Provenance Gathering from Scripts: Challenges and Opportunities

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IC/UFF

UFF

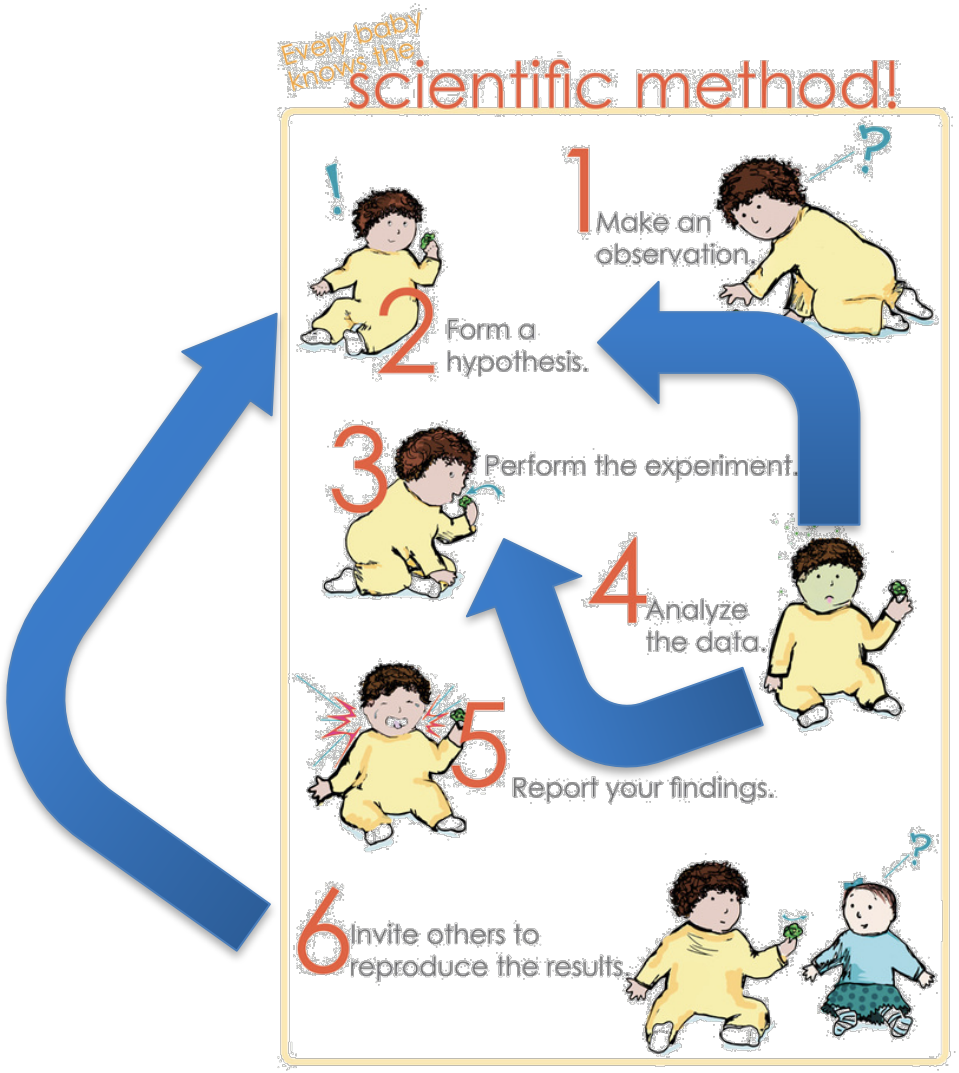
- 3.180 professors
- 66.186 students

IC

- 65 professors
- 90 PhD students
- 110 MS students
- 500 BS (CC) students
- 500 BS (IS) students
- 2.000 TSC students

It all starts with the Scientific Method

In fact, it is not linear



In the beginning

In-vivo

In-vitro

However in-vivo and in-vitro experiments are...

