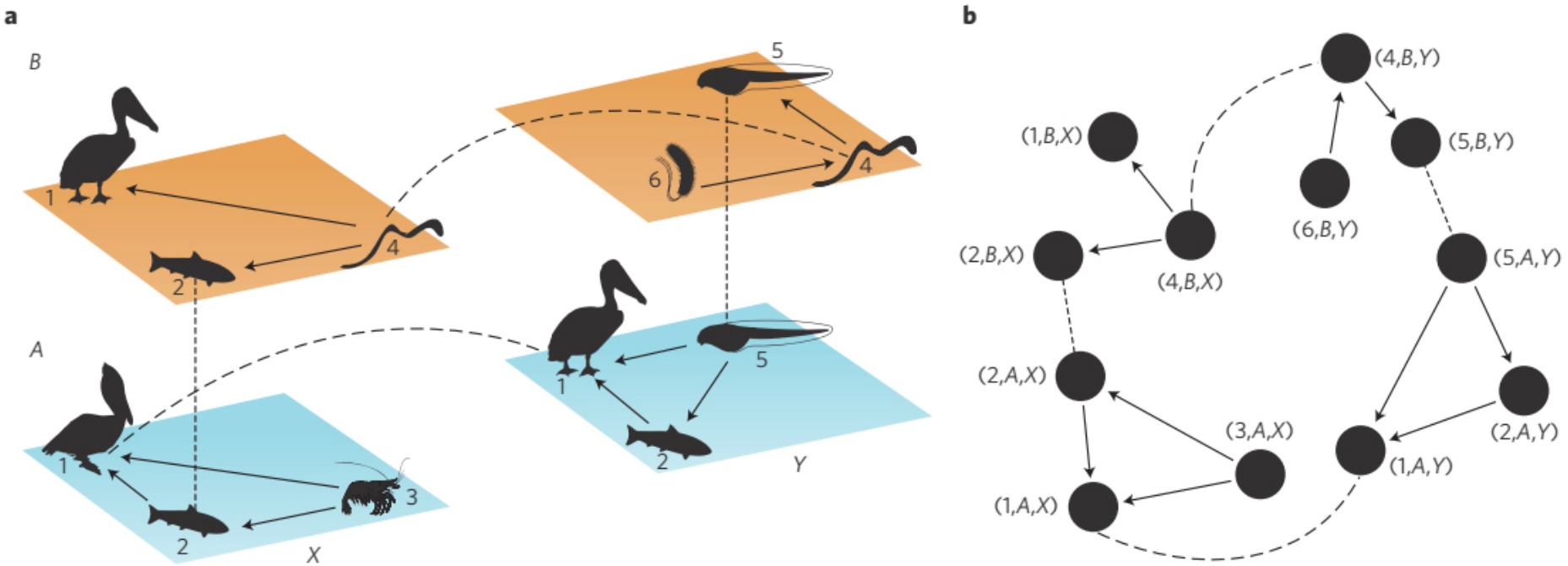
Easier reproducibility for scientists with encapsulation


