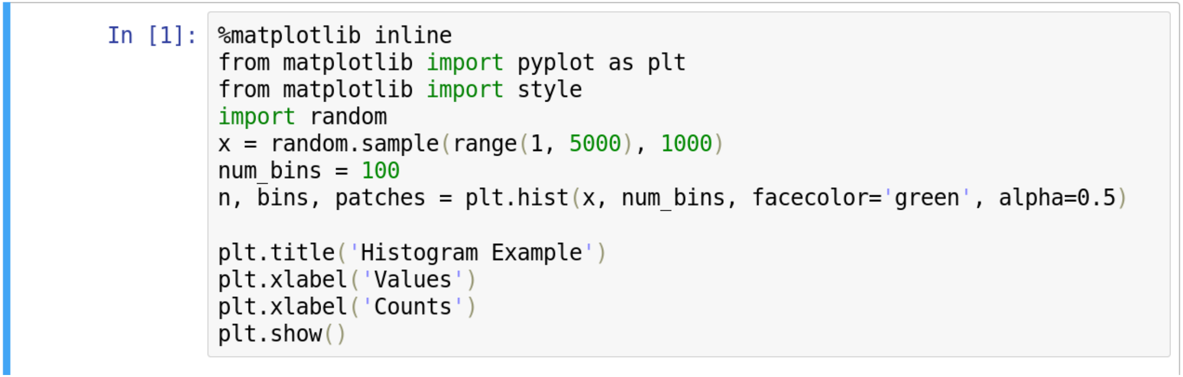
Towards reproducible Jupyter notebooks

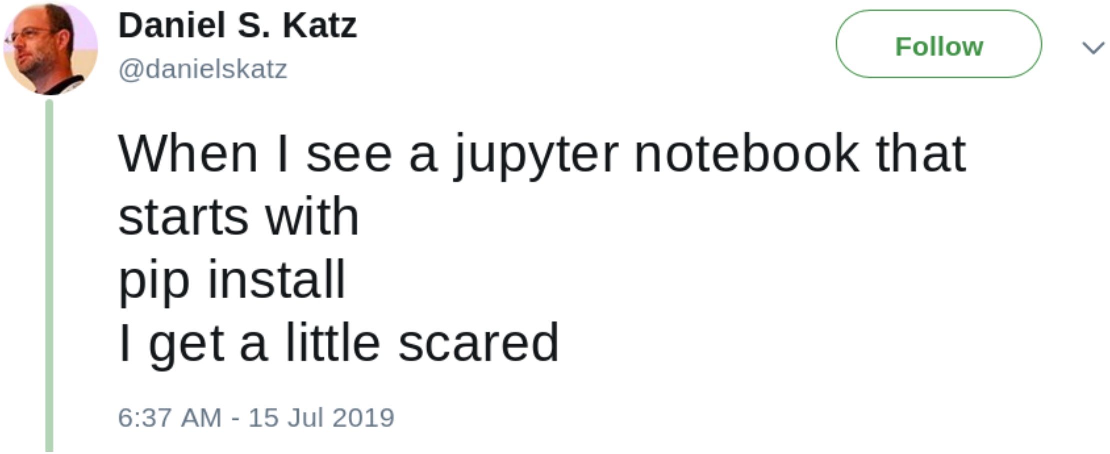
Ludovic Courtès
Pierre-Antoine Rouby

Scicloj Web Meeting
9 January 2020

Jupyter = reproducible science

Jupyter = reproducible science?