Costly

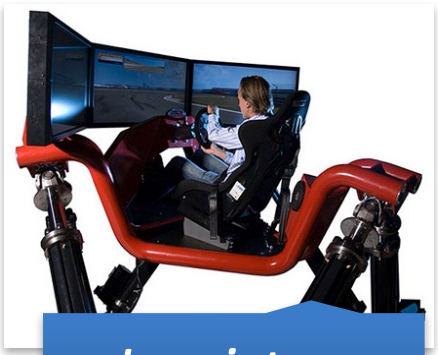
Risky

Slow

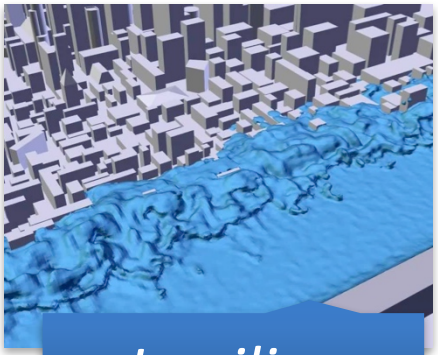
From in-vivo to *in-silico*

In-vivo

In-vitro



In-virtuo



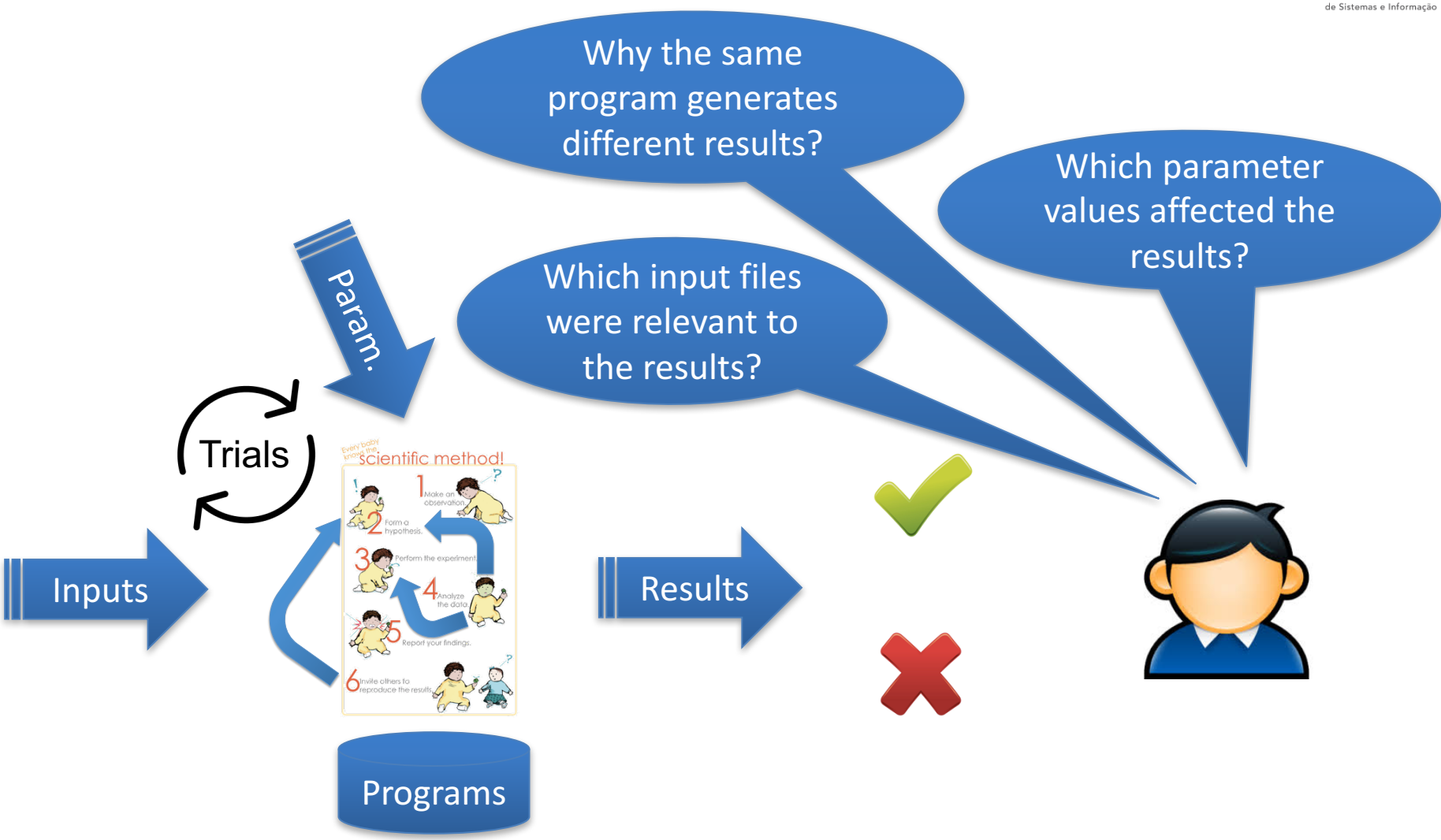
In-silico

Cost, Risk, Duration

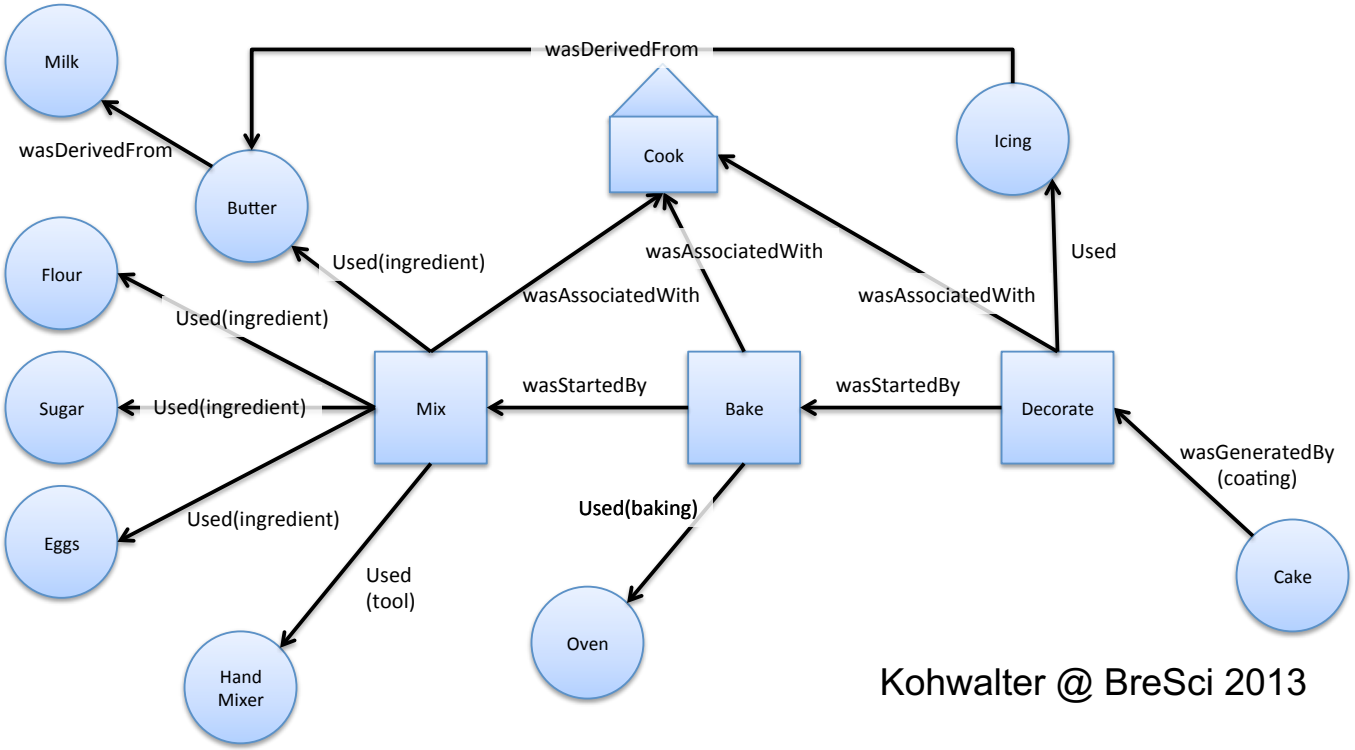
Data volume

Travassos and Barros "Contributions of in virtuo and in silico experiments for the future of empirical studies in software engineering." WSESE 2003

How to reason from the data?



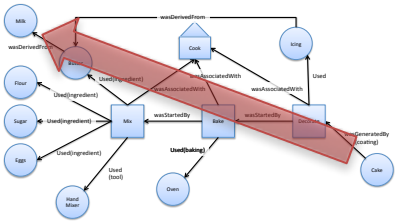
Provenance is the key!



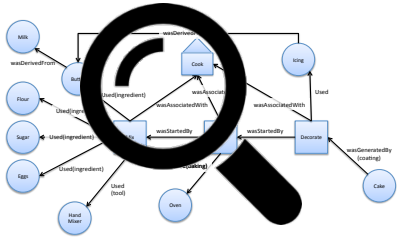
"Life can only be understood backwards; but it must be lived forwards."

Søren Kierkegaard, 1843.

Provenance is useful for…

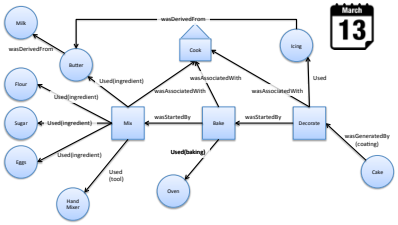


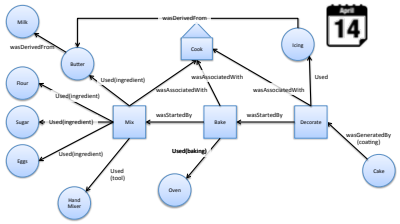
Interpreting and Understanding results

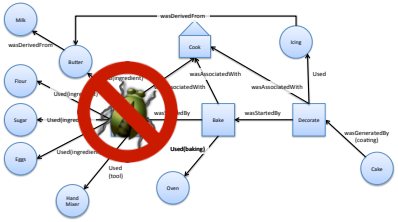


Auditing

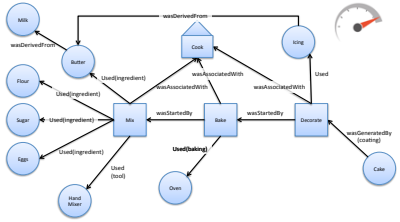
Reproducibility







Debugging

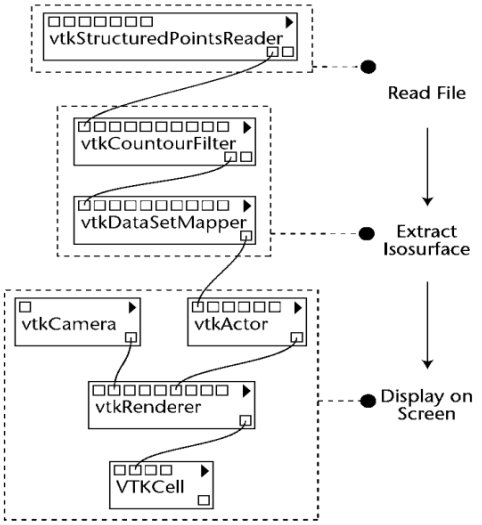


Caching

Among others applications (attribution, reuse, trustworthiness, sharing, …)

