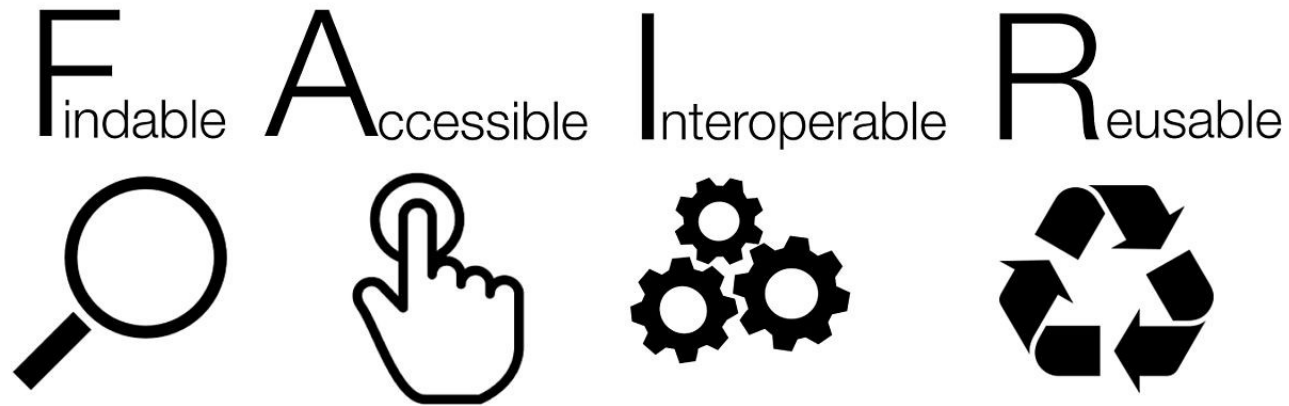
Reproducible Research in Computational Science



[Reproducible Research in Computational Science, Roger D. Peng, 2011]



FAIR Data Principles



The FAIR Guiding Principles for scientific data management and stewardship, Wilkinson et al. 2016

FAIR Data Principles:



- F1. (Meta)data are assigned a globally unique and persistent identifier
- F2. Data are described with rich metadata (defined by R1 below)
- F3. Metadata clearly and explicitly include the identifier of the data they describe
- F4. (Meta)data are registered or indexed in a searchable resource

FAIR Data Principles: A_{ccessible}



- A1. (Meta)data are retrievable by their identifier using a standardised communications protocol
 - A1.1 The protocol is open, free, and universally implementable
 - A1.2 The protocol allows for an authentication and authorisation procedure, where necessary
- A2. Metadata are accessible, even when the data are no longer available

FAIR Data Principles:



Interoperable



- I1. (Meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (Meta)data use vocabularies that follow FAIR principles
- I3. (Meta)data include qualified references to other (meta)data

FAIR Data Principles: R_{eusable}

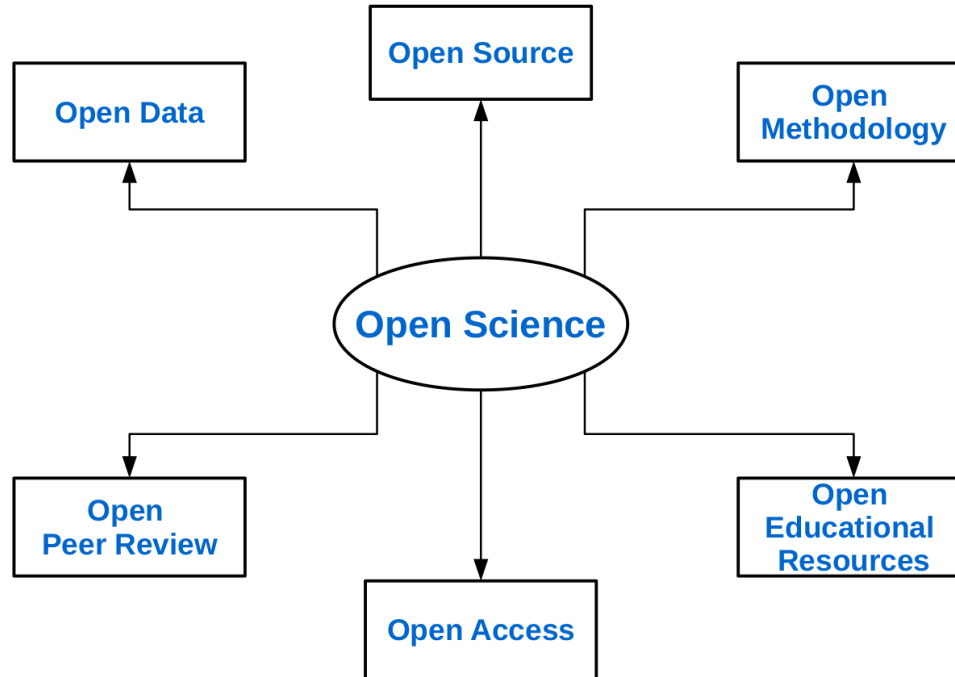


- R1. (Meta)data are richly described with a plurality of accurate and relevant attributes
 - R1.1. (Meta)data are released with a clear and accessible data usage license
 - R1.2. (Meta)data are associated with detailed provenance
 - R1.3. (Meta)data meet domain-relevant community standards



Open Science

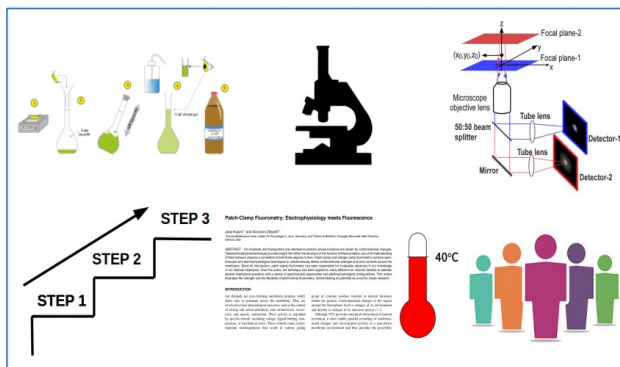
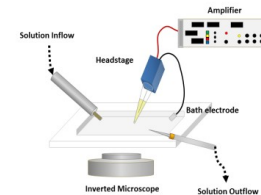
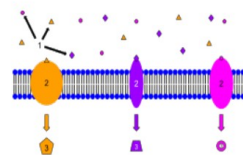
- Open science is the movement to make scientific research available to any member in society.



Open Reproducible Scientific Experiments



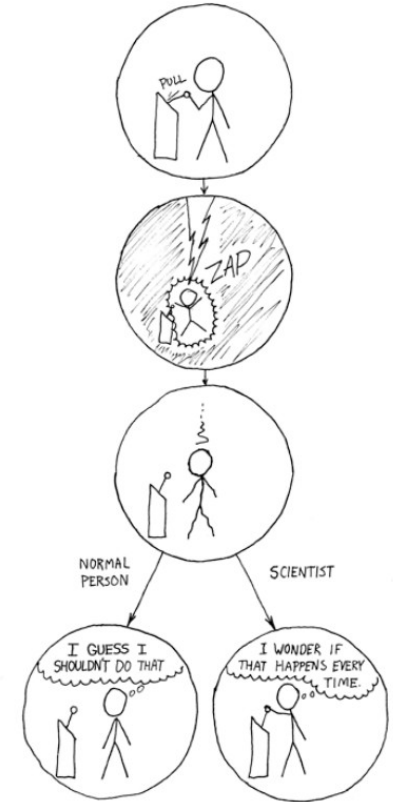
- Open Data
- Open Source
- Open Publications
- Open Experiment Materials
- Open Hardware
- Open Instruments
- Open Notebook Science
- Open Methodology
- Open Steps
- Open Data Standards
- Open Workflows
- Open File Formats



Factors behind irreproducible research



- Proprietary Data Standards and File Formats
- Availability of hardware
- Unavailability of Experiment Materials
- Not enough description in methodology
- Missing steps
- Human error
- Data and Software used to generate original results unavailable
- Difficulty in running computational steps
- Takes time



*Image Source: <https://xkcd.com/242/>

Why Reproducible Research?

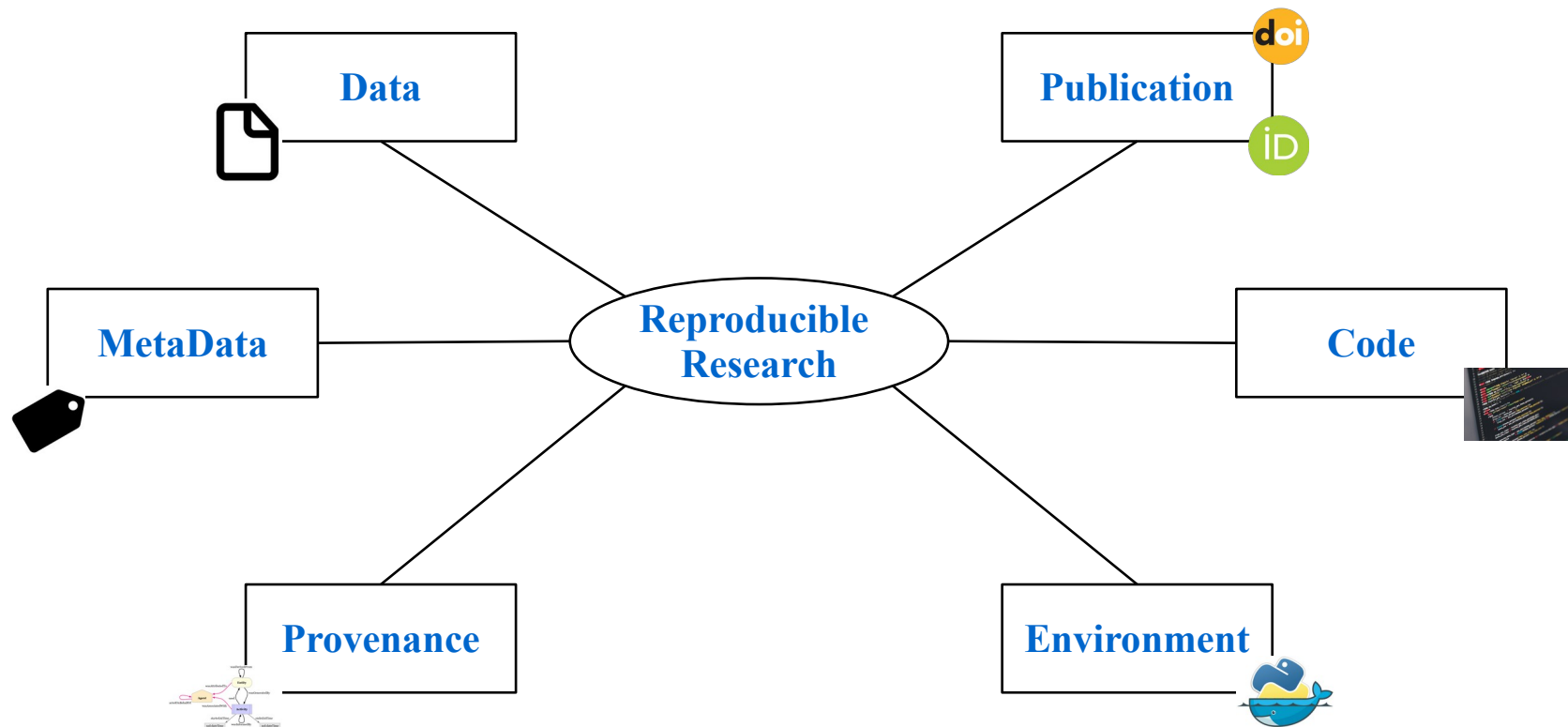
- Reproducible Research benefits
 - YOU
 - The research community



Image Source: <https://doi.org/10.6084/m9.figshare.5577340.v1>

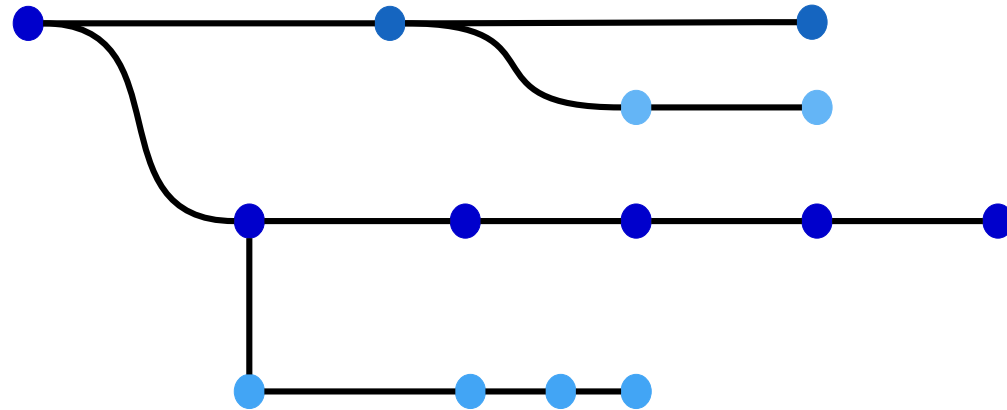


How do you make your work more reproducible?



Data Provenance

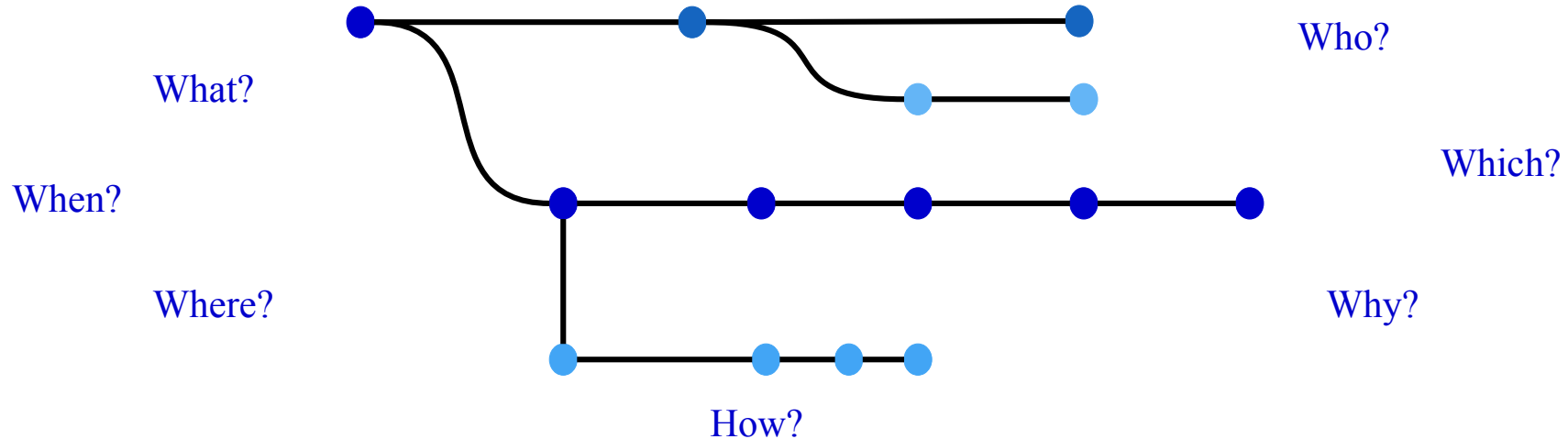
- The source or origin of an object; its history