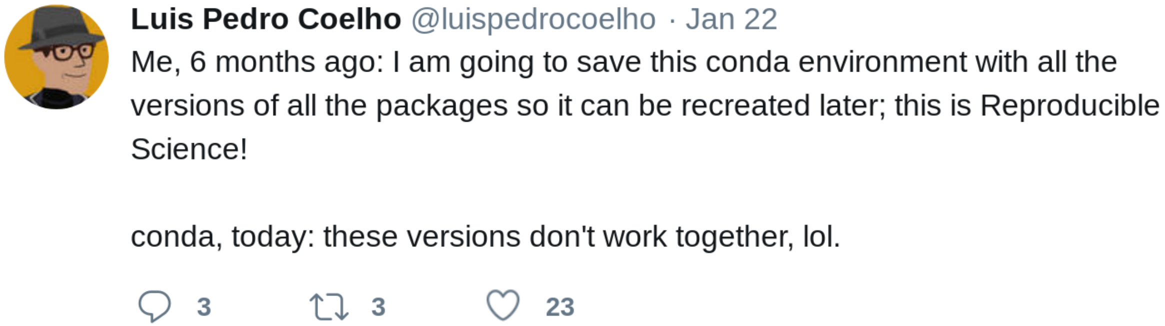

```
In [1]: %matplotlib inline
        from matplotlib import pyplot as plt
        from matplotlib import style
        import random
        x = random.sample(range(1, 5000), 1000)
        num_bins = 100
        n, bins, patches = plt.hist(x, num_bins, facecolor='green', alpha=0.5)

        plt.title('Histogram Example')
        plt.xlabel('Values')
        plt.xlabel('Counts')
        plt.show()
```



Daniel S. Katz
@danielskatz

When I see a jupyter notebook that starts with
pip install
I get a little scared

6:37 AM - 15 Jul 2019



Luis Pedro Coelho @luispedrocoelho · Jan 22

Me, 6 months ago: I am going to save this conda environment with all the versions of all the packages so it can be recreated later; this is Reproducible Science!

conda, today: these versions don't work together, lol.

3 3 23

binder

Turn a Git repo into a collection of interactive notebooks

Have a repository full of Jupyter notebooks? With Binder, open those notebooks in an executable environment, making your code immediately reproducible by anyone, anywhere.

- `environment.yml` - Install a Python environment
- `Pipfile` and/or `Pipfile.lock` - Install a Python environment
- `requirements.txt` - Install a Python environment
- `setup.py` - Install Python packages
- `Project.toml` - Install a Julia environment
- `REQUIRE` - Install a Julia environment (legacy)
- `install.R` - Install an R/RStudio environment
- `apt.txt` - Install packages with apt-get
- `DESCRIPTION` - Install an R package
- `manifest.xml` - Install Stencila
- `postBuild` - Run code after installing the environment
- `start` - Run code before the user sessions starts
- `runtime.txt` - Specifying runtimes
- `default.nix` - the nix package manager
- `Dockerfile` - Advanced environments

What if notebooks were self-contained, “deployment-aware”?

```
$ guix environment --ad-hoc \
      python python-numpy python-scipy \
      -- python3
```