Provenance Gathering


```
1  import vtk
2
3  data = vtk.vtkStructuredPointsReader()
4  data.setFileName("../../../examples/data/head.120.vtk")
5
6  contour = vtk.vtkContourFilter()
7  contour.SetInput(0, data.GetOutput())
8  contour.SetValue(0, 67)
9
10 mapper = vtk.vtkPolyDataMapper()
11 mapper.SetInput(contour.GetOutput())
12 mapper.ScalarVisibilityOff()
13
14 actor = vtk.vtkActor()
15 actor.SetMapper(mapper)
16
17 cam = vtk.vtkCamera()
18 cam.SetViewUp(0,0,-1)
19 cam.SetPosition(745,-453,369)
20 cam.SetFocalPoint(135,135,150)
21 cam.ComputeViewPlaneNormal()
22
23 ren = vtk.vtkRenderer()
24 ren.AddActor(actor)
25 ren.SetActiveCamera(cam)
26 ren.ResetCamera()
27
28 renwin = vtk.vtkRenderWindow()
29 renwin.AddRenderer(ren)
30
31 style = vtk.vtkInteractorStyleTrackballCamera()
32 iren = vtk.vtkRenderWindowInteractor()
33 iren.SetRenderWindow(renwin)
34 iren.SetInteractorStyle(style)
35 iren.Initialize()
36 iren.Start()
```



Manual	General-purpose Script	SWfMS
• Error prone • Time consuming • Unviable for complex experiments	• Complex programming model • Primitive execution logs (if any)	• Visual programming interface • Controlled execution environment • Support for parallel execution • Built-in provenance support

Freire et al. "Provenance for computational tasks: A survey." CS&E 10(3) 2008

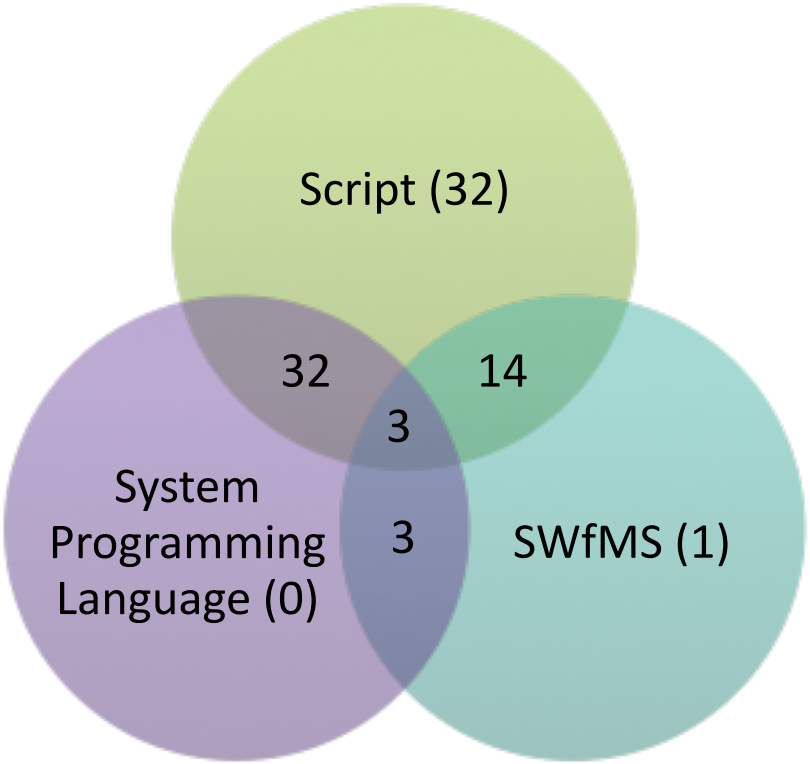
So, let's use SWfMS! ☺

Among many others…

However, lots of people still use scripts ☹

95%

of the respondents* have scripts among their preferred/more often used tools to run experiments



*Survey sent to AMC@UvA (Olabarriaga), UFRJ (Mattoso), DATAONE (newsletter), DBBras (mailing list), FIOCRUZ (Davila), USP (Traina), INRIA-Montpellier (Zenith group), LNCC (Ocana), PW 2016 TPC, SciPyLA (Telegram), Software Carpentry (mailing list), U. Nantes (Gaignard), UPENN (Davidson), receiving 85 answers.

However, lots of people still use scripts ☹

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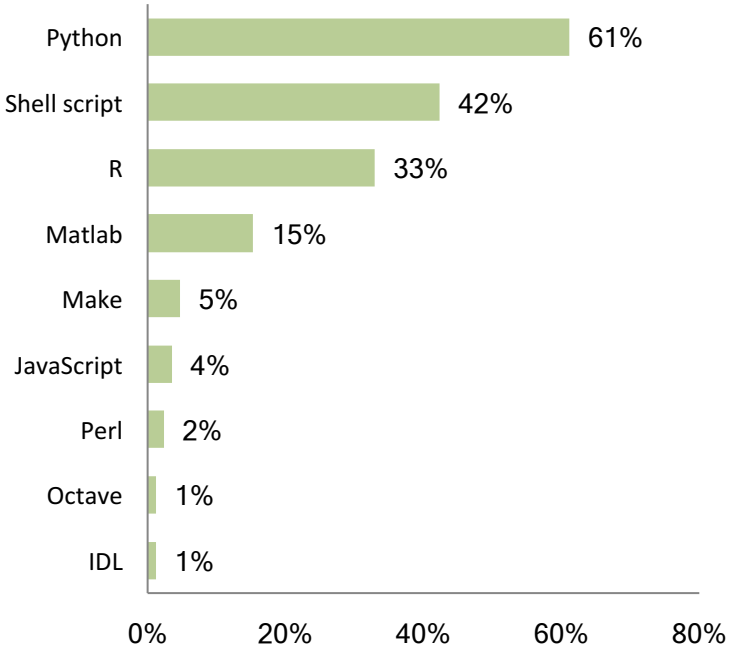
61%

of the respondents* have Python among their preferred/more often used tools to run experiments



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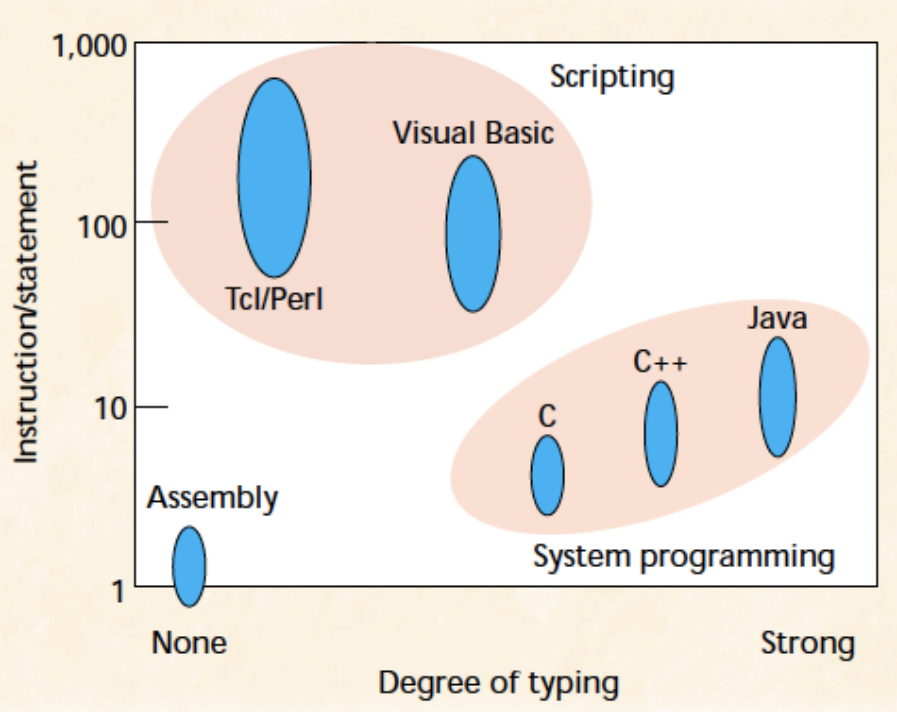
But what exactly are Scripts?