a
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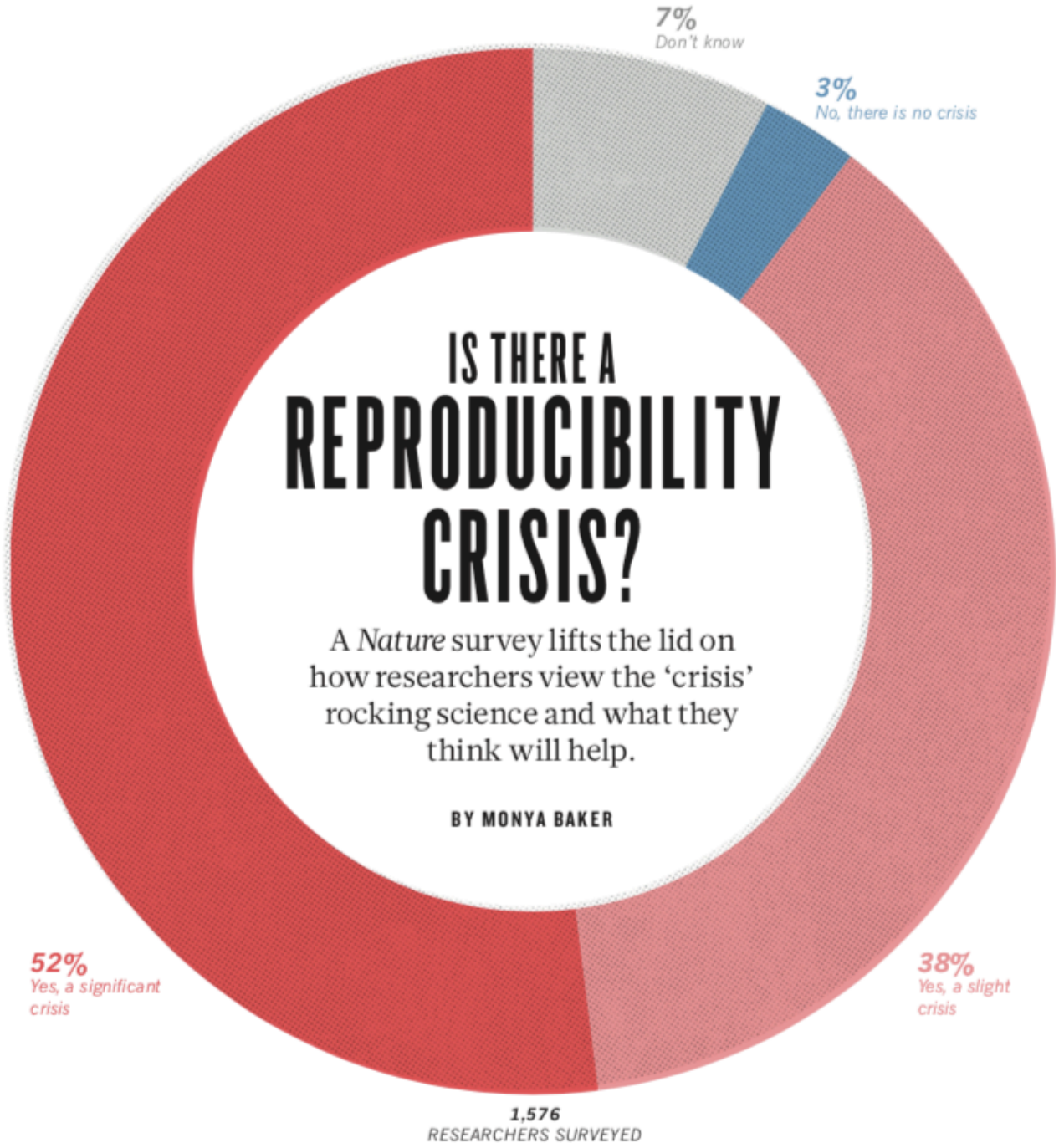
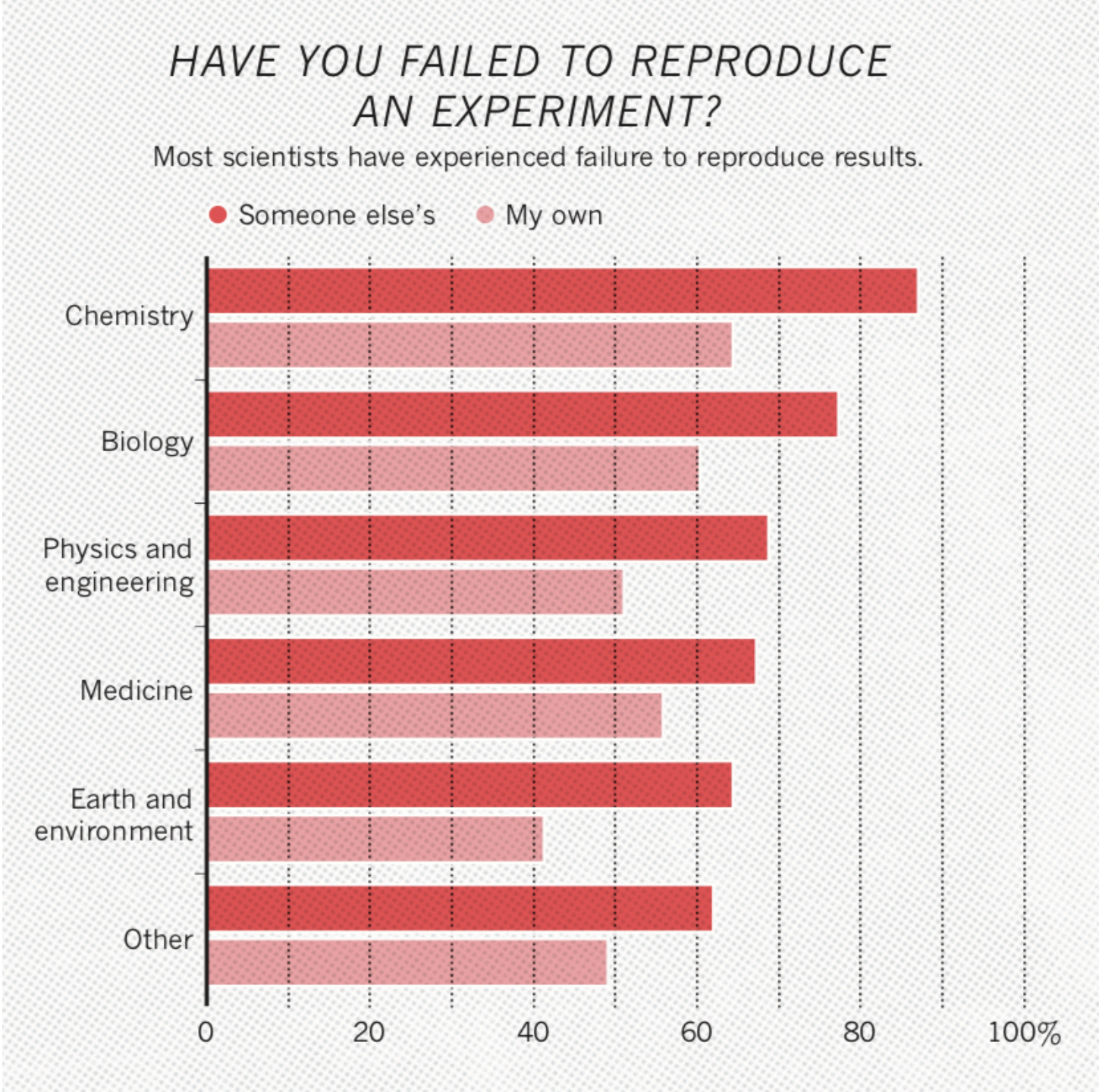
Software should not limit science.

