

Data Requested...

You request data from the authors of a study you're excited about, hoping to replicate it and build your new study on top of that one's findings.

A month later, they send you a zip file with code and data.

After a week of trying to get it to run based on their instructions, you haven't gotten the code to run without errors.

Should you still begin your study? Why / Why not?

Should you request more time to search for a new direction?

How do you know, that the files you received don't actually work as-is?

Death of the Magic Machine...

After a long holiday, you go back to collecting data, only to find that your data acquisition software won't start, and you don't know why! It's the only computer your department has with that program, and the lab member that originally set it up and modified it left long ago.

After a couple days of searching online, you finally find the key program online.

Should you use the program to collect your data?

How will this new change affect what you do with the existing data?

A little help...

Data collection is taking you all day, leaving little time for analysis, literature review, and your other projects. To help lighten the load, the department has offered to hire a part-time student assistant to help you out.

How much training will be needed before they are up to speed?

How similar will their new data look to your old data? Will this affect your study?

If the new data has collection-related problems (incompleteness, new artifacts, data loss, etc), will you catch them in time to retrain your assistant and get enough new data to recoup the loss?

Is it worth getting help, or should you work extra hours on the weekend to keep the status quo and hopefully still make your deadline?

Collaborating on the analysis...

You request help on the data analysis from a labmate, giving them your existing analysis scripts so they can build on it.

A month later, they come back with two figures--one you requested that shows the pattern you had hoped for, and another that is supposed to be the same analysis as the one done you did before, but there are now differences from your previous findings.

Whose code do you work on from that point on: your original files, or theirs?

Do you accept their figures for your manuscript or keep the one you made?

If you don't accept their code, do you make them an author on your paper?

Have you tried...

After six months of data collection and analysis, you give a presentation on your results to your lab/department, and someone suggests a change in methods or a new parameter.

What do you do with that feedback?

Do you remember what parameter you used in the first place?

How much effort will it be to change your code and re-run the analysis in the first place?

Accepted, with Revisions...

The manuscript for the computational project you've been working on for 2 years is under review, but the editors want a specific new figure before accepting your paper.

How much work will it be to make the requested changes?

Is it worth submitting to a more-lenient journal?

Do you write a rebuttal letter, explaining that it is too much work or claim that the suggestion is out of scope for your study?

Data Analysis Requested...

Your paper is finally accepted! You move on to a new laboratory and continue doing amazing work, but one day you receive an email requesting the code and data for your prior work.

Do you know where it all is?

How much effort will it be to find it?

How much of it needs to be modified before sending it out?

How long does it take for you to reply to the email?

Will it matter if you don't reply at all?

Scientific DevOps:

Designing Reproducible Data Analysis Pipelines with Containerized Workflow Managers

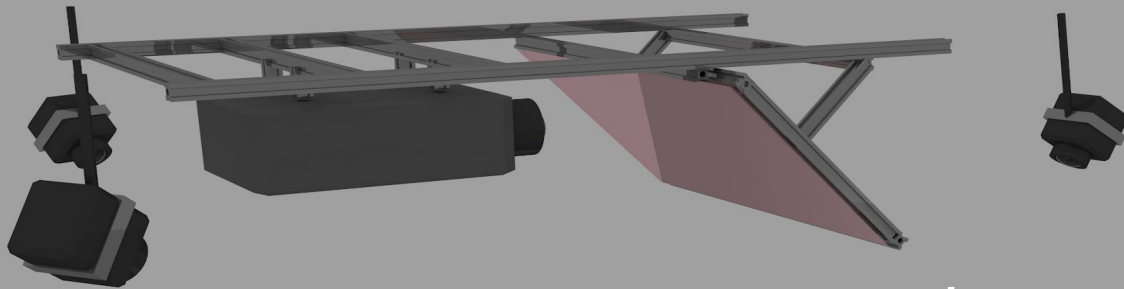
Nicholas Del Grosso

EuroScipy 2019

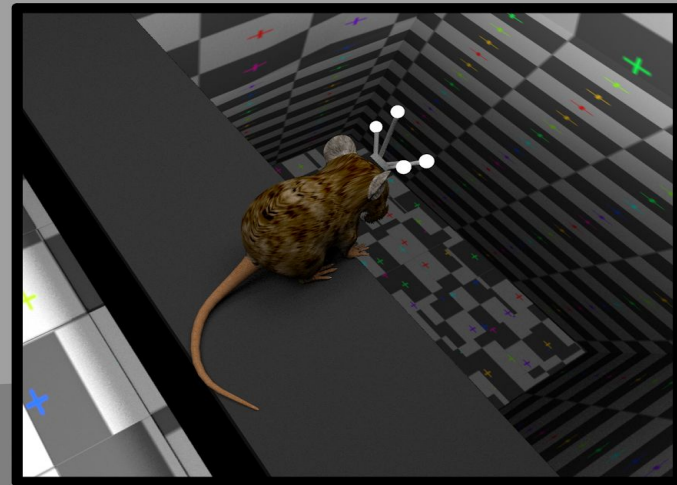
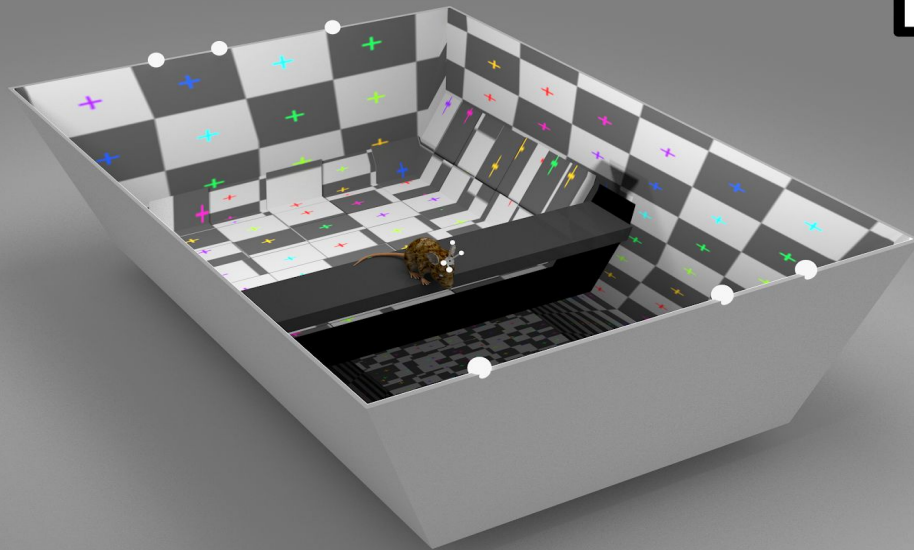
Bilbao, Spain