- There is no robust definition in the literature!
- Our to-be-improved definition:
  - "A script is a program conceived for gluing components, which may have been written in different programming languages"
- Actually, it does not matter much…
  - "When I see a bird that walks like a duck and swims like a duck and quacks like a duck, I call that bird a duck" (James Whitcomb Riley)

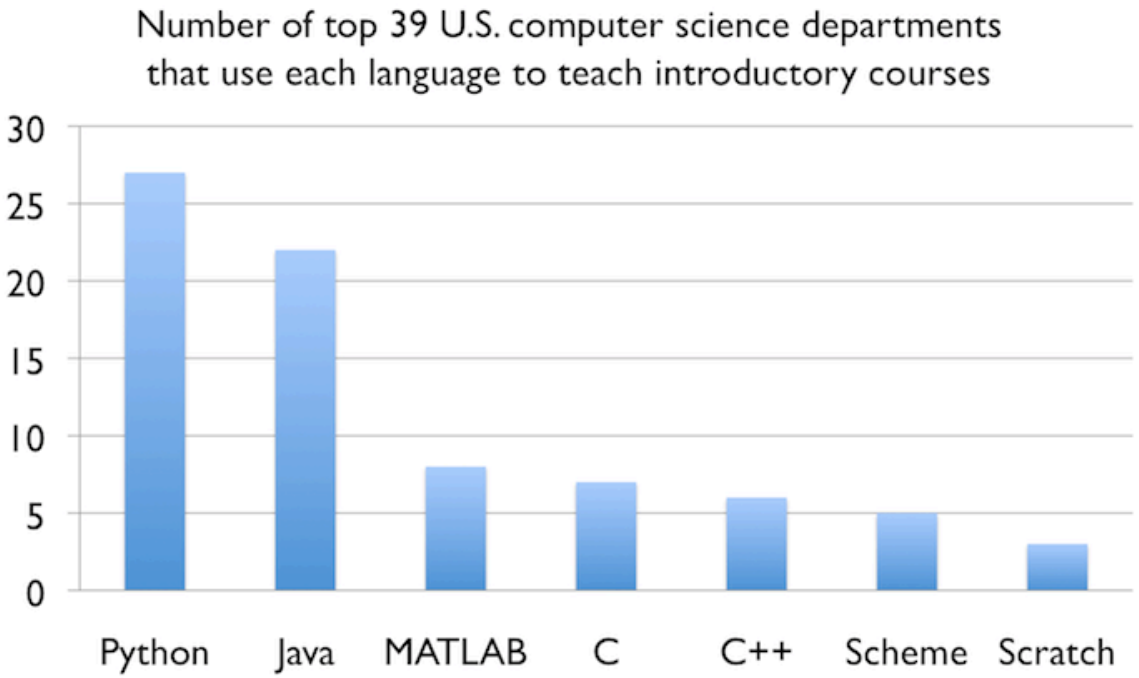
Scripts are high-level programs

- Everything is Object
- Multiparadigm
- Typeless (dynamically-typed)
- Interpreted
- Automatic memory management
- Extensive component library



Ousterhout "Scripting: Higher level programming for the 21st century." Computer 31(3) 1998

Scripts are easy to learn



Guo “Python is Now the Most Popular Introductory Teaching Language at Top U.S. Universities”, BLOG@CACM July 2014

Scripts
are easy to code

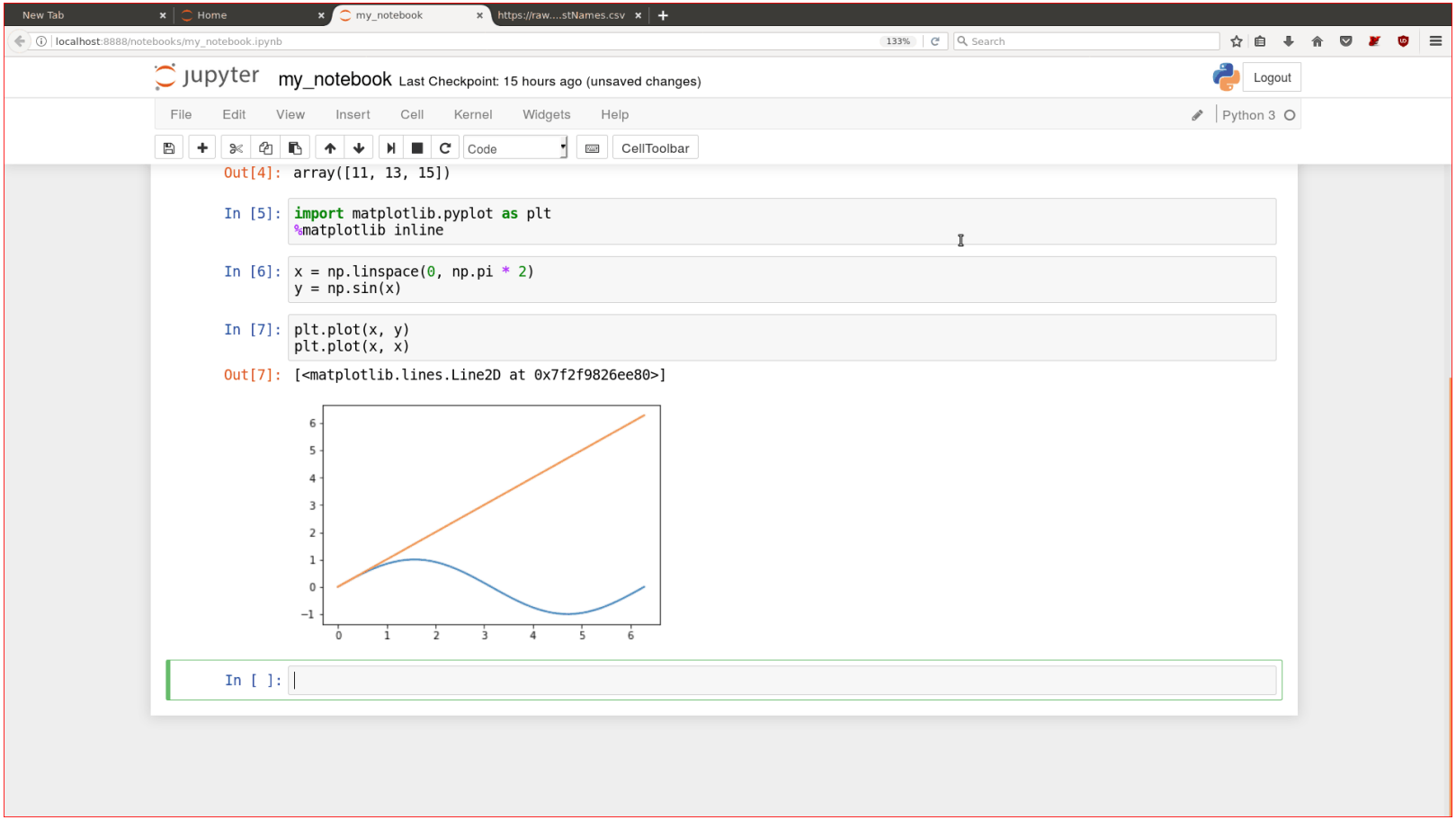
Application (contributor)	Comparison	Code ratio*	Effort ratio**	Comments
Database application (Ken Corey)	C++ version: 2 months Tcl version: 1 day		60	C++ version implemented first; Tcl version had more functionality
Computer system test and installation (Andy Belsey)	C test application: 272,000 lines, 120 months C FIS application: 90,000 lines, 60 months Tcl/Perl version: 7,700 lines, 8 months	47	22	C version implemented first; Tcl/Perl version replaced both C applications
Database library (Ken Corey)	C++ version: 2-3 months Tcl version: 1 week		8-12	C++ version implemented first
Security scanner (Jim Graham)	C version: 3,000 lines Tcl version: 300 lines	10		C version implemented first; Tcl version had more functionality
Display oil well production curves (Dan Schenck)	C version: 3 months Tcl version: 2 weeks		6	Tcl version implemented first
Query dispatcher (Paul Healy)	C version: 1,200 lines, 4-8 weeks Tcl version: 500 lines, 1 week	2.5	4-8	C version implemented first, uncommented; Tcl version had comments, more functionality
Spreadsheet tool	C version: 1,460 lines Tcl version: 380 lines	4		Tcl version implemented first
Simulator and GUI (Randy Wang)	Java version: 3,400 lines, 3-4 weeks Tcl version: 1,600 lines, <1 week	2	3-4	Tcl version had 10 to 20 percent more functionality and was implemented first