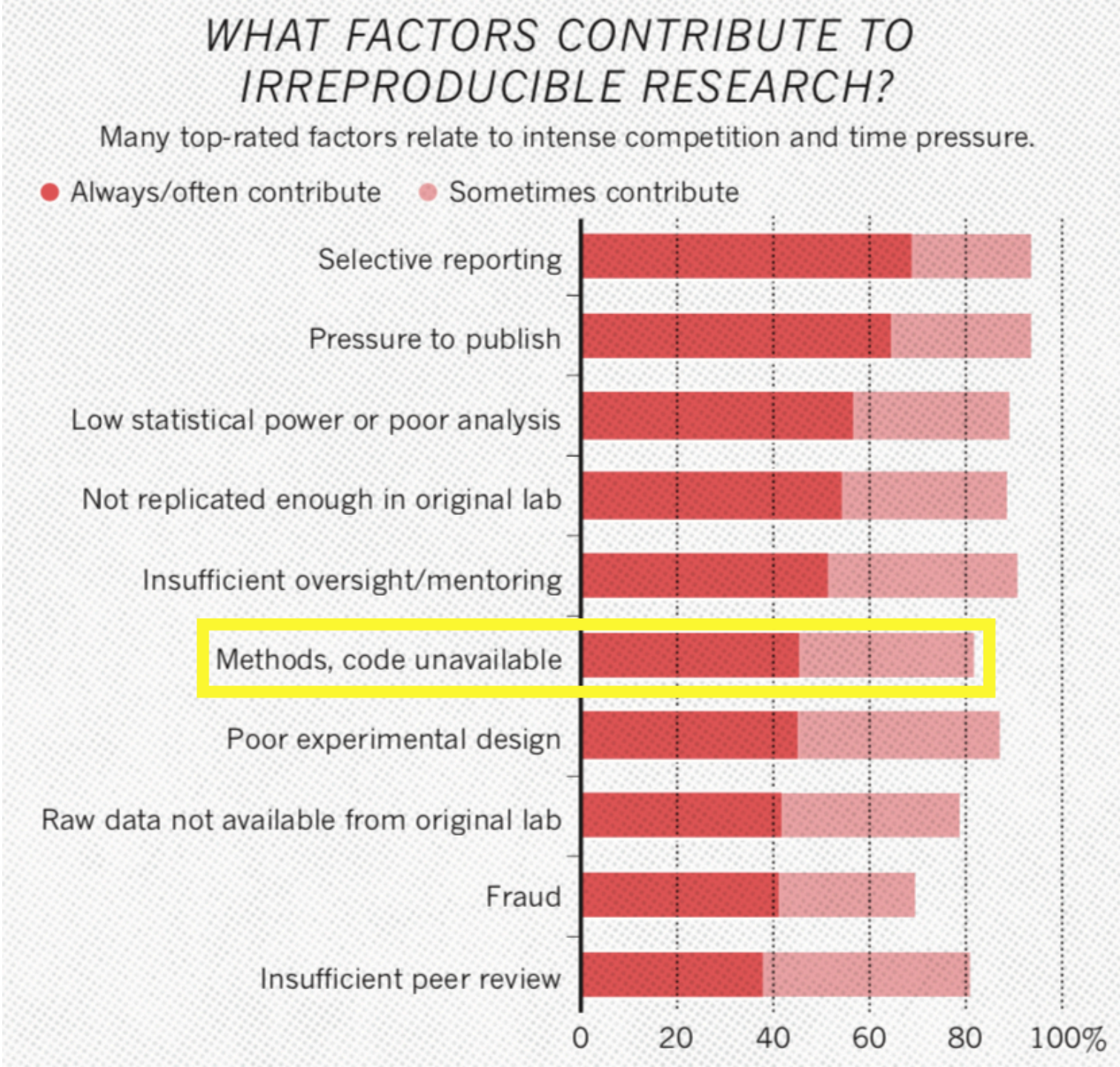


IS THERE A REPRODUCIBILITY CRISIS?

A *Nature* survey lifts the lid on how researchers view the 'crisis' rocking science and what they think will help.