Guix

+

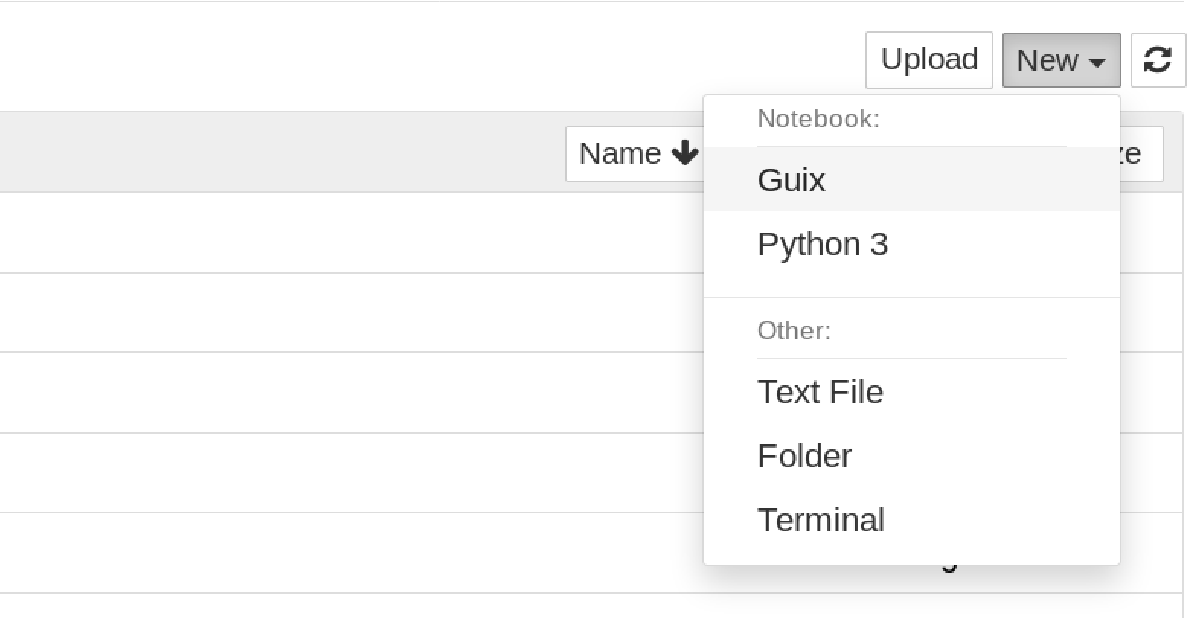
jupyter

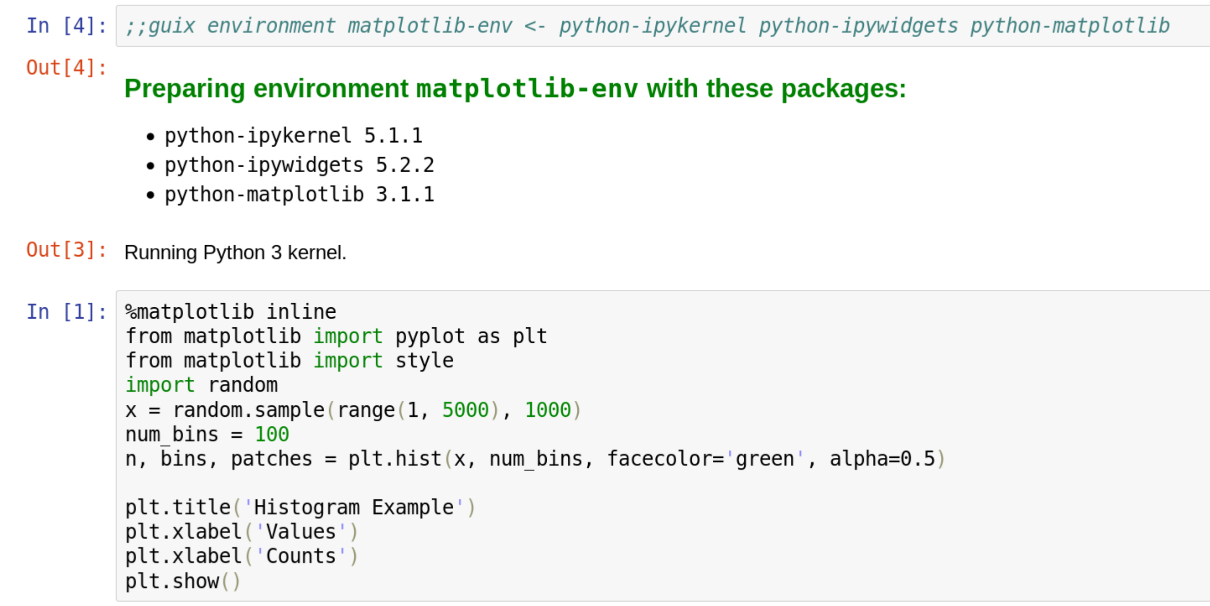
Guix

+

jupyter

https://hpc.guix.info/blog/2019/10/towards-reproducible-jupyter-notebooks


Upload
New
Name
Notebook:
Guix
Python 3
Other:
Text File
Folder
Terminal



```
In [4]: ;;guix environment matplotlib-env <- python-ipykernel python-ipywidgets python-matplotlib
```