* Code ratio is the ratio of lines of code for the two implementations (<1 means the system programming language required more lines).

** Effort ratio is the ratio of development times. In most cases the two versions were implemented by different people.

Ousterhout “Scripting: Higher level programming for the 21st century.” Computer 31(3) 1998

Scripts are interactive



http://n-s-f.github.io/2017/03/25/r-to-python.html

Scripts-based initiatives for science miss provenance

noWorkflow

not only Workflow

- **Transparently** capture **provenance from Python scripts** at **fine grain**
- Consider multiple executions (**trials**)
- Provide **visualizations** for provenance analysis
- Allows **querying** provenance in different languages

Installing and running

Instead of running

```
$ python experiment.py
```

Install noWorkflow (once)

```
$ pip install noworkflow[all]
```

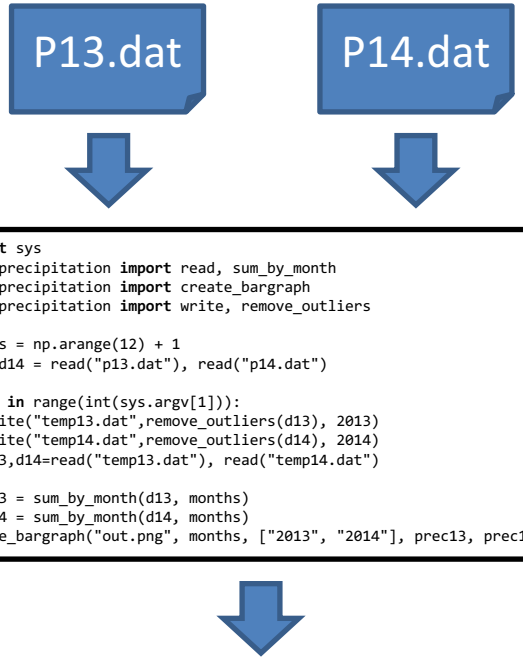
And run

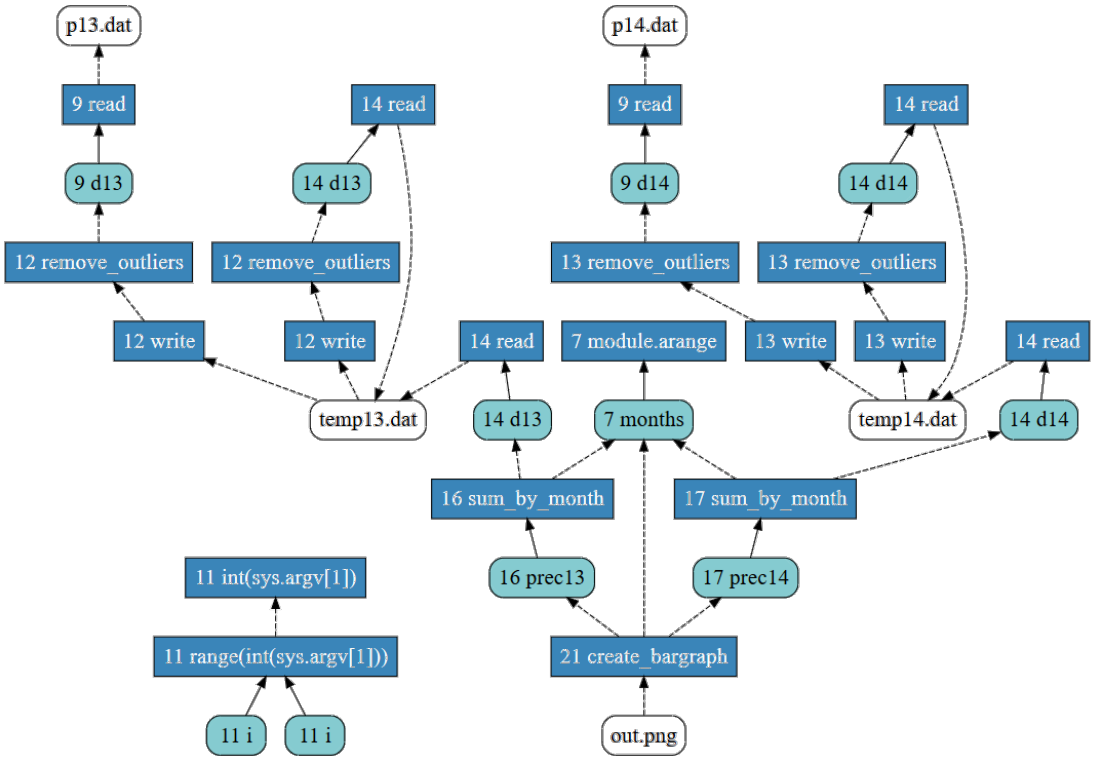
```
$ now run experiment.py
```

experiment.py

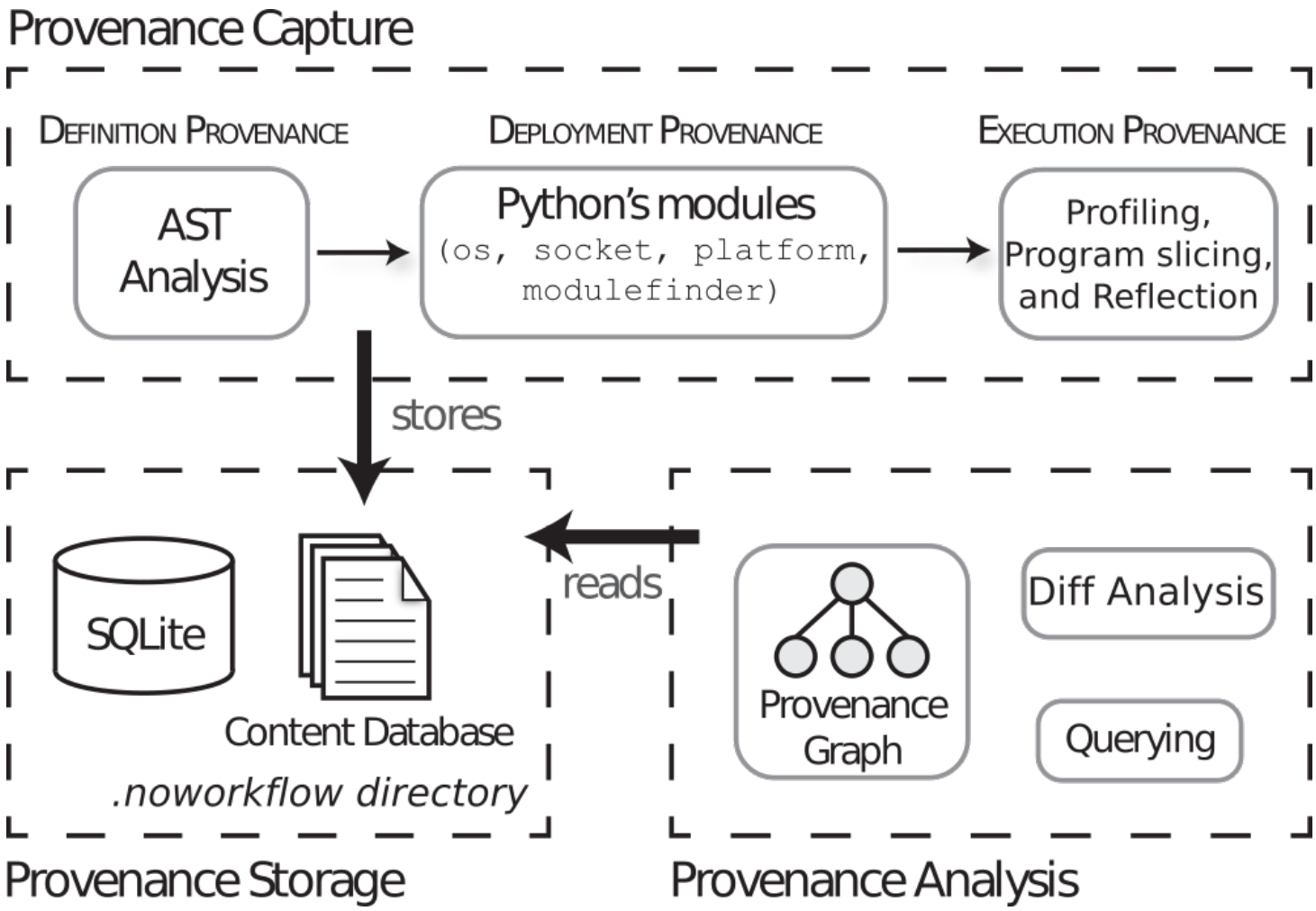
```
import sys
from precipitation import read, sum_by_month
from precipitation import create_bargraph
from precipitation import write, remove_outliers

months = np.arange(12) + 1
d13, d14 = read("p13.dat"), read("p14.dat")

for i in range(int(sys.argv[1])):
   write("temp13.dat",remove_outliers(d13), 2013)
   write("temp14.dat",remove_outliers(d14), 2014)
