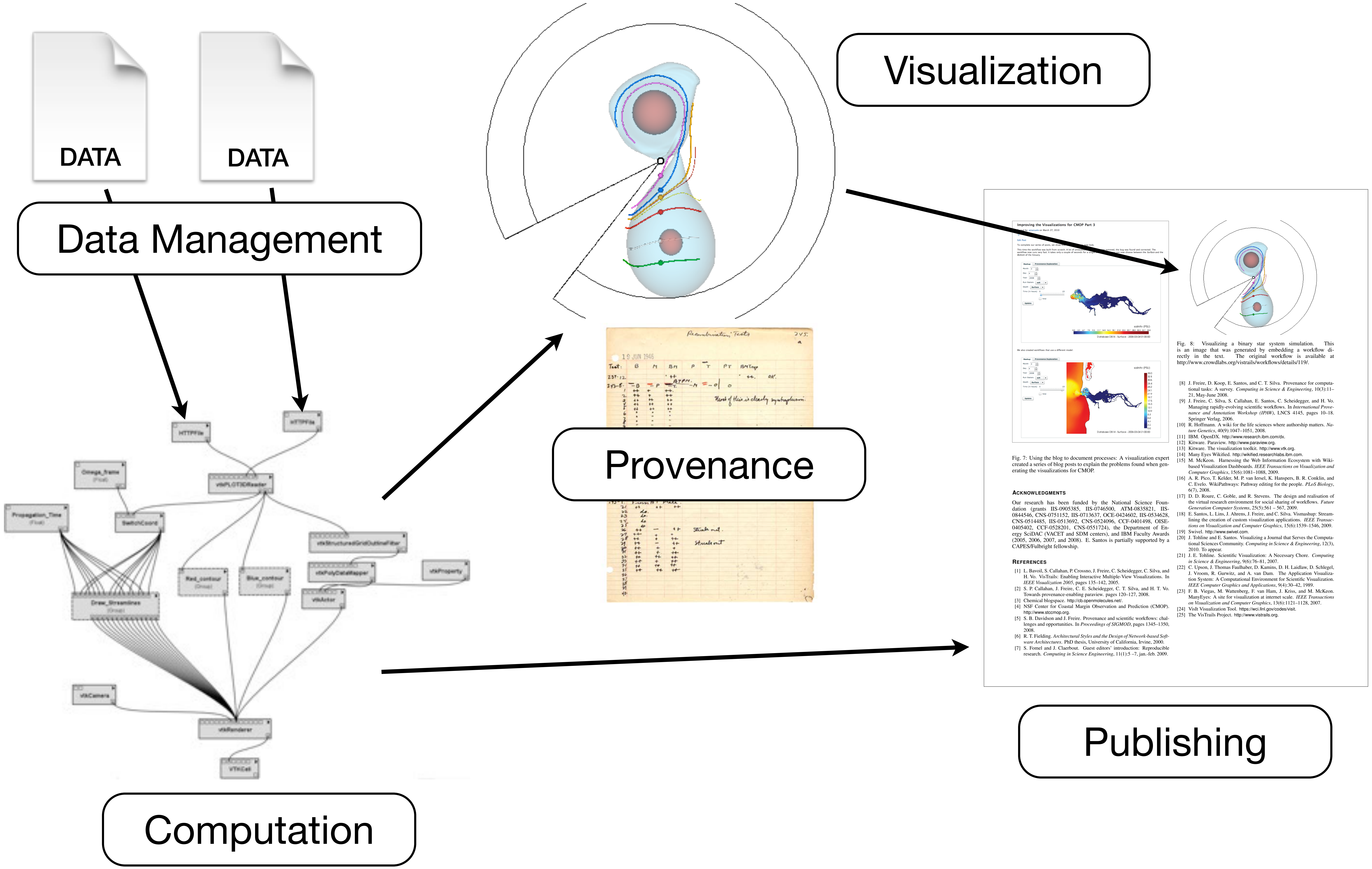
Advanced Data Management (CSCI 640/490)

Reproducibility

Dr. David Koop

Provenance in Computational Science



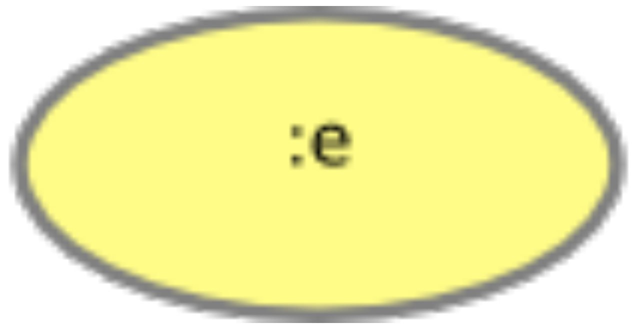
Provenance Capture Mechanisms

- **Workflow-based**: Since workflow execution is controlled, keep track of all the workflow modules, parameters, etc. as they are executed
- **Process-based**: Each process is required to write out its own provenance information (not centralized like workflow-based)
- **OS-based**: The OS or filesystem is modified so that any activity it does it monitored and the provenance subsystem organizes it
- Tradeoffs:
    - Workflow- and process-based have better abstraction
    - OS-based requires minimal user effort once installed and can capture "hidden dependencies"

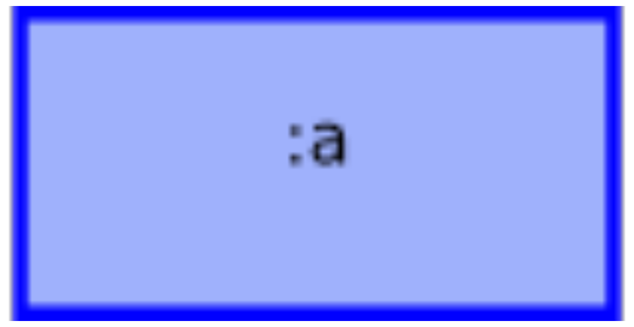
Prospective and Retrospective Provenance

- Prospective provenance is what was specified/intended
  - a workflow, script, list of steps
- Retrospective provenance is what actually happened
  - actual data, actual parameters, errors that occurred, timestamps, machine information
- **Do not need** prospective provenance to have retrospective provenance!
- Recipe for a cake vs. Baking a cake

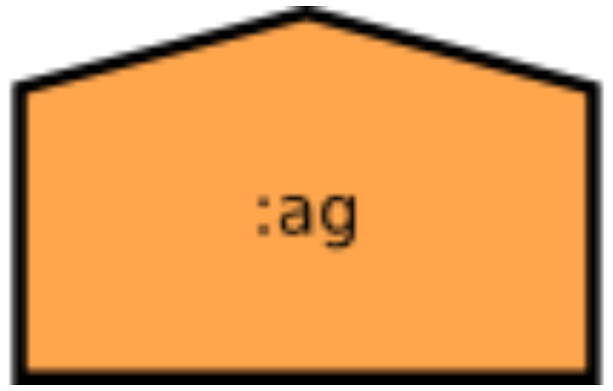
PROV: Three Key Classes



An **entity** is a physical, digital, conceptual, or other kind of thing with some fixed aspects; entities may be real or imaginary.



An **activity** is something that occurs over a period of time and acts upon or with entities; it may include consuming, processing, transforming, modifying, relocating, using, or generating entities.



An **agent** is something that bears some form of responsibility for an activity taking place, for the existence of an entity, or for another agent's activity.

[Moreau et al., 2014]

Database Provenance

- Motivation: Data warehouses and curated databases
  - Lots of work
  - Provenance helps check correctness
  - Adds value to data by how it was obtained
- Three Types:
  - Why (Lineage): Associate each tuple t present in the output of a query with a set of tuples present in the input
  - How: Not just existence but routes from tuples to output (multiple contrib.'s)
  - Where: Location where data is copied from (may have choice of different tables)

[Cheney et al., 2007]

Why Provenance

Agencies

	name	based_in	phone
t_1:	BayTours	San Francisco	415-1200
t_2:	HarborCruz	Santa Cruz	831-3000

ExternalTours

	name	destination	type	price
t_3:	BayTours	San Francisco	cable car	$50
t_4:	BayTours	Santa Cruz	bus	$100
t_5:	BayTours	Santa Cruz	boat	$250
t_6:	BayTours	Monterey	boat	$400
t_7:	HarborCruz	Monterey	boat	$200
t_8:	HarborCruz	Carmel	train	$90

```
Q1:
SELECT a.name, a.phone
FROM Agencies a, ExternalTours e
WHERE a.name = e.name AND e.type='boat'
```

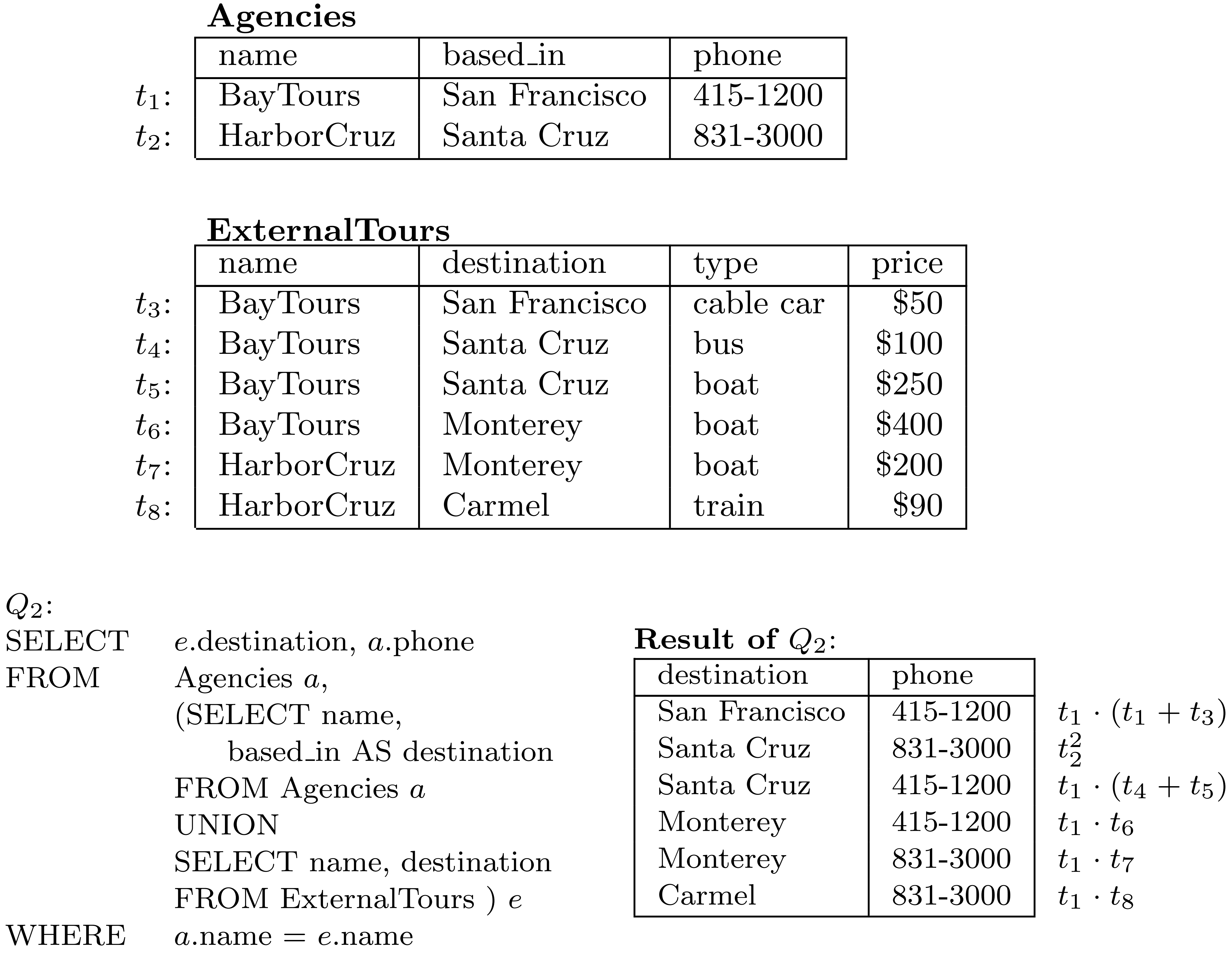
Result of Q_1:

name	phone
BayTours	415-1200
HarborCruz	831-3000

- Lineage of `(HarborCruz, 831-3000)`: `{Agencies(t2),ExternalTours(t7)}`
- Lineage of `(BayTours, 415-1200)`: `{Agencies(t1), ExternalTours(t5,t6)}`
- This is not really precise because we don't need both `t5` and `t6`—only one is ok

[Cheney et al., 2007]

How Provenance



Agencies

	name	based_in	phone
t_1:	BayTours	San Francisco	415-1200
t_2:	HarborCruz	Santa Cruz	831-3000

ExternalTours

	name	destination	type	price
t_3:	BayTours	San Francisco	cable car	$50
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t_6:	BayTours	Monterey	boat	$400
t_7:	HarborCruz	Monterey	boat	$200
t_8:	HarborCruz	Carmel	train	$90

Q_2:

```
SELECT   e.destination, a.phone
FROM     Agencies a,
         (SELECT name,
             based_in AS destination
         FROM Agencies a
         UNION
         SELECT name, destination
         FROM ExternalTours ) e
WHERE    a.name = e.name
```