The Semantics of Data Provenance

- W7 model: Provenance is defined as a n-tuple

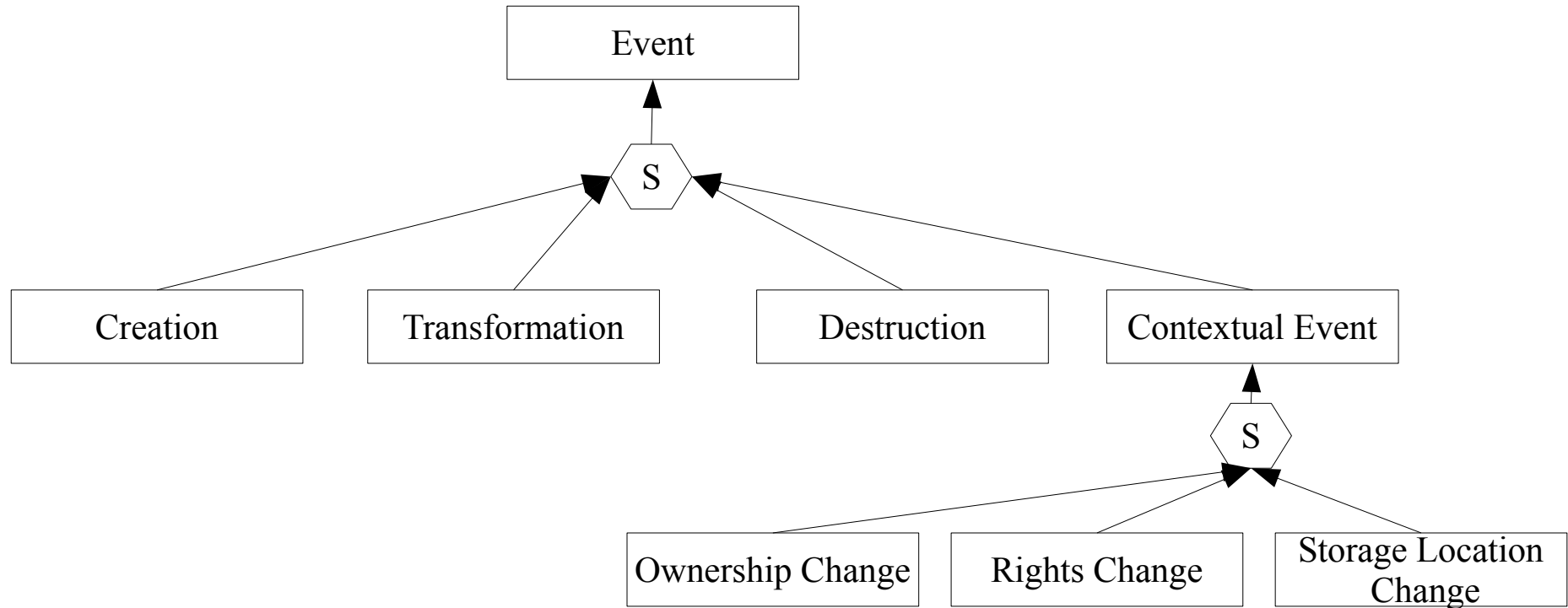
P = (WHAT, WHEN, WHERE, HOW, WHO, WHICH, WHY)





Semantics of 'What' Provenance

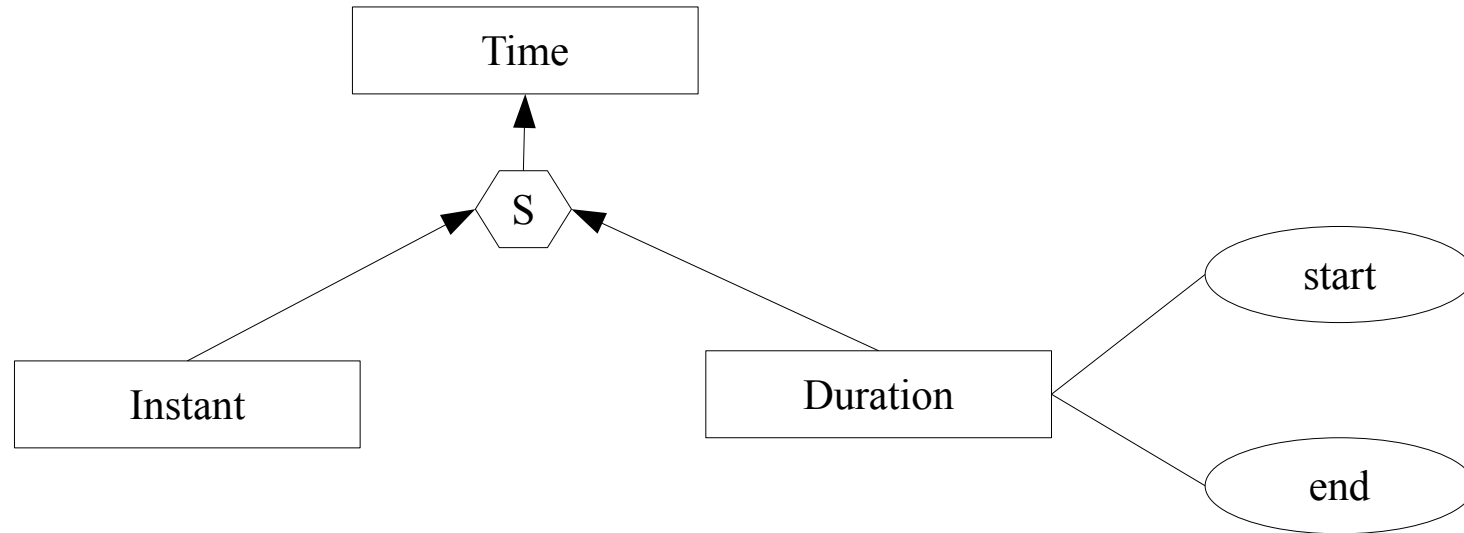
WHAT is a sequence of events that affect a data object during its life time.





Semantics of 'When' Provenance

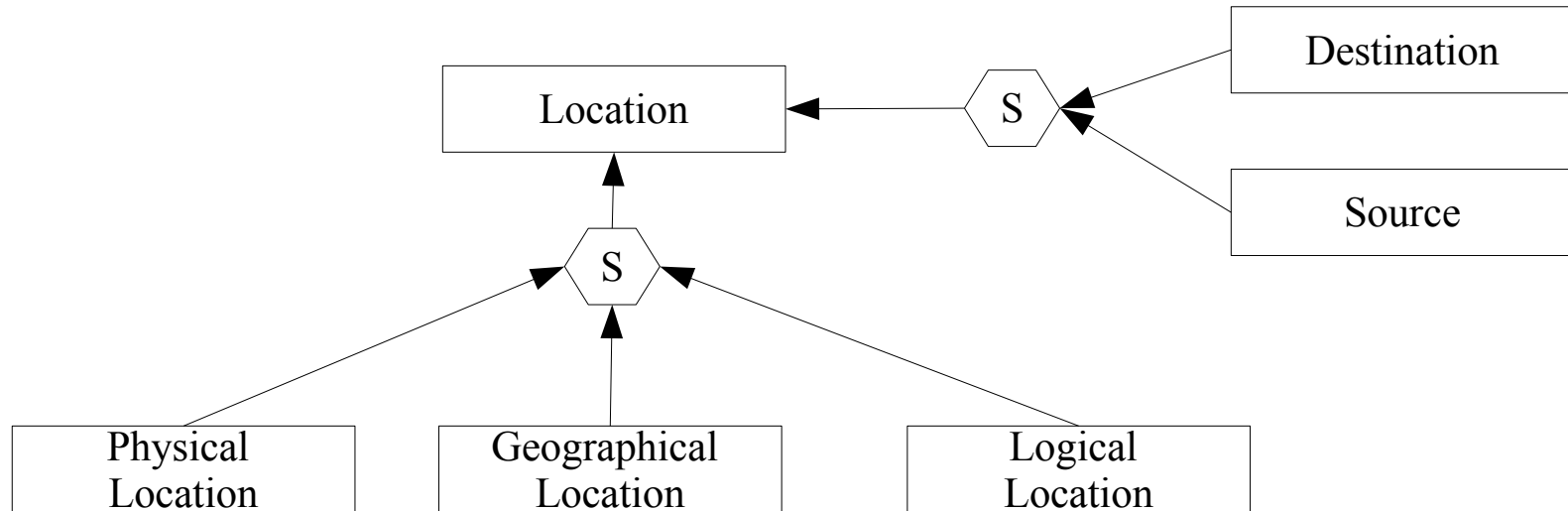
WHEN represents a set of timestamps associated with various provenance events.





Semantics of 'Where' Provenance

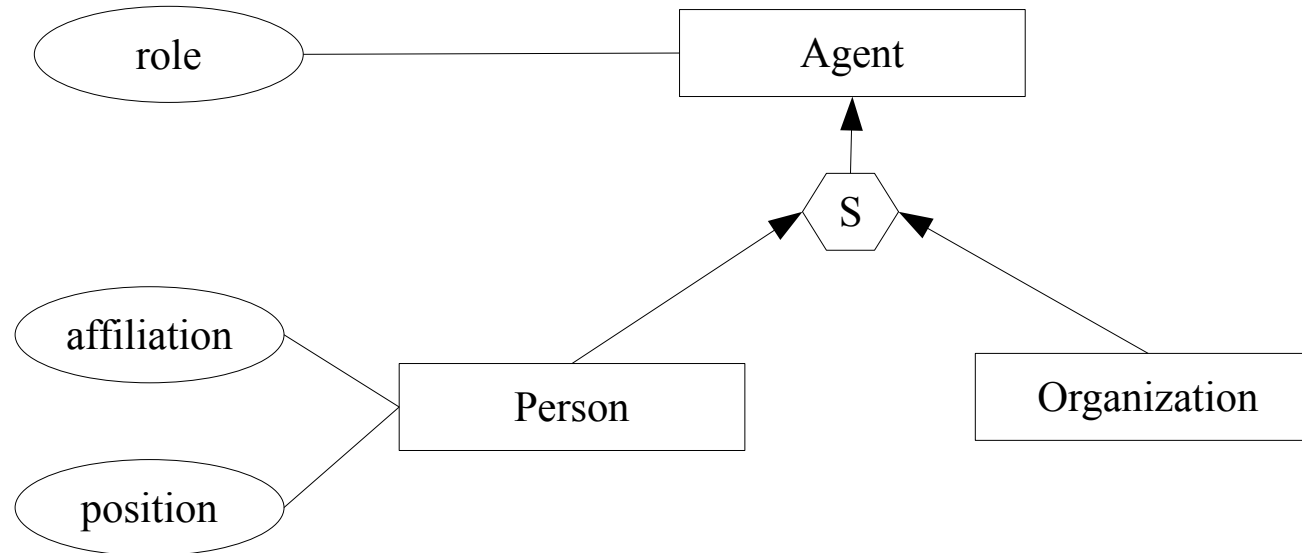
WHERE denotes a set of locations where various events happen.





Semantics of 'Who' Provenance

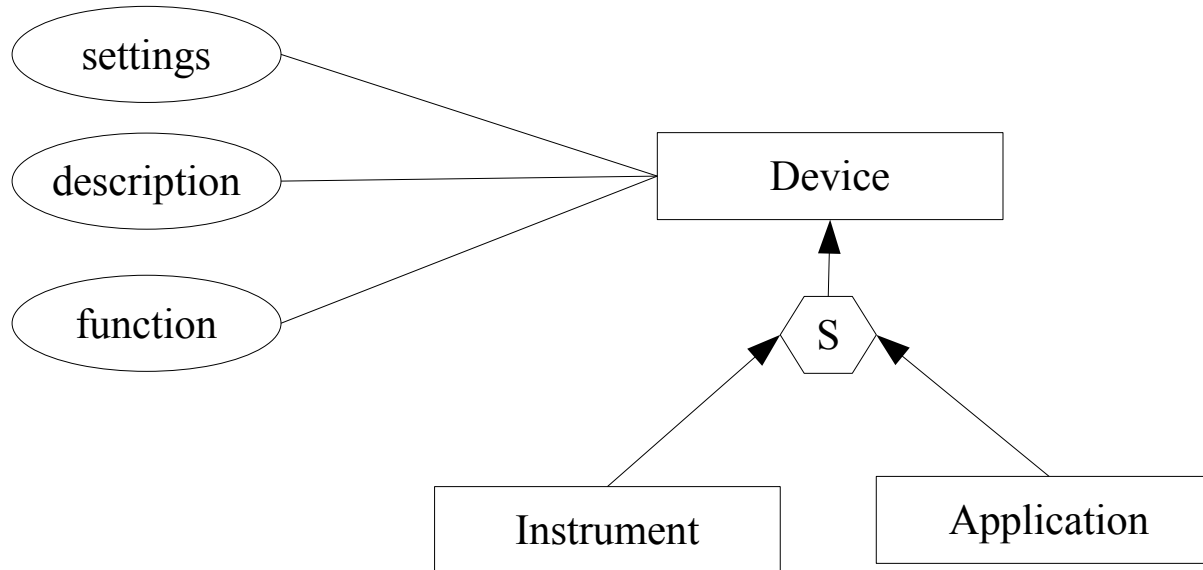
WHO is a triple (AGENT, ROLE, RL)





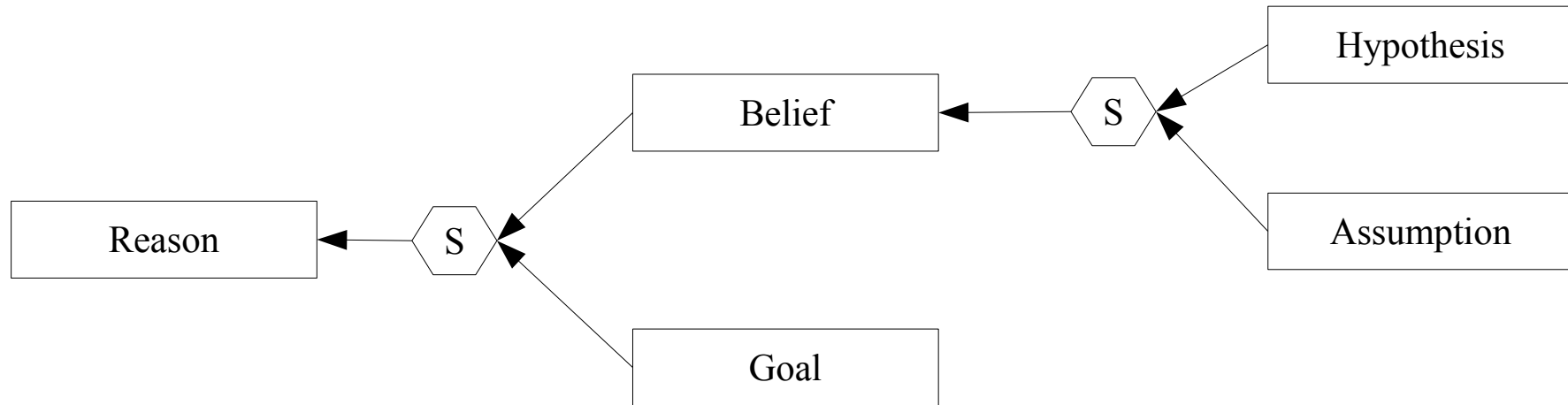
Semantics of 'Which' Provenance

WHICH is a tuple (DEVICE, SETTINGS, DESCRIPTION, FUNCTION, S, D, F).



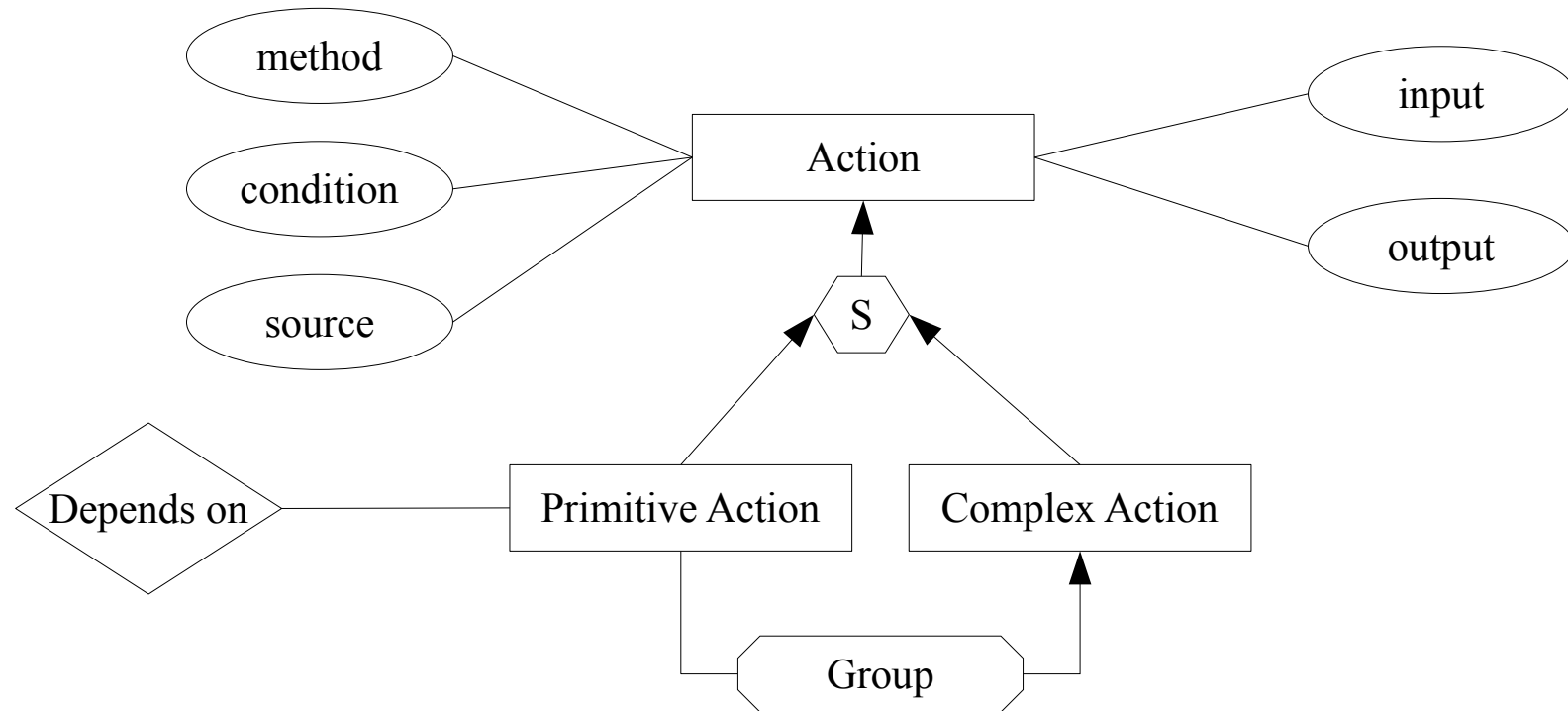
Semantics of 'Why' Provenance

WHY represents a set of reasons for various provenance events



Semantics of 'How' Provenance

HOW is defined as a tuple (ACTION, PRECONDITIONS, METHODS, INPUTS, OUTPUTS, SOURCES, P, M, I, O, S)



Benefits of Provenance Tracking



- Ensuring transparency and accountability in research.
- Facilitating collaboration and knowledge sharing.
- Enhancing the credibility of research results.