These Slides Available at:

github.com/nickdelgrosso/devops_talk_euroscipy2019



Closed-Loop Research and Software Development

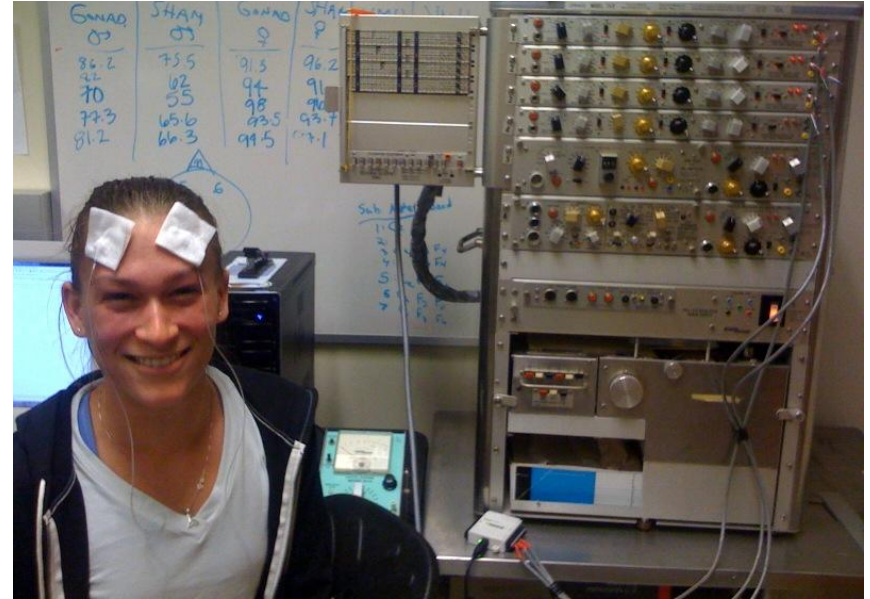


Early Inspiration



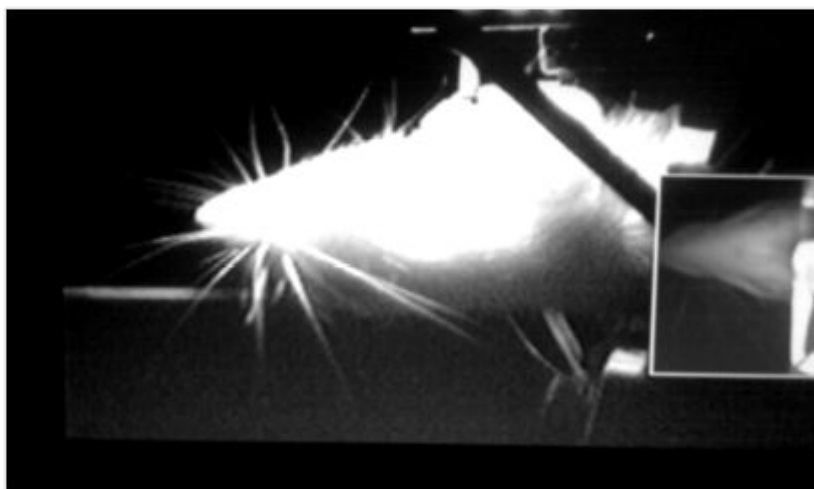
“Teenager moves video icons
just by imagination.”

-Leuthard and Blakely, 2006



“College Student Learns MATLAB and LabVIEW to
build DAQ System for EEG-based BCI.
Fails to ground 20-year-old recording equipment.”

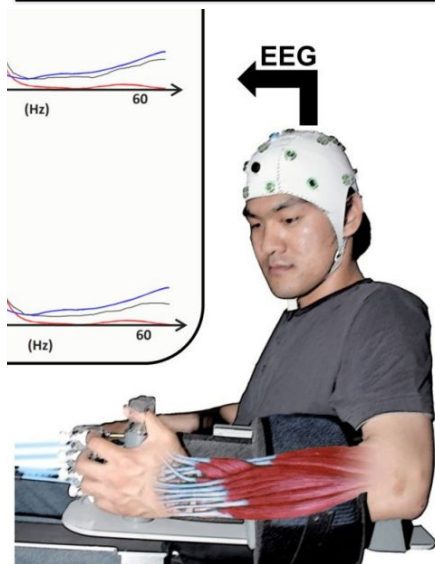
-Nick Del Grosso, 2009



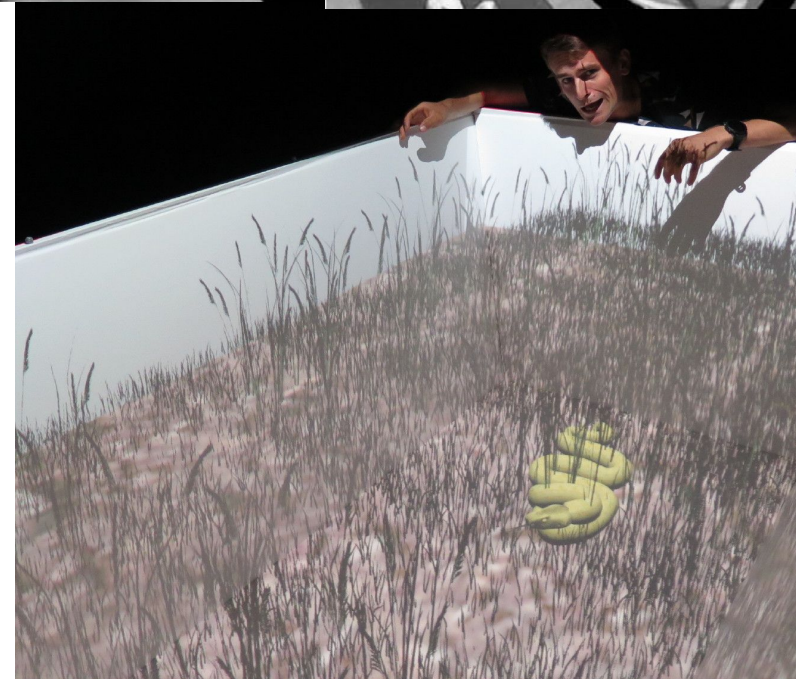
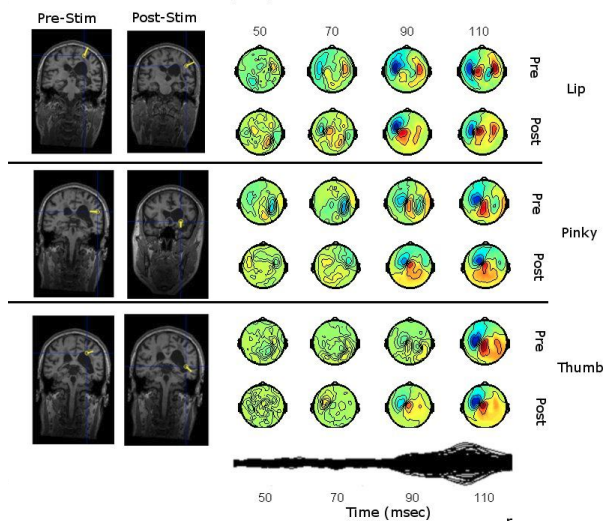
7a



7c



Paretic (Left) Side Stimulation





Nicholas A. Del Grosso

nickdelgrosso

A Passionate Neuroscientist and Pythonista

📍 Munich, Germany

✉ [Sign in to view email](#)



Block or report user

Organizations



Overview

Repositories **125**

Projects **0**

Stars **147**

Followers **70**

Following **26**

Pinned

 [ratcave/ratcave](#)

A Simple Python 3D Graphics Engine extension for Pyglet, Psychopy, and PyGame.