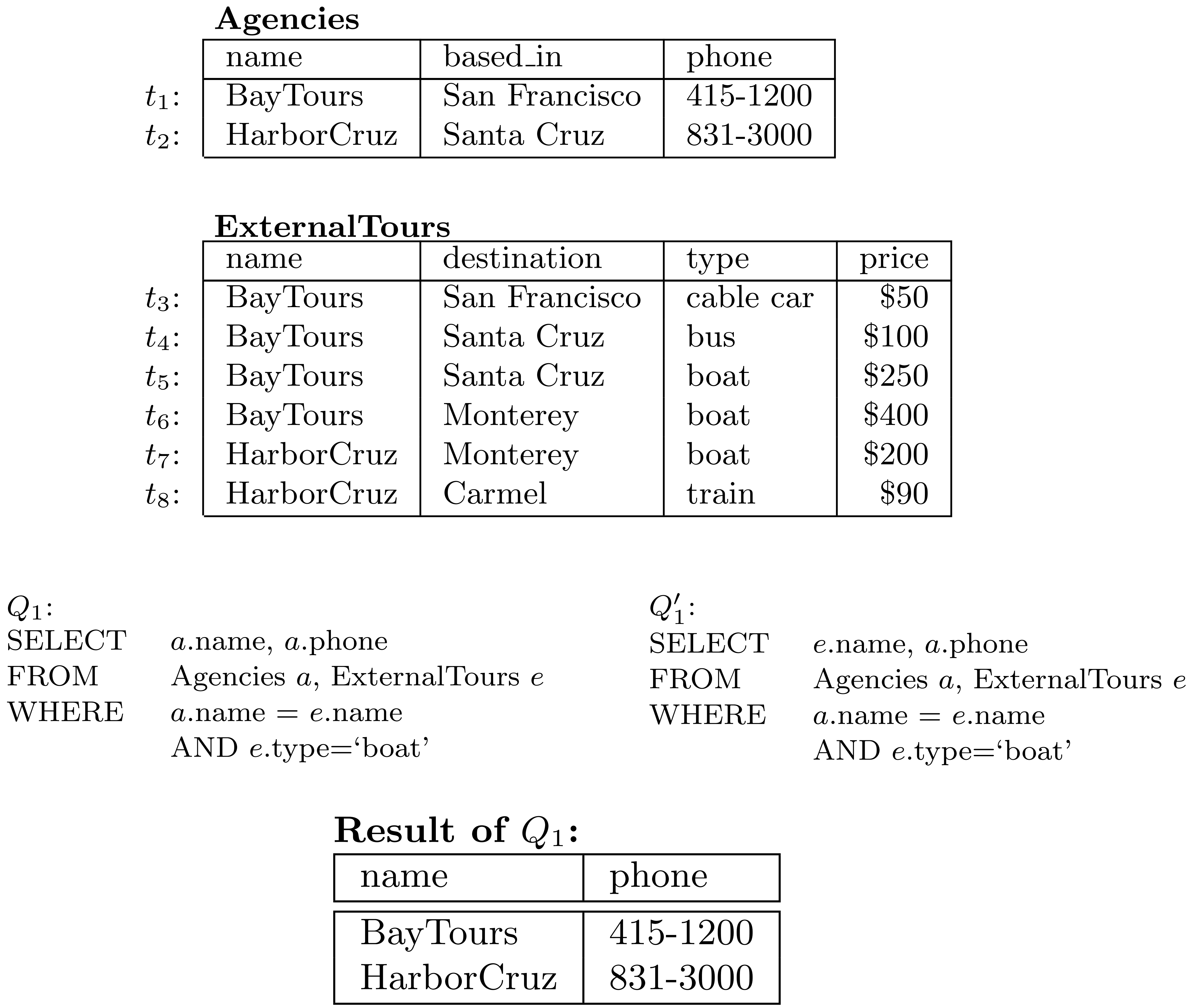
Result of Q_2:

destination	phone	
San Francisco	415-1200	$t_1 \cdot (t_1 + t_3)$
Santa Cruz	831-3000	t_2^2
Santa Cruz	415-1200	$t_1 \cdot (t_4 + t_5)$
Monterey	415-1200	$t_1 \cdot t_6$
Monterey	831-3000	$t_1 \cdot t_7$
Carmel	831-3000	$t_1 \cdot t_8$

- How provenance gives more detail about how the tuples provide witnesses to the result
- Prov of `(San Francisco, 415-1200)`: `{{t1}, {t1,t3}}`
- `t1` contributes **twice**
- Uses provenance semirings (the "polynomial" shown on the right)

[Cheney et al., 2007]

Where Provenance



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Q_1:

```
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```

Q'_1:

```
SELECT   e.name, a.phone
FROM     Agencies a, ExternalTours e
WHERE    a.name = e.name
         AND e.type='boat'
```

Result of Q_1:

name	phone
BayTours	415-1200
HarborCruz	831-3000

- Where provenance traces to specific locations, not the tuple values
- Q and Q' give the same result but the name comes from different places
- Prov of `HarborCruz` in second output: `(t2, name)`
- Important in annotation-propogation

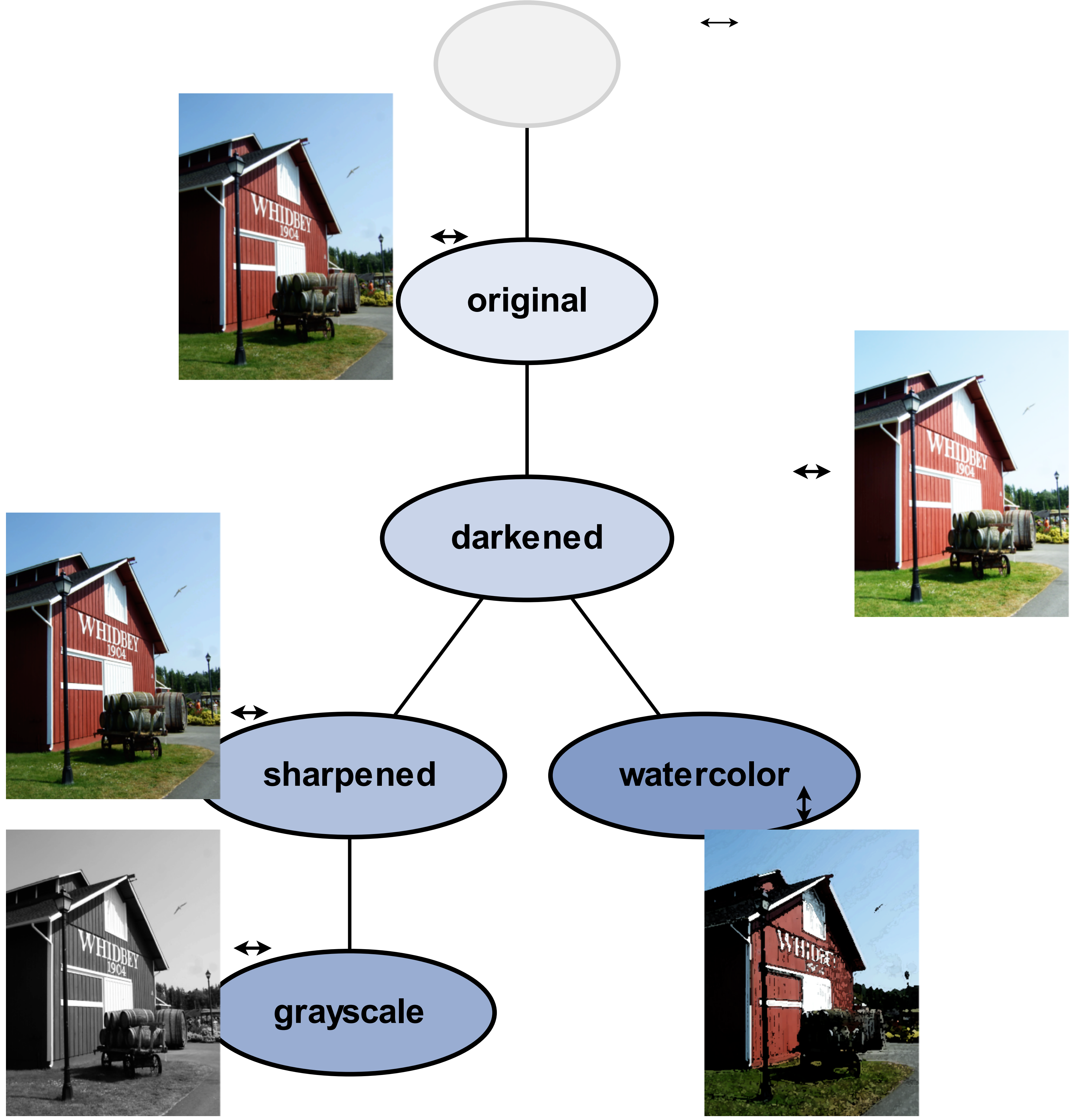
[Cheney et al., 2007]

VisTrails

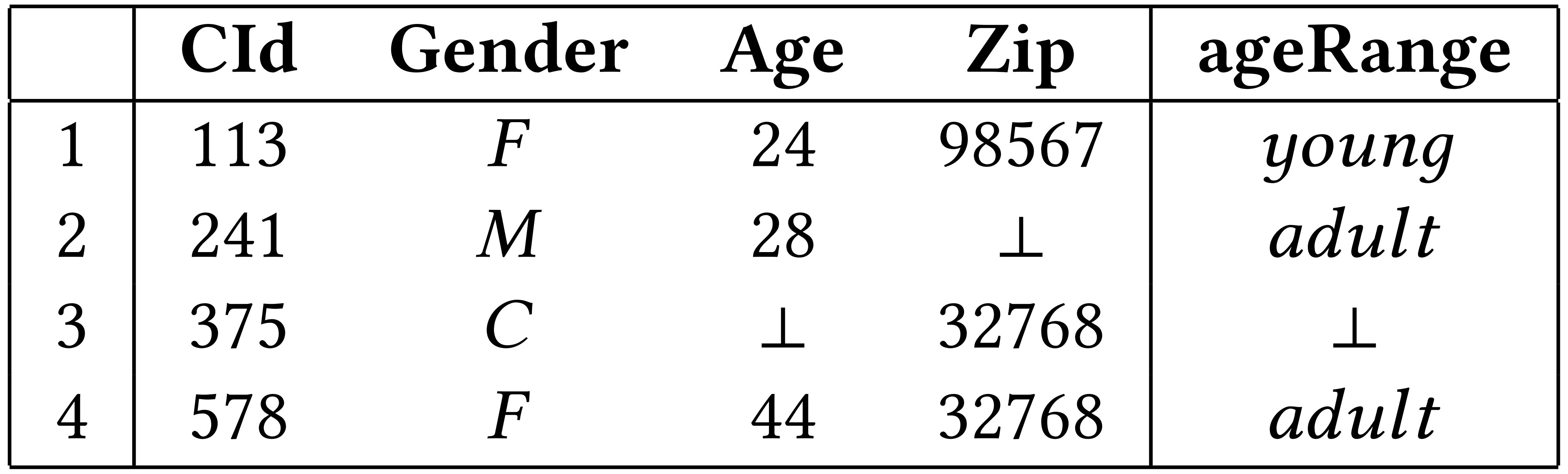
- Comprehensive provenance infrastructure for computational tasks
- Focus on exploratory tasks such as simulation, visualization, and data analysis
- Transparently tracks provenance of the discovery process—from data acquisition to visualization
    - The trail followed as users generate and test hypotheses
    - Users can refer back to any point along this trail at any time
- Leverage provenance to streamline exploration
- Focus on usability—build tools for scientists

Version Trees for Evolution Provenance

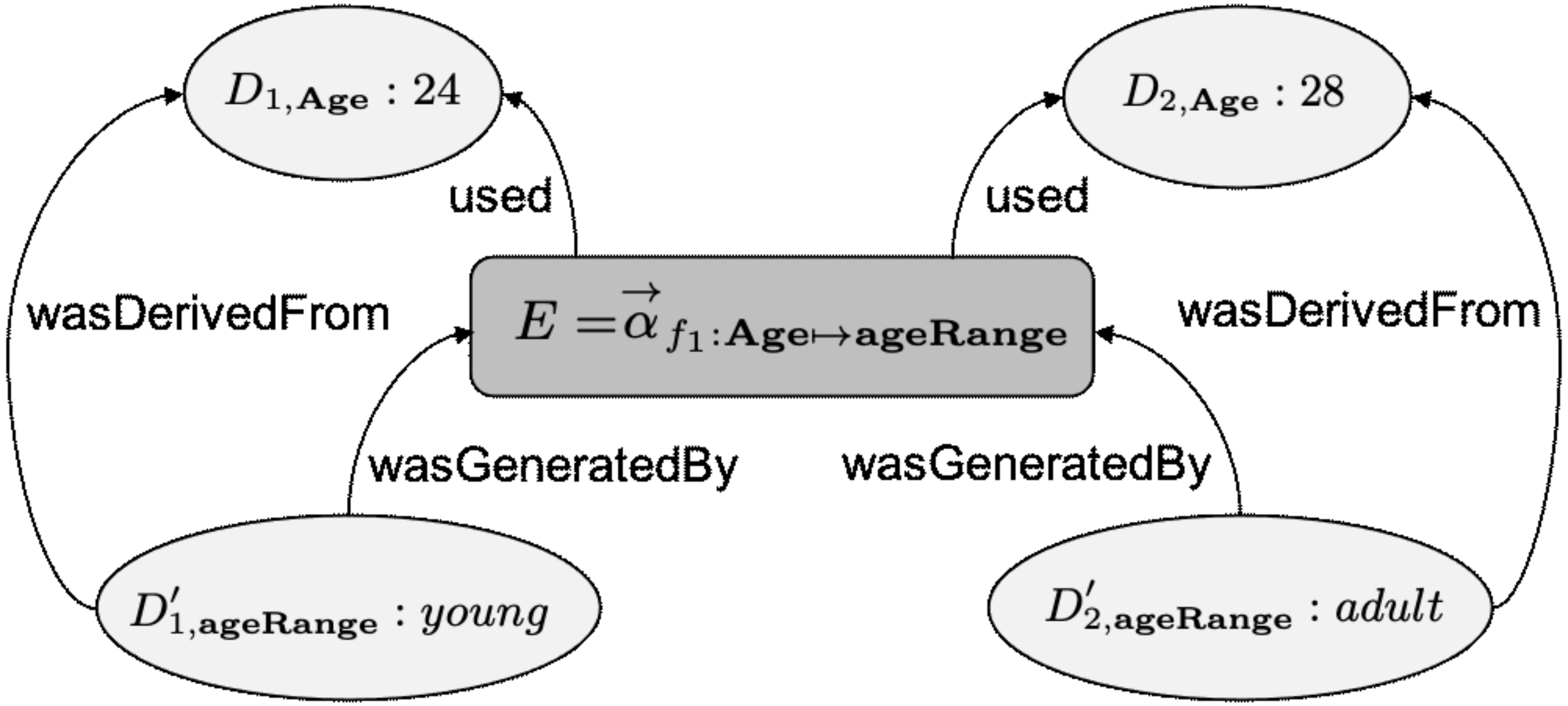
- Undo/redo stacks are **linear**!
- We **lose history** of **exploration**
- Old Solution: User saves files/state
- VisTrails Solution:
  - **Automatically** & **transparently** capture entire history as a **tree**
  - Users can tag or annotate each version
  - Users can go back to **any** version by selecting it in the tree



Data Provenance for Data Science



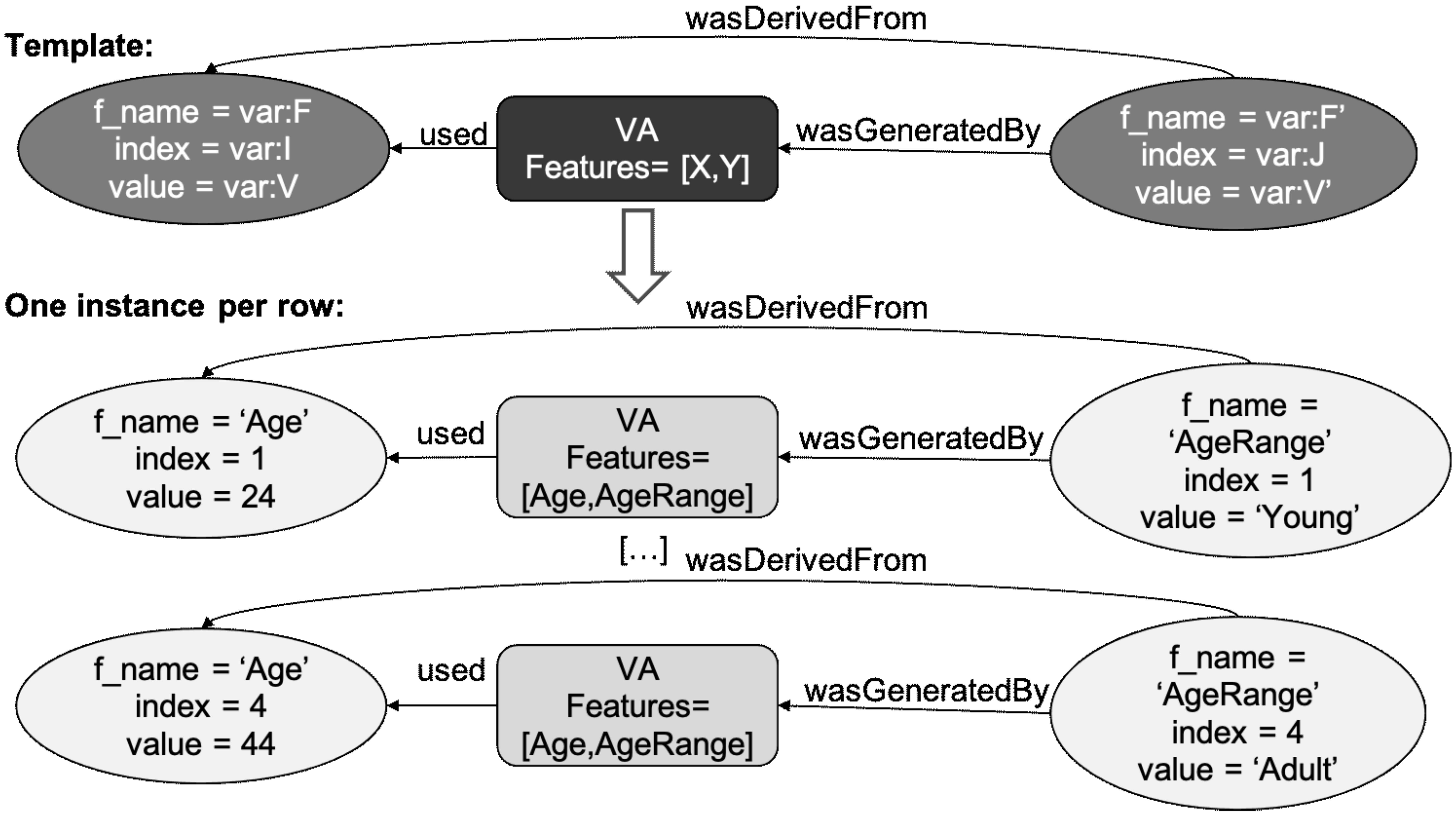
	CId	Gender	Age	Zip	ageRange
1	113	*F*	24	98567	*young*
2	241	*M*	28	⊥	*adult*
3	375	*C*	⊥	32768	⊥
4	578	*F*	44	32768	*adult*



$D_{1,\mathbf{Age}} : 24$
$D_{2,\mathbf{Age}} : 28$
used
used
wasDerivedFrom
$E = \vec{\alpha}_{f_1:\mathbf{Age}\mapsto\mathbf{ageRange}}$
wasDerivedFrom
wasGeneratedBy
wasGeneratedBy
$D'_{1,\mathbf{ageRange}} : young$
$D'_{2,\mathbf{ageRange}} : adult$

[A. Chapman et al., 2020]

Provenance Templates



[A. Chapman et al., 2020]

Assignment 5

- Chicago Bike Sharing Data
  - Spatial Analysis
  - Temporal Analysis
  - Graph Database (neo4j)

Final Exam

- Wednesday, May 10, **8:00**-9:50pm, PM 253
- Similar format
- More comprehensive (questions from topics covered in Test 1 & 2)
- Will also have questions from graph/spatial/temporal data, provenance, reproducibility, machine learning

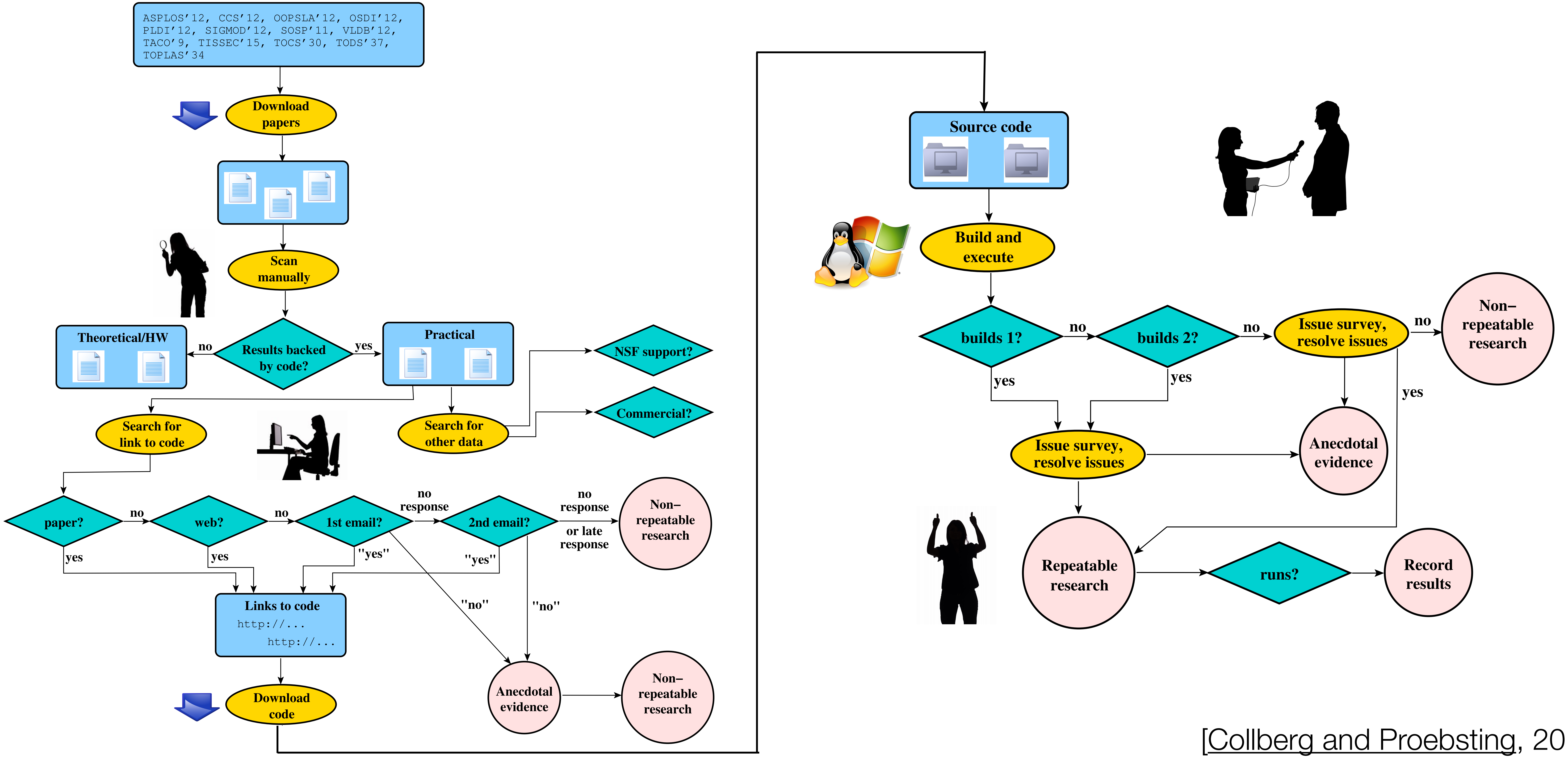
The State of Repeatability in Computer Systems Research

C. Collberg and T. Proebsting
CACM 2016

State of Repeatability in Computer Systems

- "Cool paper! Can you send me the system?"
- How hard is it to just re-execute published experiments
- Most people say they will share their code and data are available…
- Weak repeatability: Do authors make the source code used to create the results in their article available, and will it build?

Experiment



ASPLOS'12, CCS'12, OOPSLA'12, OSDI'12, PLDI'12, SIGMOD'12, SOSP'11, VLDB'12, TACO'9, TISSEC'15, TOCS'30, TODS'37, TOPLAS'34

Download papers

Scan manually

Theoretical/HW

no

Results backed by code?

yes

Practical

NSF support?

Commercial?

Search for link to code

Search for other data

paper?

no

web?

no

1st email?

no response

2nd email?

no response

or late response

Non–repeatable research

yes

yes

"yes"

"yes"

"no"

"no"

Links to code

http://...

http://...

Download code

Anecdotal evidence

Non–repeatable research

Source code

Build and execute

builds 1?

no

builds 2?

no

Issue survey, resolve issues

no

Non–repeatable research

