

Provenance-based Semantic Approach for the Reproducibility of Scientific Experiments

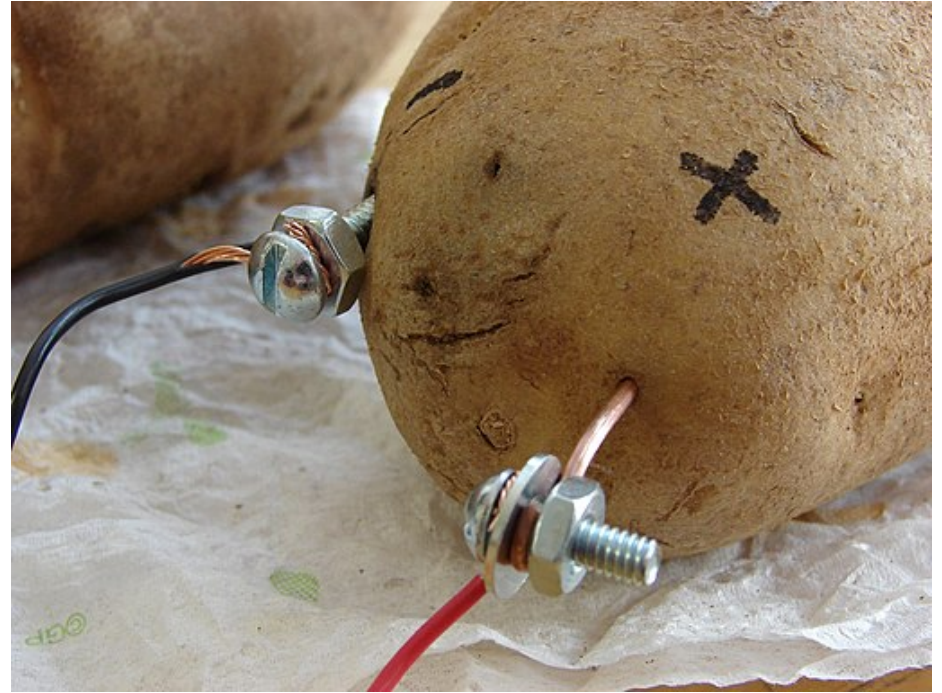
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Friedrich-Schiller University, Jena, Germany

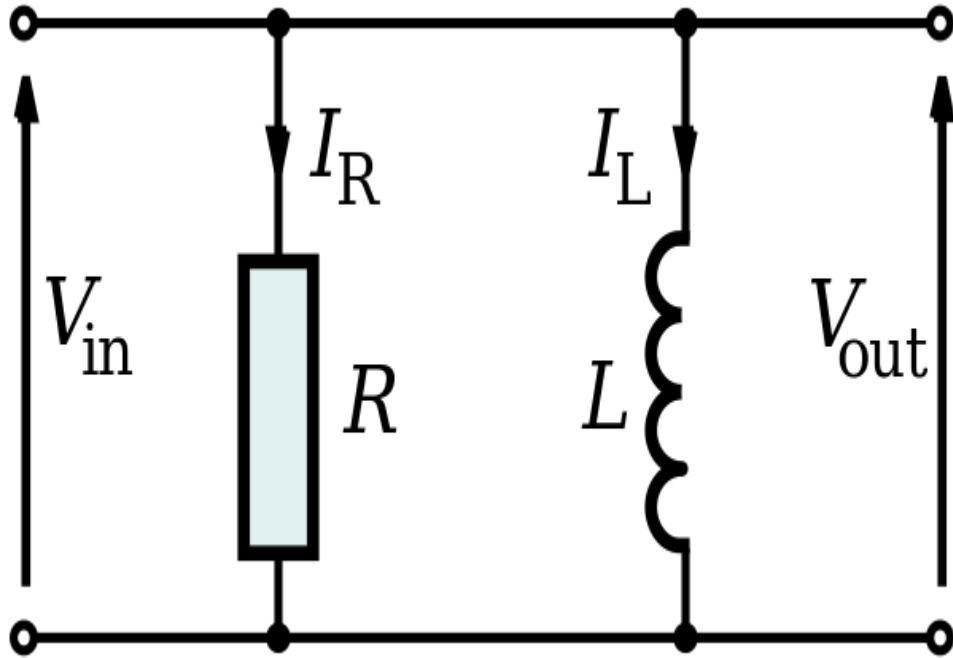
27 September 2018



Experiments



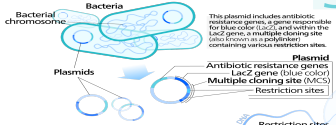
Experiments



Experiments

gene cloning

1 Small, circular DNA molecules called plasmids are removed from bacterial cells. These plasmids serve as vectors—molecules which will carry genes of interest.



