

Shareable Science:

Analysis, Archiving, and Authoring for Collaboration

Elizabeth DuPre

 [@emdupre](https://twitter.com/emdupre)

7 August, 2019

Science today





Olah & Carter (2017). Research Debt. *Distill.*

An outline for this morning

- Community-based project management
- A practical introduction to pyBIDS
- Authoring for collaboration
- A practical introduction to Jupyter Notebooks and JupyterLab



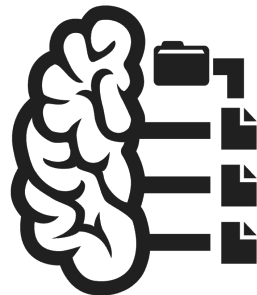
An outline for this morning

- Community-based project management
- A practical introduction to pyBIDS
- Authoring for collaboration
- A practical introduction to Jupyter Notebooks and JupyterLab



BIDS & the TIER Protocol


*Community-based standards
for project management*



BIDS
BRAIN IMAGING DATA STRUCTURE



Brain Imaging Data Structure



Teaching Integrity in Empirical Research



Community-based project management standards



Community-based project management standards



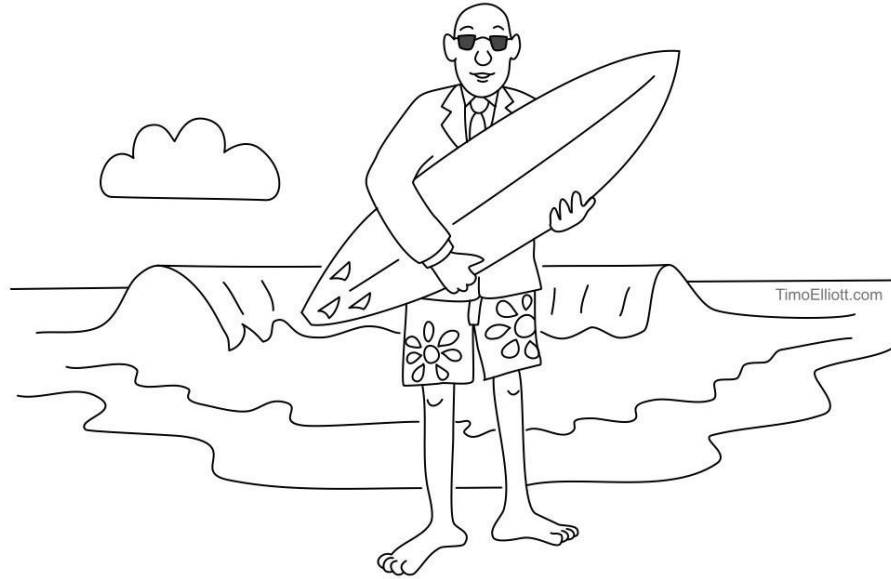
Community-based project management standards

Meet Professor Smith



With thanks to [Chris Gorgolewski](#)