Python ★ 58 🍴 19

 [MS_Booker](#)

A simple web app for booking mass spec machines

Python ★ 1 🍴 2

 [ratcave/wavefront_reader](#)

A basic Wavefront .obj and .mtl reader module for Python

Python ★ 7 🍴 7

 [ratcave/natnetclient](#)

Python NatNet Client for retrieving NaturalPoint's Optitrack data from Motive software using depacketization.

Python ★ 8 🍴 10

 [helptranslator](#)

Translates the Python help text to any language, for helping with programming learning.

Python ★ 6

 [dzne_python_workshop](#)

Jupyter Notebook 🍴 1

424 contributions in the last year

My Latest Concern: The Replication Crisis

Essay

Power size new Why Most Published Research Findings Are False

John P. A. Ioannidis

Katherine S. Button^{1,2}, John P. A. Ioannidis³, Claire Mokrysz¹, Brian A. Jonathan Flint⁵, Emma S. J. Robinson⁶ and Marcus R. Munafò¹

Abstract | A study with low statistical power has a reduced chance of detecting

False-Positive Psychology: Undisclosed Flexibility in Data Collection and Analysis Allows Presenting Anything as Significant

Joseph P. Simmons¹, Leif D. Nelson², and Uri Simonsohn¹



And More Recently: The Reproducibility Crisis

PERSPECTIVE

OPEN ACCESS

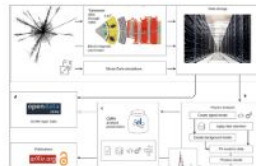
15 NOV 2018

Nature Physics

Open is not enough

The solutions adopted by the high-energy physics community to foster reproducible research are examples of best practices that could be embraced more widely. This first experience suggests that reproducibility requires going beyond openness.

Xiaoli Chen, Sünje Dallmeier-Tiessen ... Sebastian Neubert



WORLD VIEW

24 MAY 2018

Nature

Before reproducibility must come preproducibility

Instead of arguing about whether results hold up, let's push to provide enough information for others to

Philip B. Stark

EDITORIAL

18 APR 2018

Nature



Checklists work to improve science

Nature authors say a reproducibility checklist is a step in the right direction, but more needs to be done.



WORLD VIEW

16 MAY 2018

Nature

Give every paper a read for reproducibility

I was hired to ferret out errors and establish routines that promote rigorous research, says Catherine Winchester.

Catherine Winchester



COMMENT

24 AUG 2017

Nature

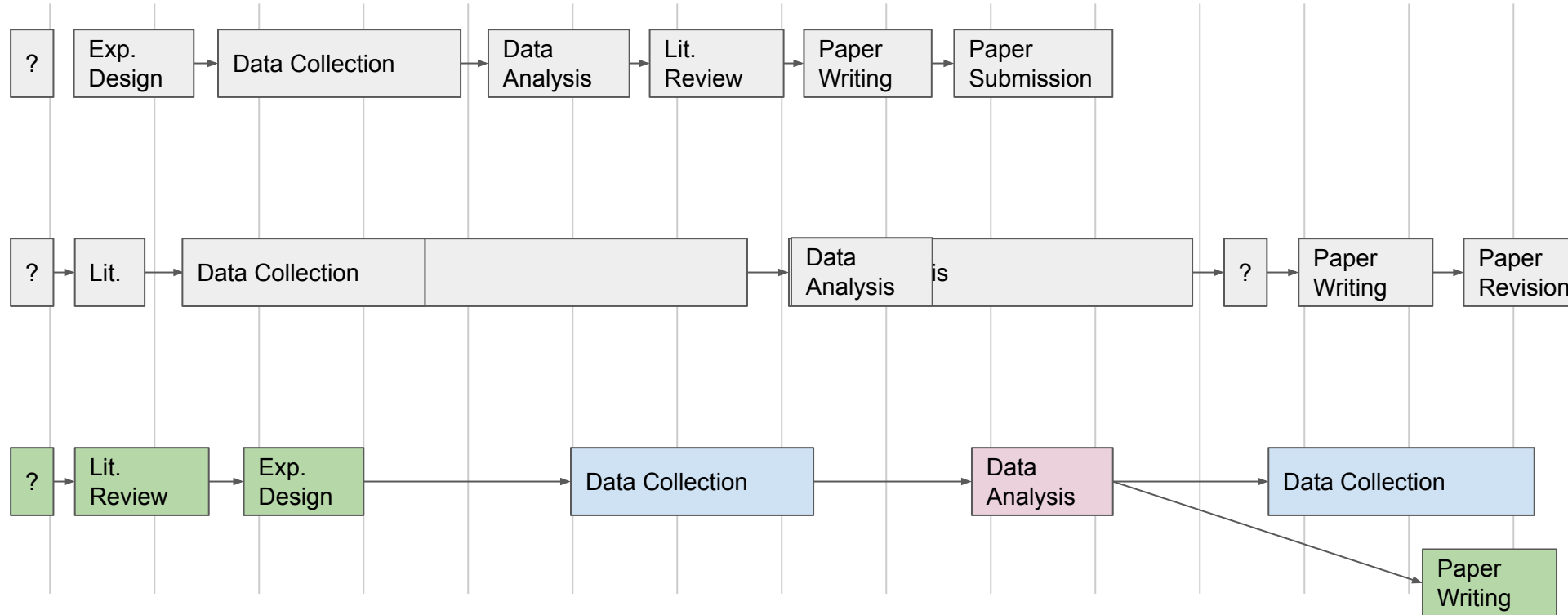
A long journey to reproducible results

Replicating our work took four years and 100,000 worms but brought surprising discoveries, explain Gordon L. Lithgow, Maria Driscoll and Patrick Phillips



Wastes in of Lean Product Development

(Effects of Waterfalls and Siloed Knowledge)



DevOps is...

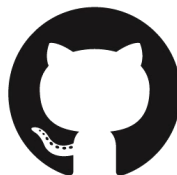
- Management principles adapted from the Lean community to software deployment: an application of the scientific method, queuing theory, and systems design to productivity.
- A set of software tools to help a team work toward constant, usable learning and build while maintaining a productive environment.
- The recognition that software development is an integral part of an organization.
- the observation that much wasted effort is produced by short-sightedness within individual steps in a pipeline.
- An observation that all steps contribute toward the achievement of some goal.