2 DNA containing the gene of interest is also taken from its cell.



3 A restriction enzyme (also called a restriction endonuclease) recognizes its specific restriction site—a short sequence about 4–8 base pairs long.



4 It breaks apart the DNA, leaving overhangs called sticky ends. The restriction enzyme cuts open the circular plasmids. The same enzyme cuts out the gene of interest from its DNA molecule.



5 The sticky ends of the restriction fragments attach to each other via base pairing, forming weak hydrogen bonds. The genes of interest get included into some of the plasmids, forming recombinant plasmids. Other plasmids close right back up, remaining unchanged.



6 DNA ligase makes the bond permanent by attaching nucleotides to each other with phosphodiester bonds.



7 The plasmids are mixed with the bacteria. Some of them take up the plasmids in a process called transformation.



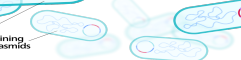
8 Plasmids with an uninterrupted LacZ gene turn their bacteria blue. In the recombinant plasmids, the inserted gene interrupts the LacZ gene, and the bacteria remain their original color. Bacteria which did not take up any plasmids also remain uncolored.



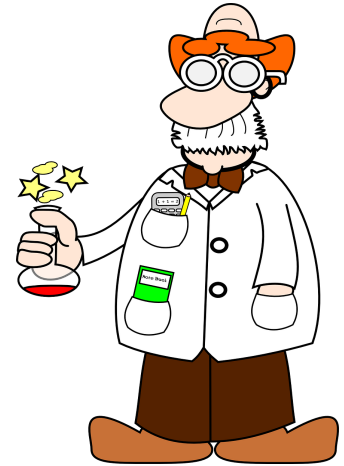
9 Antibiotics are added. Because the plasmid contains the genes for antibiotic resistance, only bacteria which took up the plasmid survive.



10 The bacteria can then be sorted by color, isolating the bacteria which took up a plasmid containing the gene of interest.



11 The uncolored bacteria can then be allowed to reproduce.



Experiments

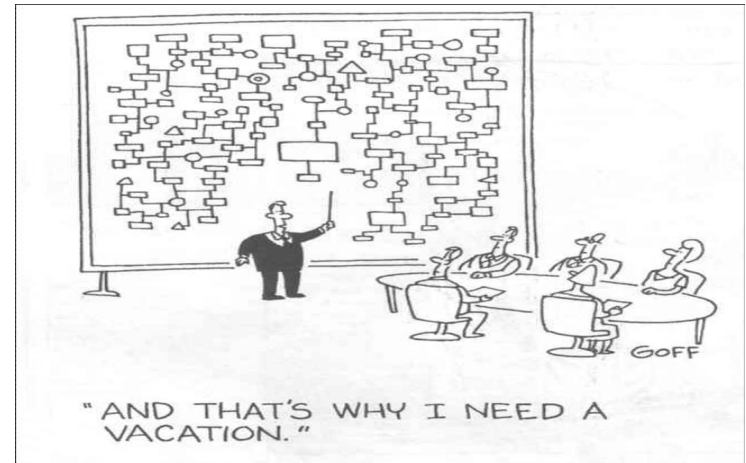


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Scientific Experiments

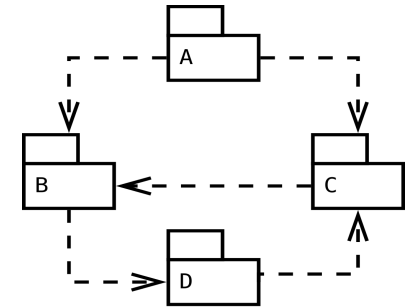
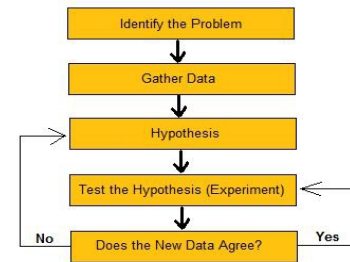
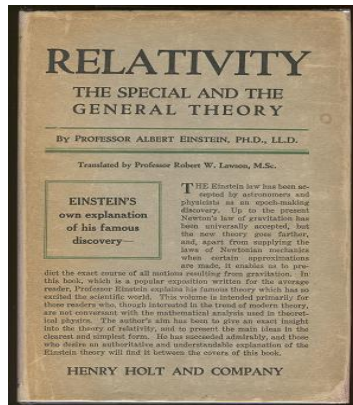
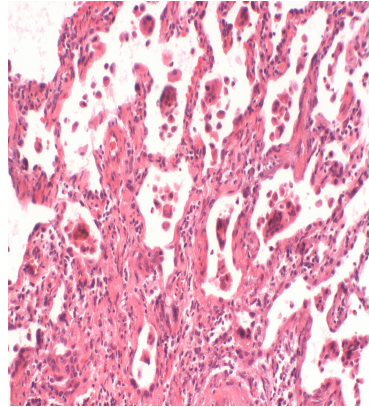
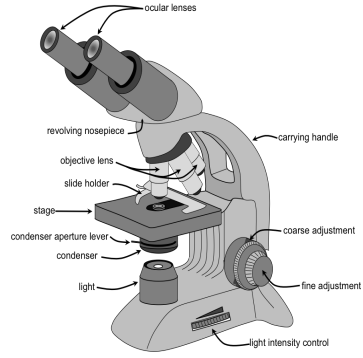
- Complex
- Several steps
- Several activities in the real world or cyberspace.
- Several people
- New technologies and entities