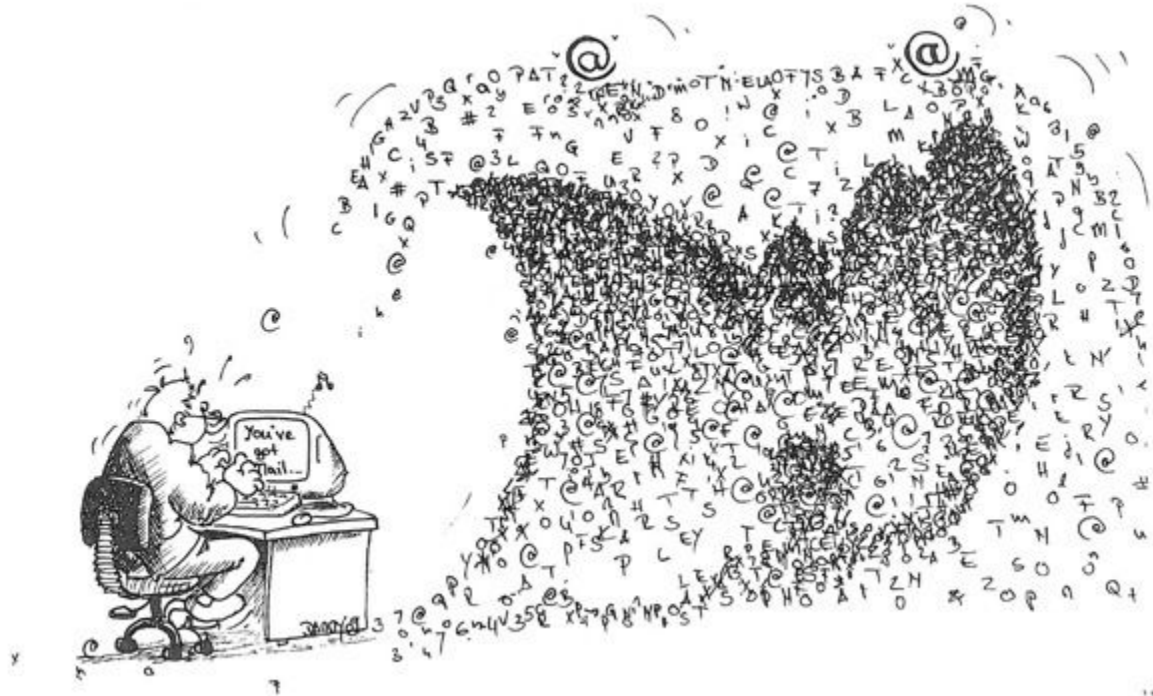
Meet Mike



A Business Analyst that lives in California.

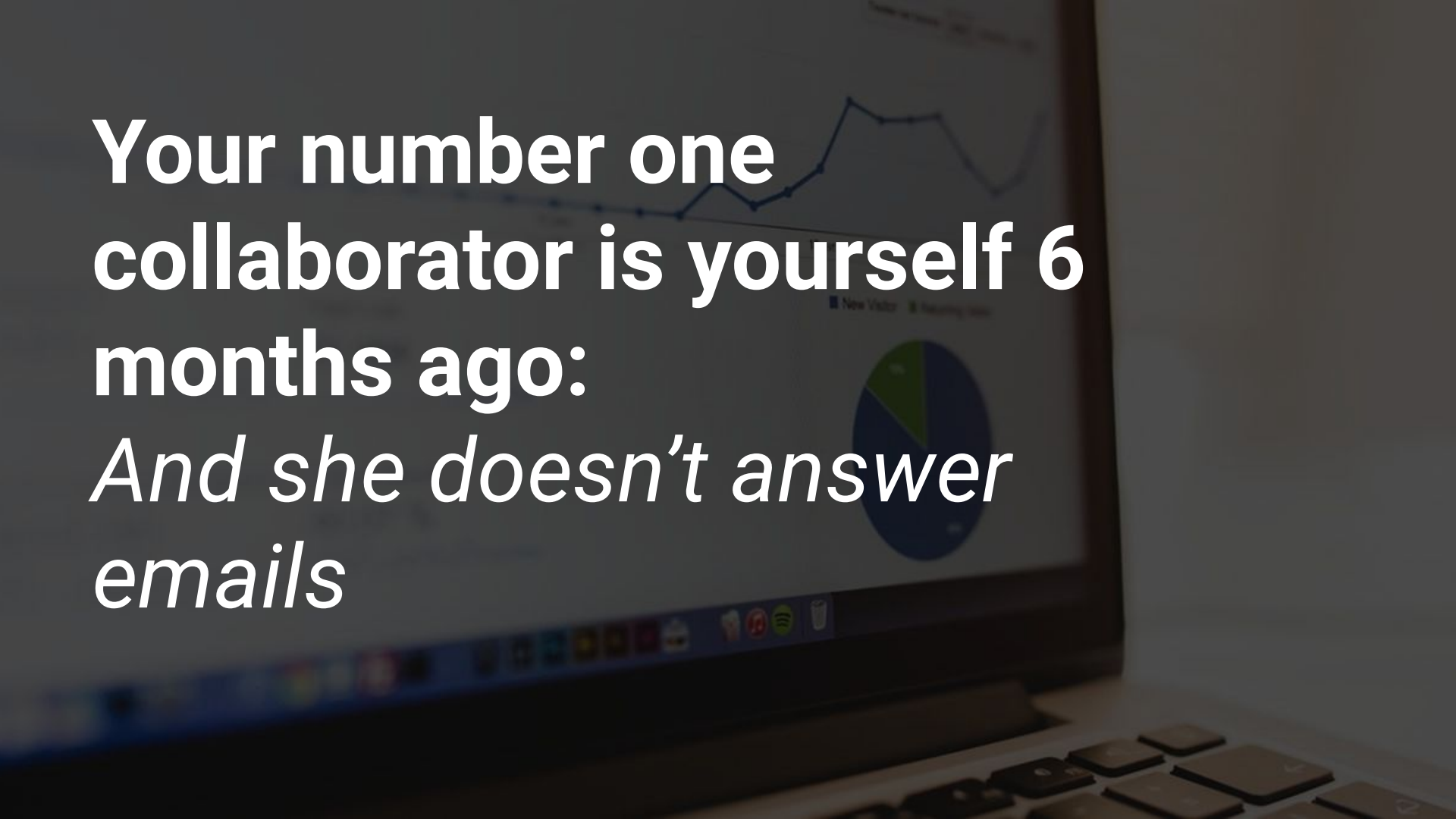
With thanks to [Chris Gorgolewski](#)