BY MONYA BAKER


HAVE YOU FAILED TO REPRODUCE AN EXPERIMENT?
Most scientists have experienced failure to reproduce results.
Someone else's
My own
Chemistry
Biology
Physics and engineering
Medicine
Earth and environment
Other
0
20
40
60
80
100%


WHAT FACTORS CONTRIBUTE TO IRREPRODUCIBLE RESEARCH?
Many top-rated factors relate to intense competition and time pressure.
Always/often contribute
Sometimes contribute
Selective reporting
Pressure to publish
Low statistical power or poor analysis
Not replicated enough in original lab
Insufficient oversight/mentoring
Methods, code unavailable
Poor experimental design
Raw data not available from original lab
Fraud
Insufficient peer review
0
20
40
60
80
100%


BLAZING
SADDLES

www.nature.com/scientificdata

SCIENTIFIC DATA

OPEN

Comment: If these data could talk

Thomas Pasquier[1], Matthew K. Lau[2], Ana Trisovic[3,4], Emery Boose[2], Ben Couturier[3], Mercè Crosas[5], Aaron M. Ellison[2], Valerie Gibson[4], Chris Jones[4] & Margo Seltzer[1]

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In the last few decades, data-driven methods have come to dominate many fields of scientific inquiry. Open data and open-source software have enabled the rapid implementation of novel methods to manage and analyze the growing flood of data. However, it has become apparent that many scientific fields exhibit distressingly low rates of repeatability and reproducibility. Although there are many dimensions to this issue, we believe that there is a lack of formalism used when describing end-to-end published results, from the data source to the analysis to the final published results. Even when authors do their best to make their research and data accessible, this lack of formalism reduces the clarity and efficiency of reporting, which contributes to issues of reproducibility. Data provenance aids both repeatability and reproducibility through *systematic* and *formal* records of the relationships among data sources, processes, datasets, publications and researchers.


The
Dataverse®
Project

Sharing and Preserving Computational Analyses for Posterity with *encapsulator*

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University of Cambridge

Matthew K. Lau and Xueyuan Han
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Reproducibility has become a recurring topic of discussion in many scientific disciplines.[1] Although it might be expected that some studies will be difficult to reproduce, recent conversations highlight important aspects of the scientific endeavor that could be improved to facilitate reproducibility. Open data and open source software are two important parts of a concerted effort to achieve reproducibility.[2] However, multiple publications point out these approaches' shortcomings,[3,4] such as the identification of dependencies, poor documentation of the installation processes, "code rot," failure to capture dynamic inputs, and technical barriers.

In prior work,[5] we pointed out that open data and open source software alone are insufficient to ensure reproducibility, as they do not capture information about the computational execution, that is, the "process" and context that produced the results using the data and code. In keeping with the "open" culture, we defined open process as the practice of both sharing the source and the input data and providing a description of the entire computational