Reproducibility

- Understandability
- Data Provenance
- Non computational and computational part of an experiment.

Non-Computational Parts



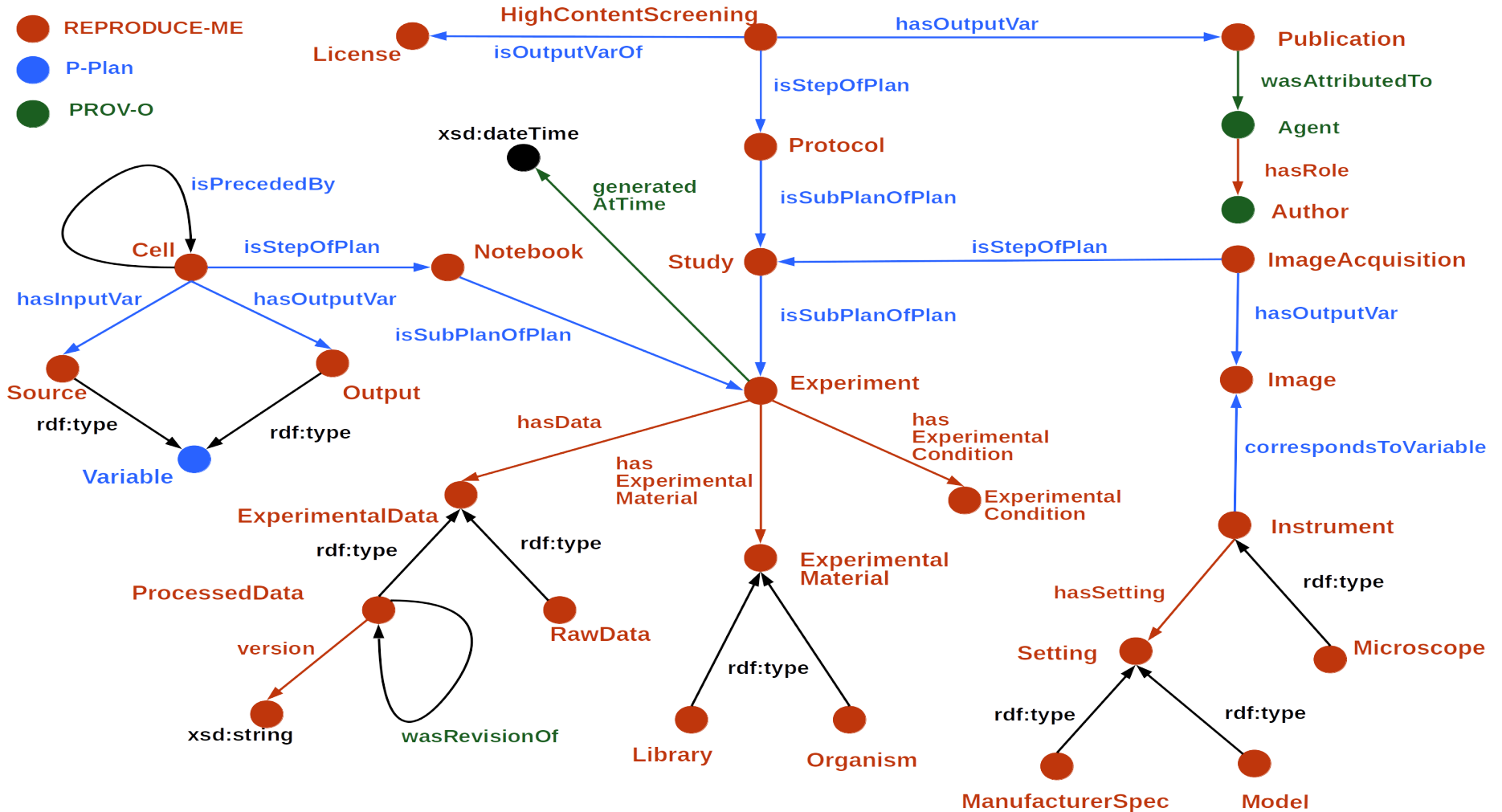
Aim

- Connect all these parts together.
- Semantically describe the provenance of the complete execution of a scientific experiment in a structured form using linked data