Version Control: Essential Tool #1

- Takes snapshots of a folder, creating a timeline of changes to that folder.
- Has tools for copying that timeline and making alternative timelines.
- Asks users to describe, in their own words, the point of each snapshot.



Version Control System



GitHub

**Code Hosting Website &
Social Network**



GitLab

Code Hosting Tool

Scientific DevOps:

Designing Reproducible Data Analysis Pipelines with Containerized Workflow Managers

Nicholas Del Grosso

EuroScipy 2019

Bilbao, Spain

These Slides Available at:

github.com/nickdelgrosso/devops_talk_euroscipy2019

The Three “Ways” of DevOps

1. Build Smooth Forward Flow
2. Increase Feedback
3. Foster an Environment of Continuous Improvement

Building Smooth, Forward Flow

The First Way

Data -----> Figures ----> Reader

Ambiguity -----> Certainty

- MyProject
 - README.txt

README.txt

My Project
This project makes histograms
of my awesome data!

My Project

This project makes histograms of my awesome data!

- MyProject
 - README.md

README.md

My Project

This project makes histograms of my awesome data!

Run the Analysis

```
```python
import pandas as pd
df = pd.read_csv("mydata1.csv")
fig = df.plot.hist()
fig.savefig("myresults.png")
```
```

My Project

This project makes histograms of my awesome data!

Run the Analysis

```
import pandas as pd
df = pd.read_csv("mydata1.csv")
fig = df.plot.hist()
fig.savefig("myresults.png")
```

cat README.md | codedown python | python

- MyProject
 - README.md
 - get_results.py

get_results.py

```
import pandas  
  
read_csv  
plot_histogram  
savefig
```

My Project

This project makes histograms of my awesome data!

Run the Analysis

```
python get_results.py
```

- MyProject
 - README.md
 - get_results.py

My Project

This project makes histograms of my awesome data!

Install the Dependencies

```
pip install pandas
```

```
pip install numpy
```

```
pip install matplotlib
```

Run the Analysis

```
python get_results.py
```


- MyProject
 - README.md
 - get_results.py
 - install_requirements.sh

install_requirements.sh

```
pip install pandas  
pip install numpy  
pip install matplotlib
```

My Project

This project makes histograms of my awesome data!

Install the Dependencies

```
bash install_requirements.sh
```

Run the Analysis

```
python get_results.py
```

- MyProject
 - README.md
 - get_results.py
 - requirements.txt

requirements.txt

```
pandas  
matplotlib  
numpy
```

My Project

This project makes histograms of my awesome data!

Install the Dependencies

```
pip install -r requirements.txt
```

Run the Analysis

```
python get_results.py
```

- MyProject
 - README.md
 - get_results.py
 - requirements.txt
 - requirements.lock

requirements.lock

```
cycler==0.10.0
kiwisolver==1.1.0
matplotlib==3.1.1
numpy==1.17.1
pandas==0.25.1
pyparsing==2.4.2
python-dateutil==2.8.0
pytz==2019.2
six==1.12.0
```

My Project

This project makes histograms of my awesome data!

Install the Dependencies

`pip install -r requirements.lock`

Run the Analysis

`python get_results.py`

Developers

Save the current versions of the packages:

`pip freeze > requirements.lock`

- MyProject
 - README.md
 - get_results.py
 - requirements.txt
 - requirements.lock
- (Virtual Environments)
 - myproject
 - bin
 - python
 - activate

My Project

This project makes histograms of my awesome data!

Install the Dependencies

```
conda create --name myproject python=3.7  
conda activate myproject  
pip install -r requirements.lock
```

Run the Analysis

```
conda activate myproject  
python get_results.py
```

Developers

Save the current versions of the packages:

```
pip freeze > requirements.lock
```

- MyProject
 - README.md
 - get_results.py
 - environment.yml
 - requirements.lock

My Project

This project makes histograms of my awesome data!

Install the Dependencies

```
conda create --name myproject python=3.7
```

```
conda activate myproject
```

```
conda install --file environment.yml
```

Run the Analysis

```
conda activate myproject
```

```
python get_results.py
```

Developers

Save the current versions of the packages:

```
conda list --export > requirements.lock
```

- MyProject
 - README.md
 - get_results.py
 - Pipfile
 - Pipfile.lock

My Project

This project makes histograms of my awesome data!

Install the Dependencies

```
pip install pipenv
```

```
pipenv install
```

Run the Analysis

```
pipenv shell
```

```
python get_results
```

```
cd MyProject
pipenv --python 3.7
pipenv install pandas
```

- MyProject
 - README.md
 - get_results.py
 - Pipfile
 - Pipfile.lock

My Project

This project makes histograms of my awesome data!

Install the Dependencies

`pip install pipenv`

`pipenv install`

Run the Analysis

`pipenv run get_results.py`

```
cd MyProject
pipenv --python 3.7
pipenv install pandas
pipenv lock
```

- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock

pyproject.toml

```
[tool.poetry]
name = "MyProject"
version = "0.1.0"
description = ""
authors = ["Nicholas A. Del Grosso
<delgrosso.nick@gmail.com>"]
```

```
[tool.poetry.dependencies]
python = "^3.6"
pandas = "^0.25.1"
```

```
[tool.poetry.dev-dependencies]
pytest = "^3.0"
```

My Project

This project makes histograms of my awesome data!

Install the Dependencies

`pip install poetry`

`poetry install`

Run the Analysis

`poetry shell`

`python get_results.py`

```
poetry MyProject
cd MyProject
pipenv add pandas
```


- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock

pyproject.toml

```
[tool.poetry]
name = "MyProject"
version = "0.1.0"
description = ""
authors = ["Nicholas A. Del Grosso
<delgrosso.nick@gmail.com>"]
```

```
[tool.poetry.dependencies]
python = "^3.7"
pandas = "^0.25.1"
```

```
[tool.poetry.dev-dependencies]
pytest = "^3.0"
```

My Project

This project makes histograms of my awesome data!

Install the Dependencies

`pip install poetry`

`poetry install`

Run the Analysis

`poetry run python get_results.py`



- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock

pyproject.toml

```
[tool.poetry]
name = "MyProject"
version = "0.1.0"
description = ""
authors = ["Nicholas A. Del Grosso
<delgrosso.nick@gmail.com>"]
```

```
[tool.poetry.dependencies]
python = "^3.7"
pandas = "^0.25.1"
```

```
[tool.poetry.dev-dependencies]
pytest = "^3.0"
```

My Project

This project makes histograms of my awesome data!