Out[4]:

Preparing environment `matplotlib-env` with these packages:

- `python-ipykernel 5.1.1`
- `python-ipywidgets 5.2.2`
- `python-matplotlib 3.1.1`

Out[3]: Running Python 3 kernel.

```
In [1]: %matplotlib inline
from matplotlib import pyplot as plt
from matplotlib import style
import random
x = random.sample(range(1, 5000), 1000)
num_bins = 100
n, bins, patches = plt.hist(x, num_bins, facecolor='green', alpha=0.5)

plt.title('Histogram Example')
plt.xlabel('Values')
plt.xlabel('Counts')
plt.show()
```

travel in space *and* time!

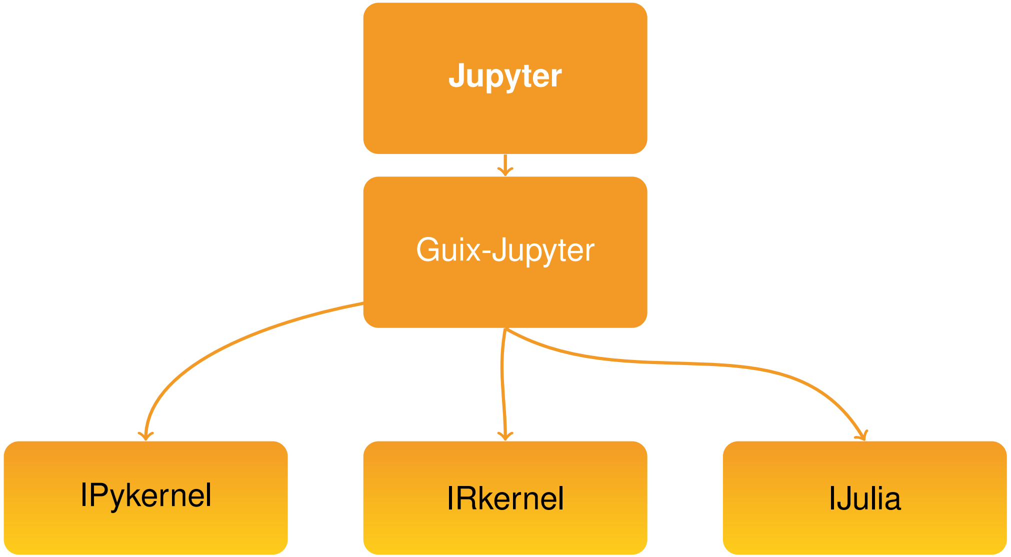
First, jump back to Guix as it existed in January 2019:

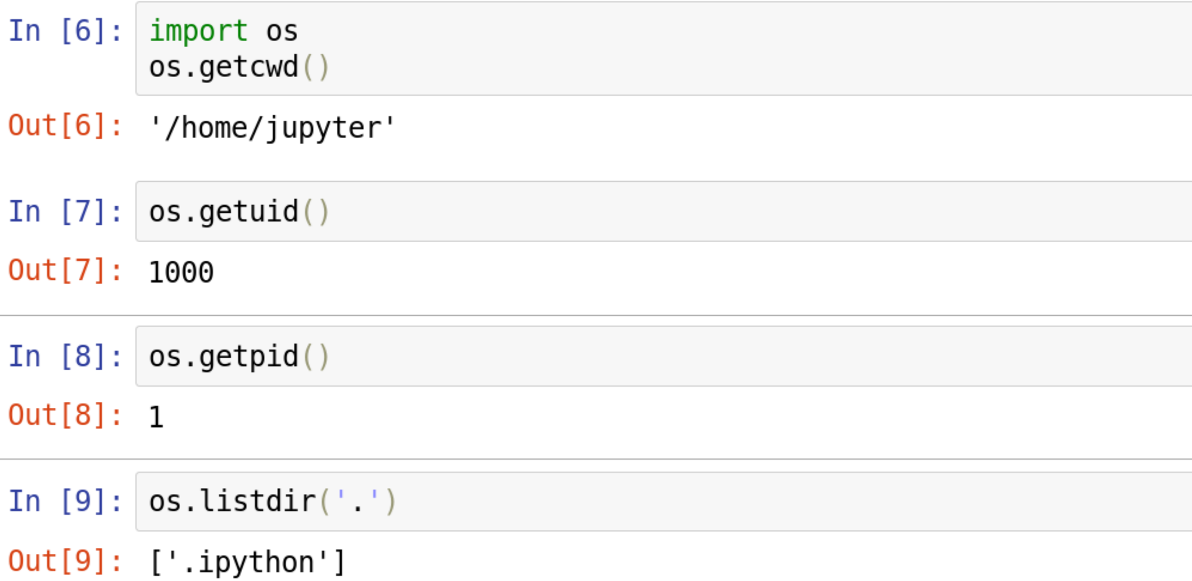
```
In [1]: ;;guix pin 0791437f972caa7e48de91ad5cb150a614f617c2
```

```
Out[1]:
```