yes

yes

yes

Issue survey, resolve issues

Anecdotal evidence

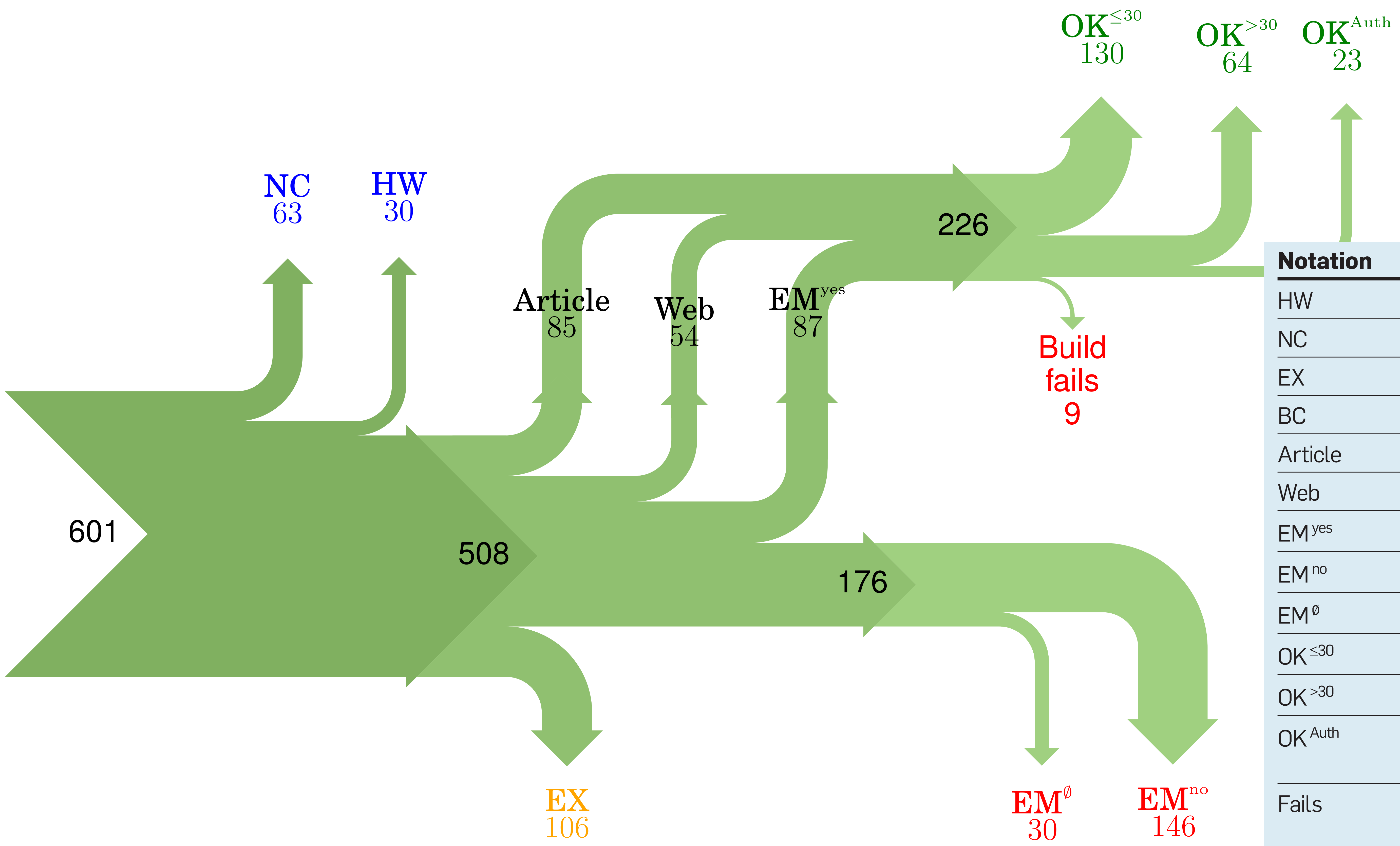
Repeatable research

runs?

Record results

[Collberg and Proebsting, 2015]

Repeatability Results



Notation	Number of papers …
HW	excluded due to replication requiring special hardware
NC	excluded due to results not being backed by code
EX	excluded due to overlapping author lists
BC	where the results are backed by code
Article	where code was found in the paper itself
Web	where code was found through a Web search
EM^{yes}	where the author provides code after receiving an email message
EM^{no}	where the author responds to an email message saying code cannot be provided
$EM^{\emptyset}$	where the author does not respond to email requests within two months
$OK^{\leq 30}$	where code is available and we succeed in building the system in ≤30 minutes
$OK^{>30}$	where code is available and we succeed in building the system in >30 minutes
OK^{Auth}	where code is available and we fail to build, and the author says the code builds with reasonable effort
Fails	where code is available and we fail to build, and the author says the code may have problems building

Figure 11: Study result. Blue numbers represent papers that were excluded from consideration, green numbers papers that are weakly repeatable, red numbers papers that are non-weakly repeatable, and orange numbers represent papers that were excluded (due to our restriction of sending at most one email to each author).

[Collberg and Proebsting, 2015]

Excuses

- "Unfortunately the current system is not mature"
- "The code was never intended to be released so it is not in any shape for general use"
- "[Our] prototype included many moving pieces that only [student] knew how to operate… he left"
- "… the server in which my implementation was stored had a disk crash … three disks crashed… Sorry for that"

[Collberg and Proebsting, 2015]

Excuses

- "…when we attempted to share it, we [spent] more time getting outsiders up to speed than on our own research"
- "… we can't share what [we] did for this paper. … this is not in the academic tradition, but this is a hazard in an industrial lab"
- "… based on earlier (bad) experience, we [want] to make sure that our implementation is not used in situations that it is not meant for"

[Collberg and Proebsting, 2015]

Excuse Classification

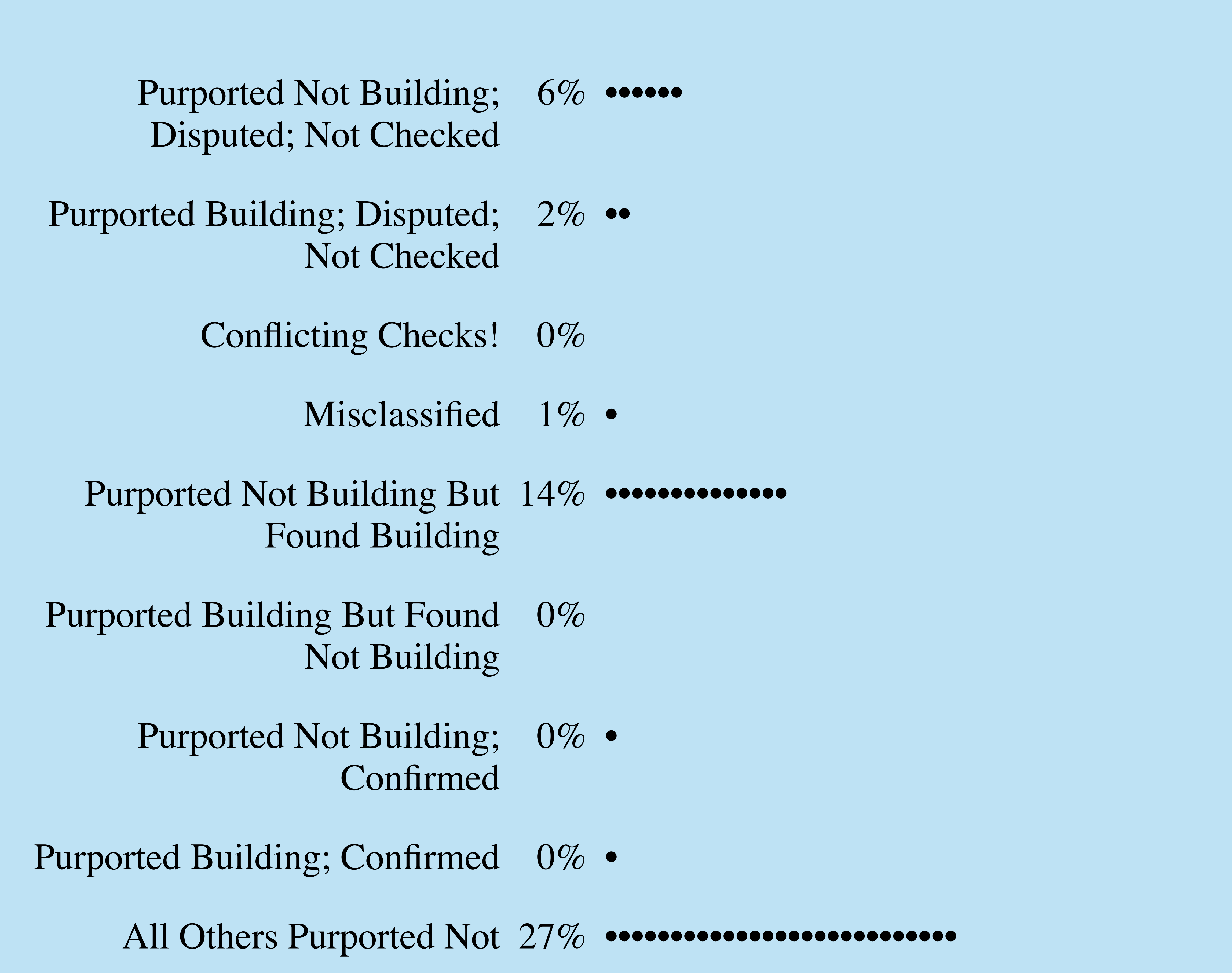
- Versioning
- Available Soon
- No Intention to Share
- Personnel Issues
- Lost Code
- Academic Tradeoffs
- Industrial Lab Tradeoffs
- Obsolete HW/SW
- Controlled Usage
- Privacy/Security
- Design Issues

[Collberg and Proebsting, 2015]

Some of these are (partially) people problems, not technical problems

Examining 'Reproducibility in Computer Science'

- Repeat the experiment in reproducibility!
- Differences from original
- Shows issues with trying to classify experiments



[S. Krishnamurthi et al.]

Recommendations

- Fund repeatability engineering
- Require sharing contracts

Location	• email address and/or web site
Resource	• **types**: code, data, media, documentation • **availability**: no access, access, NDA access • **expense**: free, non-free, free for academics • **distribution form**: source, binary, service • **expiration date** • **license** • **comment**
Support	• **kinds**: resolve installation issues, fix bugs, upgrade to new language and operating system versions, port to new environments, improve performance, add features • **expense**: free, non-free, free for academics • **expiration date**