Install the Dependencies

(Runs on Ubuntu 16.4. I haven't tested it on Windows.)

```
pip install poetry
poetry install
```

Run the Analysis

```
poetry run python get_results.py
```



- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock
 - Singularity

Dockerfile



```
FROM python:3.7-slim
```

```
WORKDIR /MyProject
```

```
COPY . /MyProject
```

```
RUN pip install poetry
```

```
RUN poetry install
```

```
CMD [ 'bash' ]
```

Singularity Recipe



```
Bootstrap: docker
```

```
From: python:3.7-slim
```

```
%files
```

```
./pyproject.toml .
```

```
./poetry.lock .
```

```
%post
```

```
pip install poetry
```

```
poetry install
```

- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock
 - Singularity
 - myproject.simg

My Project

This project makes histograms of my awesome data!

Install the Dependencies

1. install [singularity](#)

Run the Analysis

```
singularity shell myproject.simg  
python scripts/get_results.py
```

Building the Singularity Image

```
sudo singularity build myproject.simg Singularity
```

- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock
 - Singularity
 - myproject.simg

My Project

This project makes histograms of my awesome data!

Install the Dependencies

1. install [singularity](#)

Run the Analysis

singularity run myproject.simg

...

```
%runscript  
python get_results.py
```

- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock
 - Singularity
 - myproject.simg

My Project

This project makes histograms of my awesome data!

Install the Dependencies

1. install [singularity](#)
2. Get the data.

Run the Analysis

```
singularity run myproject.simg
```

- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock
 - Singularity
 - myproject.simg

- /data
 - raw
 - d1.csv
 - d2.csv



RENKU

Collaborative Data Science

**Talk to Chandrasekhar
Ramakrishnan and Rok Roškar
for more info, here at the
conference!**



GIN

Modern Research Data Management for Neuroscience

Quilt

Manage data like code

Quilt versions and deploys data

- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock
 - Singularity
 - myproject.simg

- /data
 - raw
 - d1.csv
 - d2.csv

My Project

This project makes histograms of my awesome data!

Install the Dependencies

1. install [singularity](#)

Run the Analysis

```
singularity run -B DataFolder:/data myproject.simg
```


- MyProject
 - README.md
 - get_results.py
 - pyproject.toml
 - poetry.lock
 - Singularity
 - myproject.simg

- /data
 - raw
 - d1.csv
 - d2.csv

My Project

This project makes histograms of my awesome data!

Install the Dependencies

1. install [singularity](#)

Run the Analysis

singularity run myproject.simg

```
...
```

```
%files
```

```
DataFolder /data
```

- MyProject
 - README.md
 - pyproject.toml
 - poetry.lock
 - Singularity
 - myproject.simg
 - scripts
 - get_results.py

- /data
 - raw
 - d1.csv
 - d2.csv

My Project

This project makes histograms of my awesome data!

Install the Dependencies

1. install [singularity](#)

Run the Analysis

```
singularity run myproject.simg
```

```
...
```

```
%files
```

```
DataFolder /data
```

Shrinking Your Batch Size

The First Way: Part 2

```
raw_files = glob("data/raw/data_*.csv")
processed_files = []

for raw_file in raw_files:
    session = path.basename(path.splitext(raw_file)[0]).split('_')[-1]
```

Preprocess Data

```
df = pd.read_csv(raw_file)
df2 = do_process(df)
os.makedirs("data/processed", exist_ok=True)
process_file = f"data/processed/data_{session}.h5"
df2.to_hdf(processed_file, '/')
processed_files.append(processed_file)
```

Make histograms

```
fig = df2["Variable"].plot.hist()
os.makedirs("results/hists", exist_ok=True)
fig.savefig(f"results/hists/hist_{session}.svg")
```

Make Figure1

```
df_all = pd.concat([pd.read_hdf(f, '/') for f in processed_files])
os.makedirs("results", exist_ok=True)
df_all.plot(x='Time', y='Happiness').savefig("results/figure1.svg")
```

get_results.py

```
raw_files = glob("data/raw/data_*.csv")
```

```
processed_files = []
```

```
for raw_file in raw_files:
```

```
    session = path.basename(path.splitext(raw_file)[0]).split('_')[-1]
```

Preprocess Data

```
df = pd.read_csv(raw_file)
```

```
df2 = do_process(df)
```

```
os.makedirs("data/processed", exist_ok=True)
```

```
process_file = f"data/processed/data_{session}.h5"
```

```
df2.to_hdf(processed_file, '/')
```

```
processed_files.append(processed_file)
```

Make histograms

```
fig = df2["Variable"].plot.hist()
```

```
os.makedirs("results/hists", exist_ok=True)
```

```
fig.savefig(f"results/hists/hist_{session}.svg")
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Make Figure1

```
df_all = pd.concat([pd.read_hdf(f, '/') for f in processed_files])
```

```
os.makedirs("results", exist_ok=True)
```

```
df_all.plot(x='Time', y='Happiness').savefig("results/figure1.svg")
```

get_results.py

Preprocess Data

```
for raw_file in glob("data/raw/data_*.csv"):
    session = path.basename(path.splitext(raw_file)[0]).split('_')[-1]
    df = pd.read_csv(raw_file)
    df2 = do_process(df)
    os.makedirs("data/processed", exist_ok=True)
    processed_file = f"data/processed/data_{session}.h5"
    df2.to_hdf(processed_file, '/')
```

Make Histograms

```
for processed_file in glob("data/processed/data_*.h5"):
    session = path.basename(path.splitext(raw_file)[0]).split('_')[-1]
    df = pd.read_hdf(processed_file, '/')
    fig = df["Variable"].plot.hist()
    os.makedirs("results/hists", exist_ok=True)
    fig_file = f"results/hists/hist_{session}.svg"
    fig.savefig(fig_file)
```

Make Figure 1

```
files = glob("data/processed/data_*.h5")
df_all = pd.concat([pd.read_hdf(f, '/') for f in files])
fig1 = df_all.plot(x='Time', y='Happiness')
os.makedirs("results", exist_ok=True)
fig1.savefig("results/figure1.svg")
```

get_results.py

Preprocess Data

```
inputs = [f"/data/raw/data_{session}.csv" for session in sessions]
outputs = [f"/data/processed/data_{session}.h5" for session in sessions]
os.makedirs("/data/processed", exist_ok=True)
for input, output in zip(inputs, outputs):
    df = pd.read_csv(input)
    df2 = do_process(df)
    df2.to_hdf(output, '/')

```

Make Histograms

```
inputs = [f"/data/processed/data_{session}.h5" for session in sessions]
outputs = [f"results/hists/hist_{session}.svg" for session in sessions]
os.makedirs("results/hists", exist_ok=True)
for input, output in zip(inputs, outputs):
    df = pd.read_hdf(input, '/')
    fig = df["Variable"].plot.hist()
    fig.savefig(output)

```

get_results.py

Make Figure1

```
inputs = [f"/data/processed/data_{session}.h5" for session in sessions]
output = "results/figure1.svg"
os.makedirs("results", exist_ok=True)
df_all = pd.concat([pd.read_hdf(input, '/') for input in inputs])
df_all.plot(x='Time', y='Happiness').savefig(output)

```