Meet Mike's project folders



With thanks to [Chris Gorgolewski](#)

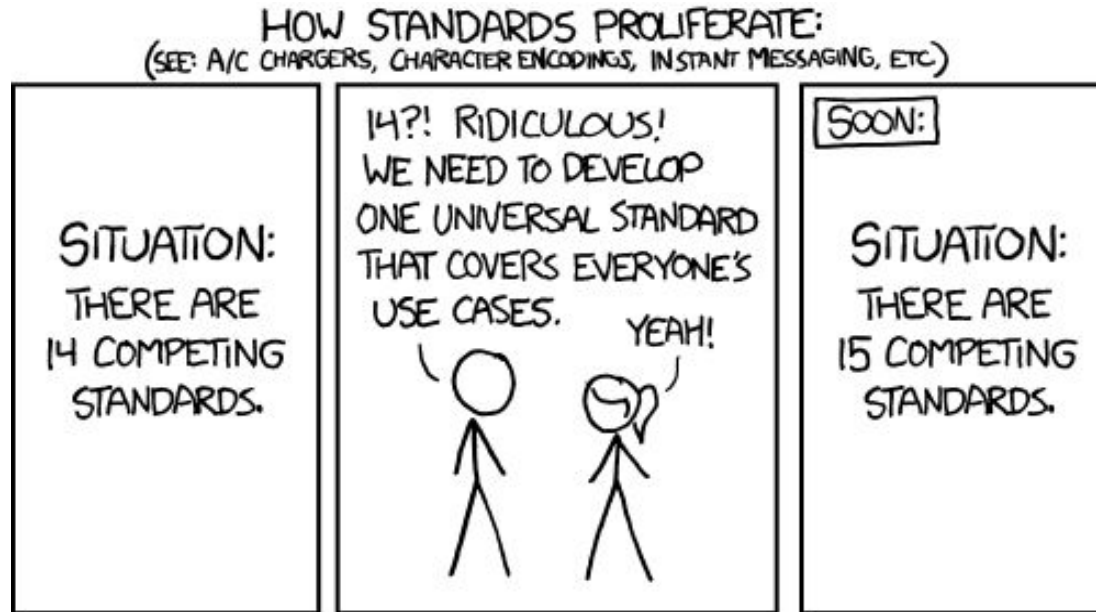
**Your number one
collaborator is yourself 6
months ago:**
*And she doesn't answer
emails*





Community-based project management standards

Houston, we have a problem





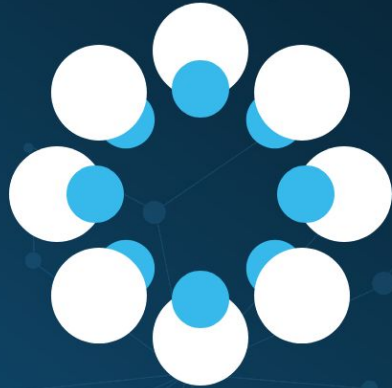
Community-based standards

- Developed **openly**
- Strive for **consensus** in decision-making
- Designed to **empower** and equip community members