   d13,d14=read("temp13.dat"), read("temp14.dat")

prec13 = sum_by_month(d13, months)
prec14 = sum_by_month(d14, months)
create_bargraph("out.png", months, ["2013", "2014"], prec13, prec14)
```

Result and Provenance





Architecture



Definition provenance (function definitions)

```
import csv
import json
threshold = 15
def run_simulation(data_a,
data_b):
    global threshold
    ...
def csv_read(f):
    fc = open(f, 'rU')
    ...
def extract_column(data, column):
    x = float(data[column])
    ...
def plot(x, y):
    ...
    plt.savefig("output.png")
```

AST analysis

sha1: aaf5d6

```
def run_simulation(data_a, data_b):
    global threshold
    ...
```

Arguments: data_a, data_b
Global: threshold
…

sha1: d91403

```
def csv_read(f):
    fc = open(f, 'rU')
    ...
```

Arguments: f
Calls: open
…

Definition provenance (function definitions)

Function definitions

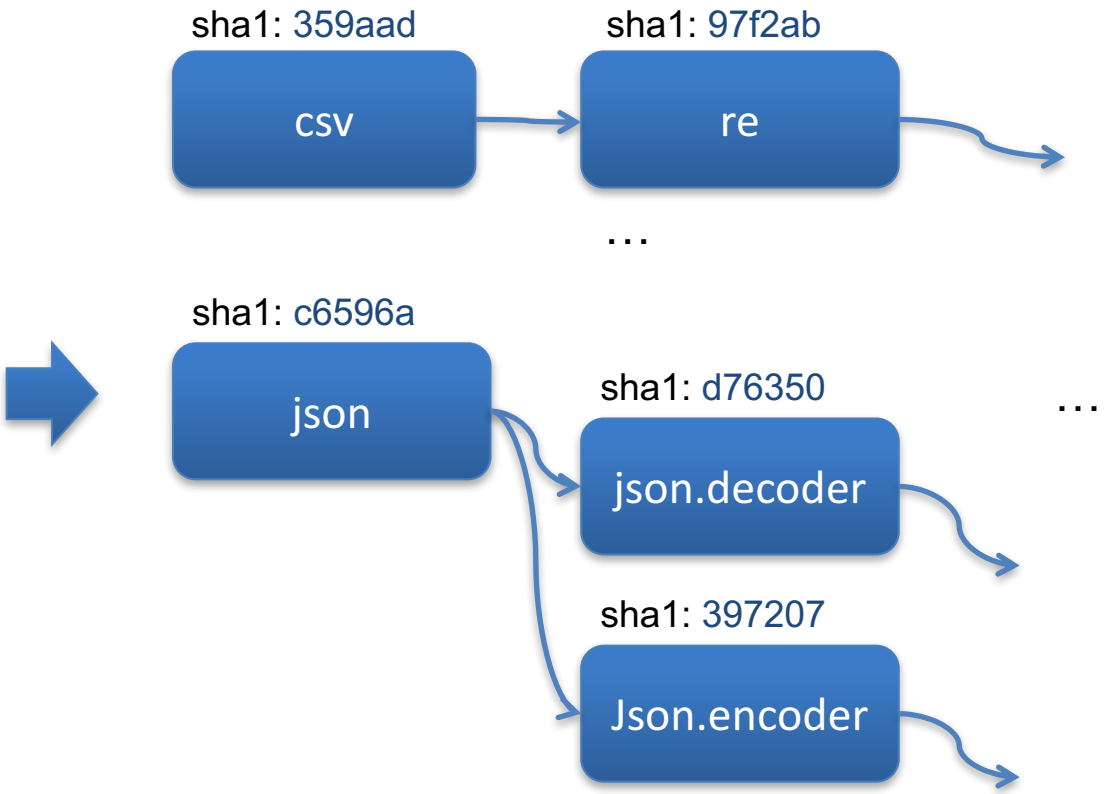
id	name	code_hash	trial_id
1	plot	ae65a2036cfcfeb70bc75646f...	1
2	run_simulation	aaf5d621671bda46f6f91d66...	1
3	extract_column	36fca5011c32e5bc8fe2309c...	1
4	csv_read	d914038c94dcbd4bfa656c1e...	1

Arguments, Global variables, and Function calls

id	name	type	function_def_id
1	x	ARGUMENT	1
2	y	ARGUMENT	1
3	data_a	ARGUMENT	2
4	data_b	ARGUMENT	2
5	threshold	GLOBAL	2
6	data	ARGUMENT	3
7	column	ARGUMENT	3
8	float	FUNCTION	3
9	f	ARGUMENT	4
10	open	FUNCTION	4