Provenance Tracking Tools



- **Version Control Systems**
 - Tools: Git, SVN
 - Tracks changes to source code, documents, and other project files.
 - Enables collaboration and versioning.
 - Records commit history, including user, date, and changes made.
- **Workflow Management Tools**
 - Tools: Apache Taverna, Galaxy, Kepler
 - Manages and tracks the entire research workflow.
 - Captures dependencies, inputs, and outputs.
 - Provides a visual representation of the workflow.



Provenance Tracking Tools

- **Provenance Representation**

- Tools: W3C PROV, Open Provenance Model (OPM)
- Standardizes representation of provenance information.
- Captures data and user provenance in a machine-readable format.
- Facilitates interoperability between different tools and systems.

- **Specialized Tools**

- Tools: Docker (<https://www.docker.com/>), ReproZip (<https://www.reprozip.org/>)
- Captures the computational environment and execution traces.
- Creates reproducible packages containing code, data, and dependencies.
- Ensures easy sharing and reproduction of computational experiments.



Open science contributions: Responding to 6W1H questions of data provenance

1 Semantic Description of Scientific Experiments

- **The REPRODUCE-ME Data Model & Ontology**
Semantic Description of Scientific experiments including Scripts and Computational Notebooks
- **The ReproduceMeON**
An Ontology Network for Reproducibility of Scientific Studies

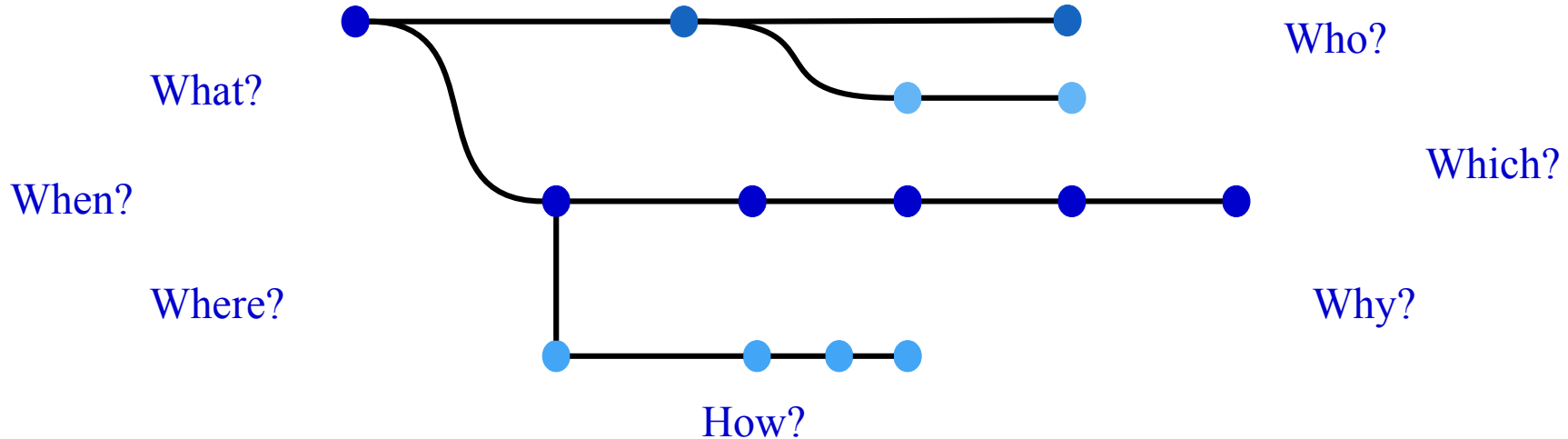
2 Support of computational reproducibility

- **ProvBook**
Provenance capture, visualize, represent and difference of results
- **MLProvLab**
Provenance capture, visualize, represent and difference of ML notebooks
- **ReproduceMeGit**
A tool for analyzing the reproducibility of Jupyter Notebooks
- **FAIR Jupyter**
Knowledge Graph for the reproducibility of Jupyter Notebooks

Representing 6W1H Provenance of Experiments

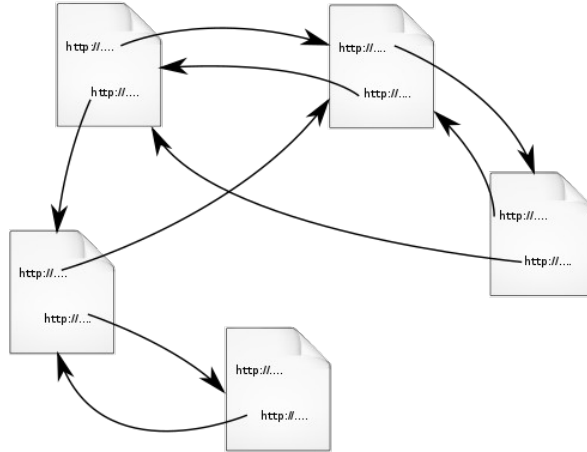


How should I represent the provenance of my experiments?

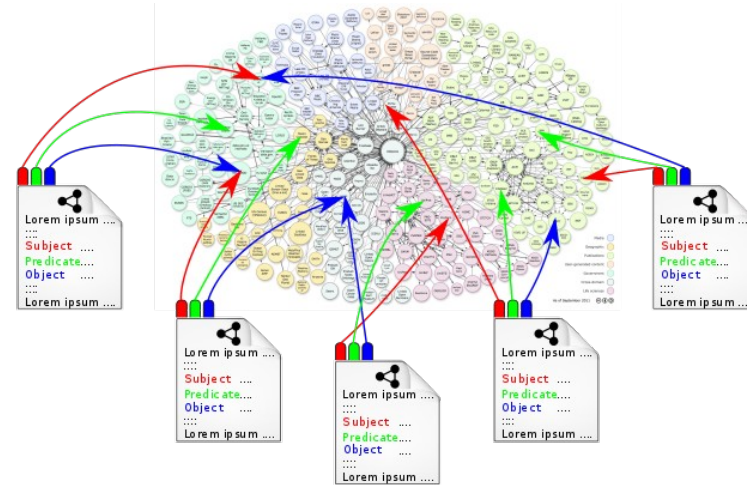


The REPRODUCE-ME Data Model & Ontology

Semantic Web



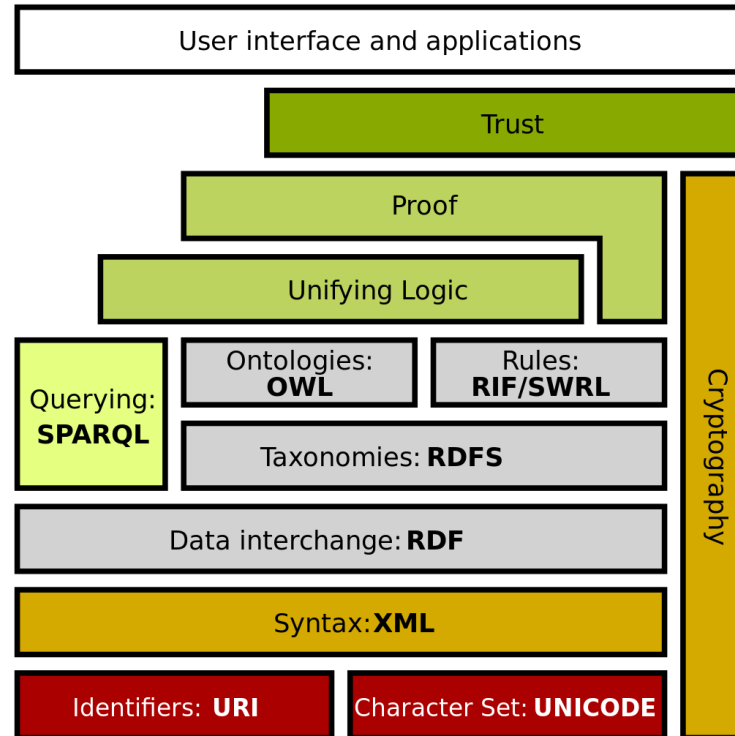
The traditional web -
A web of documents



The semantic web -
*A web of human and machine
readable content employing linked data*



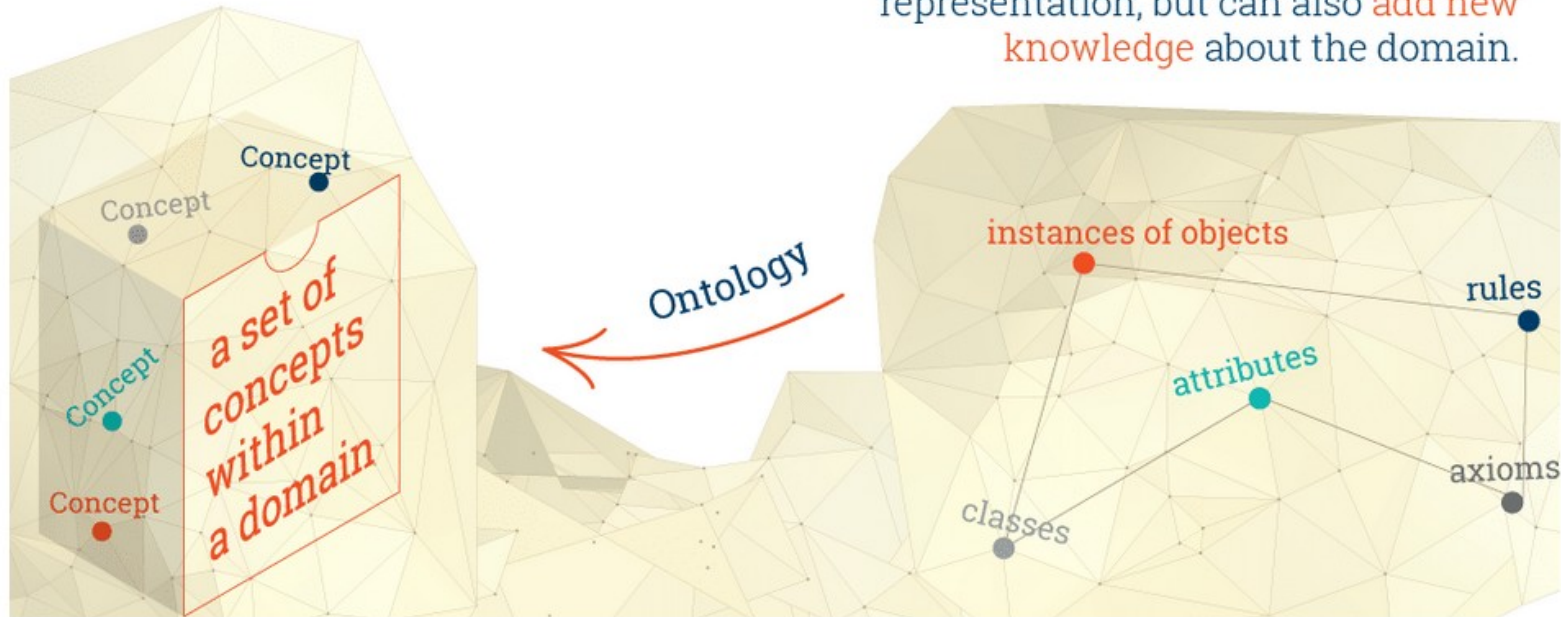
Semantic Web



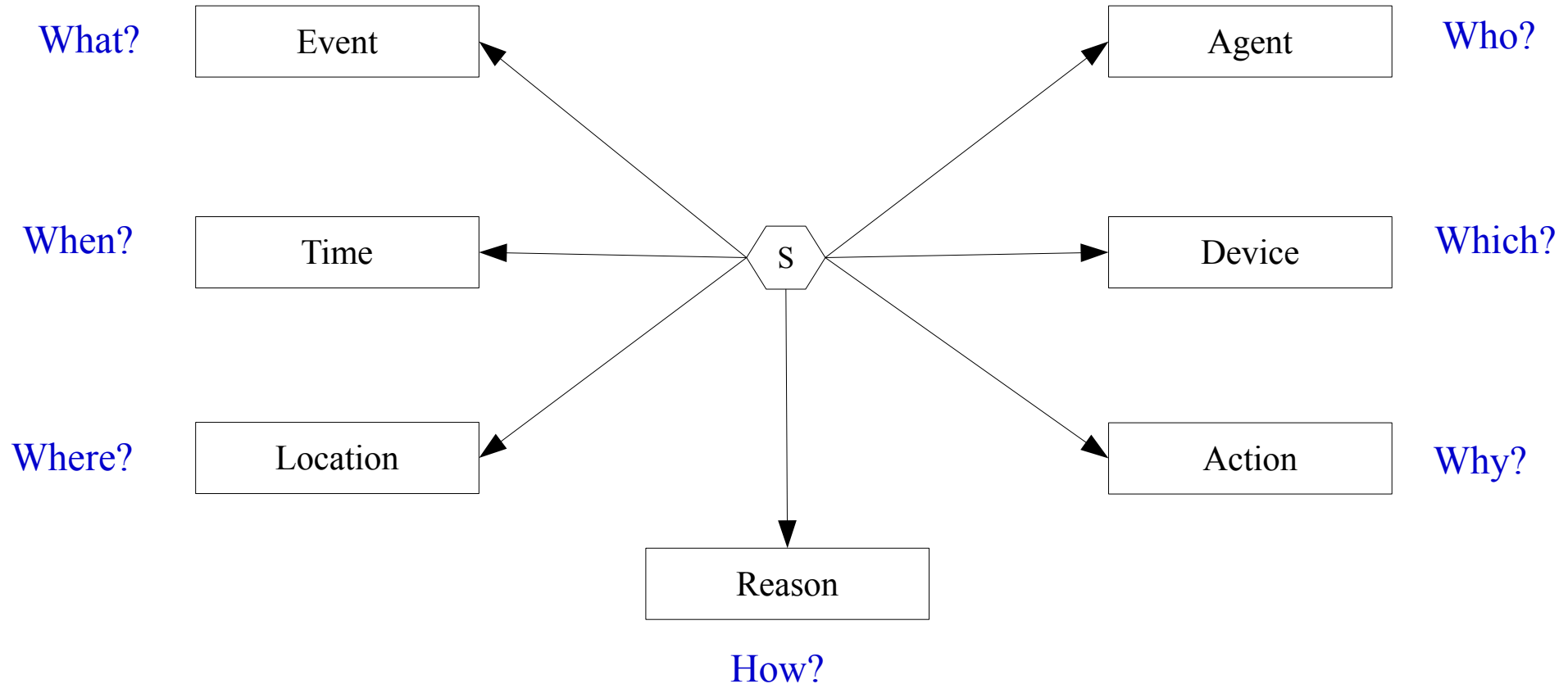
Ontologies

- An ontology is a formal, explicit specification of a shared conceptualization.
[Studer et al., 1998]

Ontologies do not only introduce a sharable and reusable knowledge representation, but can also add new knowledge about the domain.