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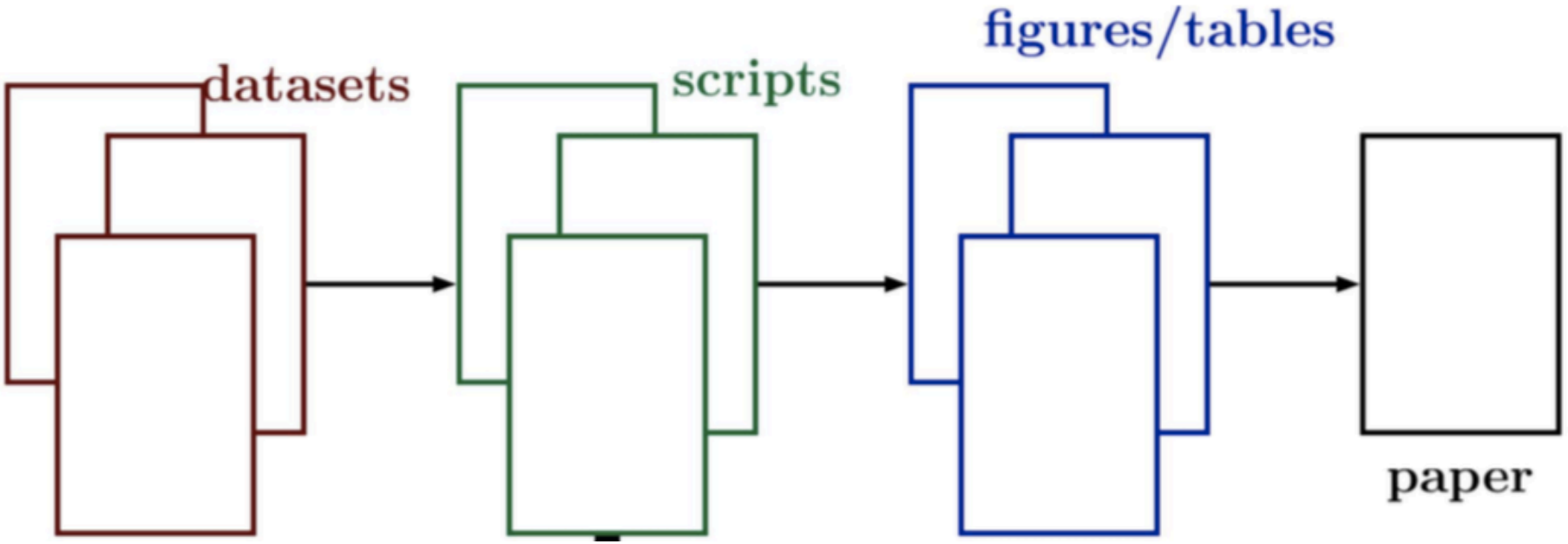
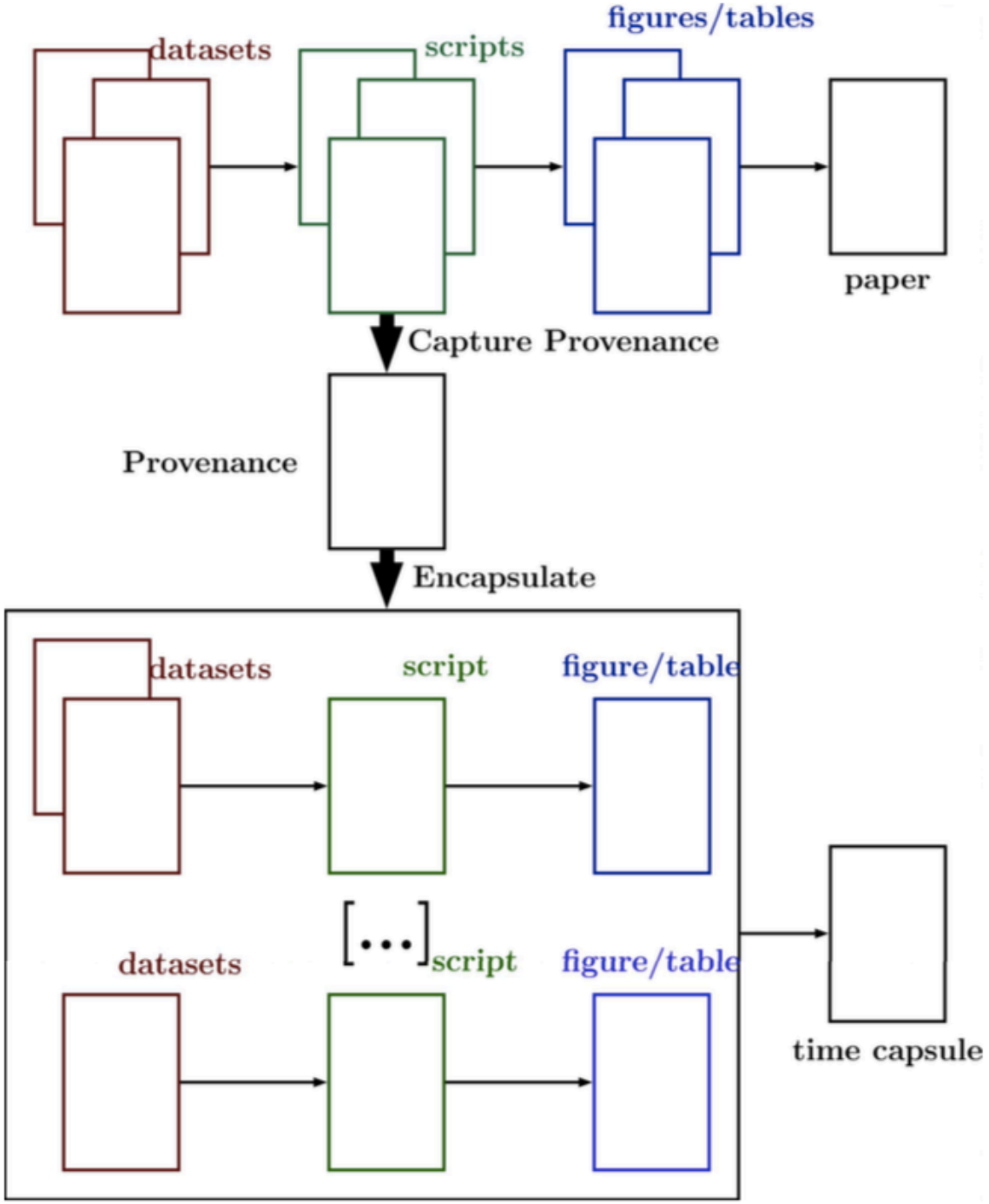
Encapsulator