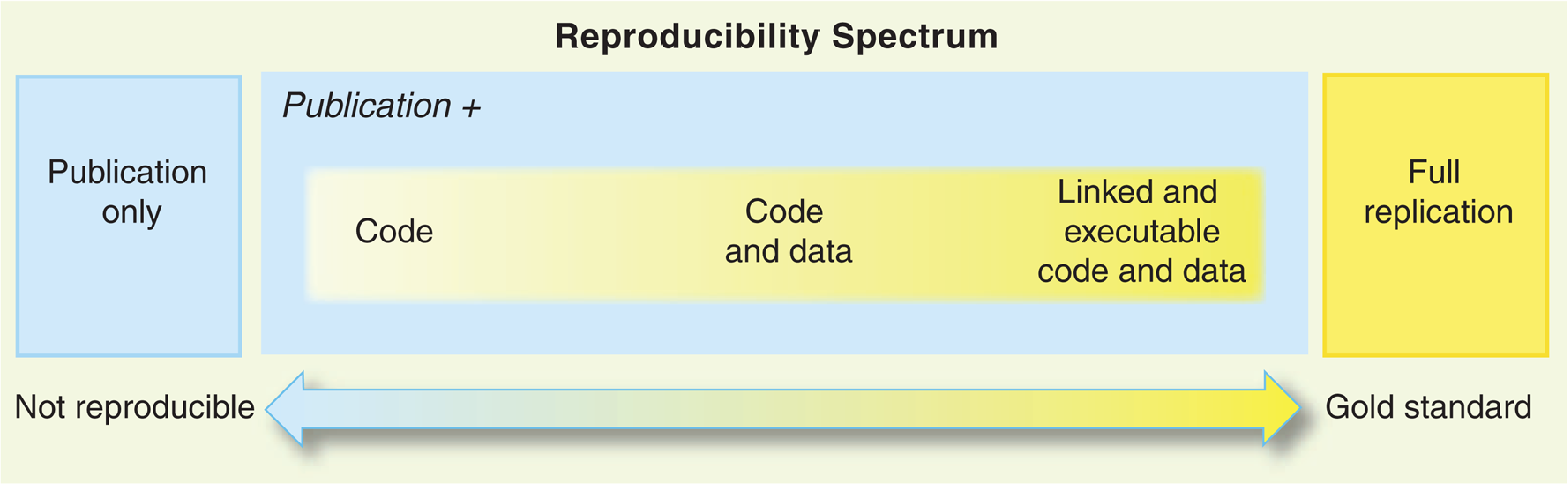
[Collberg and Proebsting, 2015]

Reproducible Research

- Science is verified by replicating work independently
- Replication Issues:
  - Requires many resources to replicate (Sloan Digital Sky Survey)
  - Requires significant computing power (Climate Model Simulation)
  - Requires too much time or very specific circumstances (Environment Epidemiology)
- Reproducibility
  - Replication of the analysis based on the collected data (not replicating the data collection itself)
  - Better if we have the actual code or available executables

[R. D. Peng]

Reproducibility Spectrum



Reproducibility Spectrum

Publication only

Publication +

Code

Code and data

Linked and executable code and data

Full replication

Not reproducible

Gold standard

[R. D. Peng]

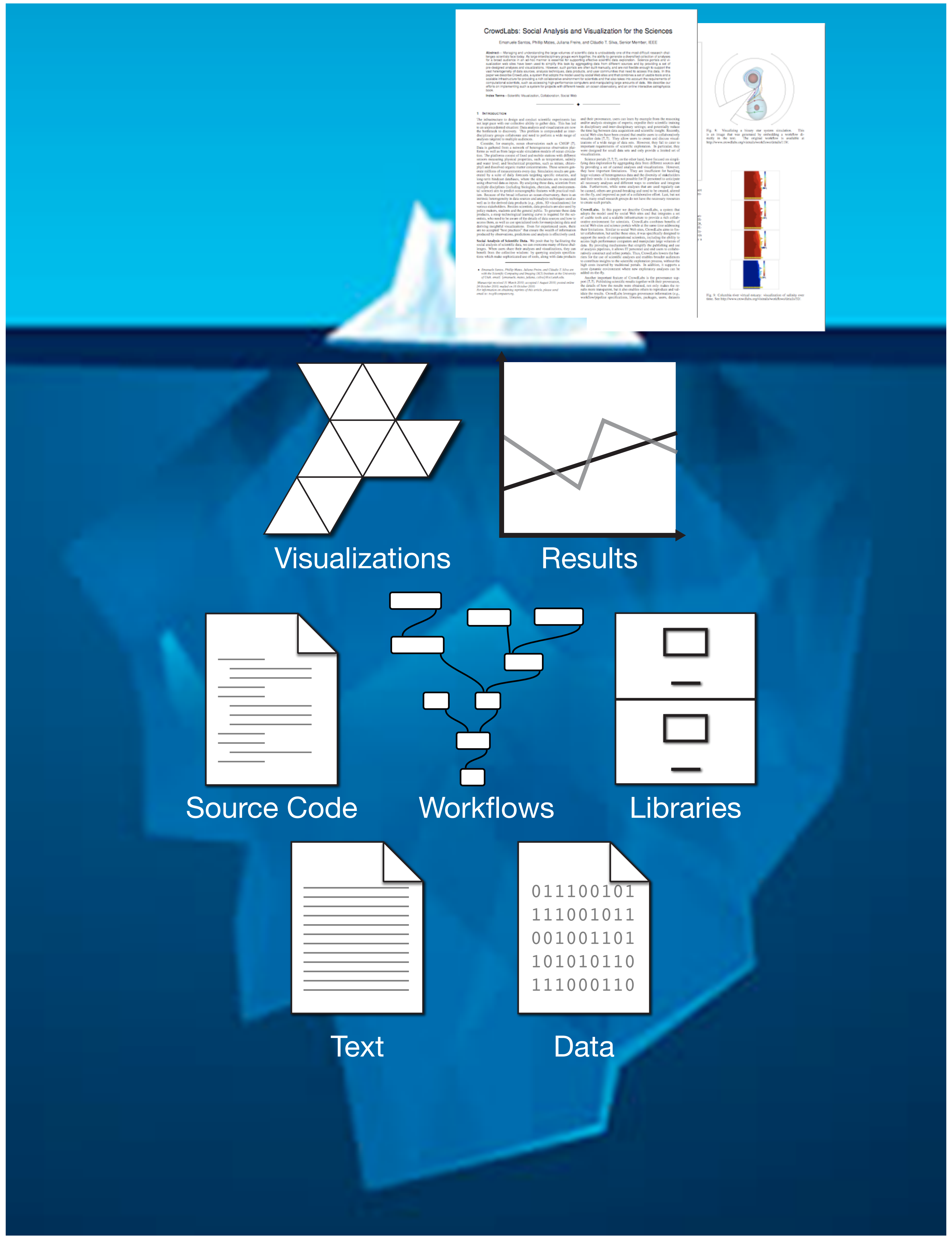
Published Papers

- “It’s impossible to verify most of the results that computational scientists present at conference and in papers.” [Donoho et al., 2009]
- “Scientific and mathematical journals are filled with pretty pictures of computational experiments that the reader has no hope of repeating.” [LeVeque, 2009]
- “Published documents are merely the advertisement of scholarship whereas the computer programs, input data, parameter values, etc. embody the scholarship itself.” [Schwab et al., 2007]

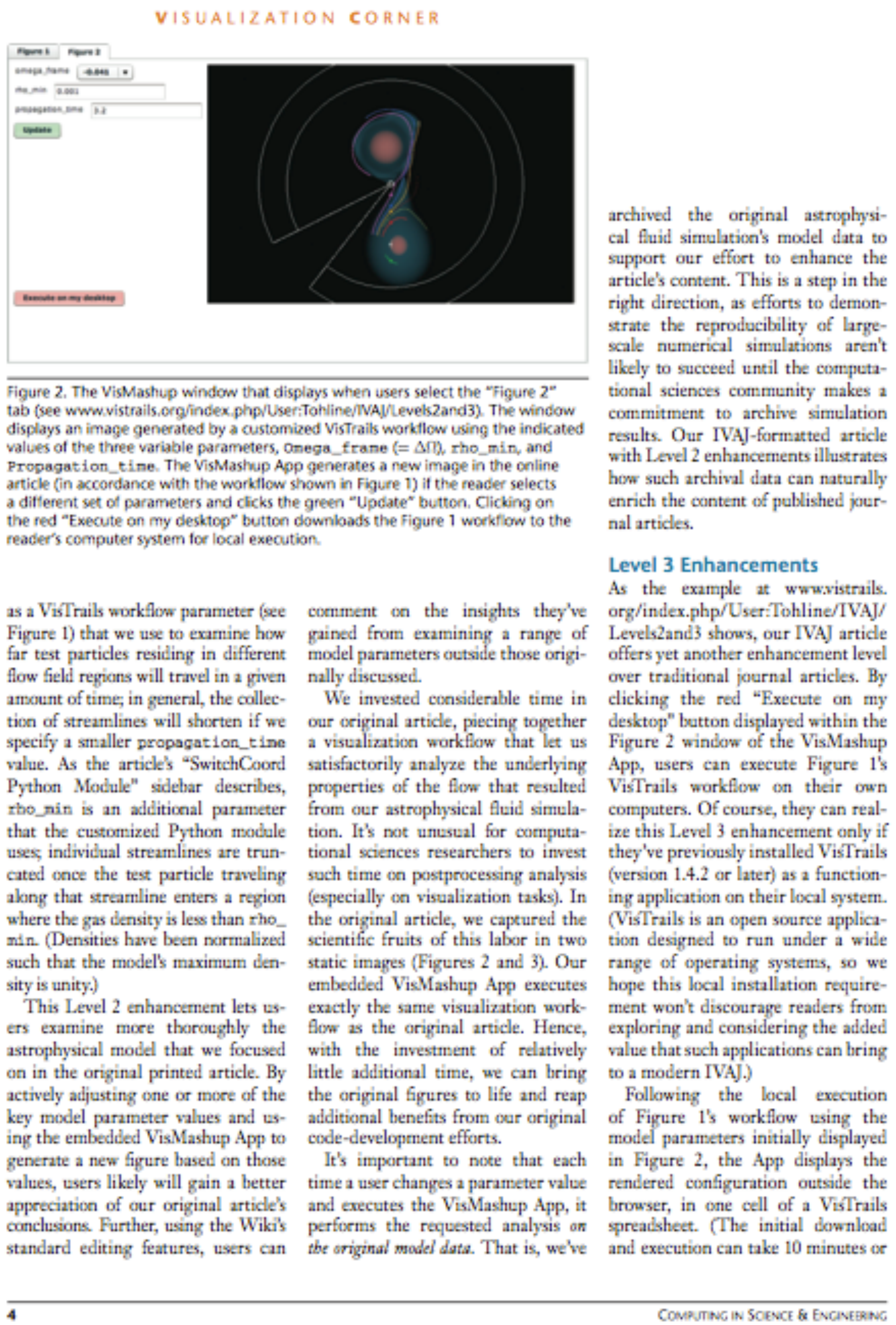
Problem: Incomplete Publications

- A paper cannot include all relevant details of the science
  - Large volumes of data
  - Complex processes
  - Code dependencies

- This makes publishing complete results more difficult!



Reproducible/Executable Papers



omega_frame -0.041

rho_min 0.001

propagation_time 3.2

Figure 2. The VisMashup window that displays when users select the "Figure 2" tab (see www.vistrails.org/index.php/User:Tohline/IVAJ/Levels2and3). The window displays an image generated by a customized VisTrails workflow using the indicated values of the three variable parameters, `Omega_frame` (= ΔΩ), `rho_min`, and `Propagation_time`. The VisMashup App generates a new image in the online article (in accordance with the workflow shown in Figure 1) if the reader selects a different set of parameters and clicks the green "Update" button. Clicking on the red "Execute on my desktop" button downloads the Figure 1 workflow to the reader's computer system for local execution.

as a VisTrails workflow parameter (see Figure 1) that we use to examine how far test particles residing in different flow field regions will travel in a given amount of time; in general, the collection of streamlines will shorten if we specify a smaller `propagation_time` value. As the article's "SwitchCoord Python Module" sidebar describes, `rho_min` is an additional parameter that the customized Python module uses; individual streamlines are truncated once the test particle traveling along that streamline enters a region where the gas density is less than `rho_min`. (Densities have been normalized such that the model's maximum density is unity.)

This Level 2 enhancement lets users examine more thoroughly the astrophysical model that we focused on in the original printed article. By actively adjusting one or more of the key model parameter values and using the embedded VisMashup App to generate a new figure based on those values, users likely will gain a better appreciation of our original article's conclusions. Further, using the Wiki's standard editing features, users can comment on the insights they've gained from examining a range of model parameters outside those originally discussed.