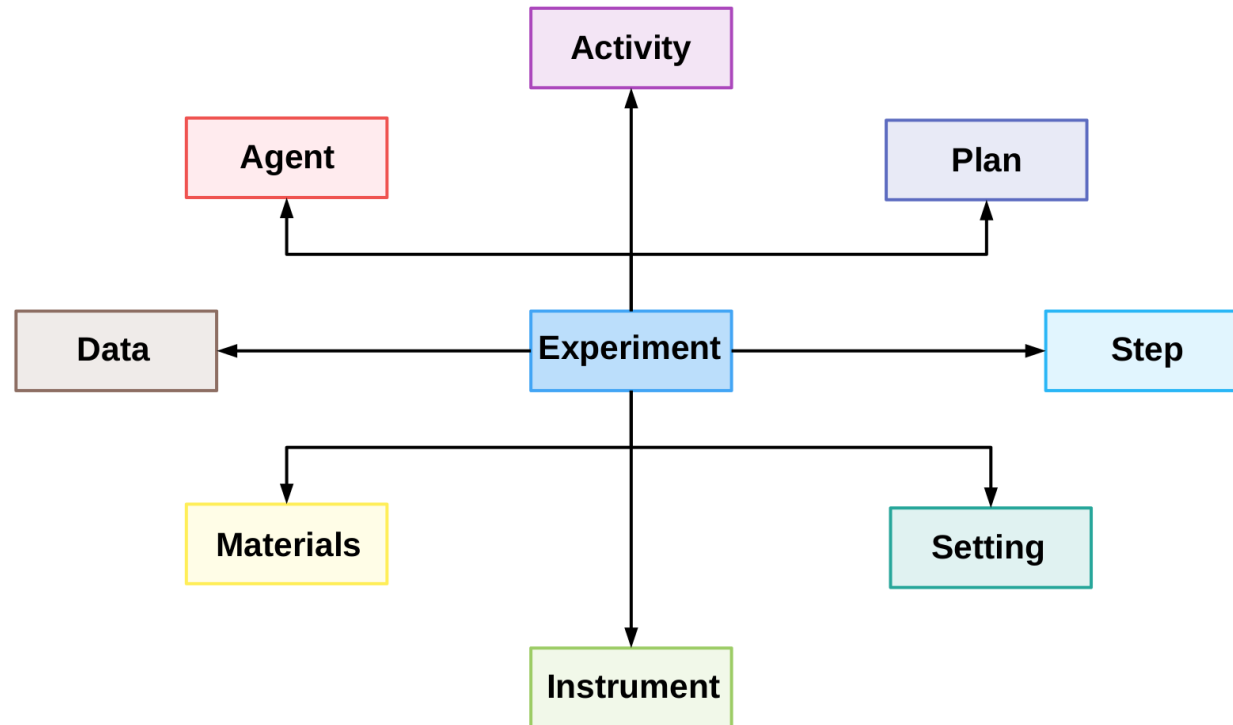
Representation of semantics of provenance



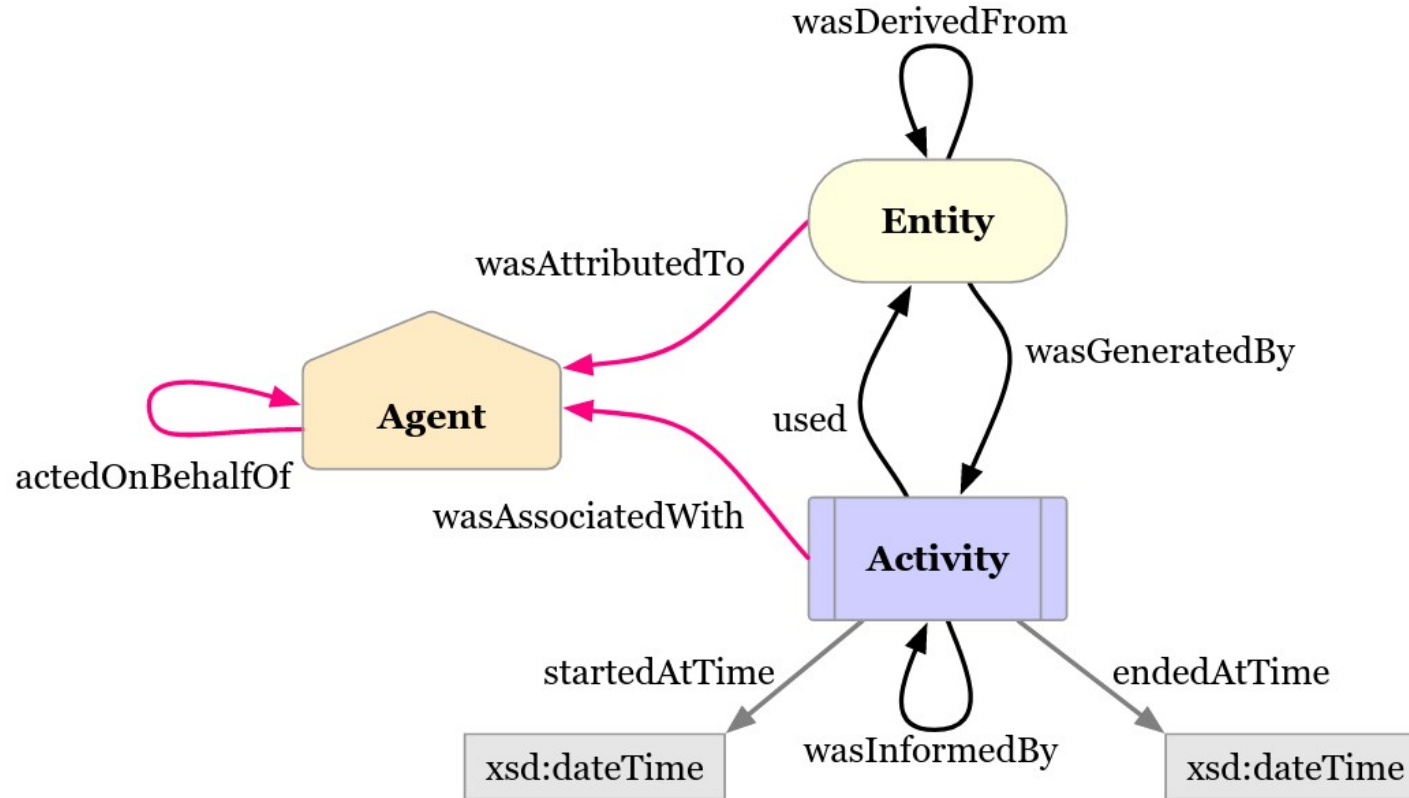
The REPRODUCE-ME Data Model

Experiment is defined as an n-tuple

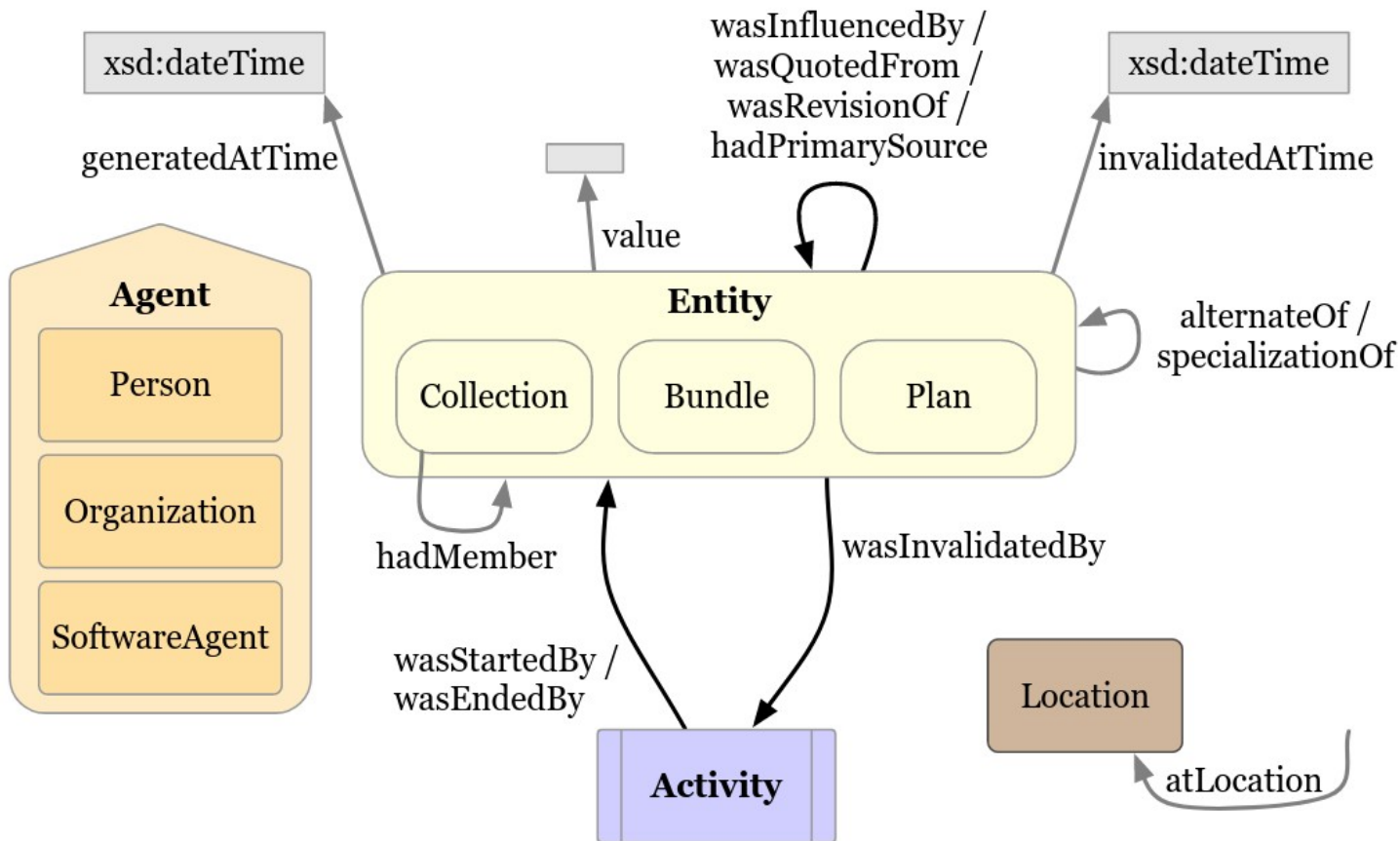
$$E = (\text{Data, Agent, Activity, Plan, Step, Setting, Instrument, Material})$$



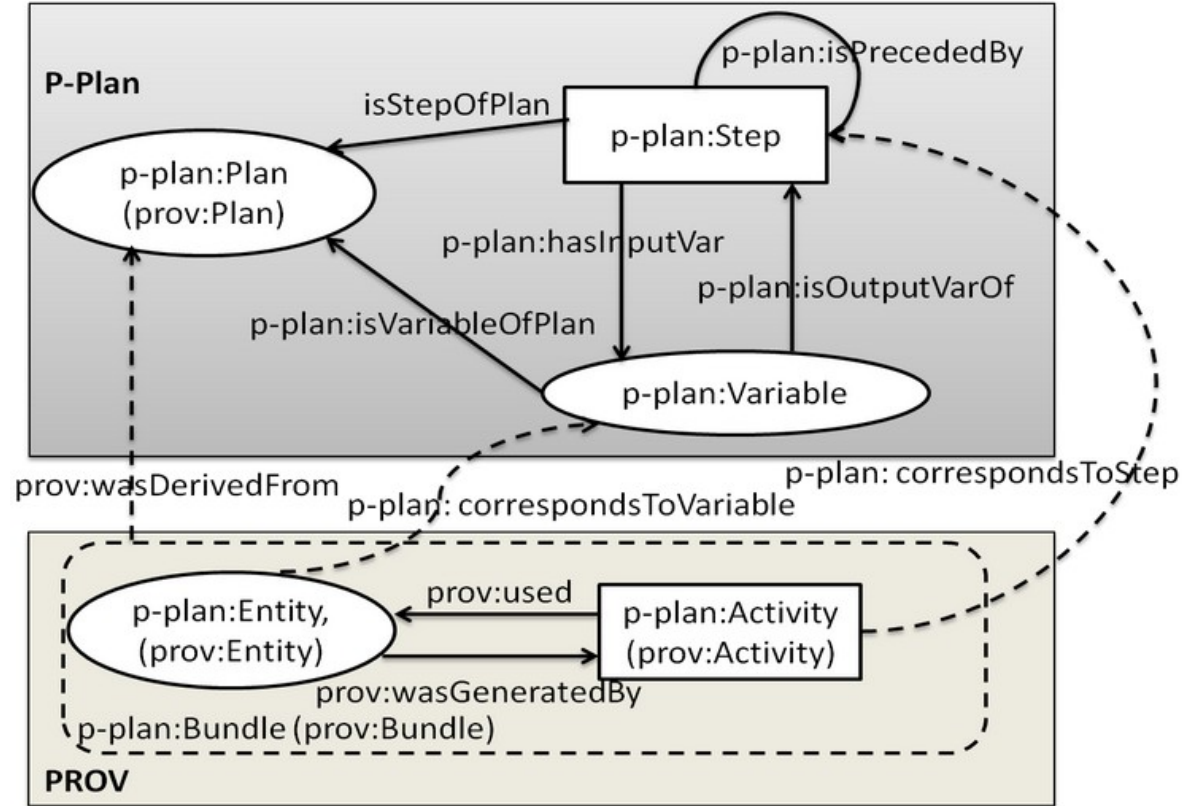
PROV-O: Ontology to represent provenance



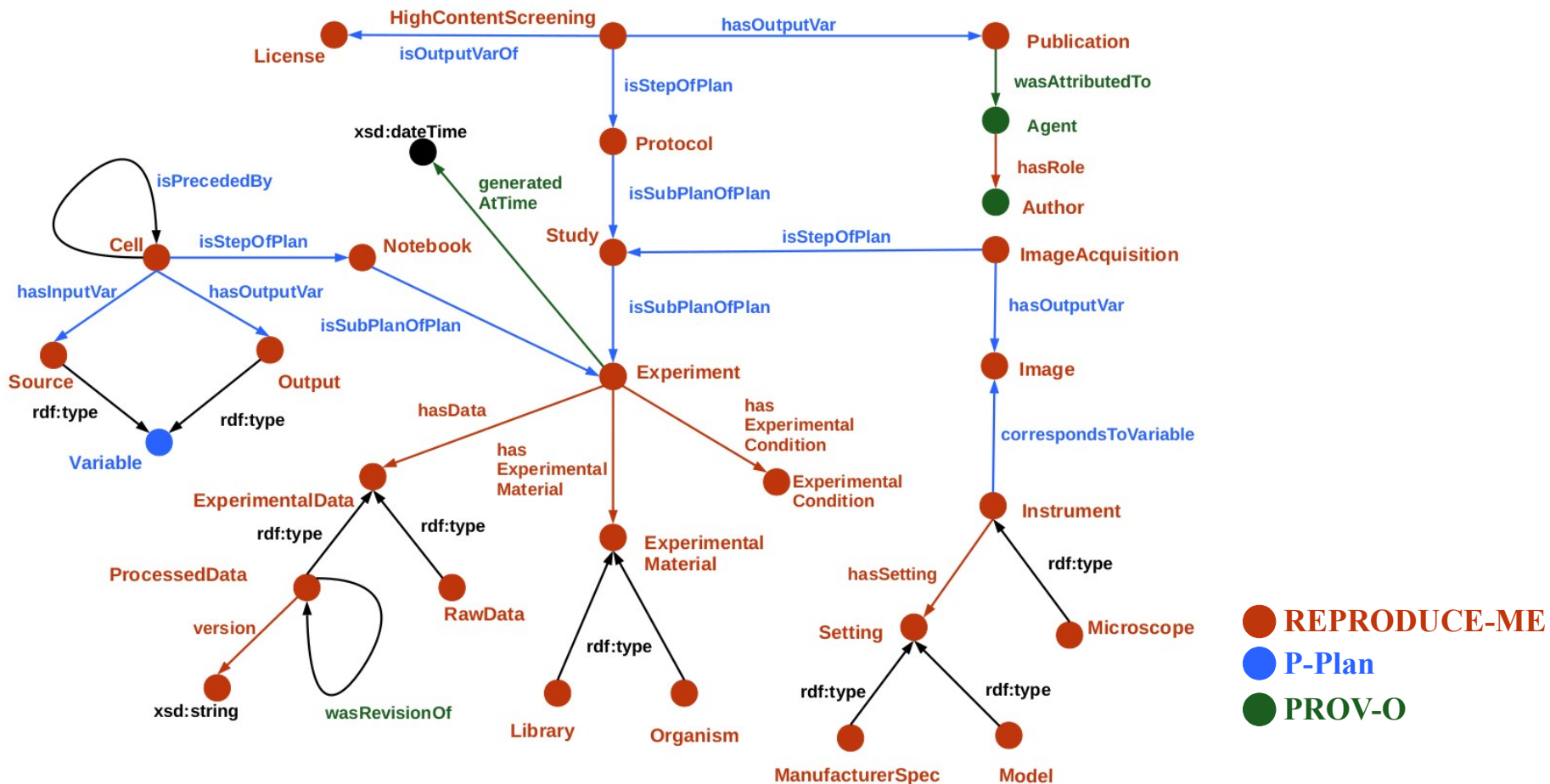
PROV-O: Ontology to represent provenance