Purpose: Simplify computational reproducibility

1. Create a data “capsule” (code + data + environment)
2. Increase transparency with “cleaned” code


datasets
scripts
figures/tables
paper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scripts
figures/tables
paper
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Provenance
Encapsulate
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script
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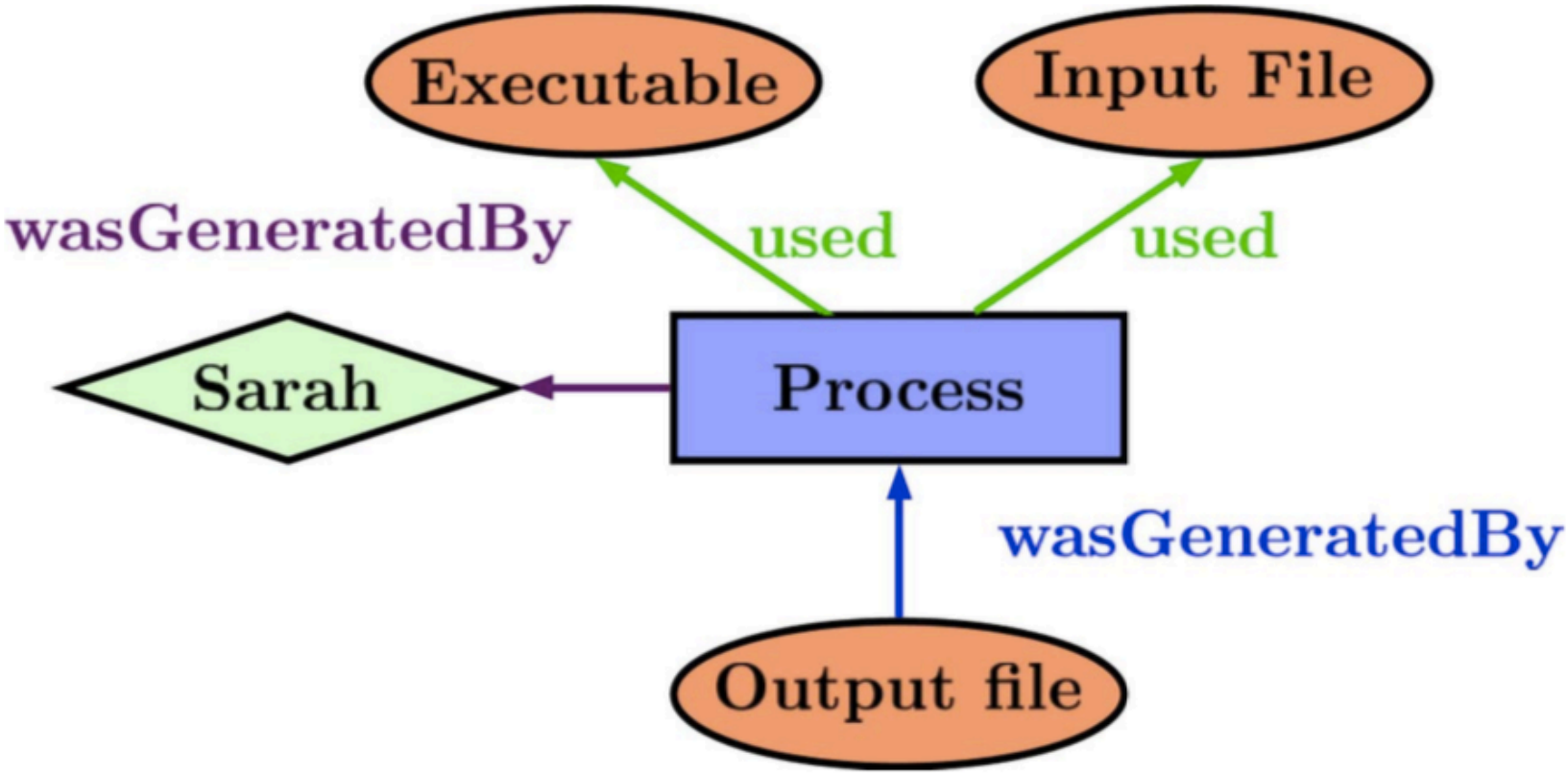
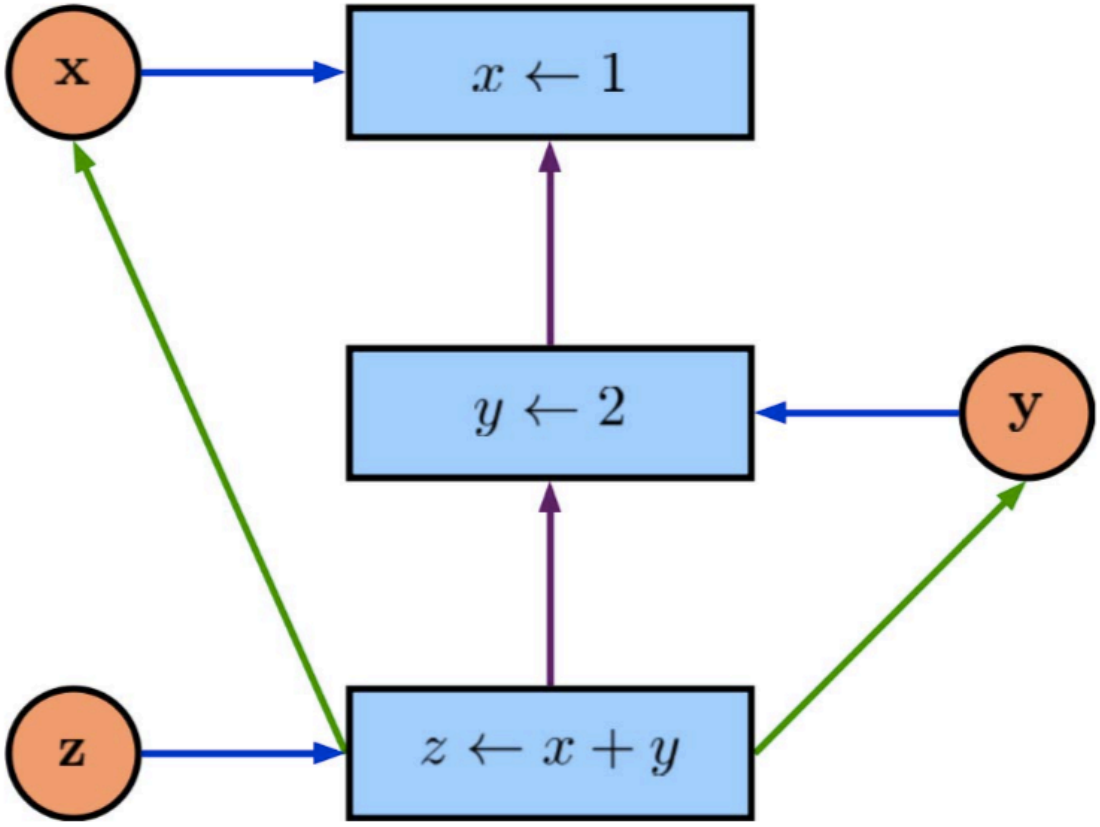
time capsule