A (quick) case study

Open Science Framework

A scholarly commons to connect the entire research cycle



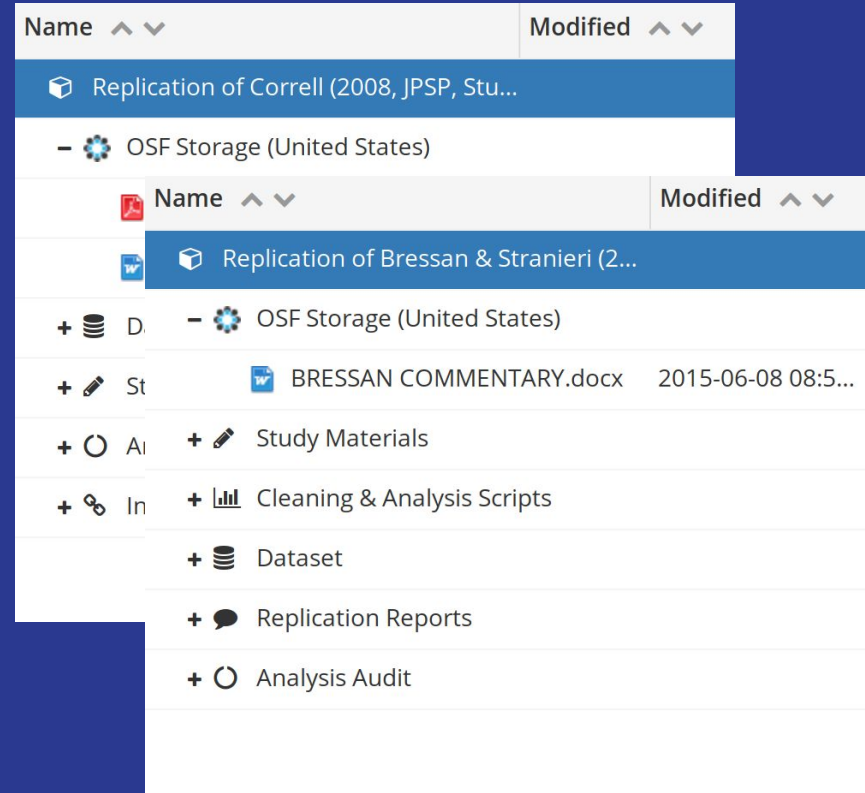
The Reproducibility Project

Name ^ v	Modified ^ v
Replication of Correll (2008, JPSP, Stu...	
- OSF Storage (United States)	
ReplicationReport_Correll2008...	2013-12-11 11:5...
ReplicationReport_incl_Metho...	2013-12-11 11:5...
+ Data	
+ Study Materials	
+ Analysis Audit	
+ Independent Direct Replication #...	

<https://osf.io/fejxb/>


The Reproducibility Project

... still did not have fully
standardized project organization !



<https://osf.io/fejxb/>

<https://osf.io/blcj6/>



Teaching Integrity in Empirical Research

Project TIER

Raw Data

A copy of **every original data file** from which you extract any of data used in your study.

Your original data files **serve as a record** of the data you began the project with.

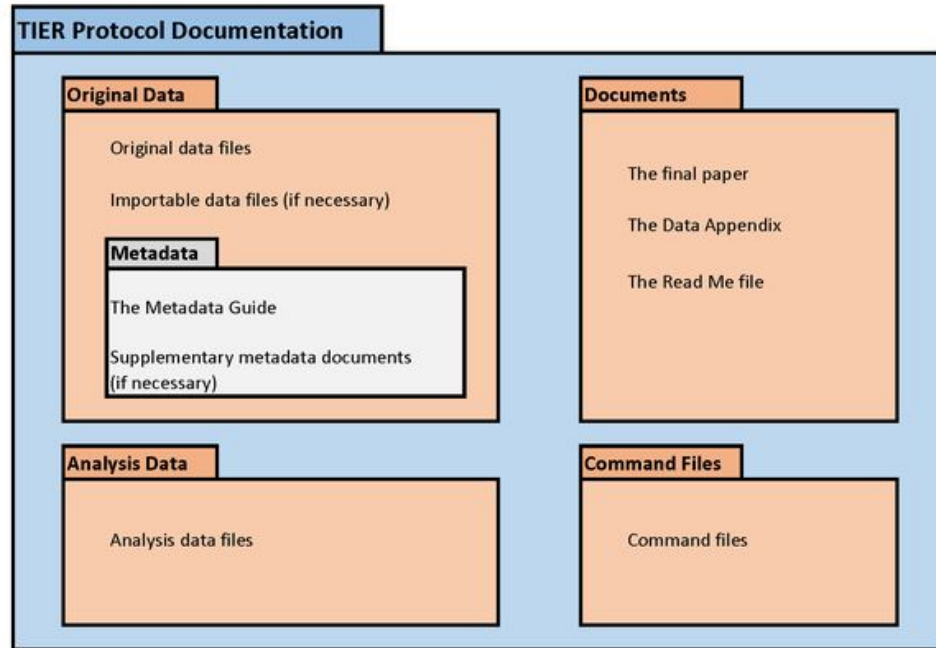
Analysis Code + Analysis Data

One or more files containing code used for the study... should **execute all the data processing and analysis necessary to replicate the study** and reproduce the reported results

Documents

Documentation to understand the study

- A copy of your final paper
- Your Data Appendix
- Your README file



The TIER Specification

TIER Protocol 3.0: Template

Public

92

...