P-Plan: Ontology to represent plans



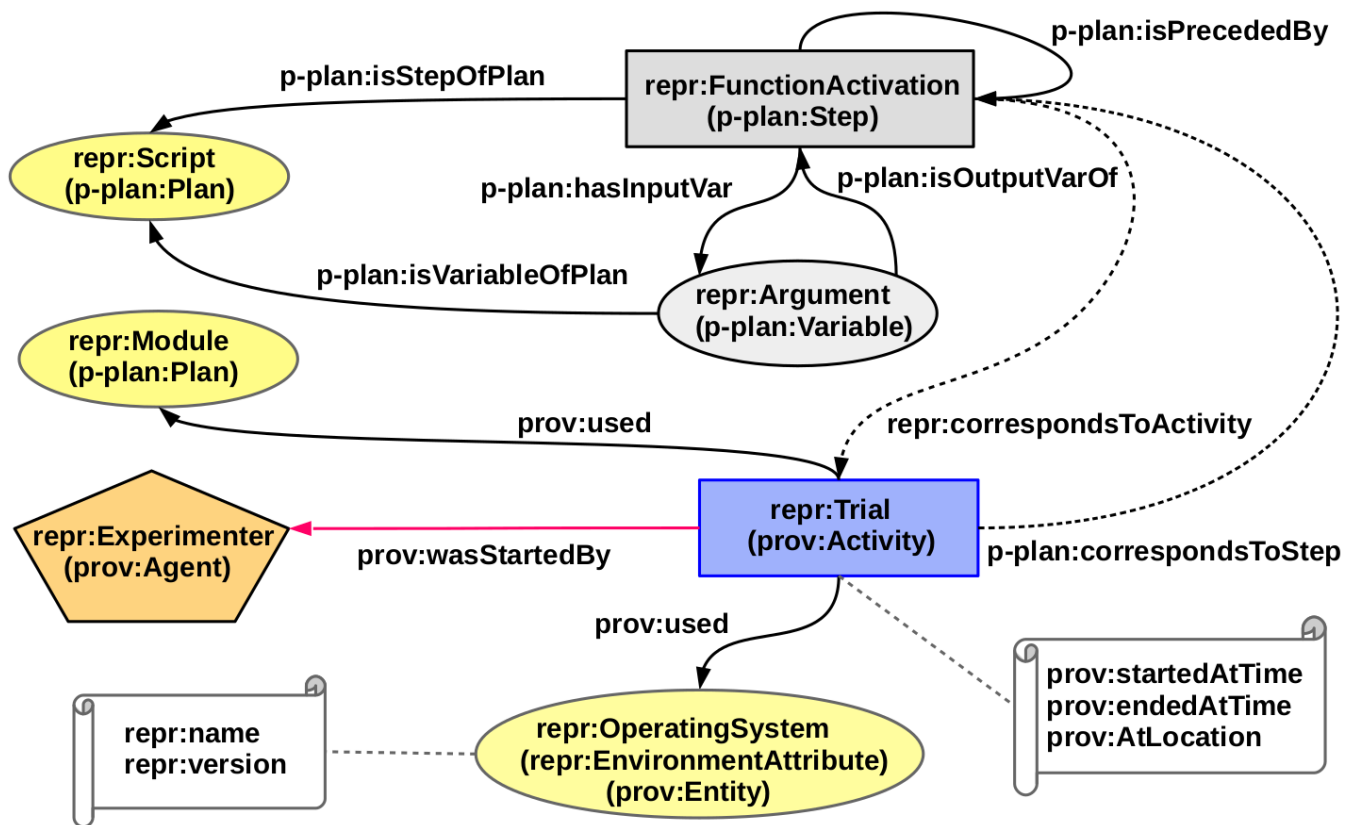
The REPRODUCE-ME Ontology



Script Provenance

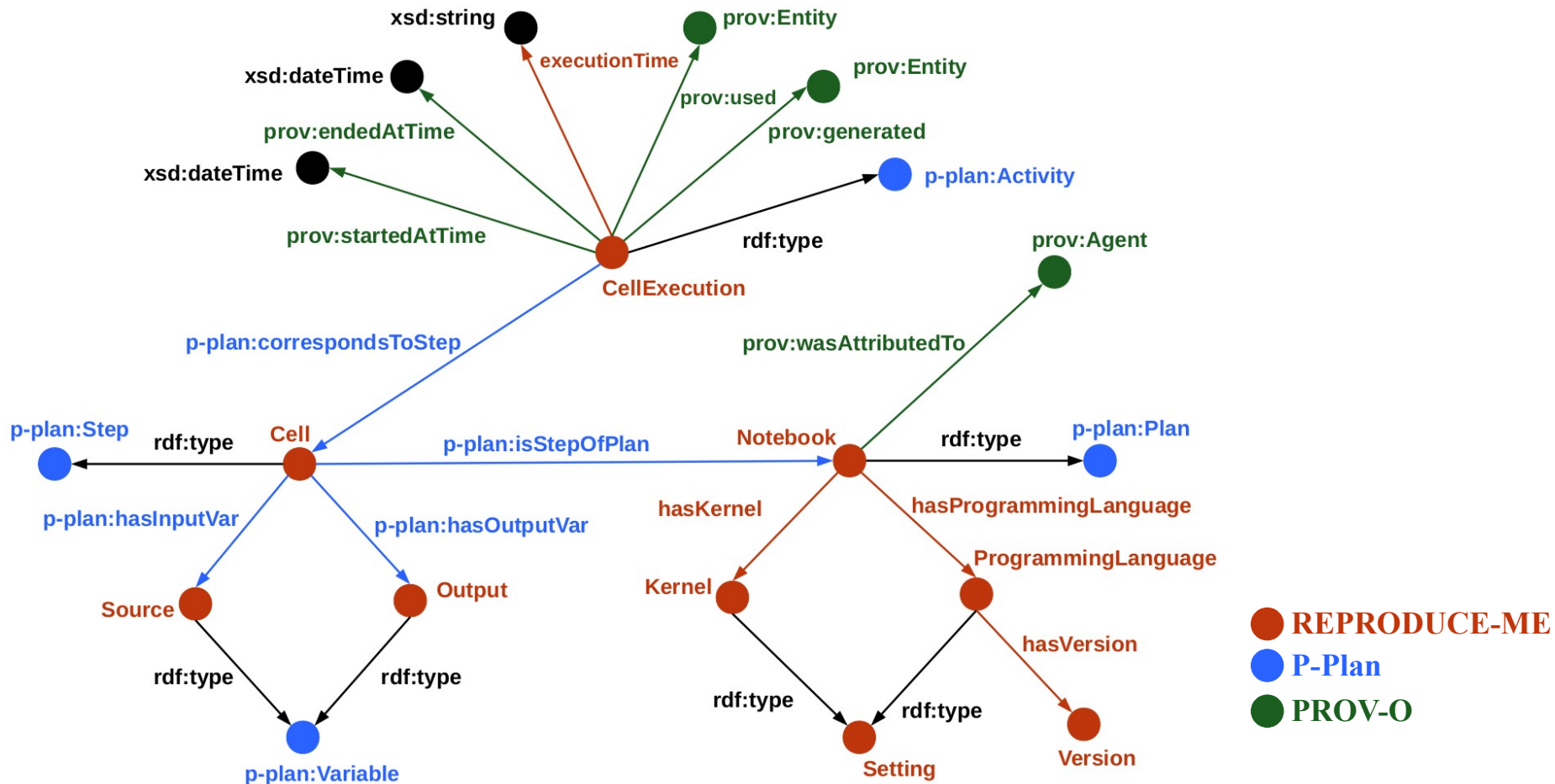


Ontology term	Remarks
<i>repr:Script</i>	<i>p-plan:Plan</i>
<i>repr:Function</i>	<i>p-plan:Plan</i>
<i>repr:Module</i>	<i>p-plan:Plan</i>
<i>repr:Version</i>	<i>repr:Setting</i>
<i>repr:Argument</i>	<i>p-plan:Variable</i>
<i>repr:Input</i>	<i>p-plan:Variable</i>
<i>repr:Output</i>	<i>p-plan:Variable</i>
<i>repr:FunctionActivation</i>	<i>p-plan:Step</i>
<i>repr:Trial</i>	<i>p-plan:Activity</i>
<i>repr:OperatingSystem</i>	<i>p-plan:Setting</i>
<i>repr:Author</i>	<i>prov:Person</i>
<i>prov:startedAtTime</i>	Data property
<i>prov:endedAtTime</i>	Data property
<i>p-plan:isPrecededBy</i>	Object property





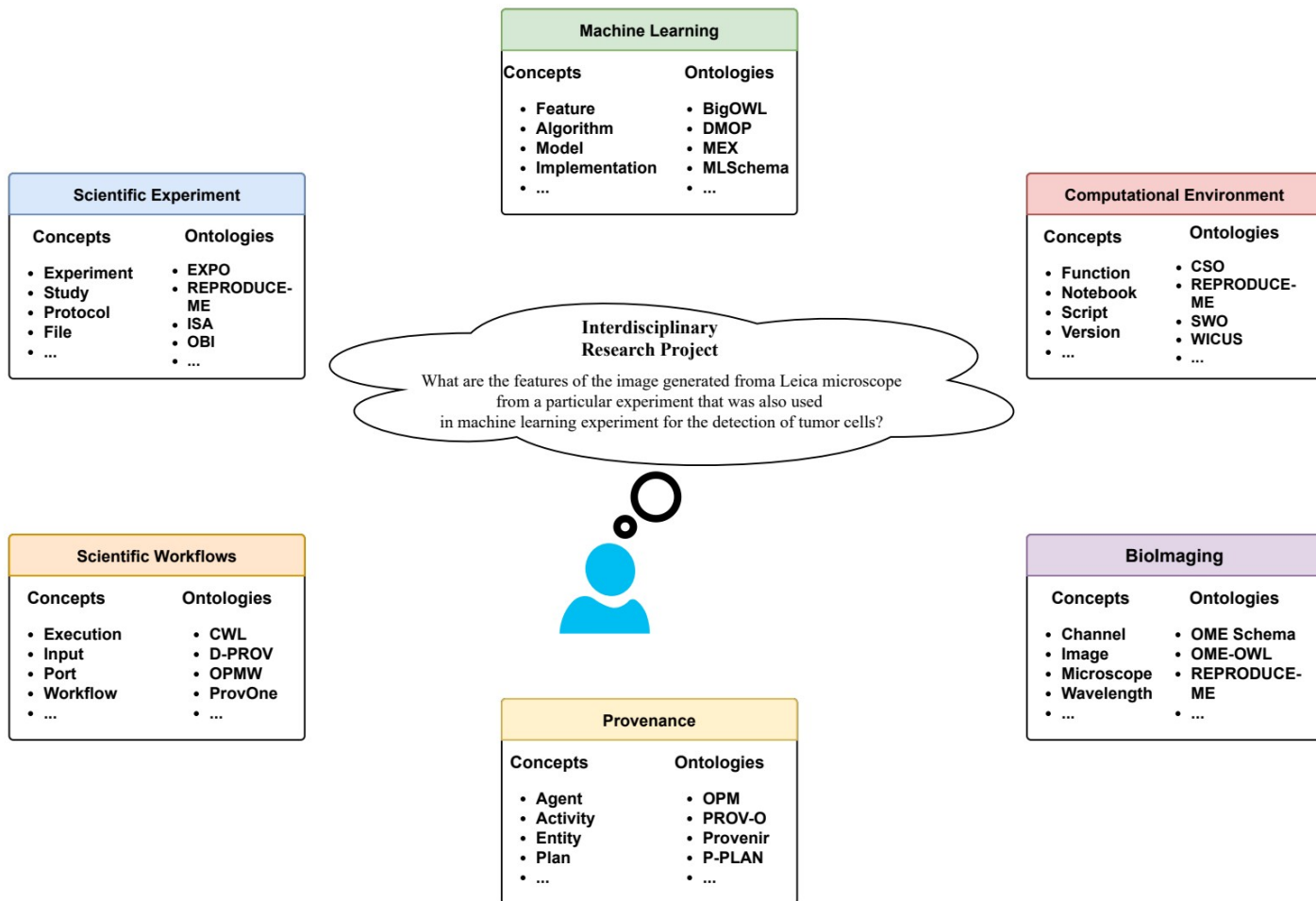
Computational Provenance



The ReproduceMe Ontology Network (ReproduceMeON)



Reproducibility related area assimilation





ReproduceMeON

- A novel approach that brings together knowledge from several domains, such as ML, provenance, and scientific computing, based on the three-layered architecture

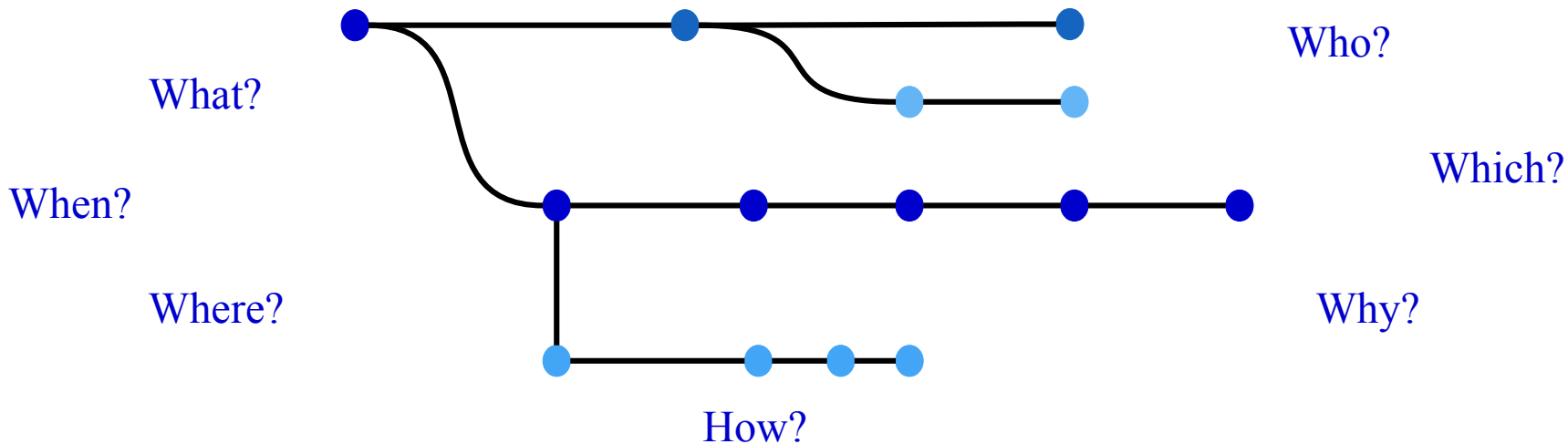




Capturing 6W1H Provenance of Computational Experiments



How should I capture and track the provenance of my computational experiments?