We invested considerable time in our original article, piecing together a visualization workflow that let us satisfactorily analyze the underlying properties of the flow that resulted from our astrophysical fluid simulation. It's not unusual for computational sciences researchers to invest such time on postprocessing analysis (especially on visualization tasks). In the original article, we captured the scientific fruits of this labor in two static images (Figures 2 and 3). Our embedded VisMashup App executes exactly the same visualization workflow as the original article. Hence, with the investment of relatively little additional time, we can bring the original figures to life and reap additional benefits from our original code-development efforts.

It's important to note that each time a user changes a parameter value and executes the VisMashup App, it performs the requested analysis *on the original model data*. That is, we've archived the original astrophysical fluid simulation's model data to support our effort to enhance the article's content. This is a step in the right direction, as efforts to demonstrate the reproducibility of large-scale numerical simulations aren't likely to succeed until the computational sciences community makes a commitment to archive simulation results. Our IVAJ-formatted article with Level 2 enhancements illustrates how such archival data can naturally enrich the content of published journal articles.

Level 3 Enhancements

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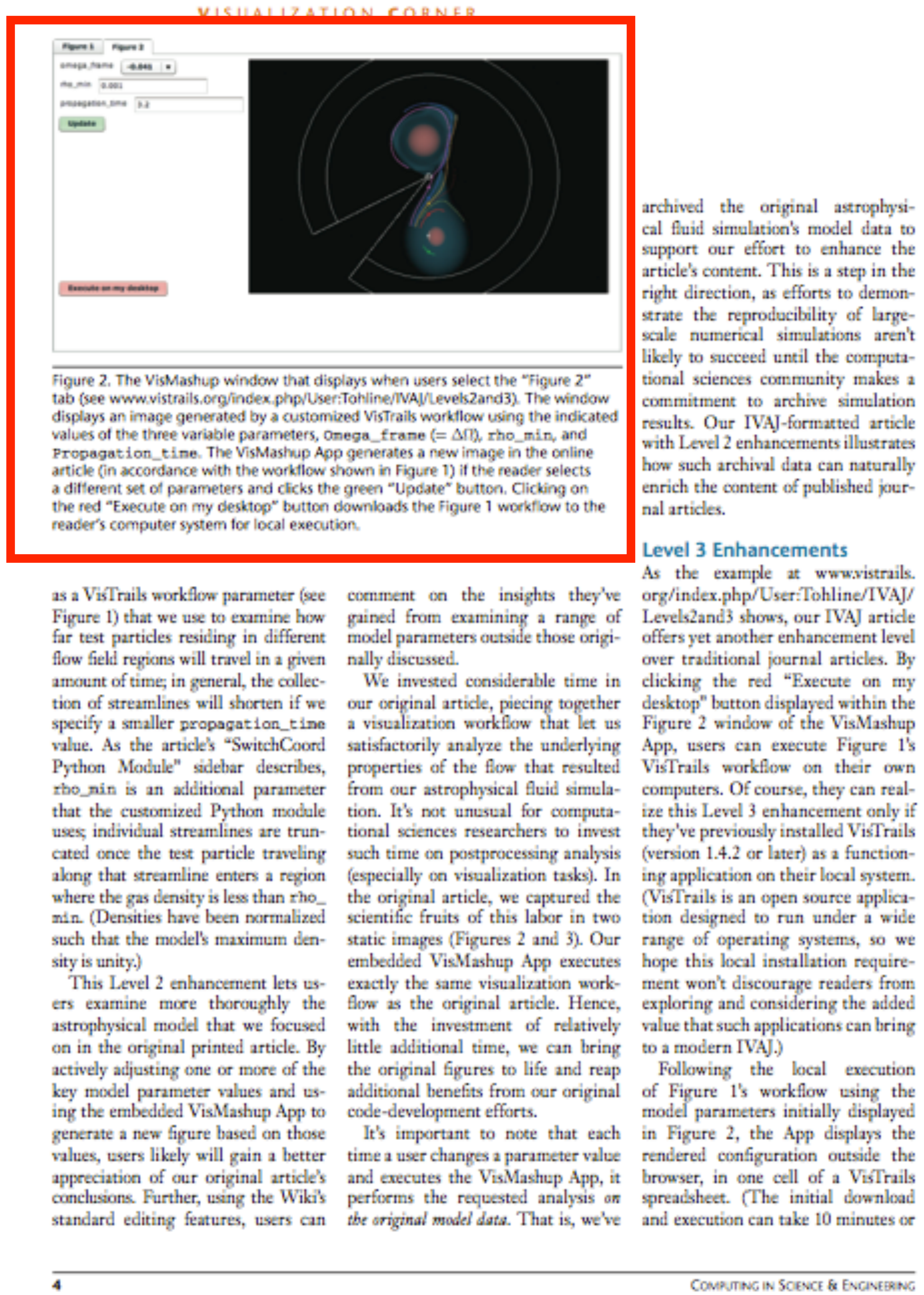
Following the local execution of Figure 1's workflow using the model parameters initially displayed in Figure 2, the App displays the rendered configuration outside the browser, in one cell of a VisTrails spreadsheet. (The initial download and execution can take 10 minutes or

Reproducible/Executable Papers



VISUALIZATION CORNER

omega_frame -0.840
rho_min 0.001
propagation_time 3.2

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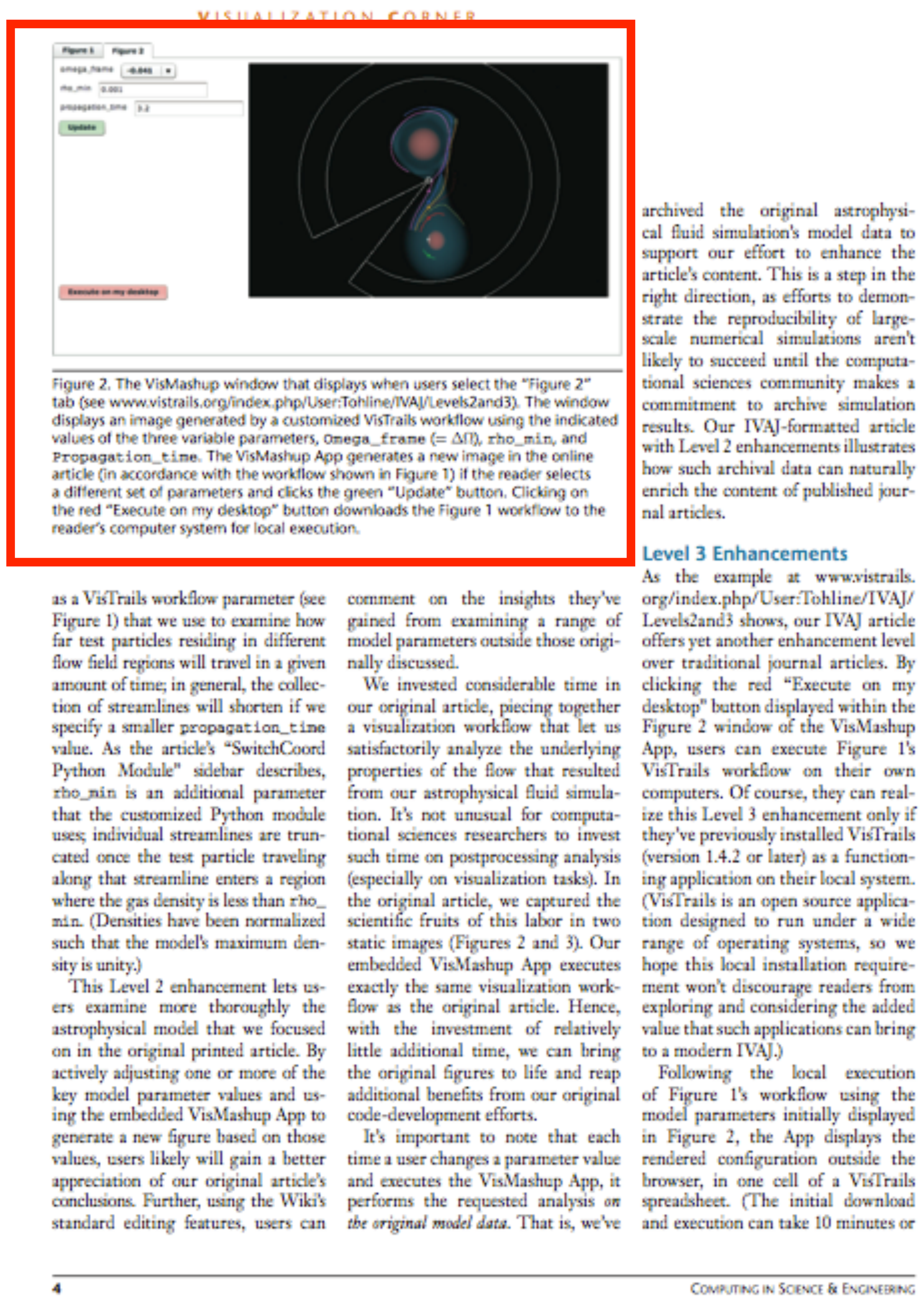
4 COMPUTING IN SCIENCE & ENGINEERING

Reproducible/Executable Papers



VISUALIZATION CORNER

Figure 1 | Figure 2

omega_frame -0.041

rho_min 0.001

propagation_time 3.2

Update

Execute on my desktop

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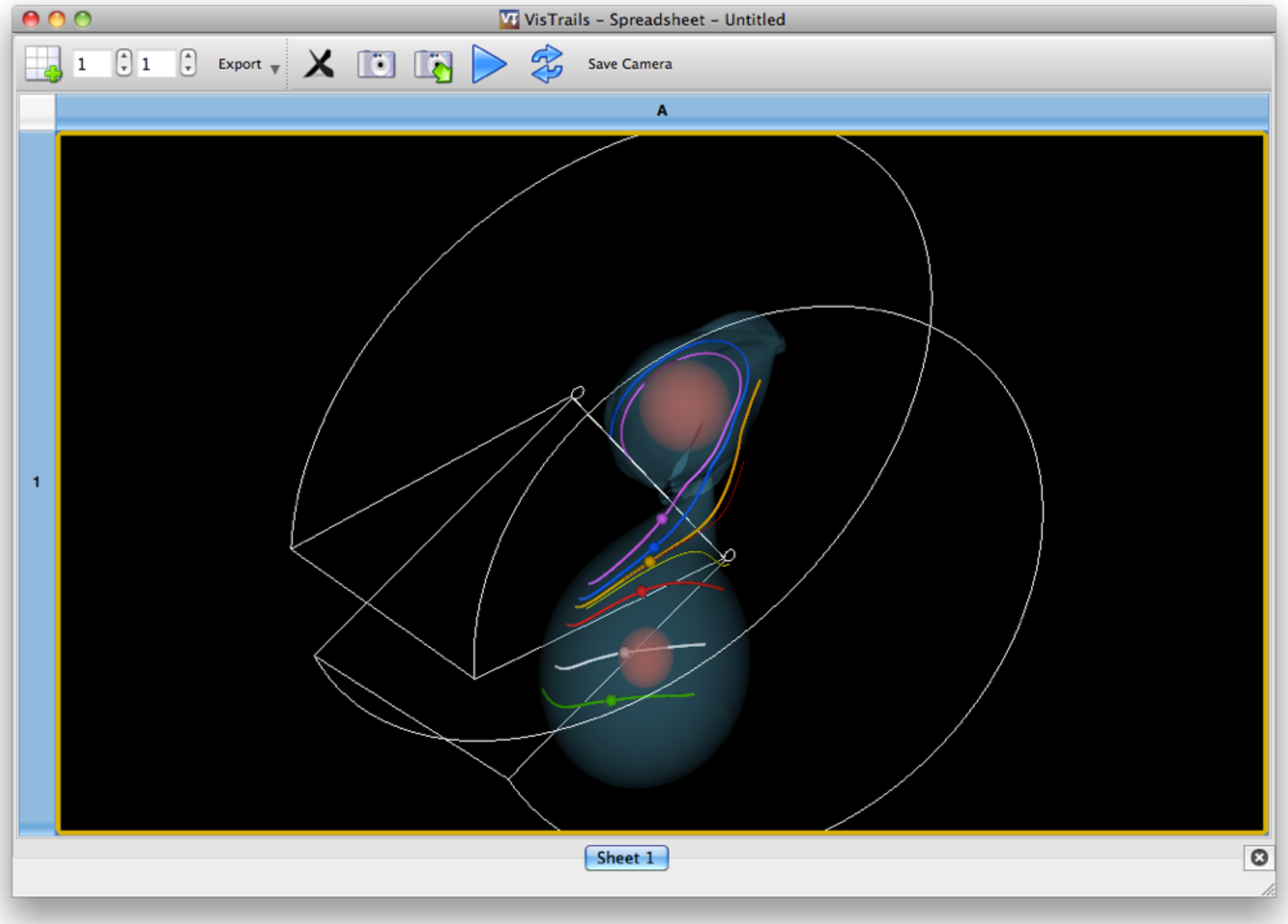
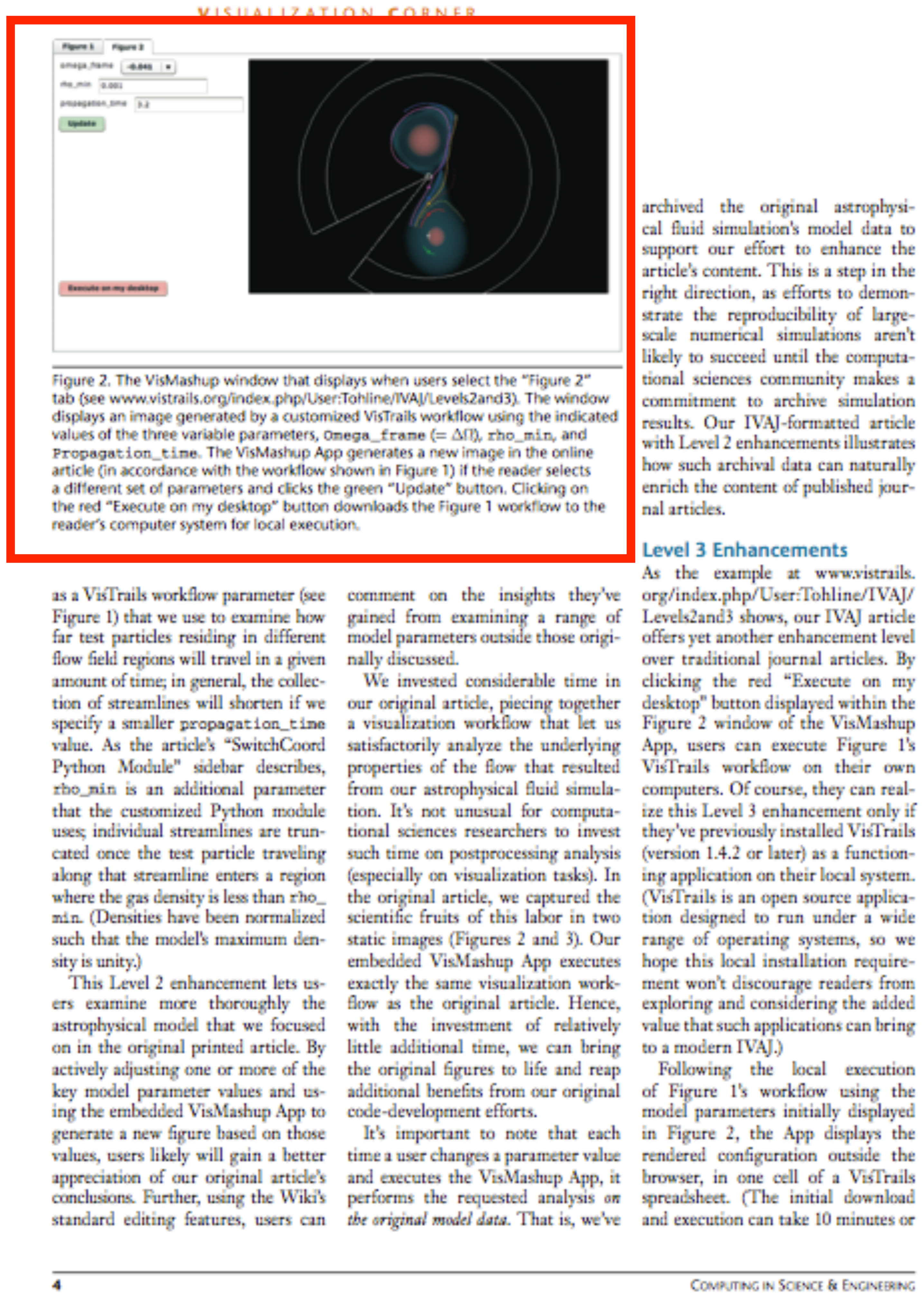
Following the local execution of Figure 1's workflow using the model parameters initially displayed in Figure 2, the App displays the rendered configuration outside the browser, in one cell of a VisTrails spreadsheet. (The initial download and execution can take 10 minutes or

4

COMPUTING IN SCIENCE & ENGINEERING



Reproducible/Executable Papers



VISUALIZATION CORNER

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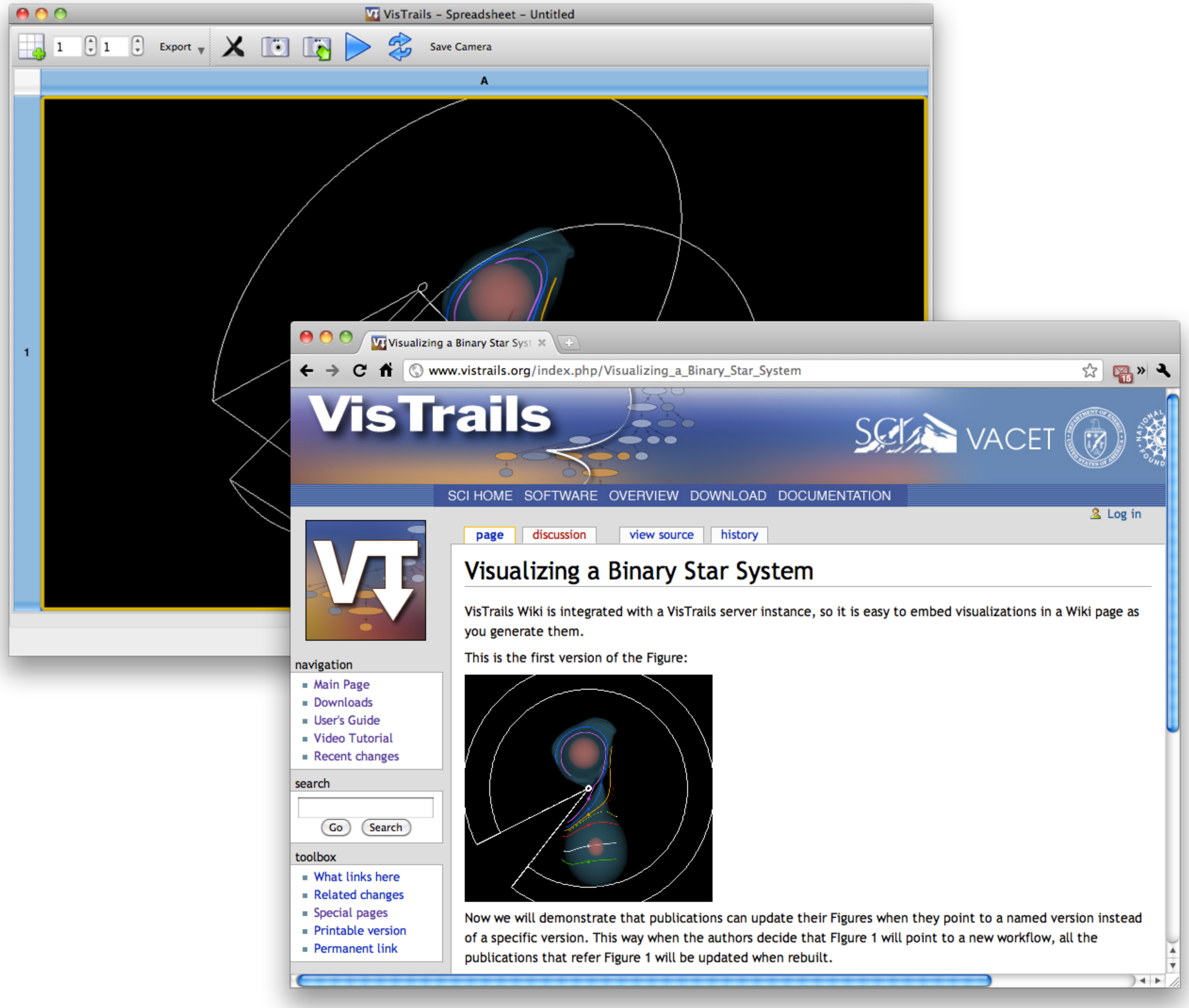
Computing in Science & Engineering



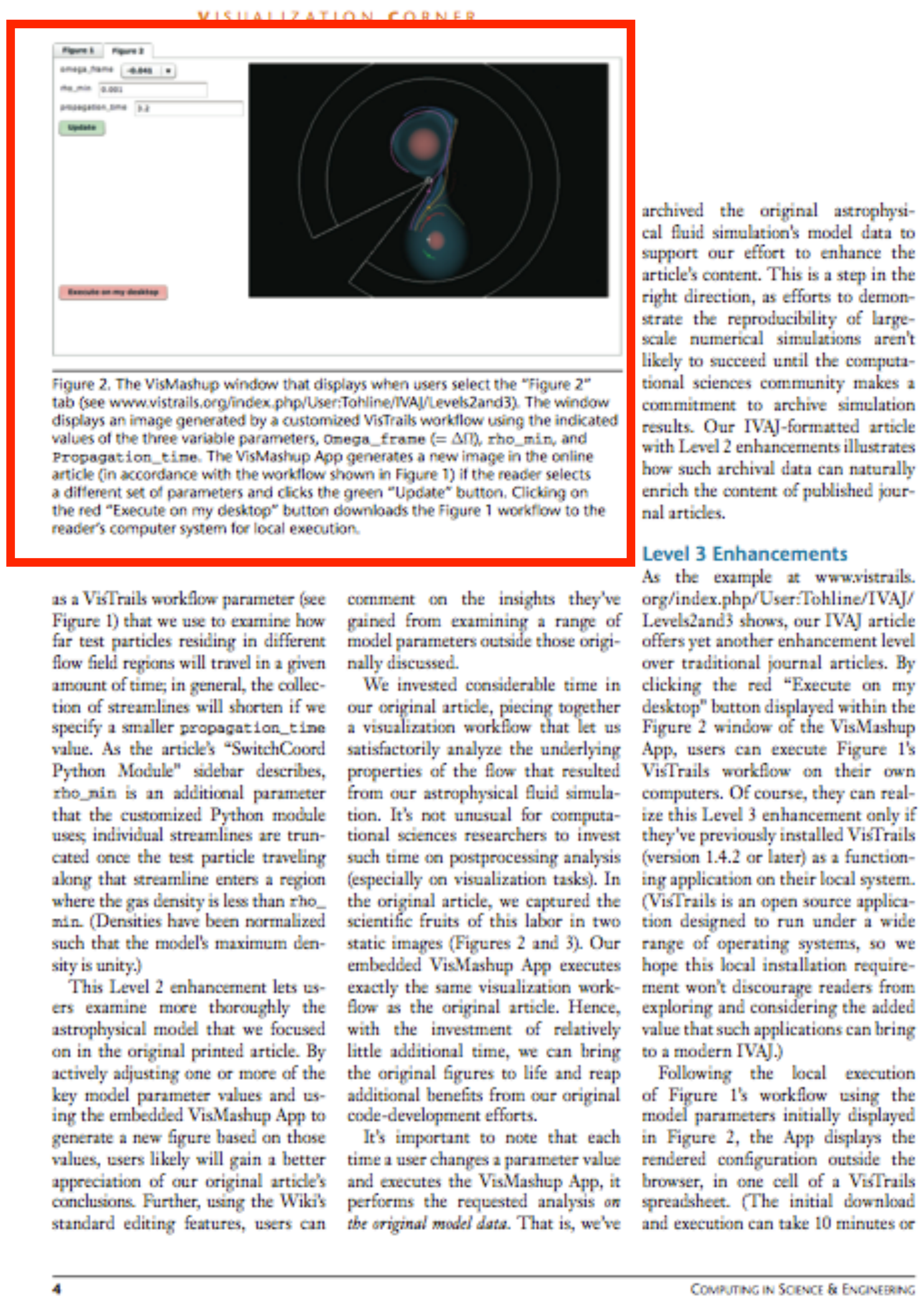
Visualizing a Binary Star System

VisTrails Wiki is integrated with a VisTrails server instance, so it is easy to embed visualizations in a Wiki page as you generate them.

This is the first version of the Figure:

Now we will demonstrate that publications can update their Figures when they point to a named version instead of a specific version. This way when the authors decide that FIgure 1 will point to a new workflow, all the publications that refer Figure 1 will be updated when rebuilt.