Contributors: [Norm Medeiros](#), [Richard Ball](#)

Forked from osf.io/7g6cn on 2016-09-16 12:43 PM

Date created: 2016-09-08 11:17 PM | Last Updated: 2018-01-22 11:36 AM

Identifiers: DOI [10.17605/OSF.IO/YBZXE](https://doi.org/10.17605/OSF.IO/YBZXE) | ARK [c7605/osf.io/ybzx](https://n2t.org/ark:/c7605/osf.io/ybzx)

Category:  Project

Description: This project is designed to support Haverford College economics majors who produce empirical theses. The structure is based on the TIER Documentation Protocol. Additional information about Project TIER is available at <http://projecttier.org>

Wiki



This template was constructed for use by individuals who wish to follow the TIER Protocol for conducting and documenting an empirical research project.

Information about the [TIER Protocol](#), and in particular about [how to use this template](#), can be found on the [Project TIER website](#).

Citation



Tags

Project TIER

<https://osf.io/ybzx/>

Articles in this section

Create DOIs

Generate Citations

Create Custom
Citations

Tag Your Project

Tag Your Registration

Create DOIs



Sara Bowman

5 months ago

Follow

In addition to its own unique, persistent URLs, OSF offers DOIs for your public research. This help guide will walk you through how to generate DOIs for public projects and registrations.

DOIs point to the current version of the project or registration. OSF does not support DOI versioning at this time.

Articles in this section

Create DOIs

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Create DOIs



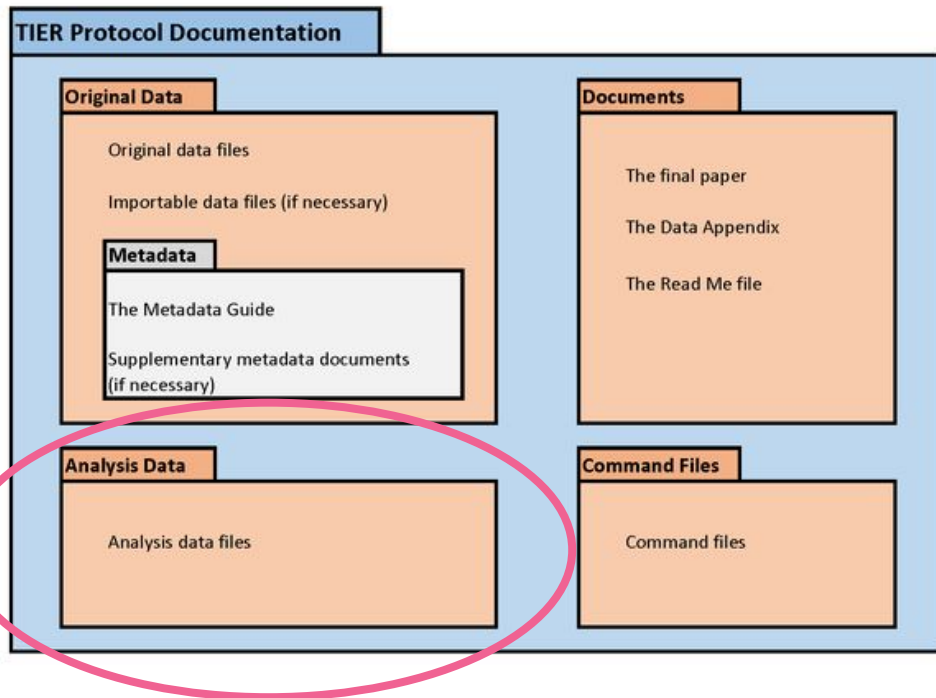
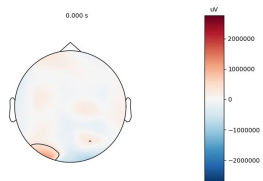
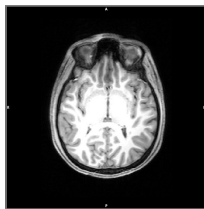
Sara Bowman

5 months ago

Follow

In addition to its own unique, persistent URLs, OSF offers DOIs for your public research. This help guide will walk you through how to generate DOIs for public projects and registrations.