Computational Reproducibility

Computational Notebooks



- Share code along with documentation
 - Project Jupyter
 - RStudio

Jupyter Notebook Facts

- Formerly known as *IPython* Notebook
- 1.7 million Jupyter notebooks on Github
- Millions of *users*
- Different *computational kernels* including Python, R, and MATLAB
- Export in different *formats* like HTML, LaTeX, PDF

Structure of a Jupyter Notebook

Labels on the left side of the notebook interface:

- Markdown Cell
- Code Cell
- Output
- Raw Cell
- Execution Count



Computational Reproducibility

- **Provenance support is limited** [Rule et al., 2018, Pimentel et al., 2019]
 - Tracking provenance when the cells are over-written and re-run
 - Track how exactly a final result has been achieved
 - Track of the experiments that have been attempted
- **“Record all intermediate results in a standardized format”**
 - One of the ten simple rules for computational reproducible research [Sandve et al., 2013]

**Provenance
Capture**

**Provenance
Representation**

**Provenance
Storage**

**Provenance
Difference**

**Provenance
Visualization**

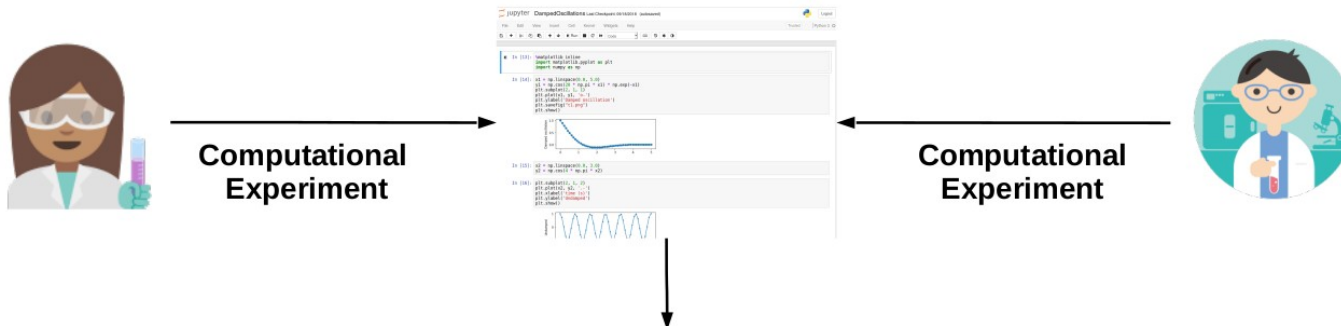


Computational Reproducibility

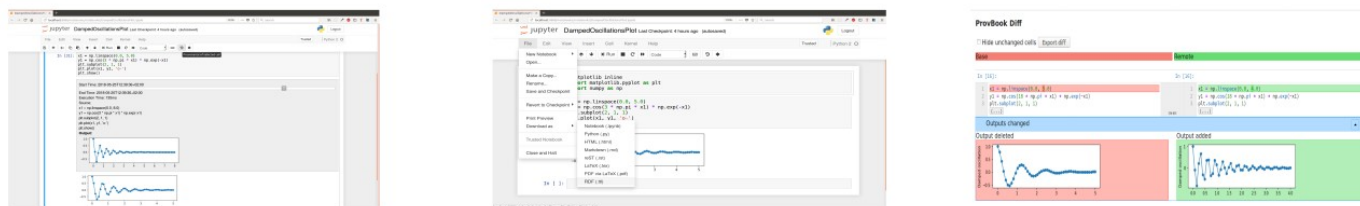
The key components for the end-to-end provenance management for computational reproducibility



ProvBook: Provenance of the Notebook



ProvBook: Provenance of the Notebook



Computational Reproducibility

ProvBook: Capture & Visualization



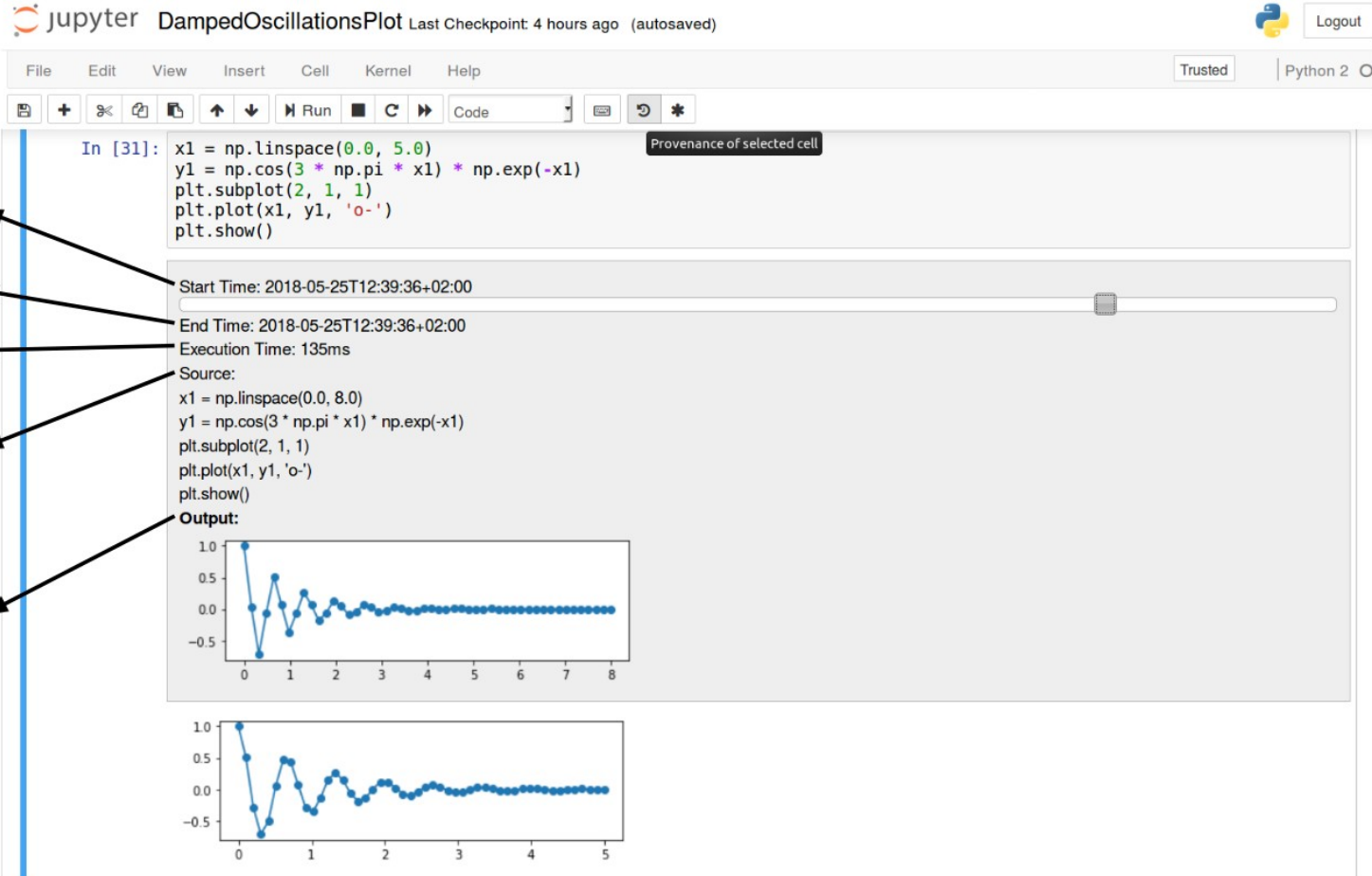
Start Time

End Time

Execution
Time

Source

Output



ProvBook: Difference



ProvBook Diff

☐ Hide unchanged cells

Export diff

Base

Remote

In [16]:

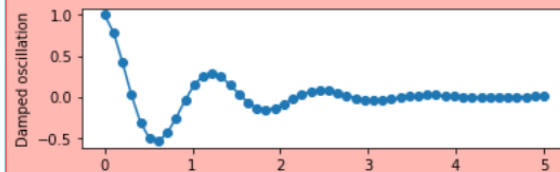
```
1 x1 = np.linspace(0.0, 5.0)
2 y1 = np.cos(18 * np.pi * x1) * np.exp(-x1)
3 plt.subplot(2, 1, 1)
  (...)
```

In [16]:

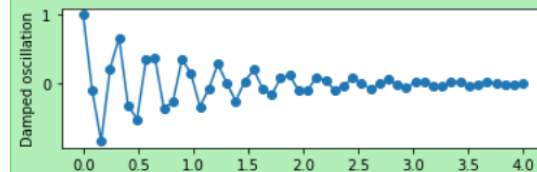
```
1 x1 = np.linspace(0.0, 4.0)
2 y1 = np.cos(18 * np.pi * x1) * np.exp(-x1)
3 plt.subplot(2, 1, 1)
  (...)
```

Outputs changed

Output deleted



Output added



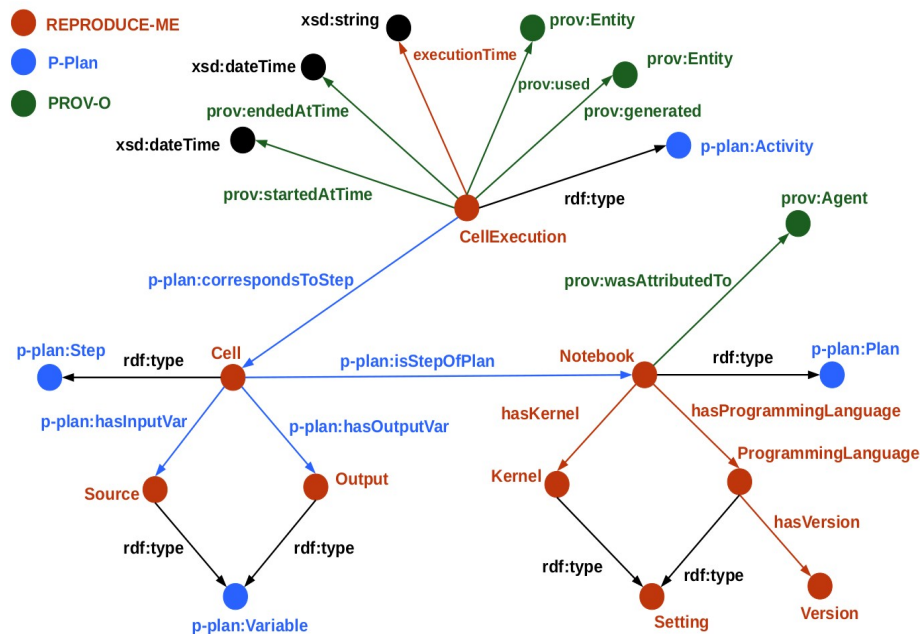


-
- Jupyter DampedOscillationsPlot Last Checkpoint: 4 hours ago (autosaved) Logout
- File Edit View Insert Cell Kernel Help Trusted Python 2 O
- New Notebook Open... Make a Copy... Rename... Save and Checkpoint Revert to Checkpoint Print Preview Download as Trusted Notebook Close and Halt
- Notebook (.ipynb) Python (.py) HTML (.html) Markdown (.md) reST (.rst) LaTeX (.tex) PDF via LaTeX (.pdf) RDF (.ttl)
- ```

import matplotlib inline
import matplotlib.pyplot as plt
import numpy as np

x = np.linspace(0.0, 5.0)
y = np.cos(3 * np.pi * x) * np.exp(-x)
plt.subplot(2, 1, 1)
plt.plot(x, y, 'o-')

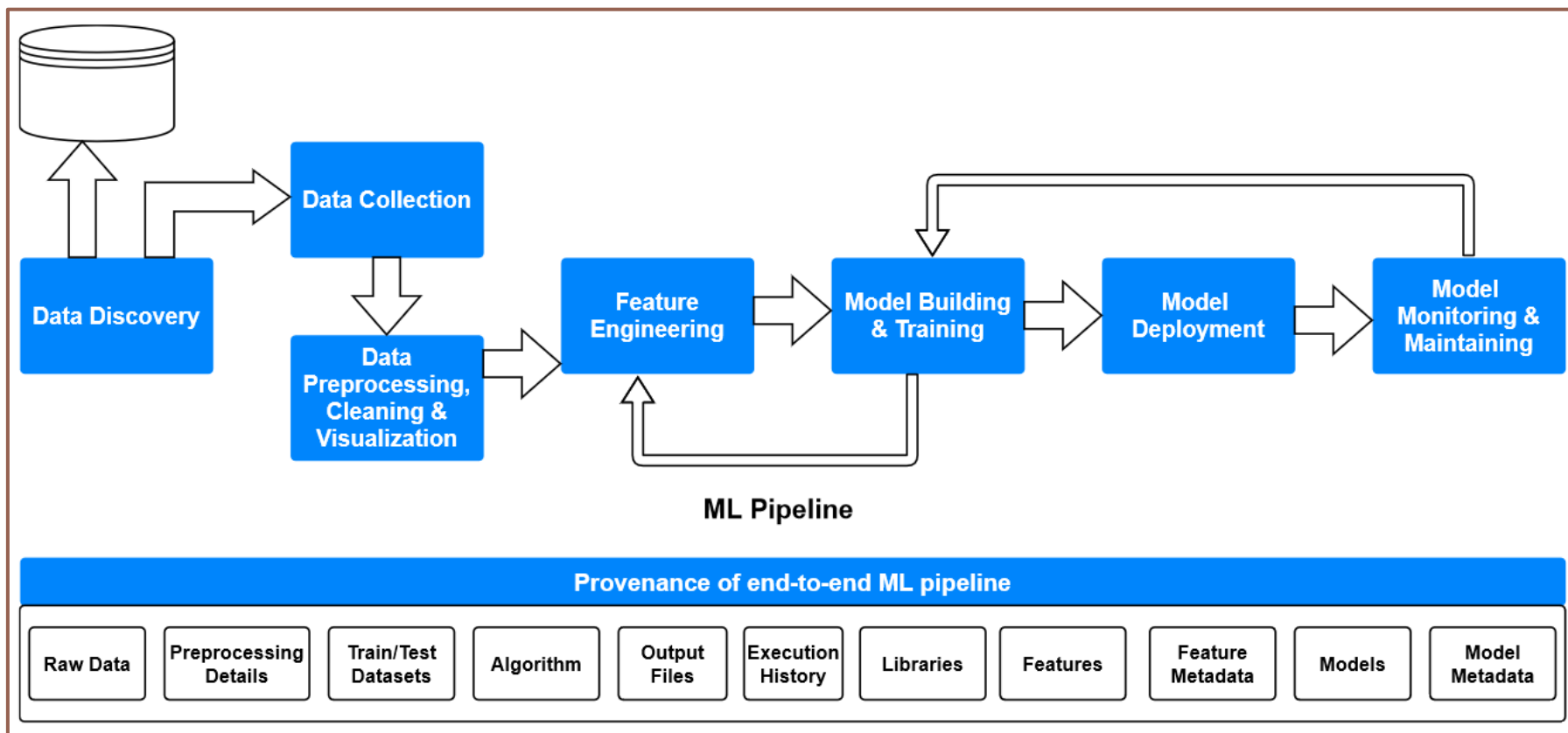
```
- 0. 3 4 5
- In [ ]:



[Samuel and König-Ries 2018a]

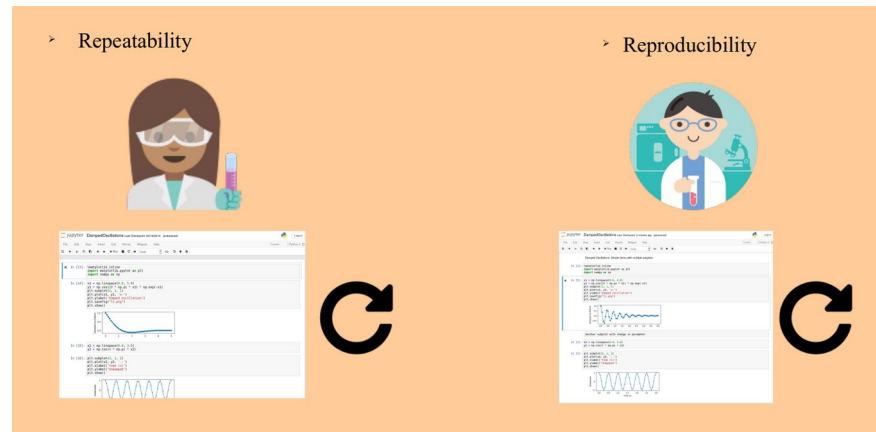


# Provenance of ML Pipelines





- Provenance management of end-to-end ML pipelines in a notebook environment
- An extension to JupyterLab
- This tool tracks, compares, manages, and visualizes provenance information
- Track, at runtime, the datasets, variables, libraries, and functions used in the notebook and their dependencies between cells.