Switched to these Guix channels:

```
guix 0791437f972caa7e48de91ad5cb150a614f617c2
```


Jupyter
Guix-Jupyter
IPykernel
IRkernel
IJulia



```
In [6]: import os
        os.getcwd()

Out[6]: '/home/jupyter'

In [7]: os.getuid()

Out[7]: 1000

In [8]: os.getpid()

Out[8]: 1

In [9]: os.listdir('.')

Out[9]: ['.ipython']
```

In [6]:
```
;;guix environment R <- r r-irkernel
```

Out[6]:

Preparing environment R with these packages:

- `r 3.6.1`
- `r-irkernel 1.0.2`

Out[5]: Running R kernel.

In [8]:
```
;;guix download https://ftp.gnu.org/gnu/coreutils/coreutils-8.30.tar.xz e831b3a86091496cdba720411f9748de8
```

Out[8]: File `coreutils-8.30.tar.xz` from https://ftp.gnu.org/gnu/coreutils/coreutils-8.30.tar.xz is now available in environment `R`.

In [2]:
```
file.info('coreutils-8.30.tar.xz')
```

A data.frame: 1 × 10

	size	isdir	mode	mtime	ctime	atime	uid	gid	uname	grname
	<dbl>	<lgl>	<octmode>	<dttm>	<dttm>	<dttm>	<int>	<int>	<chr>	<chr>
coreutils-8.30.tar.xz	5359532	FALSE	444	1970-01-01 00:00:01	2019-10-09 20:42:28	1970-01-01 00:00:01	1000	1000	jupyter	users

Imposing a Memory Management Discipline on Software Deployment

Eelco Dolstra, Eelco Visser and Merijn de Jonge
Utrecht University, P.O. Box 80089,
3508 TB Utrecht, The Netherlands
{eelco, visser, mdejonge}@cs.uu.nl

Abstract

The deployment of software components frequently fails because dependencies on other components are not declared explicitly or are declared imprecisely. This results in an incomplete reproduction of the environment necessary for proper operation, or in interference between incompatible variants. In this paper we show that these deployment hazards are similar to pointer hazards in memory models of programming languages and can be countered by imposing a memory management discipline on software deployment.

cies between the components being deployed. Dependencies on other components are not declared explicitly, causing an incomplete reproduction of the environment necessary for proper operation of the components. Furthermore, dependency information that *is* declared, is often not precise enough, allowing incompatible variants of a component to be used, or causing interference between such variants.

In this paper, we present a simple and effective solution to such deployment problems. In Section 2 we analyse the problems that occur in software deployment. We then show

Wrap-up.

Open issues

- how can we improve the **user interface**?
- should deployment be **built into Jupyter**?
- what about **interoperability**?
- ...

Guix-Jupyter =

- **self-contained** notebooks
- automatic & **reproducible deployment**
- code runs in **isolated environment**

GuixHPC

https://hpc.guix.info

ludovic.courtes@inria.fr | @GuixHPC