DOIs point to the current version of the project or registration. OSF does not support DOI versioning at this time.



The TIER Specification



Brain

Imaging

Data

Structure



**Brain Imaging Data Structure
v1.2.0**

The BIDS Specification ▾

The BIDS Starter Kit

The Brain Imaging Data Structure

This site serves as an online resource to see the current state of the Brain Imaging Data Structure (BIDS) specification. It contains information about the core specification, as well as many modality-specific extensions.

To get started, [check out the introduction](#). If you'd like more information on how to adapt your own datasets to match the BIDS specification, we recommend exploring the [bids-specification starter kit](#).

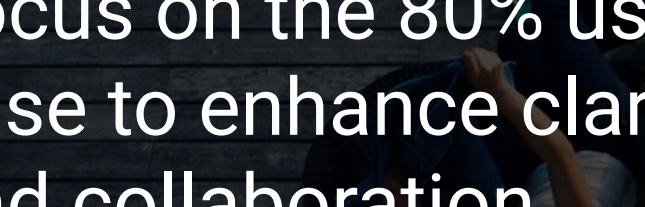


Example BIDS dataset layout

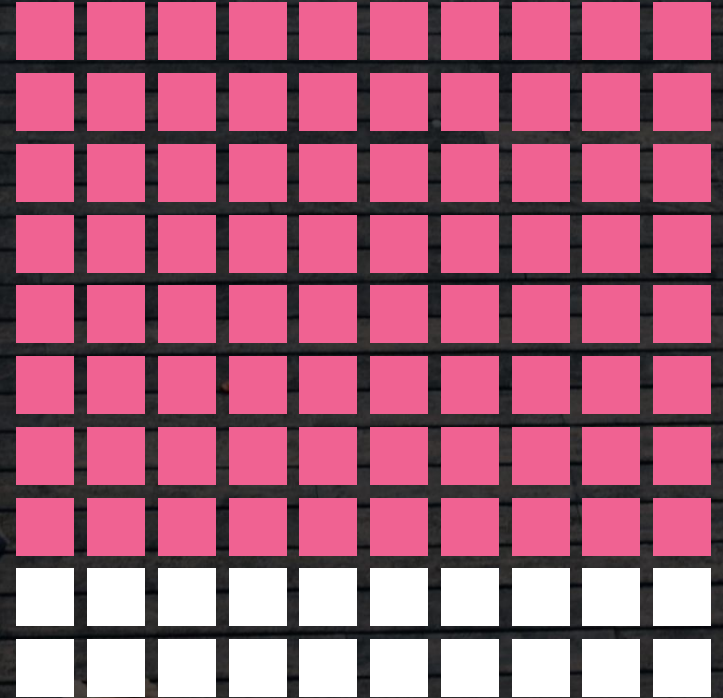
```
emdupre@ThinkPad-T480s: ~/Desktop/BIDS_dataset
File Edit View Search Terminal Help
emdupre@ThinkPad-T480s:~/Desktop/BIDS_dataset$ tree
.
├── CHANGES
├── dataset_description.json
├── participants.tsv
├── README
├── sub-01
│   └── ses-025
│       ├── dwi
│       │   ├── sub-01_ses-025_run-001_dwi.bval
│       │   ├── sub-01_ses-025_run-001_dwi.bvec
│       │   ├── sub-01_ses-025_run-001_dwi.json
│       │   ├── sub-01_ses-025_run-001_dwi.nii.gz
│       │   ├── sub-01_ses-025_run-002_dwi.bval
│       │   ├── sub-01_ses-025_run-002_dwi.bvec
│       │   ├── sub-01_ses-025_run-002_dwi.json
│       │   └── sub-01_ses-025_run-002_dwi.nii.gz
│       ├── fmap
│       │   ├── sub-01_ses-025_magnitude1.json
│       │   ├── sub-01_ses-025_magnitude1.nii.gz
│       │   ├── sub-01_ses-025_magnitude2.json
│       │   ├── sub-01_ses-025_magnitude2.nii.gz
│       │   ├── sub-01_ses-025_phasediff.json
│       │   └── sub-01_ses-025_phasediff.nii.gz
│       ├── func
│       │   ├── sub-01_ses-025_task-rest_run-001_bold.json
│       │   ├── sub-01_ses-025_task-rest_run-001_bold.nii.gz
│       │   ├── sub-01_ses-025_task-rest_run-001_events.tsv
│       │   ├── sub-01_ses-025_task-rest_run-001_sbref.json
│       │   └── sub-01_ses-025_task-rest_run-001_sbref.nii.gz
│       └── sub-01_ses-025_scans.tsv
└── task-rest_bold.json

5 directories, 25 files
emdupre@ThinkPad-T480s:~/Desktop/BIDS_dataset$
```