# Provenance Capture

Dependencies between cells

Imported and Used Modules

Execution  
Information

Variable, Class, and  
Function Definitions

Code

Outputs

Function and Object Calls

Program Structure  
(Loops, Conditions)

```
[1]: import numpy as np
 from pandas import read_csv
 from sklearn.model_selection import train_test_split
 from sklearn.metrics import classification_report
 from sklearn.metrics import confusion_matrix
 from sklearn.metrics import accuracy_score
 from sklearn.svm import SVC

[2]: # Load dataset
 url = "https://raw.githubusercontent.com/jbrownlee/Datasets/master/iris.csv"
 names = ['sepal-length', 'sepal-width', 'petal-length', 'petal-width', 'class']
 dataset = read_csv(url, names=names)
 print(dataset)
```

# Modules and Libraries



evaluation\_notebook.ipynb

+

✂

📄

📄

▶

⏮

⏪

⏩

⏭

Download

MLProvLab

☁

☁

```

[5]: X=df.drop("label",axis=1).values
 y=df["label"].values

[6]: print(X.shape)
 print(y.shape)
 print(test.shape)

(42000, 784)
(42000,)
(28000, 784)

[7]: import matplotlib.pyplot as plt
 import seaborn as sns
 plt.figure(figsize=(15,10))
 sns.set_style("darkgrid")
 sns.countplot(x="label",data=df)

[7]: <AxesSubplot:xlabel='label', ylabel='count'>

```

```

[8]: from sklearn.model_selection import train_test_split
 X_train,X_test,y_train,y_test = train_test_split(
 print(X_train.shape)
 print(X_test.shape)
 print(y_train.shape)
 print(y_test.shape)

(39900, 784)
(2100, 784)

```

Provenance: evaluation\_not

Options

Export

Environment info

Import info

Code info

General info

Help

Info about imports and modules in epoch 4

Imports from module **keras.preprocessing.image**:

Import **ImageDataGenerator** was used 1 times

Imports from module **keras.utils.np\_utils**:

Import **to\_categorical** was used 1 times

Import **matplotlib.pyplot** with alias **plt** was used 3 times

Import **numpy** version 1.19.5 with alias **np** was used 0 times

Import **os** was used 2 times

Import **pandas** version 1.2.3 with alias **pd** was used 3 times

Import **seaborn** version 0.11.1 with alias **sns** was used 2 times

Epoch 4/4

Execution 19/19

Thu, 24 Jun 2021 10:19:30 GMT

Thu, 24 Jun 2021 10:26:21 GMT

65

# Datasets



Provenance: evaluation\_note ✕

Options

Export

Environment info

Import info

Code info

General info

Help

Source **D:/Projects/mnist-evaluation/data** was first used in execution **1** in variable

Source **D:/Projects/mnist-evaluation/data/train.csv** was first used in execution **2** in variable **df**

Source **D:/Projects/mnist-evaluation/data/test.csv** was first used in execution **3** in variable **test**

# Execution Environment



Provenance: evaluation\_note X

Options

Export

Environment info

Import info

Code info

General info

Help

## Environment information of epoch 3

**Language:** python

**Version:** 3.9.2

**Mimetype:** text/x-python

**Kernel start time:** Thu, 24 Jun 2021 10:17:35 GMT

**Kernel implementation:** ipython

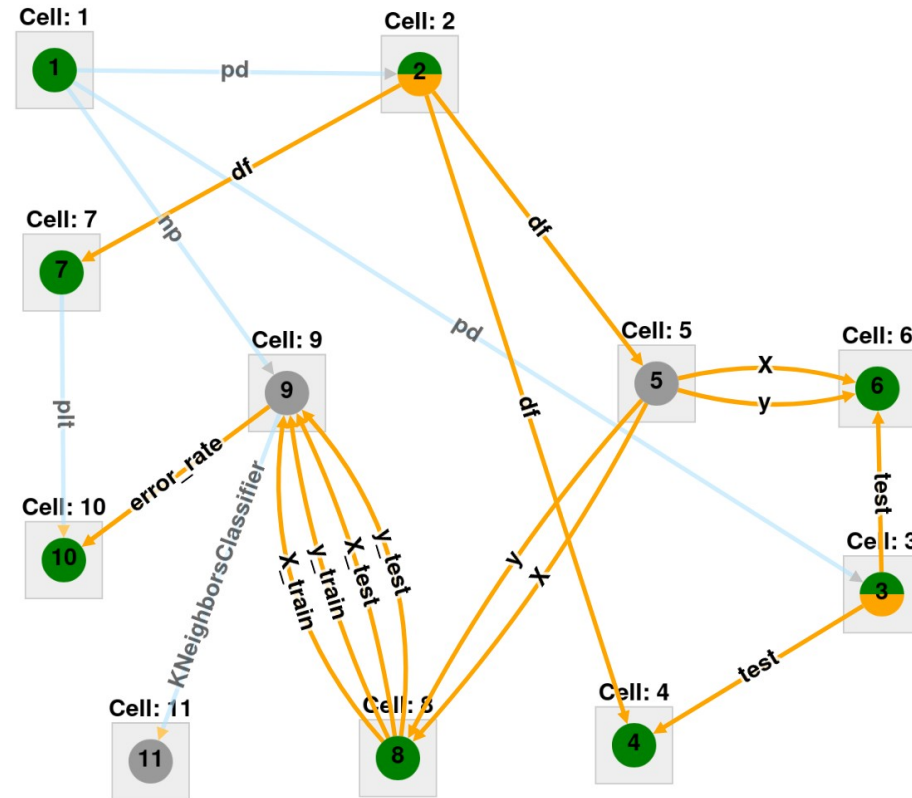
**Kernel version:** 7.22.0

**User agent:** Mozilla/5.0 (Windows NT 10.0; Win64; x64; rv:89.0) Gecko/20100101 Firefox/89.0

# MLProvLab: Provenance Visualization



|                               |        |                  |             |           |              |      |
|-------------------------------|--------|------------------|-------------|-----------|--------------|------|
| Provenance: evaluation_note X |        |                  |             |           |              |      |
| Options                       | Export | Environment info | Import info | Code info | General info | Help |

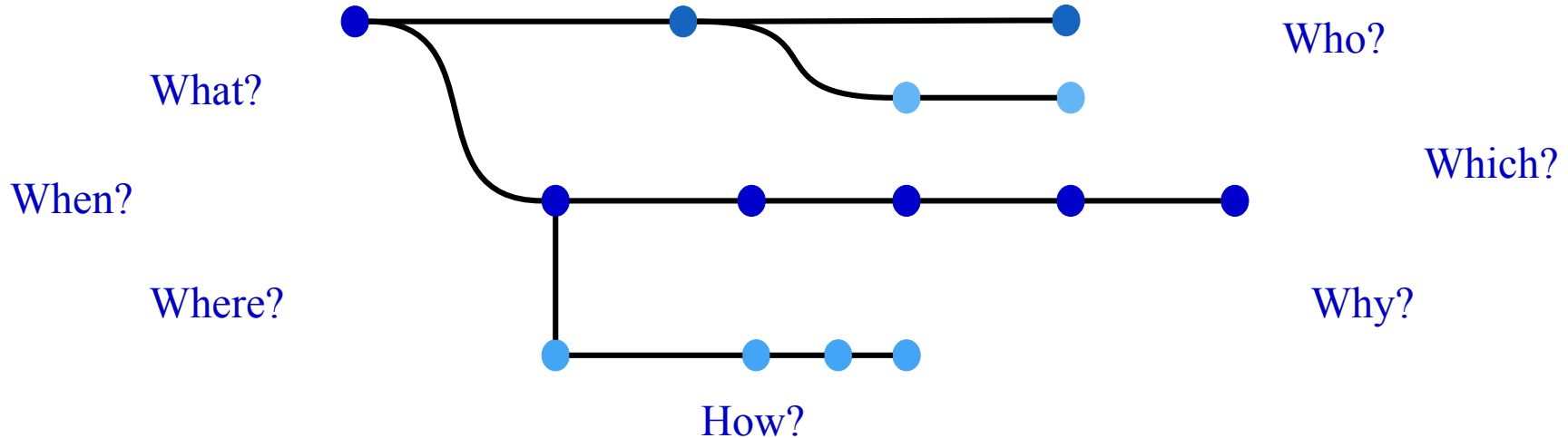




# Analyzing 6W1H Provenance of Experiments



Is it possible to reproduce and analyze  
others experiments?



# ReproduceMeGit

# ReproduceMeGit



- A visualization tool for analyzing the reproducibility of Jupyter Notebooks.
- Goals:
  - Help repository users and owners to reproduce, directly analyze and assess the reproducibility of notebooks
  - Get information on notebooks
    - that were successfully reproducible
    - that resulted in exceptions during runs
  - Analyze the notebooks:
    - the difference in the results from the original notebooks
    - provenance history of runs

## ReproduceMeGit

GitHubURL

Reproduce



# An Overview

## Reproducibility Study

Notebooks (un-)successfully  
finishing the executions

Notebooks with same or different  
results compared to the original.

Exceptions occurred in the runs  
ImportError, ModuleNotFoundError  
FileNotFoundError, IOError, SyntaxError

Provenance History in RDF  
using REPRODUCE-ME ontology

Direct access to  
Binder and ProvBook

**ReproduceMeGit**

## Structure & Usage

Repository Overview

Notebook Overview

Cells Overview

Modules Overview

Distribution of programming  
Languages and the versions used

# Computational reproducibility of Jupyter notebooks from biomedical publications



- Using fully automated workflows, we analyzed the computational reproducibility of Jupyter notebooks related to publications indexed in PubMed Central (Data till Mar 2023).

**740**  
Journals



**3,467**  
Publications



**2,660**  
Repositories

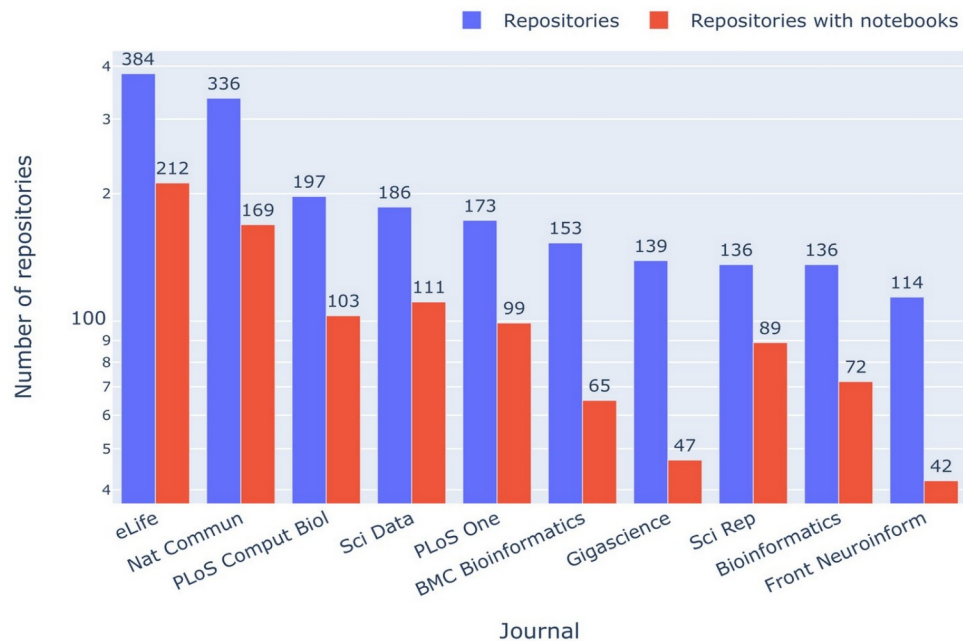


**27,271**  
Notebooks

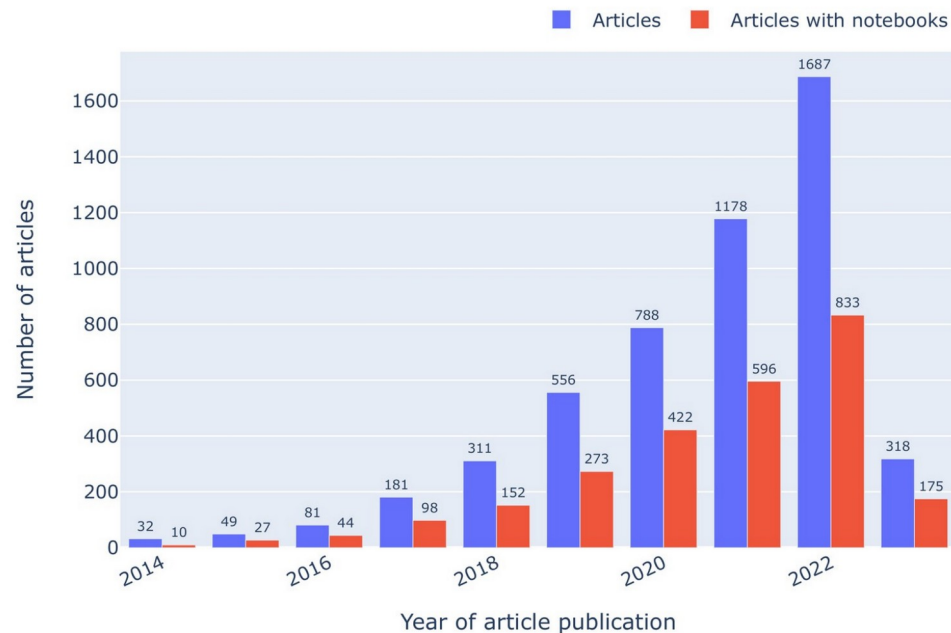


Computational reproducibility of Jupyter notebooks from biomedical publications, Sheeba Samuel and Daniel Mietchen 2024. <https://doi.org/10.1093/gigascience/giad113>

# Results

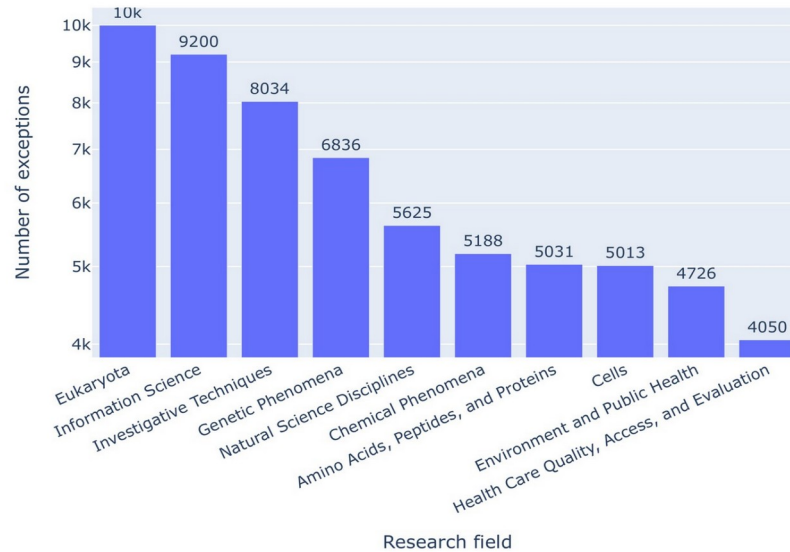


(1)

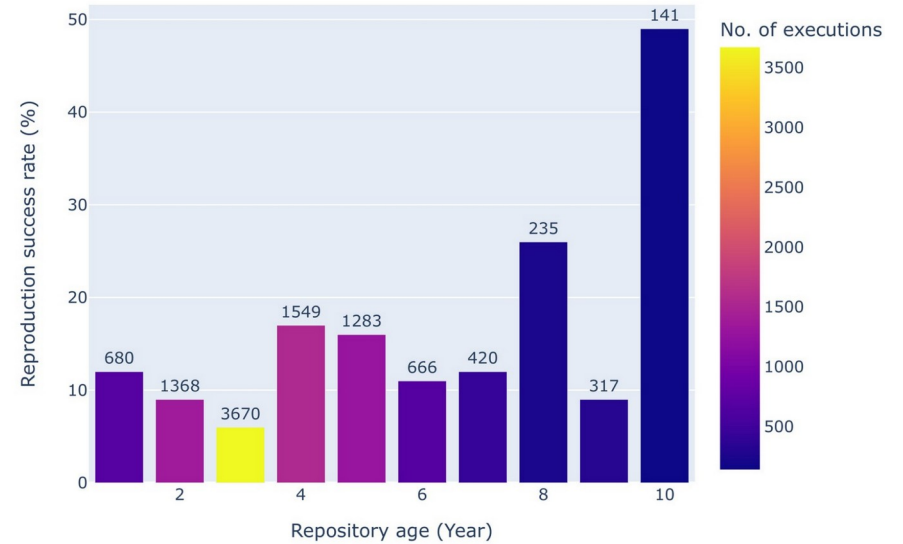


(2)

# Results



(3)



(4)