Reproducible/Executable Papers



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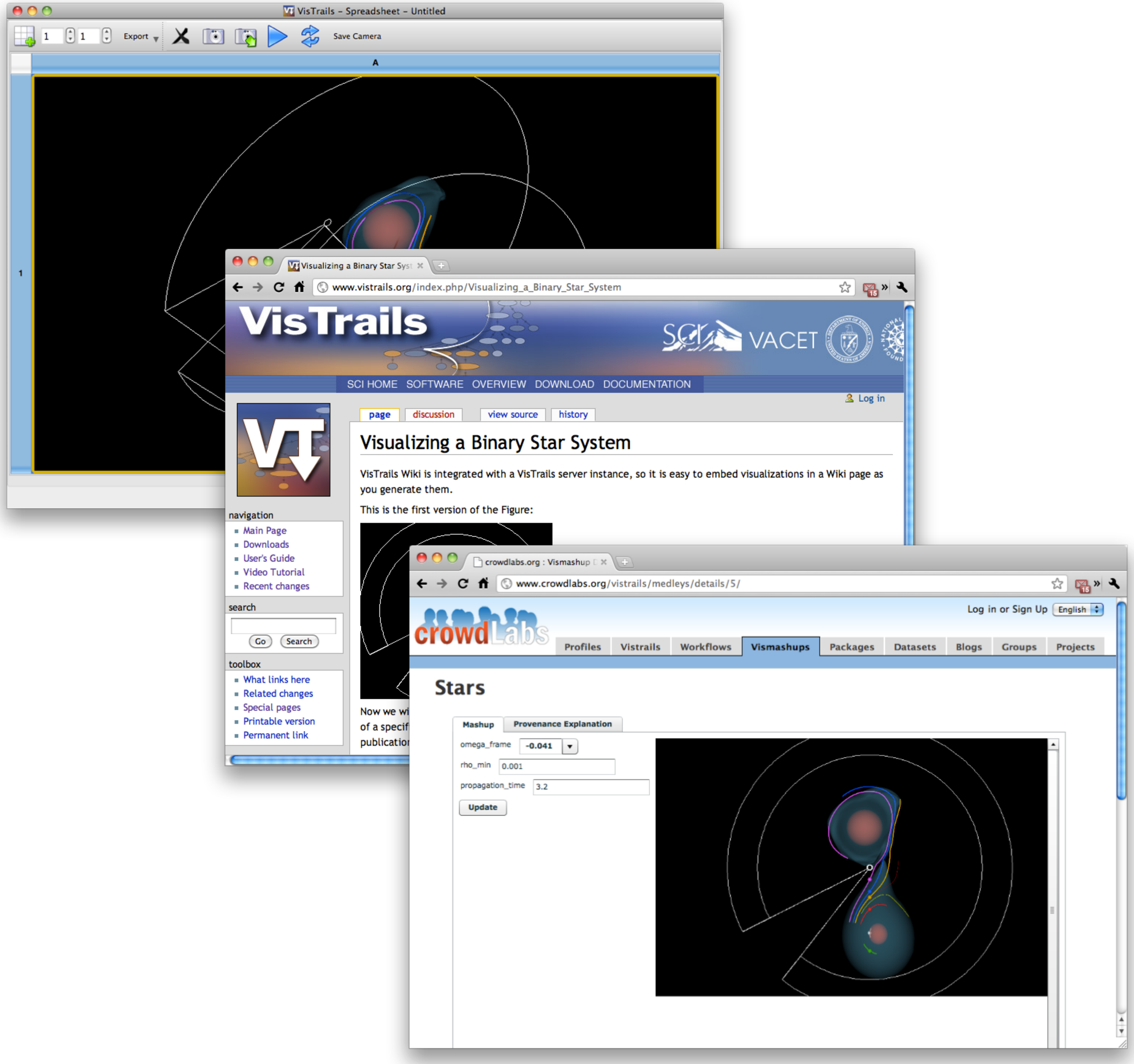
COMPUTING IN SCIENCE & ENGINEERING



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This is the first version of the Figure:

Now we wi
of a specif
publicatio

Stars

omega_frame -0.041

rho_min 0.001

propagation_time 3.2

Challenges

- Re-using results
- Adding results to publications
- Obtaining results, computations, and input from publications
- Publishing interactive experiments
- Searching executable paper collections
- Reviewers: execution environments, checking different parameters
- Longevity/maintenance
- Resource constraints:
  - analyses run on supercomputers
  - large datasets
  - privacy or intellectual property concerns

General Strategies for Reproducibility

- Preserving the Mess:
  - Just save a virtual machine
  - Trace dependencies
- Encouraging Cleanliness:
  - Use a system (e.g. Umbrella, VisTrails)
  - Use literate programming environments
  - Use code and data repositories
  - Use packaging system (ReproZip)

[Categories from H. Meng et al., 2016]

Literate Programming

- Knuth's WEB system
- Mathematica
- Code this is well-documented using comments
- Jupyter Notebooks

Data and Code Availability

- Code Repositories:
  - GitHub
  - GitLab
  - ...
- Data Repositories:
  - figshare, freebase, dryad, DataONE
  - Also many domain-specific repositories
  - http://oad.simmons.edu/oadwiki/Data_repositories

10 Rules for Reproducible Computational Research

- Rule 1: For Every Result, Keep Track of How It Was Produced
- Rule 2: Avoid Manual Data Manipulation Steps
- Rule 3: Archive the Exact Versions of All External Programs Used
- Rule 4: Version Control All Custom Scripts
- Rule 5: Record All Intermediate Results, When Possible in Standardized Formats

[Sandve et al., 2013]

10 Rules for Reproducible Computational Research

- Rule 6: For Analyses That Include Randomness, Note Underlying Random Seeds
- Rule 7: Always Store Raw Data behind Plots
- Rule 8: Generate Hierarchical Analysis Output, Allowing Layers of Increasing Detail to Be Inspected
- Rule 9: Connect Textual Statements to Underlying Results
- Rule 10: Provide Public Access to Scripts, Runs, and Results

[Sandve et al., 2013]

Rules or Benefits?

- Laws to make sure people don't cheat or lie or steal
- Is that a good incentive? You won't be mislabeled as a criminal?
- Benefits of Reproducibility
  - Reproducible programs can be compared
  - Reproducible software and results are documented
  - Reproducible software is portable
  - Reproducible experiments are cited

[J. Freire et al.]

Reproducible Experiments Classification

- Depth: how much is available?
  - figures
  - scripts
  - raw data
  - experiments
  - software system
- Portability: what machine specs are necessary?
  - same machine
  - similar machine
  - different OS
- Coverage: how much can be reproduced?

[J. Freire et al.]

(Database) Research Topics

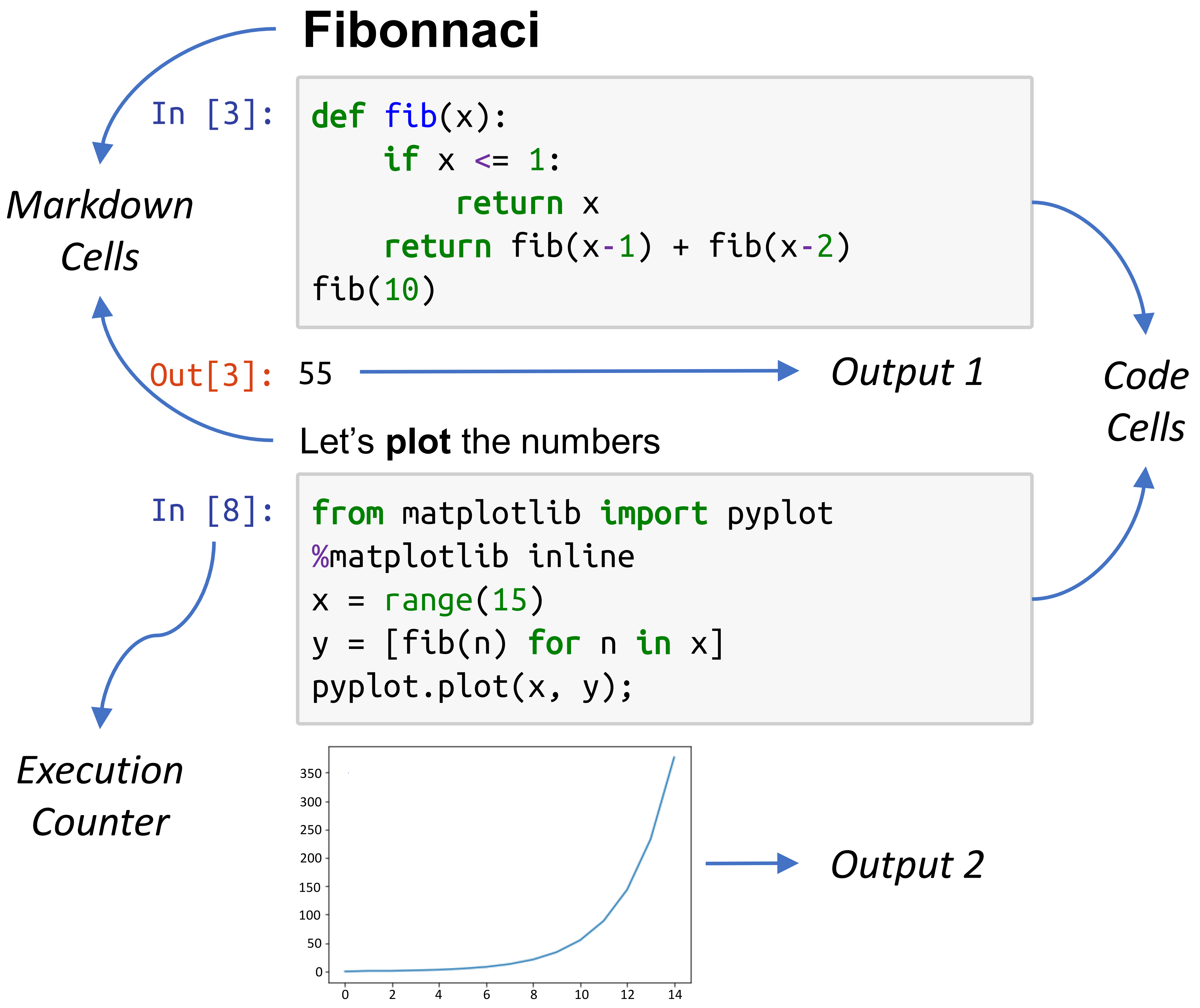
- Design and Management of Experiment Repositories
- Querying and Searching Experiments
- Mining Experiments

[J. Freire et al.]

A Large-scale Study about Quality and Reproducibility of Jupyter Notebooks

J. F. Pimentel, L. Murta, V. Braganholo, and J. Freire

Notebooks and Hidden State



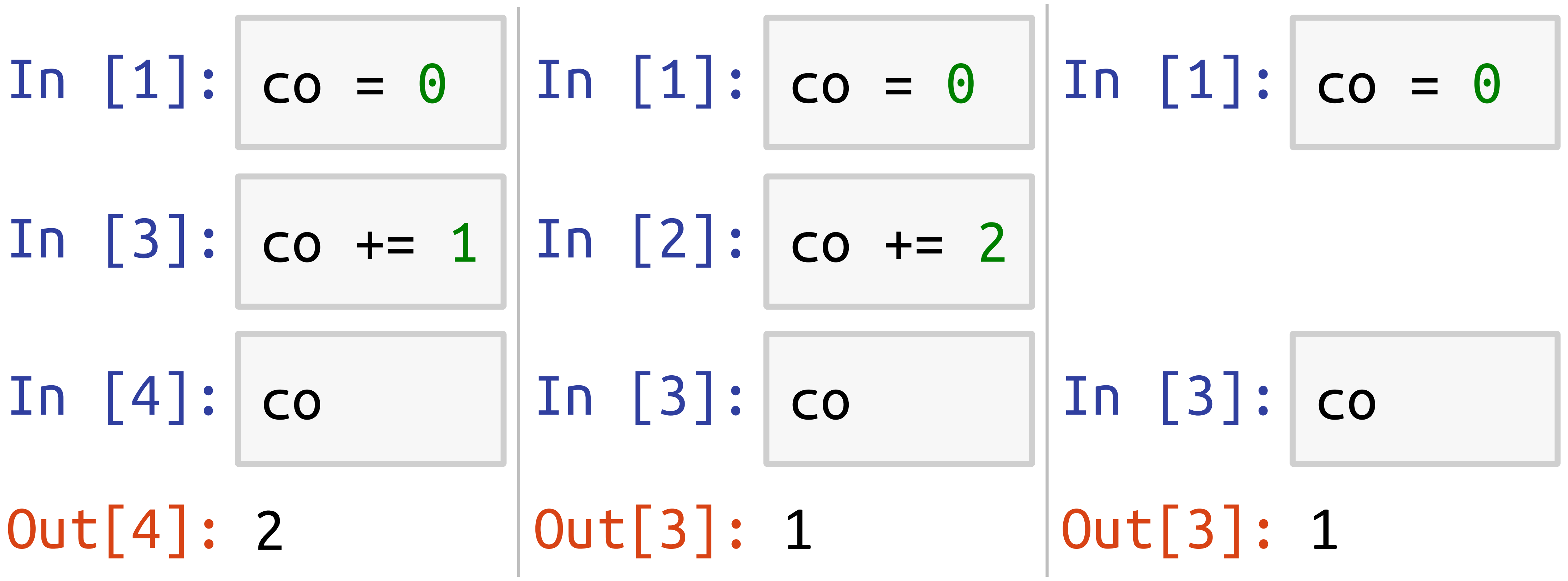
Fibonnaci