Provenance-based Semantic Approach

- The REPRODUCE-ME ontology extended from W3C vocabulary PROV-O and P-Plan.
- describe a scientific experiment along with its steps, input and output variables and their relationship with each other.
- The ontology is here: <https://w3id.org/reproduceme>

Provenance-based Semantic Approach



ProvBook

- An extension of Jupyter Notebook, to capture and view the provenance over the course of time.

The screenshot displays a Jupyter Notebook interface for a file named 'DampedOscillationsPlot'. The browser address bar shows 'localhost:8888/notebooks/notebooks/DampedOscillationsPlot.ipynb'. The notebook header includes the Jupyter logo, the filename, and a 'Last Checkpoint: 4 hours ago (autosaved)' status. A 'Logout' button is visible in the top right. The menu bar includes 'File', 'Edit', 'View', 'Insert', 'Cell', 'Kernel', and 'Help'. The toolbar contains icons for file operations, a 'Run' button, and a 'Code' dropdown menu. A tooltip 'Provenance of selected cell' is positioned over the code cell.

```
In [31]: x1 = np.linspace(0.0, 5.0)
         y1 = np.cos(3 * np.pi * x1) * np.exp(-x1)
         plt.subplot(2, 1, 1)
         plt.plot(x1, y1, 'o-')
         plt.show()
```

Start Time: 2018-05-25T12:39:36+02:00
End Time: 2018-05-25T12:39:36+02:00
Execution Time: 135ms
Source:
x1 = np.linspace(0.0, 8.0)
y1 = np.cos(3 * np.pi * x1) * np.exp(-x1)
plt.subplot(2, 1, 1)
plt.plot(x1, y1, 'o-')
plt.show()

Output:

The output consists of two plots. The top plot shows a damped oscillation with the x-axis ranging from 0 to 8. The y-axis ranges from -0.5 to 1.0. The plot shows a blue line with circular markers that starts at (0, 1.0) and decays towards zero as x increases. The bottom plot shows a similar damped oscillation with the x-axis ranging from 0 to 5. The y-axis ranges from -0.5 to 1.0. The plot shows a blue line with circular markers that starts at (0, 1.0) and decays towards zero as x increases.

ProvBook Difference

- Difference between input and output of each execution.

ProvBook Diff

Hide unchanged cells

Base

Remote

In [16]:

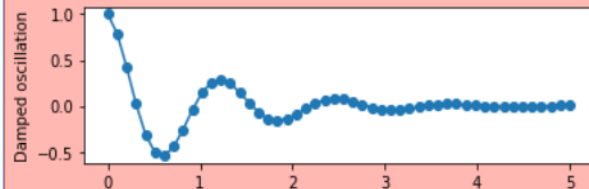
```
1 x1 = np.linspace(0.0, 5.0)
2 y1 = np.cos(18 * np.pi * x1) * np.exp(-x1)
3 plt.subplot(2, 1, 1)
(...)
```

In [16]:

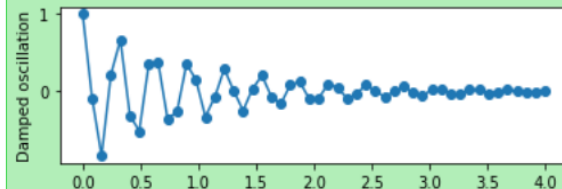
```
1 x1 = np.linspace(0.0, 4.0)
2 y1 = np.cos(18 * np.pi * x1) * np.exp(-x1)
3 plt.subplot(2, 1, 1)
(...)
```

Outputs changed

Output deleted



Output added



<https://w3id.org/reproduceme/research/>

Acknowledgement

- Christoph Biskup, Kathrin Groeneveld, Tom Kache, Teresa Langenstück (ReceptorLight B1 project)
- Prof. Martin Bücken, Frank Taubert, Daniel Walther

References

- <https://www.w3.org/TR/prov-o/>
- <http://purl.org/net/p-plan>
- Image Courtesy: Wikipedia

Thanks

- Questions???
- Find more information here:
- <https://w3id.org/reproduceme>
- <https://w3id.org/reproduceme/research>