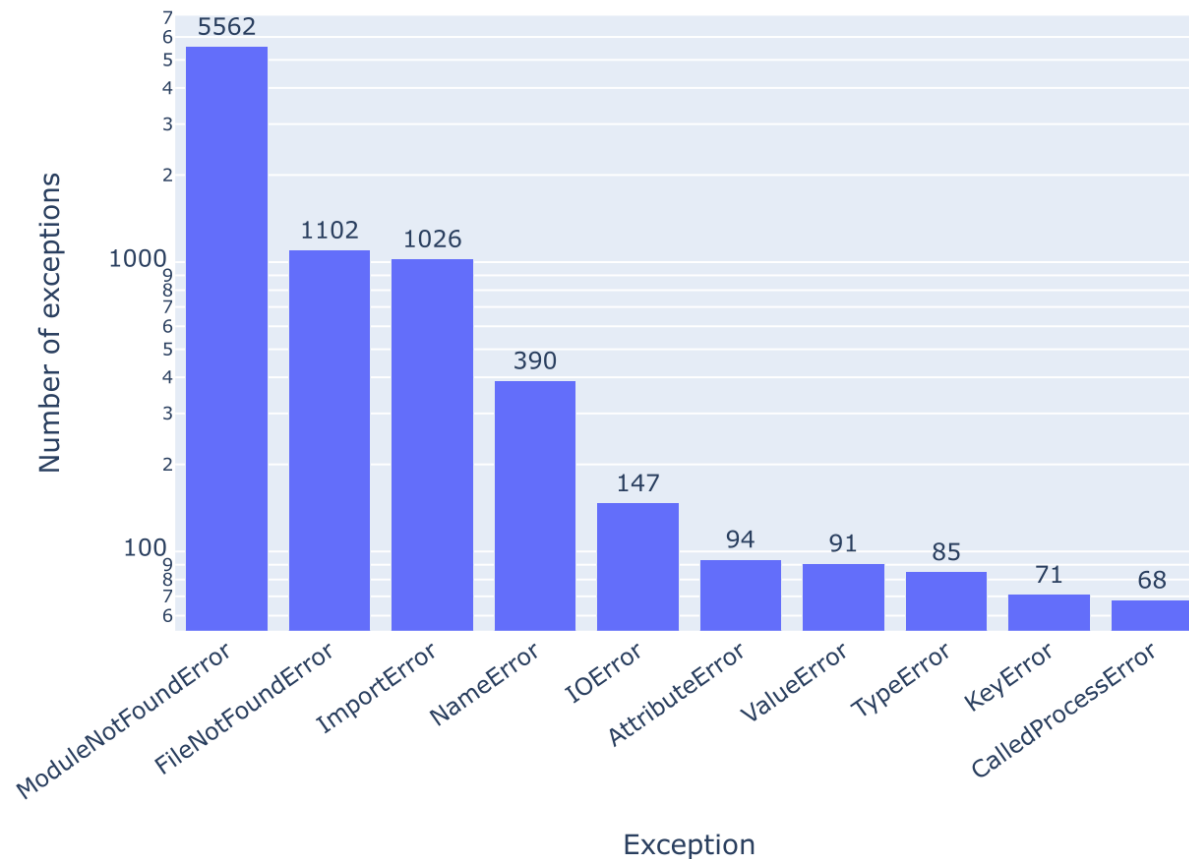


# Results: Programming Languages

| Notebook language | Rerun  | Initial run | Ratio rerun/initial |
|-------------------|--------|-------------|---------------------|
| Matlab            | 134    | 9           | 14.9                |
| Julia             | 295    | 59          | 5.0                 |
| Unknown           | 3,112  | 720         | 4.3                 |
| Python            | 22,578 | 8,160       | 2.8                 |
| R                 | 891    | 461         | 1.9                 |
| Bash              | 36     | 24          | 1.5                 |
| Sos               | 29     | 24          | 1.2                 |
| Groovy            | 95     | 95          | 1.0                 |
| Scala             | 29     | 29          | 1.0                 |
| Java              | 8      | 8           | 1.0                 |



# Results: Notebook Reproducibility





# Results: Notebook Reproducibility

| Features                                | Notebooks with different results | Notebooks with identical results |
|-----------------------------------------|----------------------------------|----------------------------------|
| Number of notebooks                     | 324 (∅ 151)                      | 879 (∅ 245)                      |
| setup.py                                | 0 (∅ 0)                          | 344 (∅ 98)                       |
| requirement.txt                         | 1 (∅ 0)                          | 353 (∅ 107)                      |
| pipfile                                 | 0 (∅ 0)                          | 0 (∅ 0)                          |
| <i>Total cells</i>                      | 23 (∅ 17.9)                      | 19.6 (∅ 17.1)                    |
| <i>Code cells</i>                       | 15.4 (∅ 12.3)                    | 11.3 (∅ 9.8)                     |
| <i>Markdown cells</i>                   | 7.6 (∅ 5.6)                      | 8.3 (∅ 6.7)                      |
| <i>Ratio of Markdown vs. code cells</i> | 0.49 (∅ 0.46)                    | 0.73 (∅ 0.68)                    |
| <i>Empty cells</i>                      | 0.9 (∅ 0.7)                      | 0.7 (∅ 0.7)                      |
| <i>Differences</i>                      | 6.3 (∅ 5.3)                      | 0 (∅ 0)                          |
| <i>Execution time (s)</i>               | 18.3 (∅ 22.1)                    | 57.6 (∅ 16.4)                    |
| <i>Execution time per code cell (s)</i> | 1.88 (∅ 1.80)                    | 5.09 (∅ 1.67)                    |

# Resources



- Code : <https://github.com/fusion-jena/computational-reproducibility-pmc>
- Data : <https://doi.org/10.5281/zenodo.8226725>
- Paper : <https://doi.org/10.1093/gigascience/giad113>

# FAIR Jupyter



- A knowledge graph approach to semantic sharing and granular exploration of a computational notebook reproducibility dataset
  - Website: <https://w3id.org/fairjupyter>
  - SPARQL Endpoint:  
<https://reproduceme.uni-jena.de/#/dataset/fairjupyter/query>
  - Knowledge Graph Browser:  
<https://reproduceme.uni-jena.de/fj/>
  - Paper: <https://doi.org/10.4230/TGDK.2.2.4>



# FAIR Jupyter Knowledge Graph

190 million triples

740  
Journals



3,467  
Publications



2,660  
Repositories

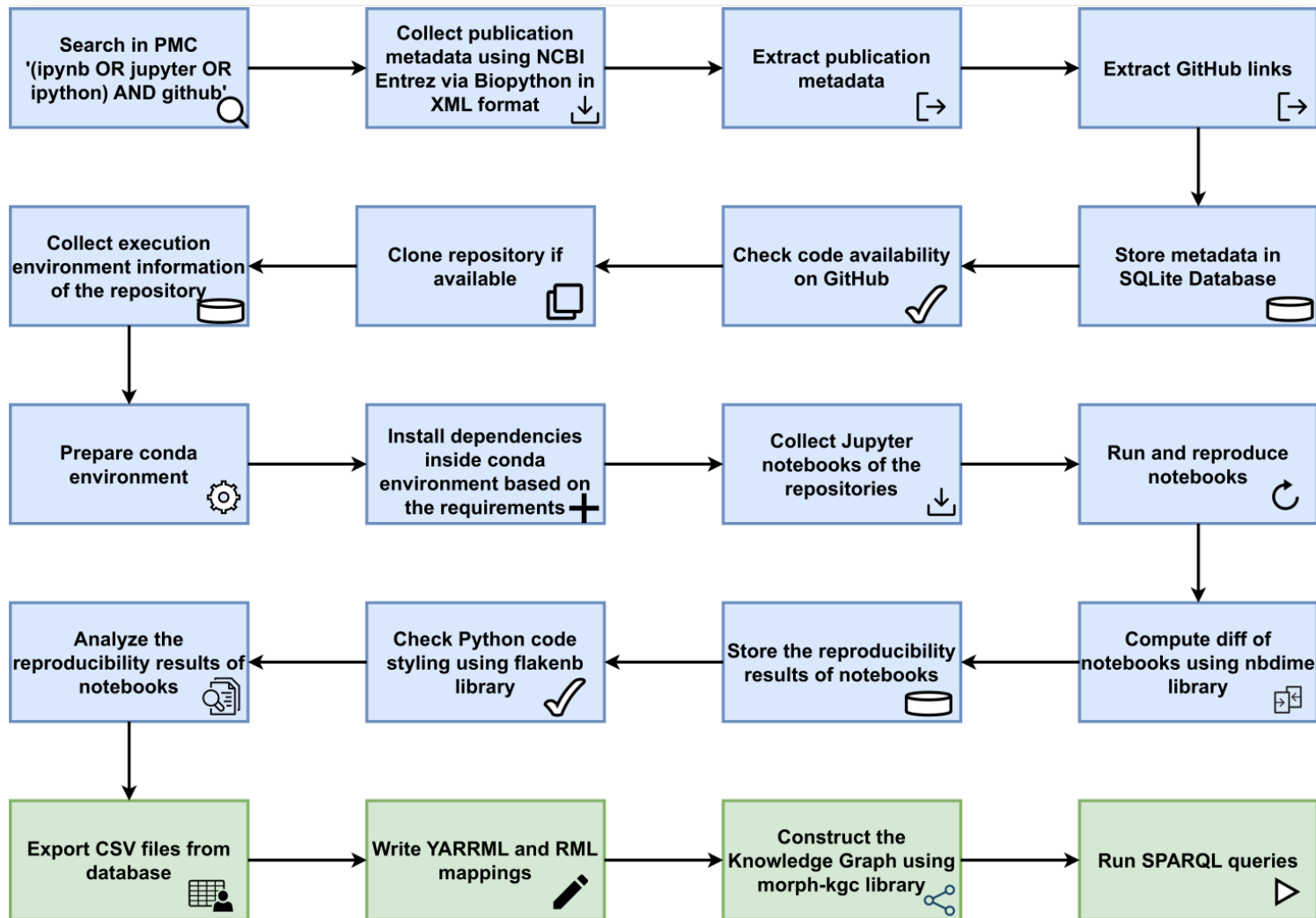


27,271  
Notebooks



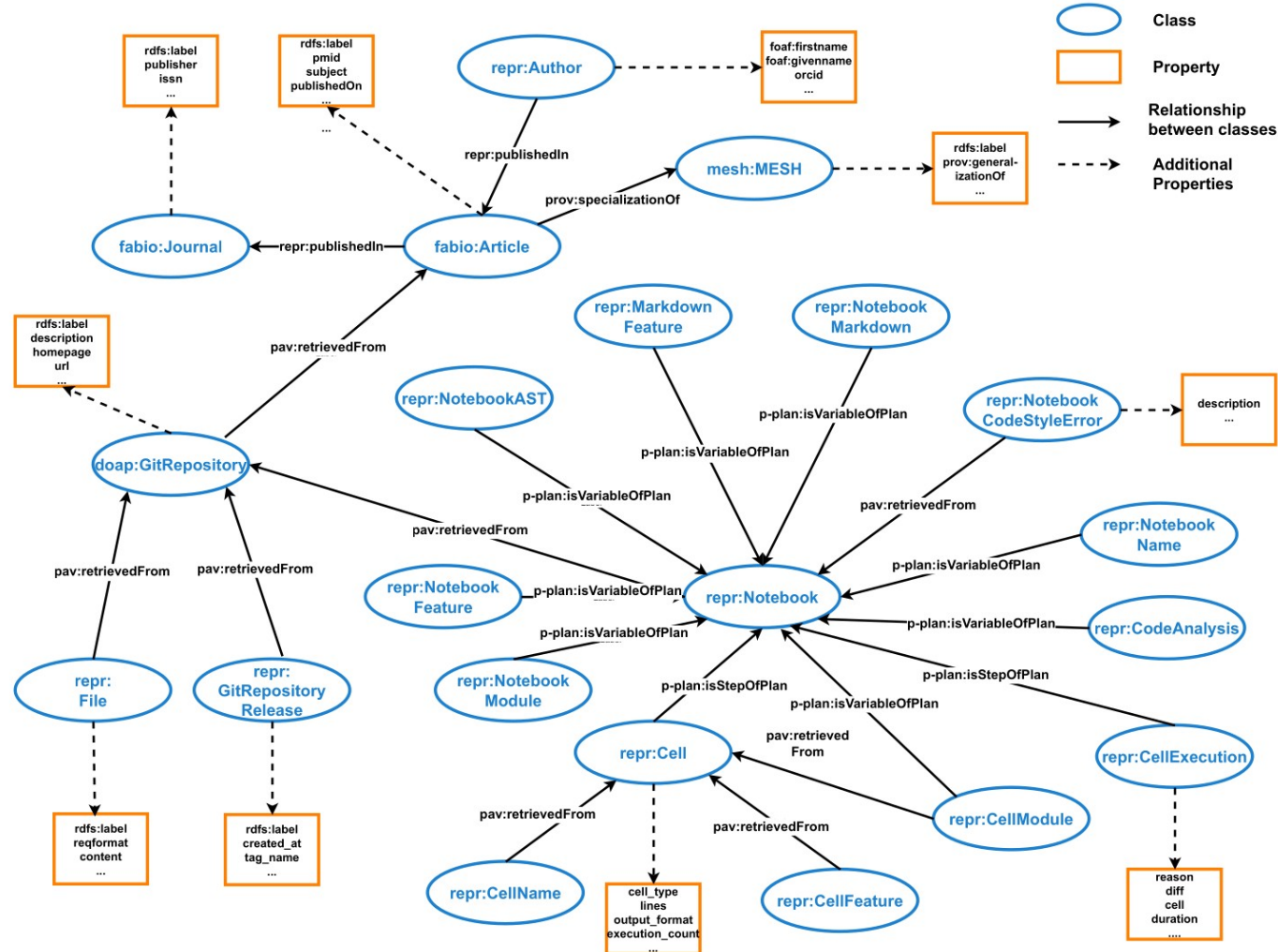


# FAIR Jupyter Workflow





# FAIR Jupyter Ontology





# FAIR Jupyter SPARQL Queries

- Local
  - Exceptions occurring in Jupyter notebooks in our corpus.
  - Notebooks by search term: 'immun' AND ('stem' OR 'differentiation')
  - Article by keywords, e.g., 'open source'
  - Most common errors in immunology
  - Most common errors in Nature journal
  - MeSH terms ranked by 'ModuleNotFoundError' frequency
  - GitHub repositories by their stargazers count
- Federated
  - Match articles between FAIR Jupyter and Wikidata via DOI

# Environmental Footprint

- Simplified calculation: carbon footprint = energy needed \* carbon intensity
- (<http://calculator.green-algorithms.org/>)



373.78 kWh

126.58 kg CO<sub>2</sub>e



# Future Trends and Challenges



- Trends:
  - Integration with AI and Machine Learning
  - Enhanced Automation in Reproducibility Workflows
  - Reproducibility as a Metric

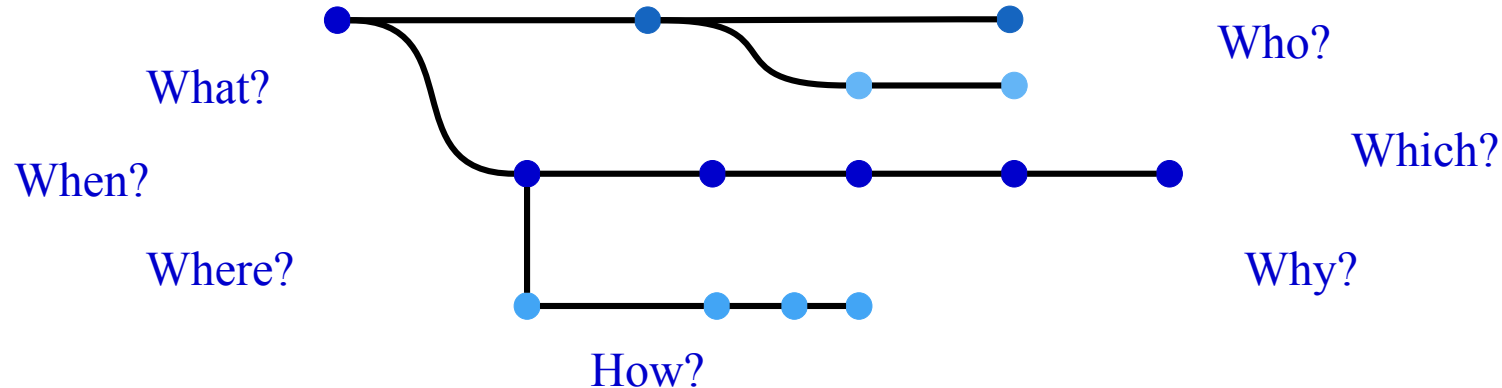


# Future Trends and Challenges

- Challenges:
  - Interdisciplinary Research and Diverse Workflows
  - Long-Term Sustainability of Reproducible Artifacts
  - Ethical Considerations in Data Sharing

# Summary

- Reproducible research benefits you and the research community
- The role of provenance, semantic web, FAIR data principles, and Open Science in reproducible research
- Solutions to 6W and 1H questions of data provenance for reproducible research
- Track, manage, and share the complete provenance of a research





# Reproducible Research Resources

- Coursera Course on Reproducible Research: <https://www.coursera.org/course/repdata>
- Guide for Reproducible Research: <https://the-turing-way.netlify.app/reproducible-research/>
- ReproHack: <https://www.reprohack.org/>
- Awesome Reproducible Research: <https://github.com/leipzig/awesome-reproducible-research>

# Thank you



sheeba.samuel@informatik.tu-chemnitz.de



@sheebasamuel



0000-0002-7981-8504

- <https://sheeba-samuel.github.io/>
- <https://vsr.informatik.tu-chemnitz.de/about/people/samuel/>