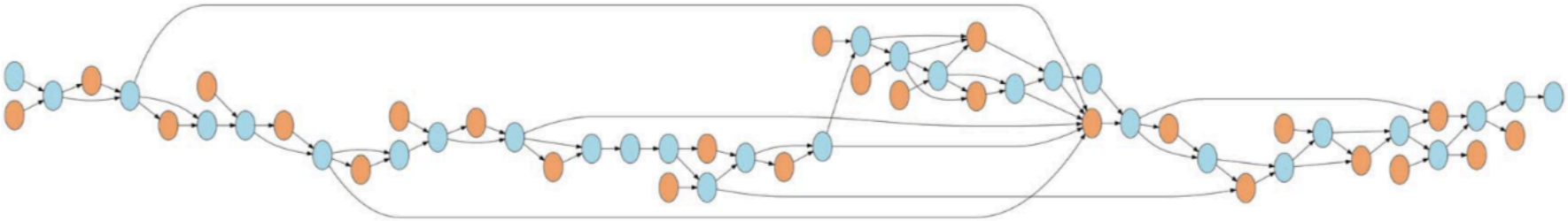
What is data provenance?

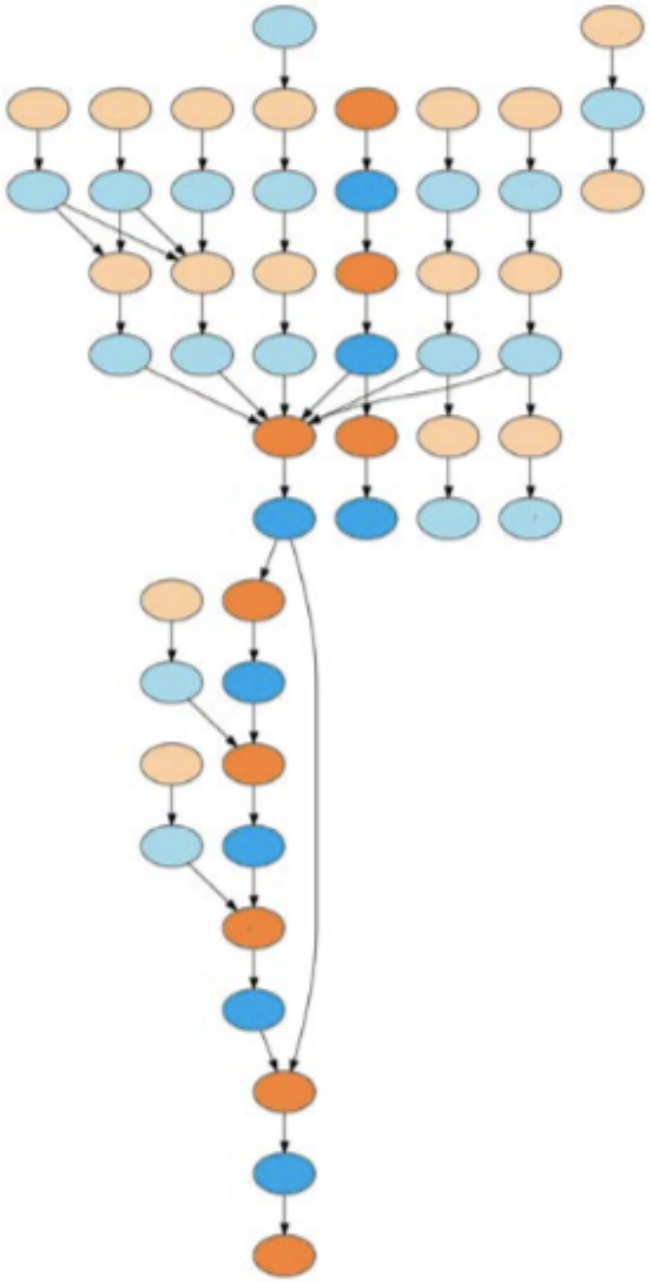


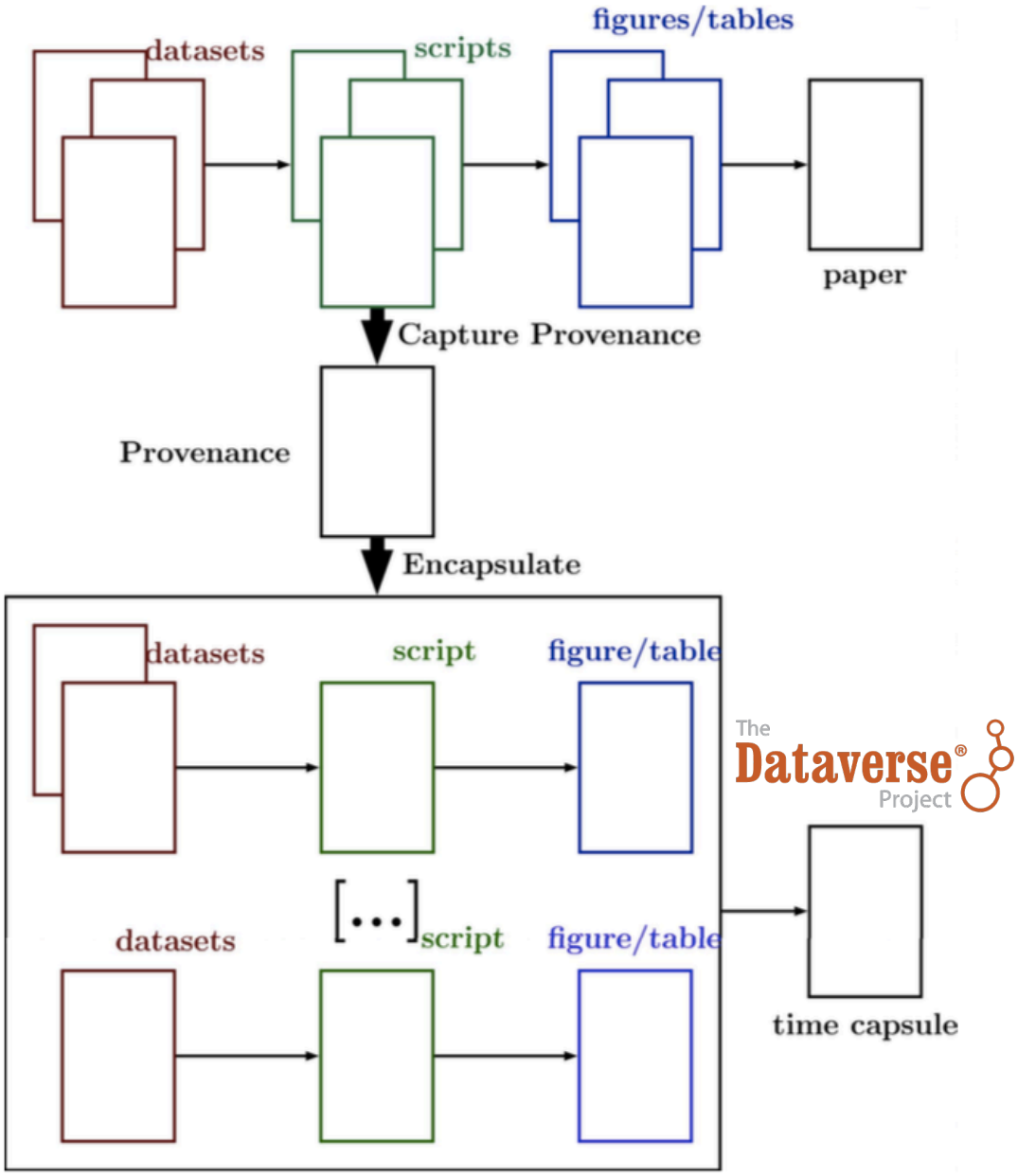
What is data provenance?



Prov. Huh. What is it good for?






figures/tables
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scripts
paper
Capture Provenance
Provenance
Encapsulate
datasets
script
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[...]
datasets
script
figure/table
time capsule
The
Dataverse®
Project

Challenges

- Out-of-tree Libraries
- Nondeterminism
- Capsule OS (*Linux*, *VirtualBox*)
- Language Support (*R*)
- More effective “code cleaning” (*Rclean*)

Future Directions

- Test Dataverse products
- Integration with IDEs (*RStudio*)
- Container Support (e.g. *Docker*)
- Domain-Specific Environments

Email: ***matthewklau@fas.harvard.edu***

Github: MKLau

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More details about those projects are available at https://projects.iq.harvard.edu/provenance-at-harvard.