```
In [3]: def fib(x):
            if x <= 1:
                return x
            return fib(x-1) + fib(x-2)
        fib(10)

Out[3]: 55
```

Let's **plot** the numbers

```
In [8]: from matplotlib import pyplot
        %matplotlib inline
        x = range(15)
        y = [fib(n) for n in x]
        pyplot.plot(x, y);
```



```
In [1]: co = 0

In [3]: co += 1

In [4]: co

Out[4]: 2
```

```
In [1]: co = 0

In [2]: co += 2

In [3]: co

Out[3]: 1
```

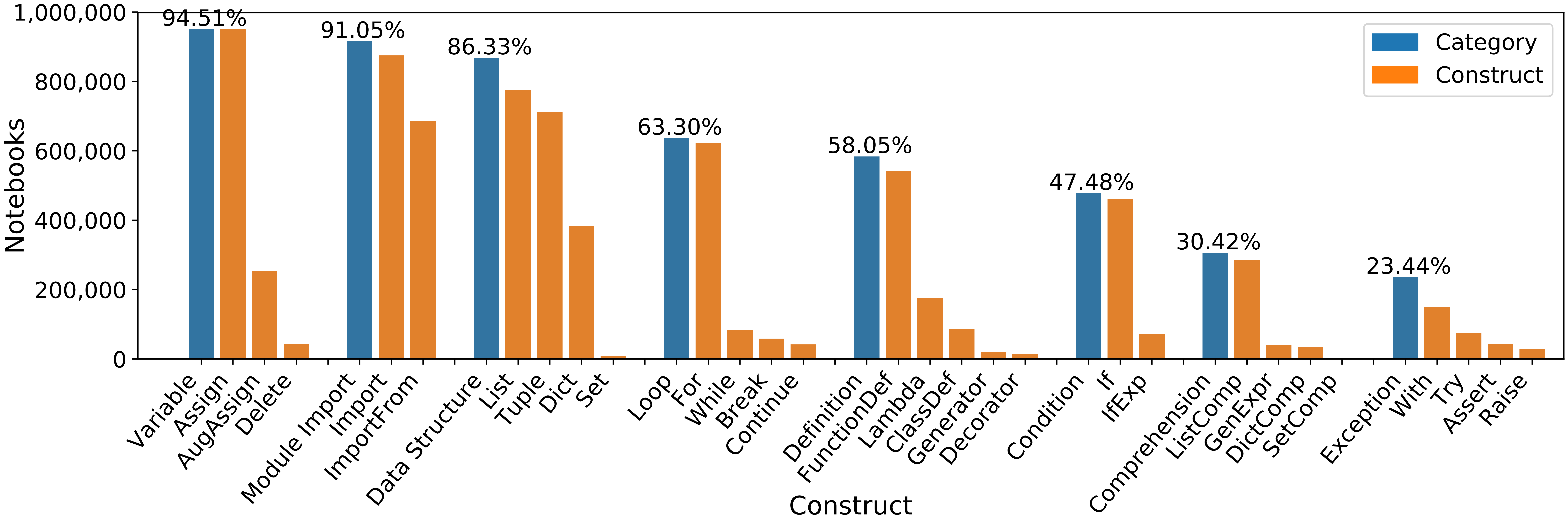
```
In [1]: co = 0

In [3]: co

Out[3]: 1
```

[Pimentel et al., 2019]

Notebook Composition



[Pimentel et al., 2019]

Notebook Reproducibility

- Use notebooks from Github (~1 million)
    - Unambiguous cell order? 81.99%
- Study notebook dependencies
    - Dependencies Available? 13.72%
    - Dependencies Install? 5.03%
- Study notebook executability
    - Execute: 24.11% of unambiguous cell order
    - Matched results: 4.03%

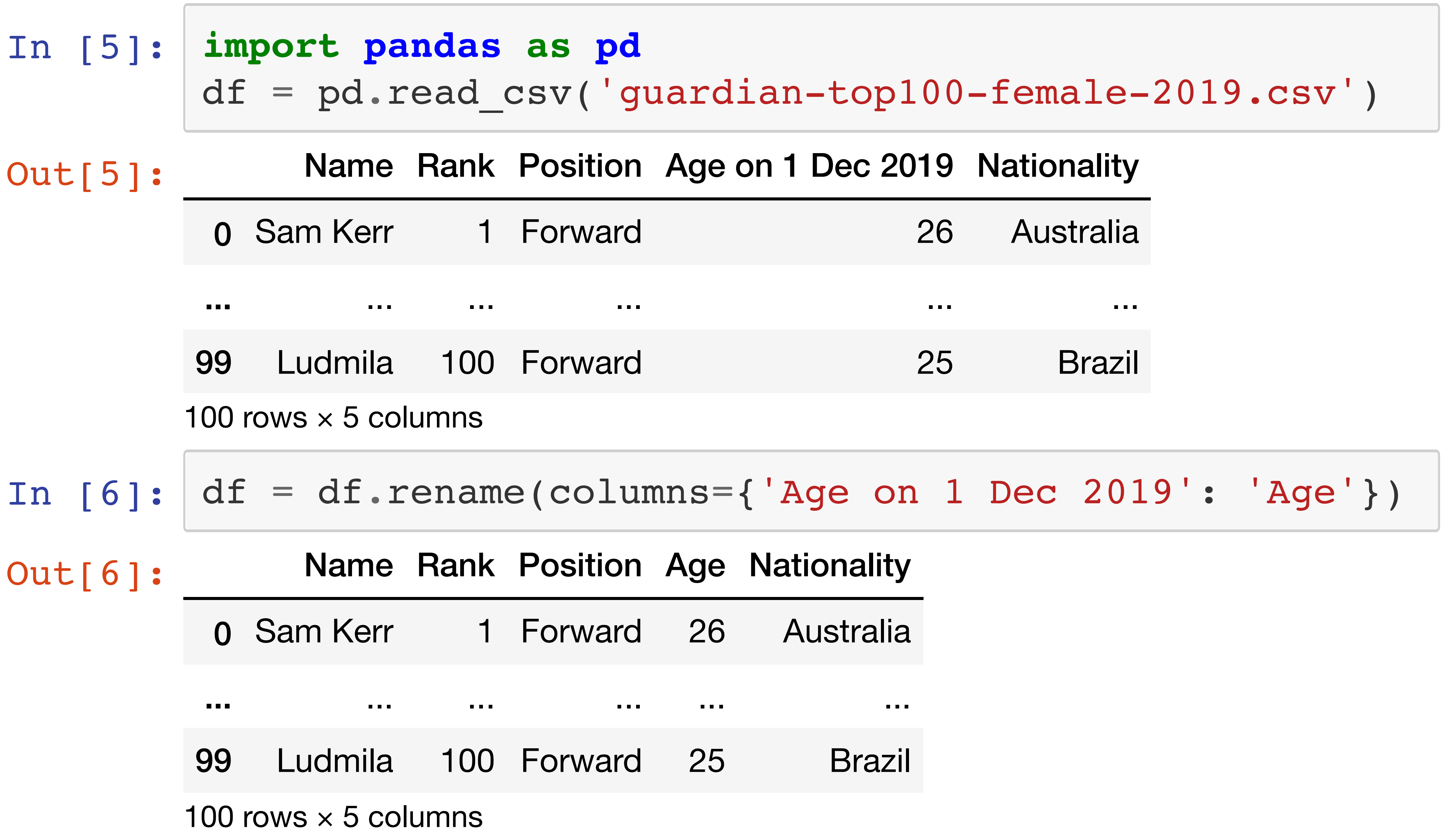
[Pimentel et al., 2019]

Best Practices

- Use short titles with a restrict charset (A-Z a-z 0-9 . -) for notebook files and markdown headings for more detailed ones in the body
- Pay attention to the bottom of the notebook. Check whether it can benefit from descriptive markdown cells or can have code cells executed or removed
- Abstract code into functions, classes, and modules and test them
- Declare the dependencies in requirement files & pin versions of all packages
- Use a clean environment to test if dependencies are properly declared
- Put imports at the beginning of notebooks
- Use relative paths for accessing data in the repository
- Re-run notebooks top to bottom before committing

[Pimentel et al., 2019]

Problem: What is df at any point in time?

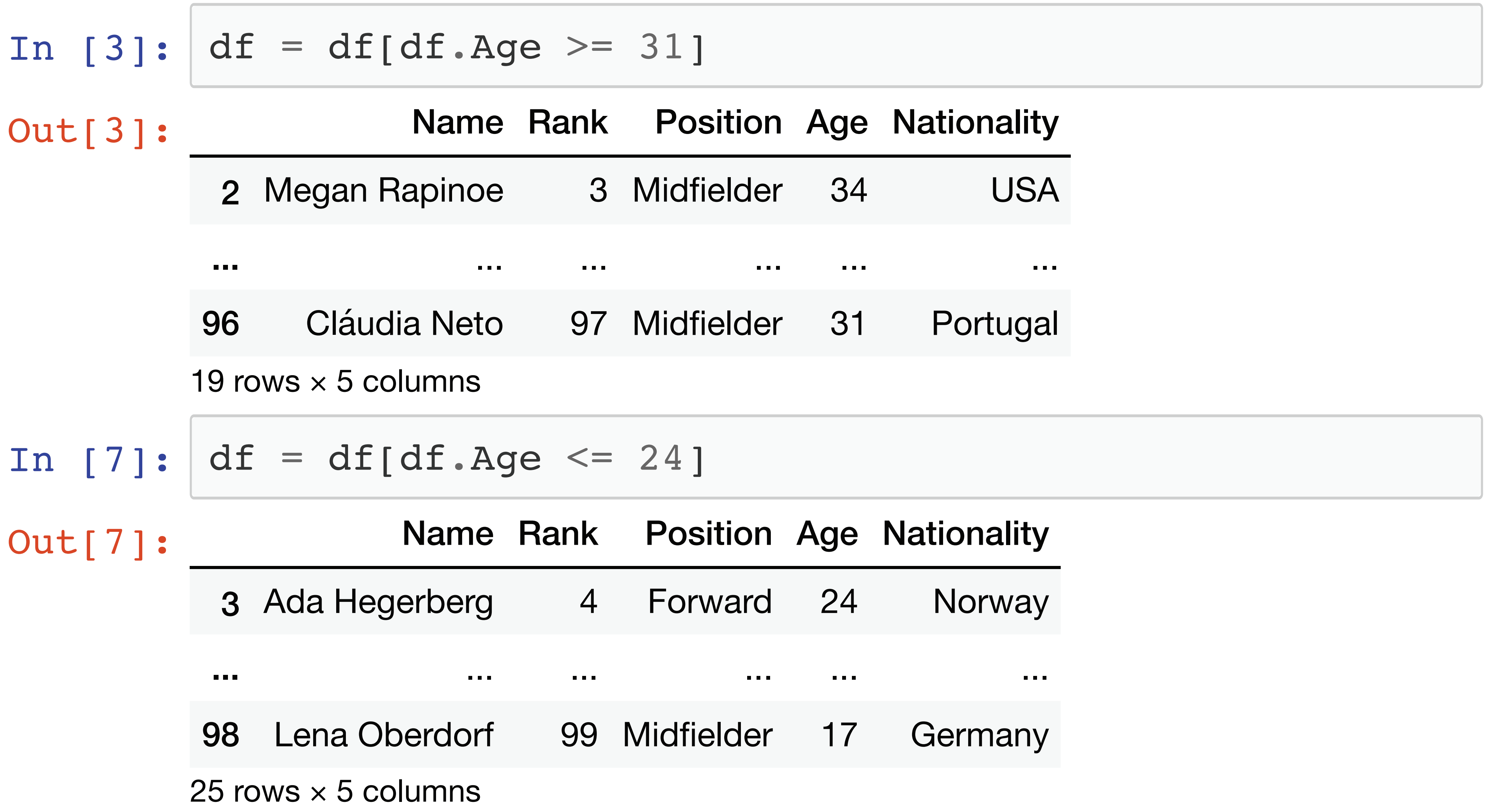


```
In [5]: import pandas as pd
        df = pd.read_csv('guardian-top100-female-2019.csv')

Out[5]:
          Name  Rank  Position  Age on 1 Dec 2019  Nationality
 0    Sam Kerr     1   Forward                 26    Australia
...        ...   ...       ...                ...          ...
99    Ludmila    100   Forward                 25       Brazil
100 rows × 5 columns
```

```
In [6]: df = df.rename(columns={'Age on 1 Dec 2019': 'Age'})

Out[6]:
          Name  Rank  Position  Age  Nationality
 0    Sam Kerr     1   Forward   26    Australia
...        ...   ...       ...  ...          ...
99    Ludmila    100   Forward   25       Brazil
100 rows × 5 columns
```



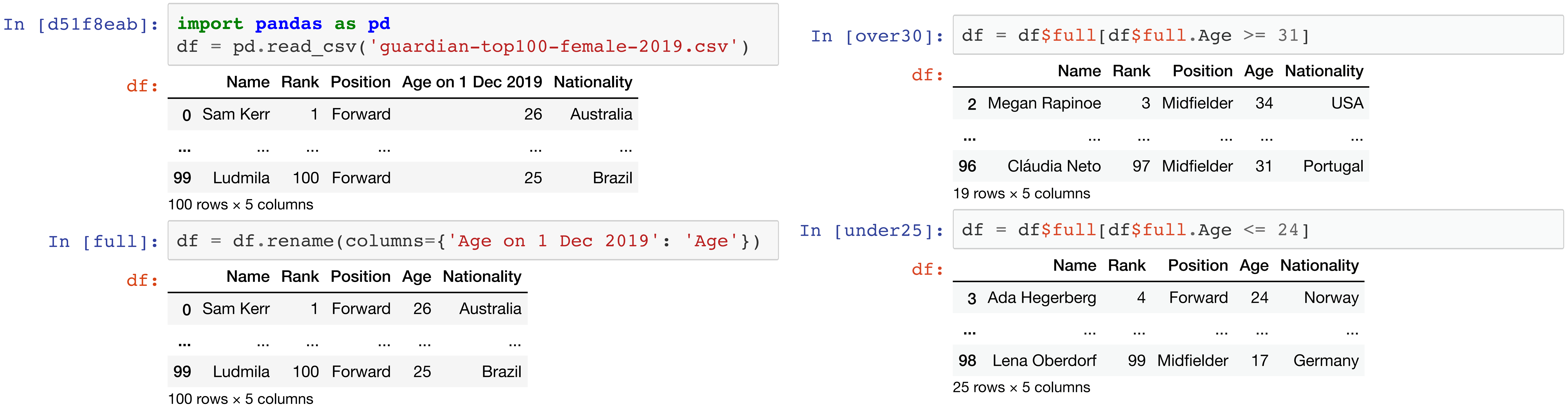
```
In [3]: df = df[df.Age >= 31]

Out[3]:
              Name  Rank    Position  Age  Nationality
 2   Megan Rapinoe     3  Midfielder   34          USA
...            ...   ...         ...  ...          ...
96     Cláudia Neto   97  Midfielder   31     Portugal
19 rows × 5 columns
```

```
In [7]: df = df[df.Age <= 24]

Out[7]:
              Name  Rank    Position  Age  Nationality
 3  Ada Hegerberg      4     Forward   24       Norway
...            ...   ...         ...  ...          ...
98   Lena Oberdorf    99  Midfielder   17      Germany
25 rows × 5 columns
```

Dataflow Notebooks: Resolve Notebook Ambiguities



```
In [d51f8eab]: import pandas as pd
               df = pd.read_csv('guardian-top100-female-2019.csv')
```

df:

	Name	Rank	Position	Age on 1 Dec 2019	Nationality
0	Sam Kerr	1	Forward	26	Australia
...	...	...	...	...	...
99	Ludmila	100	Forward	25	Brazil

100 rows × 5 columns

```
In [full]: df = df.rename(columns={'Age on 1 Dec 2019': 'Age'})
```

df:

	Name	Rank	Position	Age	Nationality
0	Sam Kerr	1	Forward	26	Australia
...	...	...	...	...	...
99	Ludmila	100	Forward	25	Brazil

100 rows × 5 columns

```
In [over30]: df = df$full[df$full.Age >= 31]
```

df:

	Name	Rank	Position	Age	Nationality
2	Megan Rapinoe	3	Midfielder	34	USA
...	...	...	...	...	...
96	Cláudia Neto	97	Midfielder	31	Portugal

19 rows × 5 columns

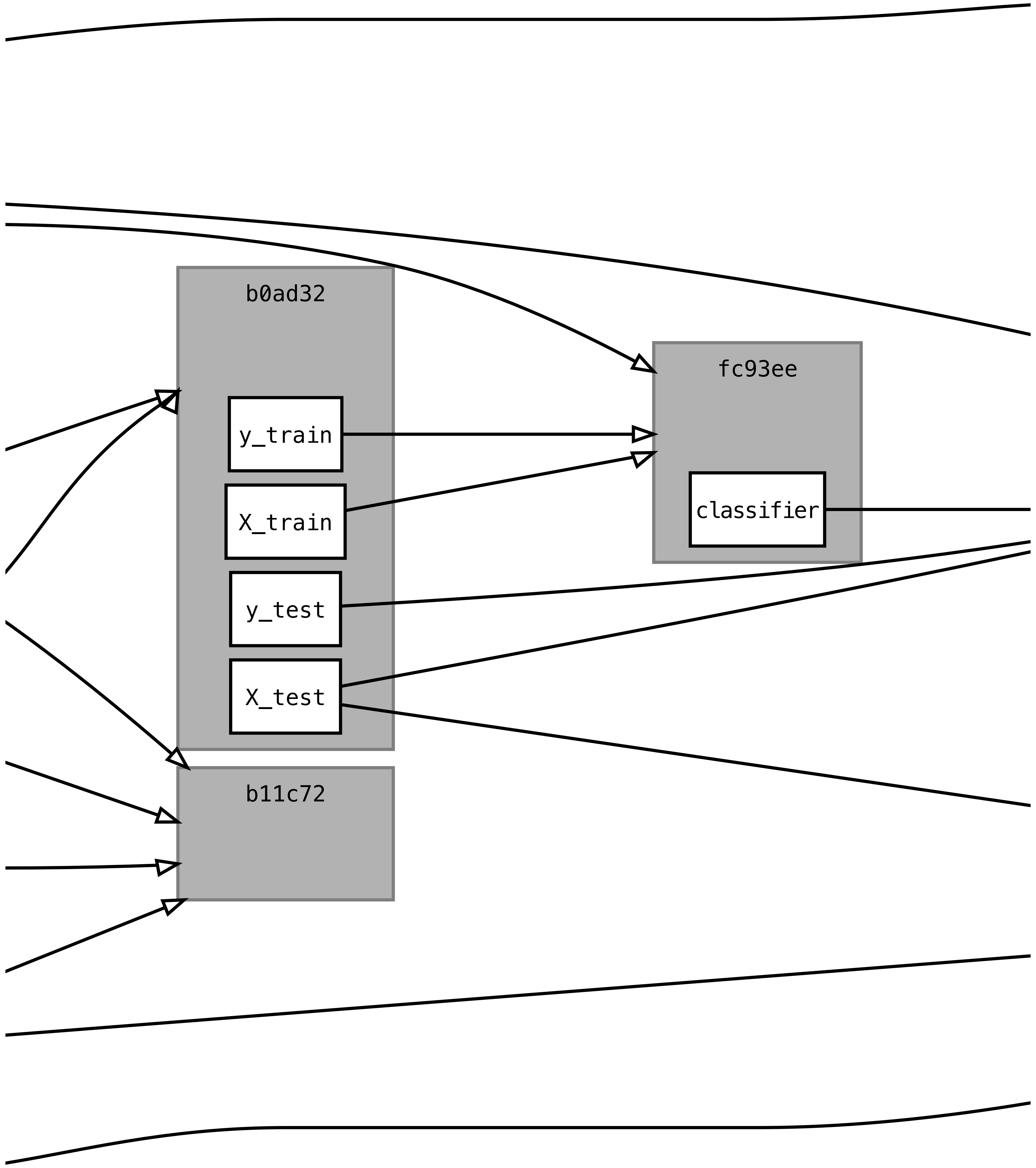
```
In [under25]: df = df$full[df$full.Age <= 24]
```

df:

	Name	Rank	Position	Age	Nationality
3	Ada Hegerberg	4	Forward	24	Norway
...	...	...	...	...	...
98	Lena Oberdorf	99	Midfielder	17	Germany

25 rows × 5 columns

Dataflow Notebooks: Dependency Graph



- Shows connections between cells
- Can see which cells would be affected by a change
- Same colors indicate which parts of the graph are stale
- Linked to the notebook
  - Hover to show a cell's code
  - Can also execute in the graph