Focus on the 80% use case to enhance clarity and collaboration



Focus on the 80% use case to enhance clarity and collaboration



<> Code

🔔 Issues 47

🔗 Pull requests 8

📁 Projects 2

📖 Wiki

📊 Insights

Filters ▾

🔍 is:issue is:open

🏷 Labels 24

📅 Milestones 0

New issue



🔔 47 Open ✓ 46 Closed

Author ▾

Labels ▾

Projects ▾

Milestones ▾

Assignee ▾

Sort ▾



🔔 [ENH] Update task and continuous recording metadata for EEG/MEG/iEEG EEG MEG iEEG

#209 opened 7 days ago by effigies



🔔 Proposal: BEP PRs should come from branches on the main repository community

#203 opened 13 days ago by effigies

💬 4



🔔 BEP Template community

#201 opened 15 days ago by effigies

💬 1



🔔 [FIX] Improvements to the "entity table" good first issue help wanted

#200 opened 18 days ago by choldgraf



🔔 [Infra] Add dates to releases in Spec infrastructure

#199 opened 19 days ago by sappelhoff



🔔 [ENH] Proposal for multidimensional array file format

#197 opened 20 days ago by tyarkoni



🔔 MRI: new metadata tag "ElementSpatialSize" (and may be more) to facilitate access to .nii.gz header information

#196 opened 21 days ago by yarikoptic





You?

We need your expertise !
Join the [BIDS community](#)
[on GitHub](#)

Welcome to the BIDS Starter Kit



How to get started with the Brain Imaging Data Structure

A community-curated collection of tutorials, wikis, and templates to get you started with creating BIDS compliant datasets.

[BIDS Homepage](#) | [Wiki](#) | [Standard](#) | [Tutorials](#) | [Chat](#) | [Forum](#)

Click to view the intro video!



Select a [BIDS dataset](#) to validate

No directory selected.

Note: Selecting a dataset only performs validation. Files are never uploaded.

life



Summary

- 192 Files, 1GB
- 19 - Subjects
- 1 - Session

Available Tasks

- life

Available Modalities

- bold
- events
- T1w

Your dataset is not a valid BIDS dataset.

[view 4 errors in 164 files](#)

Error 1: [Code 55] JSON_SCHEMA_VALIDATION_ERROR

77 files

[Click here for more information about this issue](#)

Invalid JSON file. The file is not formatted according the schema.


[+ New Topic](#)

50+ results for **BIDS validator**

Sort by Relevance


BIDS Validator error: TR mismatch between NIFTI header and JSON file, and BIDS Validator is somehow finding TR=0. Best solution?

fmri bids

Jun '18 - ...a from ~700 participants. Importantly, you get NIFTIs, but not the raw DICOMs . I had to rework their file directory structure a bit to make it fully **BIDS**-compatible, but this is what I did (notably, each subject has JSON files in the same directory as the corresponding NIFTI files, but I didn't see a n...



Inconsistent errors with BIDS validator

bids bids-validator

Sep '18 - Hi All, I am trying to get a dataset to pass **BIDS** validation, but am running into a couple of errors regarding the stimuli folder that I can't seem to figure out. I am specifically understand why I d...

Advanced Search

Posted by

Categorized

All categories

Tagged

☐ All the above tags

Only return topics/posts...

☐ Matching in title only

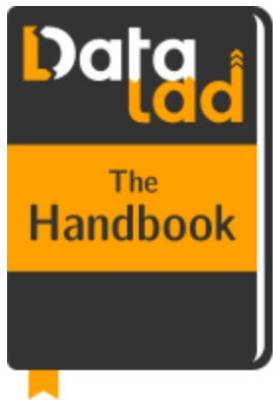
☐ I liked

☐ In my messages

☐ I read

any

Where topics



The DataLad handbook will supply you with everything you need to get started and break new grounds with DataLad.