```
sessions = [1, 2, 3]
```

rule process_data:

```
input: "/data/raw/data_{session}.csv"
```

```
output: "/data/processed/data_{session}.h5"
```

```
run:
```

```
df = pd.read_csv(input)
```

```
df2 = do_process(df)
```

```
df2.to_hdf(output, '/')
```

rule build_histograms:

```
input: "/data/processed/data_{session}.h5"
```

```
output: "results/hists/hist_{session}.svg"
```

```
run:
```

```
df = pd.read_hdf(input, '/')
```

```
fig = df["Variable"].plot.hist()
```

```
fig.savefig(output)
```

rule figure1:

```
input: expand("/data/processed/data_{session}.h5", session=sessions)
```

```
output: "results/figure1.svg"
```

```
run:
```

```
df_all = pd.concat([pd.read_hdf(input, '/') for input in inputs])
```

```
df_all.plot(x='Time', y='Happiness').savefig(output)
```

Snakefile



snakemake

```
pip install snakemake  
snakemake figure1
```


sessions = [1, 2, 3]

rule process_data:

input: "/data/raw/data_{session}.csv"

output: "data/processed/data_{session}.h5"

script: "scripts/process_data.py"

rule build_histograms:

input: "/data/processed/data_{session}.h5"

output: "results/hists/hist_{session}.svg"

script: "scripts/plot_histogram.py"

rule figure1:

input: expand("/data/processed/data_{session}.h5", session=sessions)

output: "results/figure1.svg"

script: "scripts/plot_figure1.py"

scripts/process_data.py

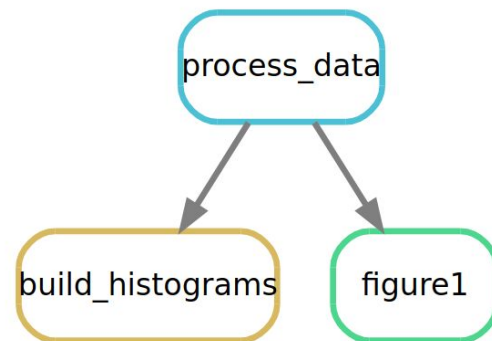
```
import pandas as pd
```

```
filename = snakemake.input[0]
```

```
df = pd.read_csv(filename)
```

```
df2 = do_process(df)
```

```
df2.write_csv(snakemake.output[0])
```



- MyProject
 - README.md
 - requirements.txt
 - Singularity
 - myproject.simg
 - .gitignore
 - **Snakefile**
 - scripts
 - process_data.py
 - plot_histogram.py
 - plot_figure1.py
 - results
- /data
 - raw
 - data_1.csv
 - data_2.csv

My Project

This project makes histograms from my data!

Before You Begin

1. install [singularity](#)

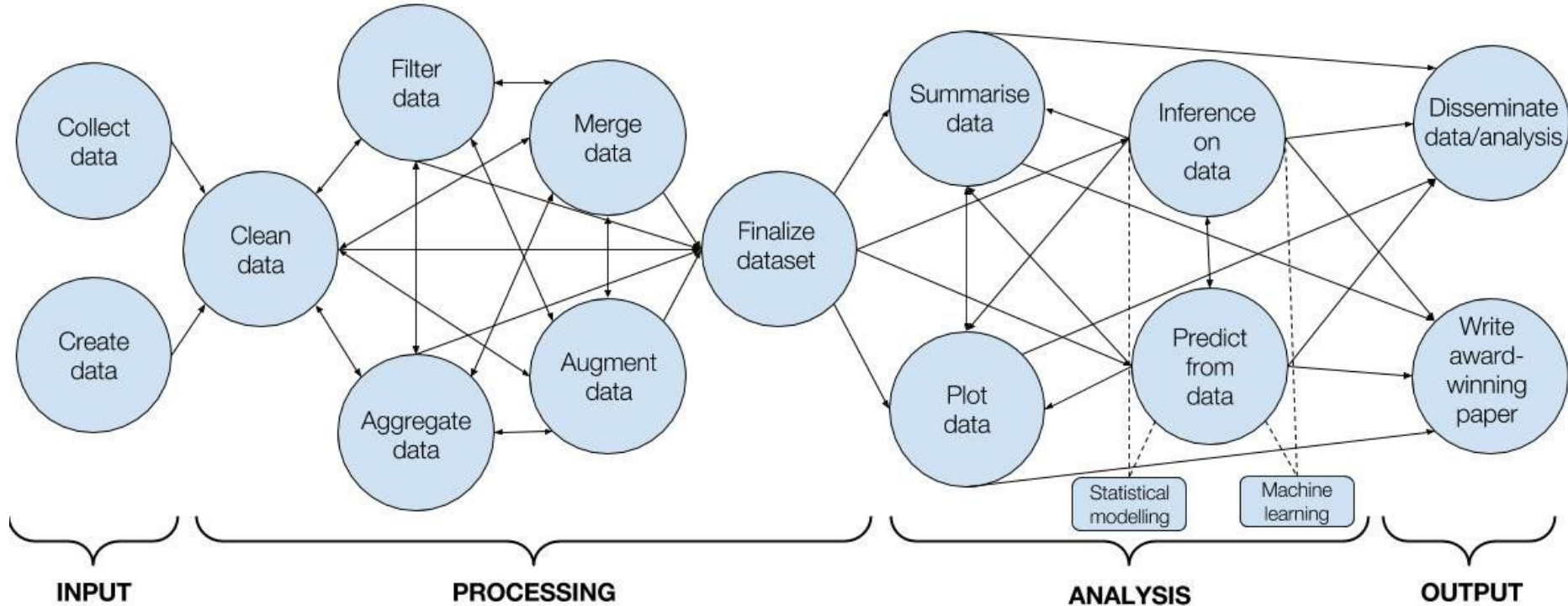
Running the Analysis Script

Run the Singularity App, connecting its /data folder to the folder you downloaded the data to.