Deployment provenance (module dependencies)

```
import csv
import json
threshold = 15
def run_simulation(data_a,
data_b):
    global threshold
    ...
def csv_read(f):
    fc = open(f, 'rU')
    ...
def extract_column(data, column):
    x = float(data[column])
    ...
def plot(x, y):
    ...
    plt.savefig("output.png")
```



Deployment provenance (module dependencies)

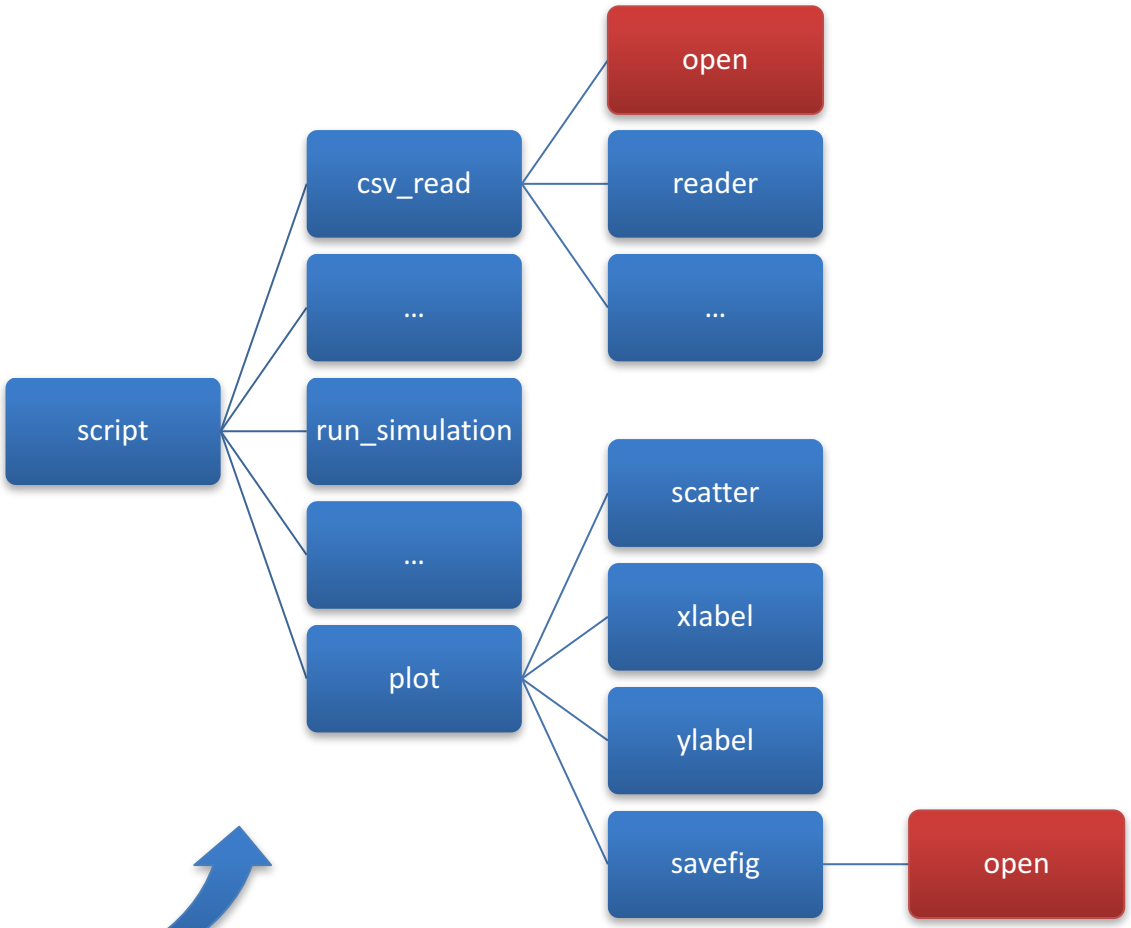
id	name	version	file	code_hash	trial_id
578	parser	0.5	/Applications/Canopy.ap...	1c3d29a3964c7ccce610...	1
266	logging	0.5.1.2	/Applications/Canopy.ap...	0f25732b370c8a9b5ef0...	1
51	PIL.JpegImagePlugin	0.6	/Users/leomurta/Library...	4c15e4929257f41438ee...	1
40	PIL.BmpImagePlugin	0.7	/Users/leomurta/Library...	81aa830d0648239fc115...	1
370	multiprocessing	0.70a1	/Applications/Canopy.ap...	29a75113696caffaaec85...	1
41	PIL.GifImagePlugin	0.9	/Users/leomurta/Library...	f32e15956af93ce5b32bf...	1
53	PIL.PngImagePlugin	0.9	/Users/leomurta/Library...	0bcca794a0059096acf6a...	1
94	_csv	1.0	/Applications/Canopy.ap...	ef4d2e093e01bdc577cba...	1
152	csv	1.0	/Applications/Canopy.ap...	359aad7eca382bb46c9a...	1
533	numpy.ma	1.0	/Users/leomurta/Library...	964546e27356efd234ce...	1
535	numpy.ma.extras	1.0	/Users/leomurta/Library...	92ed1d612e3c5fb8682e...	1
703	zlib	1.0	/Applications/Canopy.ap...	464f5b374771708a6823...	1
700	xmlrpclib	1.0.1	/Applications/Canopy.ap...	bc8883c8ae46b737b123...	1
583	platform	1.0.7	/Applications/Canopy.ap...	080d6c19c0535cea0c45...	1
95	_ctypes	1.1.0	/Applications/Canopy.ap...	e297fc0053a23eda4162...	1
153	ctypes	1.1.0	/Applications/Canopy.ap...	9631395474bf01bc81c9...	1
610	setuptools	1.1.6	/Applications/Canopy.ap...	367e53014dcff4a0e82c2...	1
39	PIL	1.1.7	/Users/leomurta/Library...	bdea292f3d7f3141d5fea...	1
44	PIL.Image	1.1.7	/Users/leomurta/Library...	c552a828c9f418951e26...	1
669	urllib	1.17	/Applications/Canopy.ap...	575f9e37b4b4c45cac90...	1
385	nose	1.2.1	/Users/leomurta/Library...	df681a5f034cf907160eb...	1

Deployment provenance (environment variables)

id	name	value	trial_id
73	OS_VERSION	Darwin Kernel Version 13.0.0:...	1
74	CS_XBS5_LP64_OFF64_LIBS		1
75	SC_AIO_PRIO_DELTA_MAX	-1	1
76	SC_THREAD_STACK_MIN	8192	1
77	TERM_PROGRAM_VERSION	326	1
78	SC_STREAM_MAX	256	1
79	OS_RELEASE	13.0.0	1
80	SC_MEMLOCK	-1	1
81	HOME	/Users/leomurta	1
82	TERM_PROGRAM	Apple_Terminal	1
83	LANG	pt_BR.UTF-8	1
84	SC_SHARED_MEMORY_OBJECTS	-1	1
85	Apple_PubSub_Socket_Render	/tmp/launch-Uo1Eq3/Render	1
86	SC_THREAD_THREADS_MAX	-1	1
87	SC_COLL_WEIGHTS_MAX	2	1
88	SC_THREAD_ATTR_STACKADDR	200112	1
89	_	/Users/leomurta/Library/Ent...	1
90	SC_THREAD_ATTR_STACKSIZE	200112	1
91	PYTHON_IMPLEMENTATION	CPython	1
92	SC_JOB_CONTROL	200112	1
93	SC_FSYNC	200112	1