```
singularity run myproject.simg
```

```
%runscript  
snakemake figure1
```

Of Courses, It Can Get Much More Complex!



def task_dot():

return {

'file_dep': ['requests.models.deps'],

'targets': ['requests.models.dot'],

'actions': [module_to_dot],

}



rule process_data:

input: "data/raw/data_{session}.csv"

output: "data/processed/data_{session}.h5"

script: process_data.py

dag = DAG('tutorial')



Airflow

**t1 = BashOperator(task_id='print_date',
bash_command='date', dag=dag)**

**t2 = BashOperator(task_id='sleep',
bash_command='sleep 5', dag=dag)**

t2.set_upstream(t1)

Because Workflow Managers Build Task Graphs, They Can Do:

- Partial Processing
- Parallel Processing
- Multi-Language Gluing
- Auto-Retrieves
- Remote Data Connections
- Workflow Monitoring
- Workflow Scheduling
- ...and much more!



Apache Taverna



Airflow



nextflow

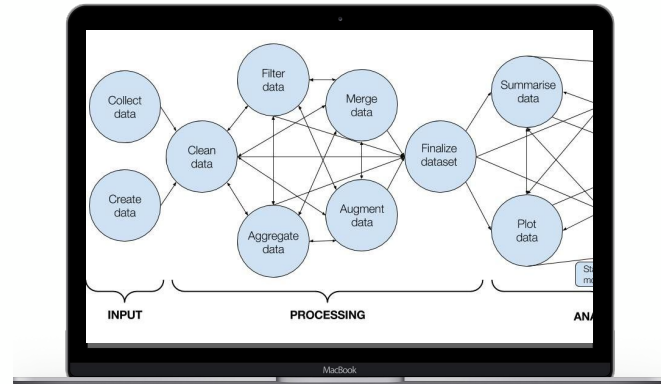


Luigi



Open for Innovation[®]

KNIME



SCIENTIFIC FILESYSTEM

```
%apphelp figure1
```

```
Figure 1 from my paper,  
showing how time spent with  
Python increases your  
happiness!
```

```
%apprun figure1
```

```
snakemake figure1
```

```
%appinstall notebook
```

```
pip install jupyterlab
```

```
%appinstall notebook
```

```
cd notebooks  
jupyter lab
```

```
%apprun overview
```

```
snakemake all -n --rulegraph
```

My Project

This project makes histograms from my data!

Before You Begin

1. install [singularity](#)

Exploring the Container

```
singularity myproject.simg help  
singularity myproject.simg apps
```

Get Figure 1

```
singularity help myproject.simg --app figure1  
singularity run myproject.simg --app figure1
```

Get a Graphical Overview of the Pipeline

```
singularity run myproject.simg --app overview
```

Interact with the Analysis Notebooks

```
singularity run myproject.simg --app notebook
```

Building Smooth, Forward Flow

The First Way

Readme Files as the human entry and first goal statement.

Version Control Systems to continually work towards goals

Package Managers to download versioned software and reduce version regressions

Environment Managers for isolating the Python interpreter

Container Systems for isolating everything.

Workflow Managers to break pipelines into smaller steps and separate out file overhead.



DataJoint™ is a free, open-source framework for programming scientific databases and computational data pipelines.

Sign up for a free tutorial database.



Getting Quick Feedback

The Second Way

Automated Testing to get feedback on the code's functionality

(PyTest, Hypothesis, Pytest-BDD)

Test-Driven Development to set goals, prioritize work, and maintain testable code.

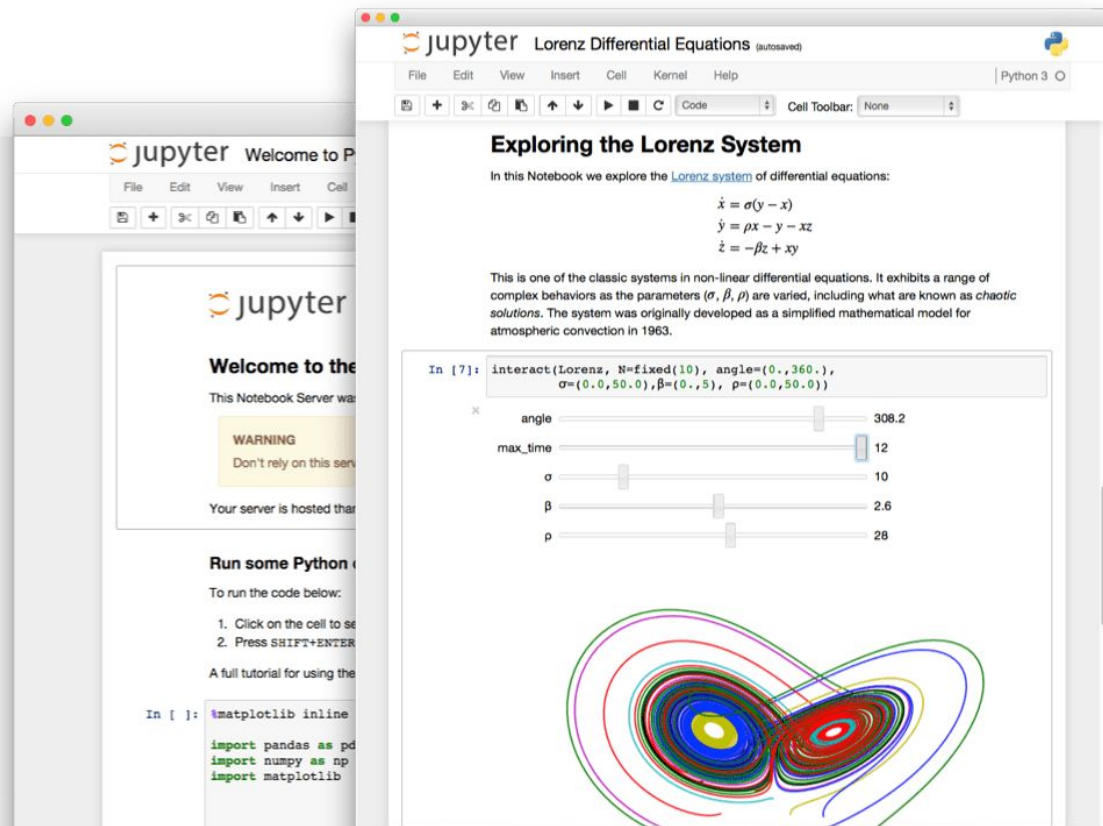
Continuous Integration to ensure constant testing off the developer's machine.

(Travis CI, Jenkins, Circle CI)

Pair Programming to get extremely rapid feedback.

Interactive Coding Environments to get immediate results for each line of code.

A Final Tool: The Jupyter Notebook and Binder



The image shows a Jupyter Notebook interface with the title "Lorenz Differential Equations (autosaved)". The notebook content includes:

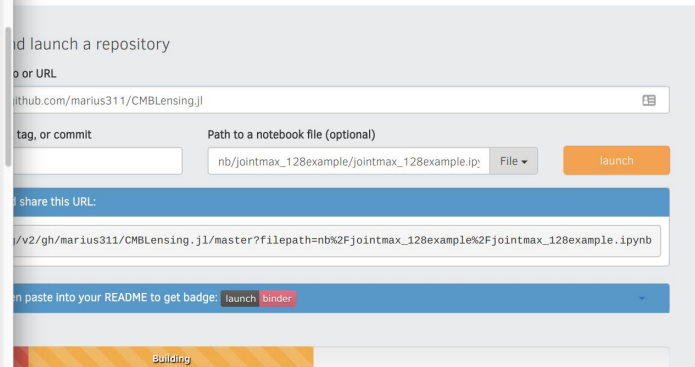
- A welcome message: "Welcome to the Jupyter Notebook Server".
- A warning box: "WARNING Don't rely on this server".
- A section titled "Run some Python code" with instructions: "1. Click on the cell to see the code. 2. Press SHIFT+ENTER".
- A code cell with the following code:

```
In [7]: %matplotlib inline
import pandas as pd
import numpy as np
import matplotlib
```
- A plot of the Lorenz attractor, showing a complex, chaotic trajectory in a 3D space.



Turn a GitHub repo into a collection of interactive notebooks

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



The image shows the Binder interface for launching a repository. It includes a form to enter a GitHub repository URL and a "Launch" button. Below the form, there is a section for sharing the URL and a "Building" status indicator.

Maintaining an Environment of Continuous Improvement

The Third Way

Opportunistic Refactoring

Pair Programming

Chaos Monkey Testing

Blameless Post-Mortems

Opportunistic Refactoring

Training Groups

Notebook Tutorials

Teaching Cohorts

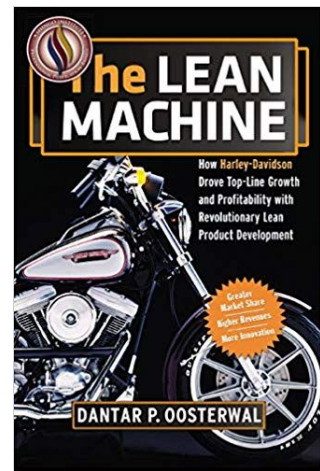
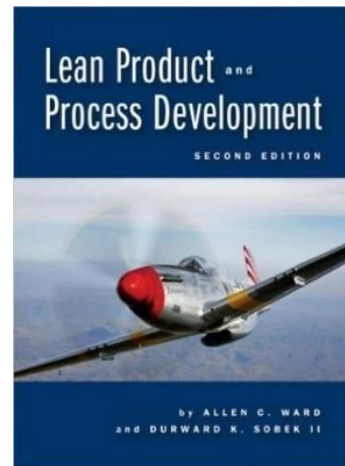
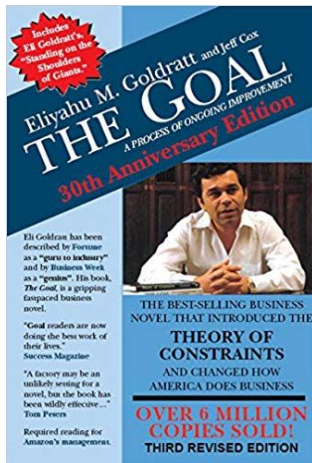
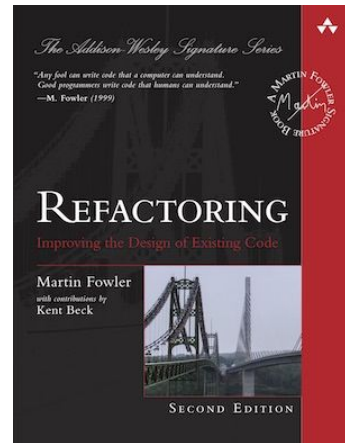
Improvement Katas

Refactoring-to-Teach

Books Recommendations: DevOps, Coding Practices, and Lean Management

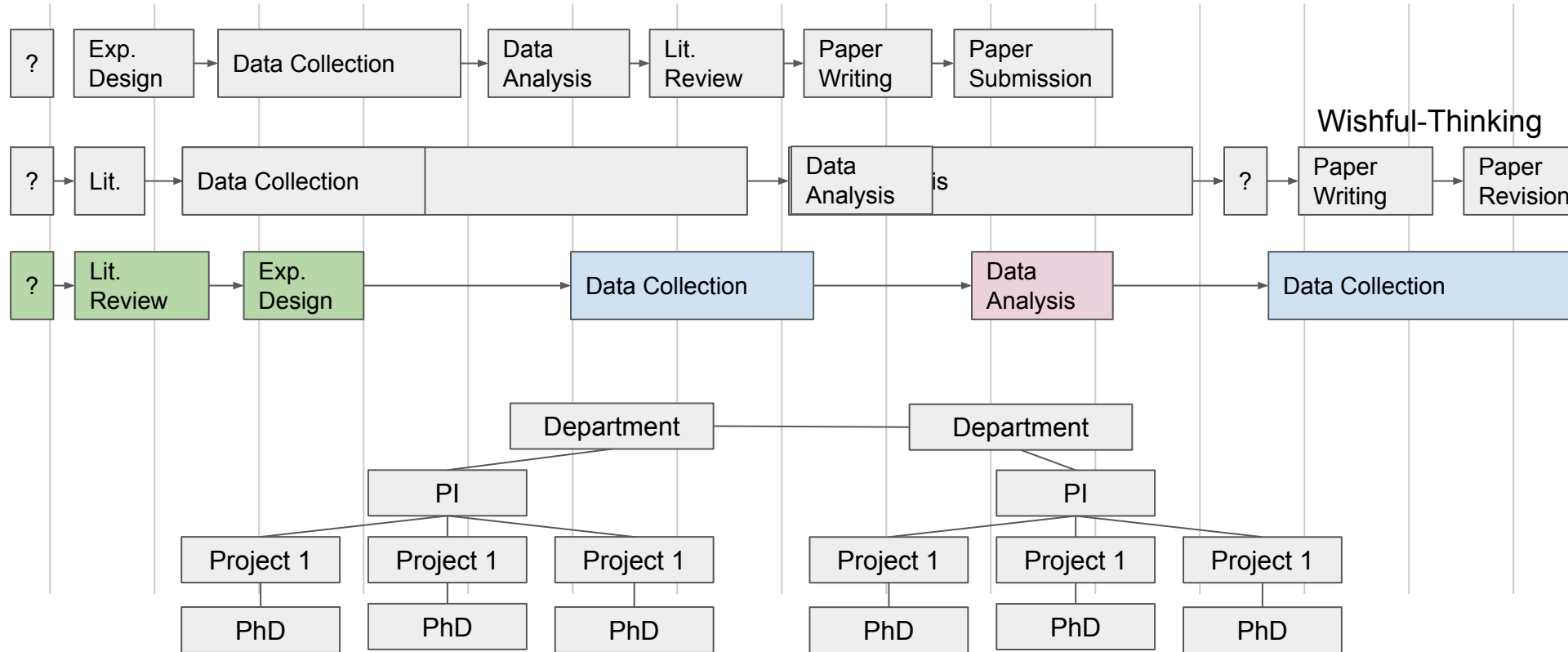
These Slides Available at:
github.com/nickdelgrosso/devops_talk_euroscipy2019

Thank you for your attention!



Wastes in of Lean Product Development

(Effects of Waterfalls and Siloed Knowledge)



Further Directions: ResearchOps and Continuous Science: Obliterating Batched Push Experimental Pipelines using Lean Product Development Models