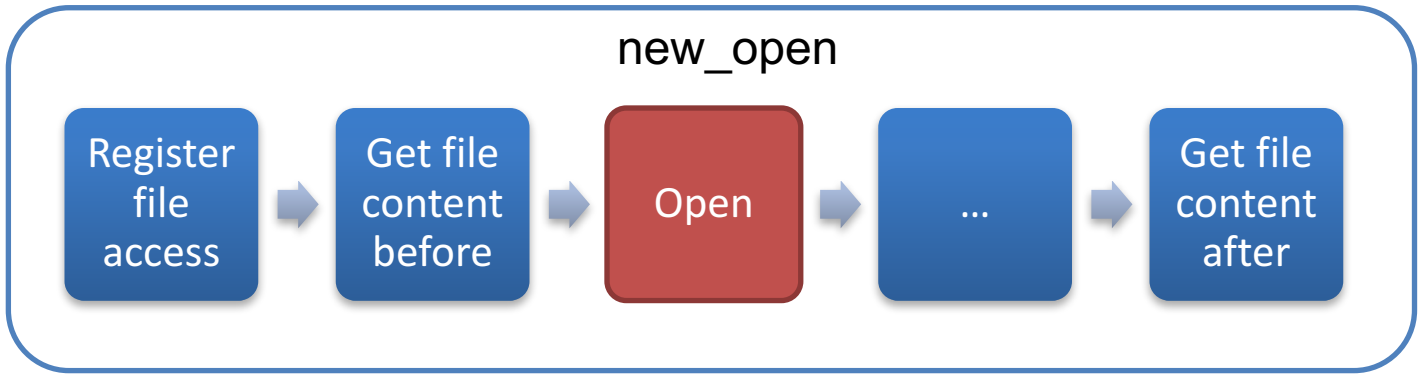
Execution provenance (function calls and file accesses)

```
import csv
import json
threshold = 15
def run_simulation(data_a,
data_b):
    global threshold
    ...
def csv_read(f):
    fc = open(f, 'rU')
    ...
def extract_column(data, column):
    x = float(data[column])
    ...
def plot(x, y):
    ...
    plt.savefig("output.png")
```



Profiling

Execution provenance (function calls and file accesses)



Monkey patching: builtins.open = self.new_open(open)

Execution provenance (function calls and file accesses)

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Function calls

id	name	line	start	finish	caller_id	trial_id
1	/Users/leo...	58	2013-11-01 ...	2013-11-01 ...		1
2	csv_read	43	2013-11-01 ...	2013-11-01 ...	1	1
3	open	17	2013-11-01 ...	2013-11-01 ...	2	1
4	reader	17	2013-11-01 ...	2013-11-01 ...	2	1
5	list.append	20	2013-11-01 ...	2013-11-01 ...	2	1

...

File accesses

id	name	mode	buffering	content_hash_before	content_hash_after	timestamp	function_call_id	trial_id
1	data1.dat	rU	default	28f4192700d9e5d...	28f4192700d9e5...	2013-11-...	3	1
2	data2.dat	rU	default	802a73cb49af958...	802a73cb49af95...	2013-11-...	187	1
3	output.png	wb	default		a305a09040143f...	2013-11-...	1102	1

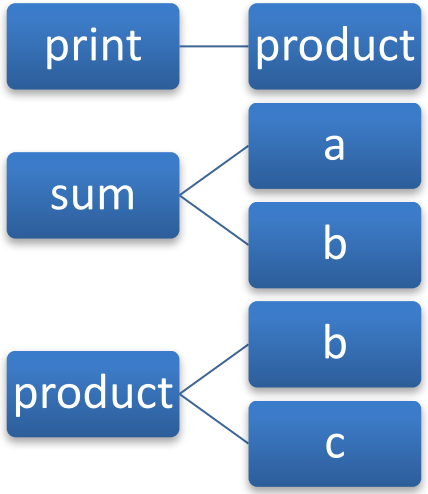
Execution provenance (data dependencies)

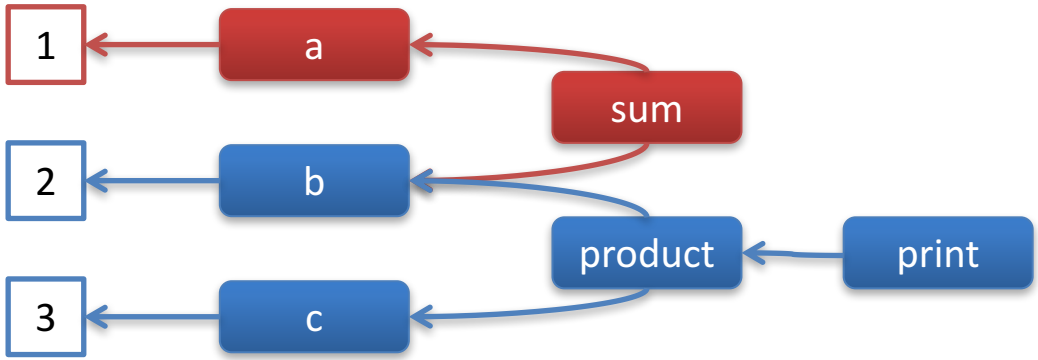
```
a = 1
b = 2
c = 3

sum = a + b
product = b * c

print(product)
```

Program slicing





Challenges and Opportunities

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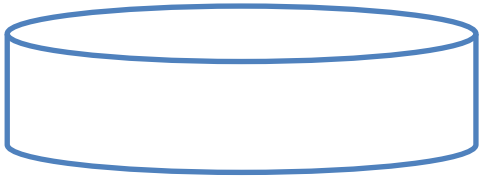
Don't limit your challenges

Challenge your limits!

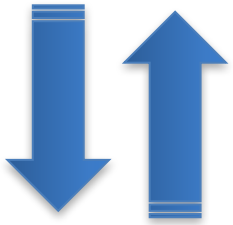
Jerry Dunn

Additional provenance sources



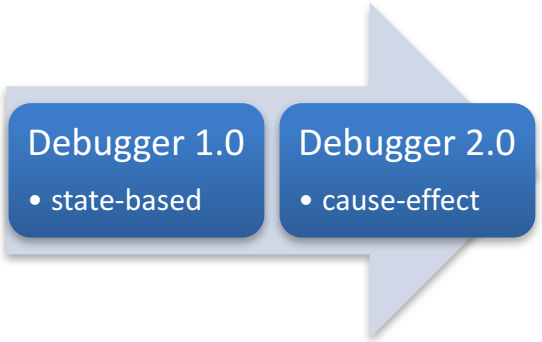
Databases

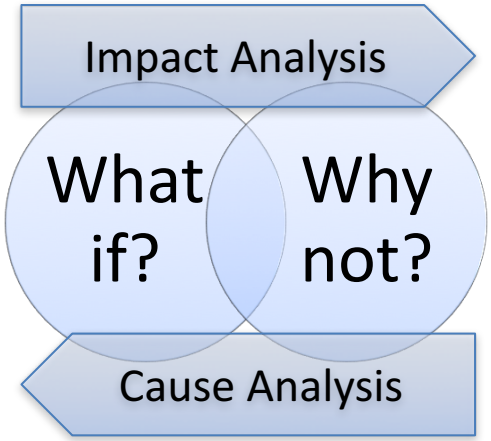
Network



New applications

Debugging



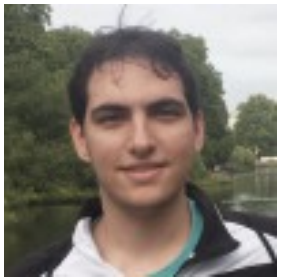


Education

Cyber security

Acknowledgments

noWorkflow main team



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Funding agencies

Provenance Gathering from Scripts: Challenges and Opportunities

Please, download noWorkflow at
http://gems-uff.github.io/noworkflow

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