The DataLad Handbook



Important:

Welcome to the DataLad handbook!

handbook.datalad.org

Checking in on Professor Smith



With thanks to [Chris Gorgolewski](#)



OpenNEURO

A free and open platform for sharing MRI,
MEG, EEG, iEEG, and ECoG data



[Sign in with Google](#)[Sign in with ORCID](#)

[Browse 219 Public Datasets](#)

OpenNeuro.org

Recent Activity

Most Active

	UCLA Consortium for Neuropsychiatric Phenomics LA5c Study
20,329	
	The Midnight Scan Club (MSC) dataset
19,376	
	Visual object recognition
10,341	
	Forrest Gump
9,449	
	Classification learning
8,599	

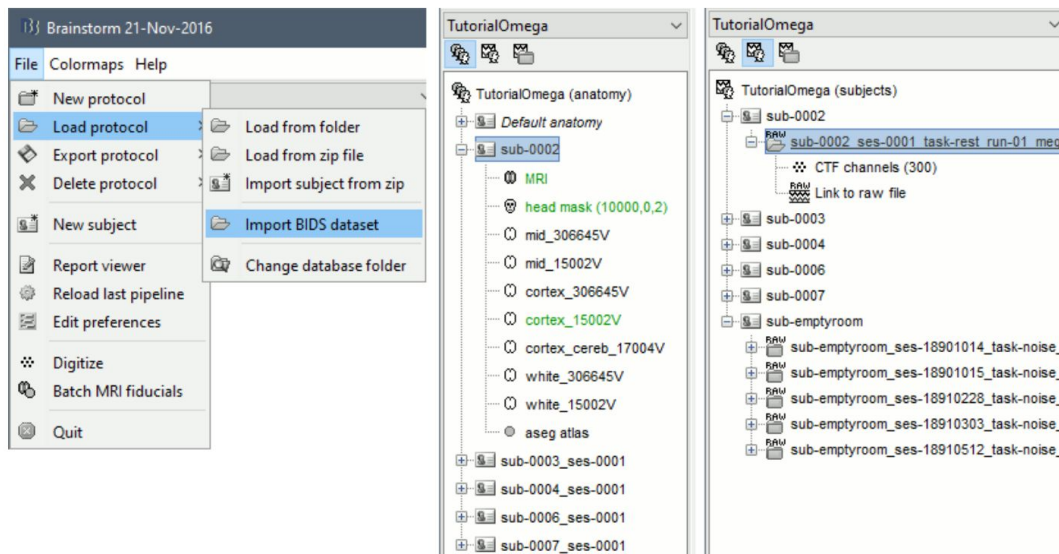
[View More...](#)

Recently Published

The Reading Brain Project L1 Adults	4 DAYS AGO
Parallel Adaptation of Symbols, Quantities, and Physical Size	10 DAYS AGO
A Probability Distribution over Latent Causes, in the Orbitofrontal Cortex	11 DAYS AGO
Spinal stimulation stepping and standing dataset	17 DAYS AGO
Handedness and Symbolic Number Representation	17 DAYS AGO

Recent activity on OpenNeuro.org

- Select the menu File > Load protocol > **Import BIDS dataset** > Select folder **OMEGA_RestingState_sample**.
- Keep the default values for all the questions that may be asked during the import process (eg. number of vertices in the cortex surfaces). Once done, you should be able to access the data for the 5 subjects in your database explorer: anatomy, and subject and noise recordings.





BIDS Apps

portable neuroimaging pipelines that understand BIDS datasets

[About](#)

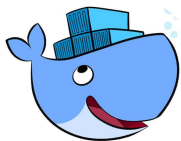
[Tutorials](#)

[Apps](#)

How it works

Containerization

Package your software to use in any computing environment.



Structured queries

Know that the provided data meets certain attributes.

```
{
  "name": "subject",
  "pattern": "{sub-\\d+}",
  "directory": "{(root)}/{subject}",
},
{
  "name": "session",
  "pattern": "{ses-\\d+}",
  "directory": "{(root)}/{subject}/{session}",
},
{
  "name": "run",
  "pattern": "{run-\\d+}"
},
{
  "name": "type",
  "pattern": "[^,;\\.\\?\\|\\." data-bbox="382 687 500 856"/>
```

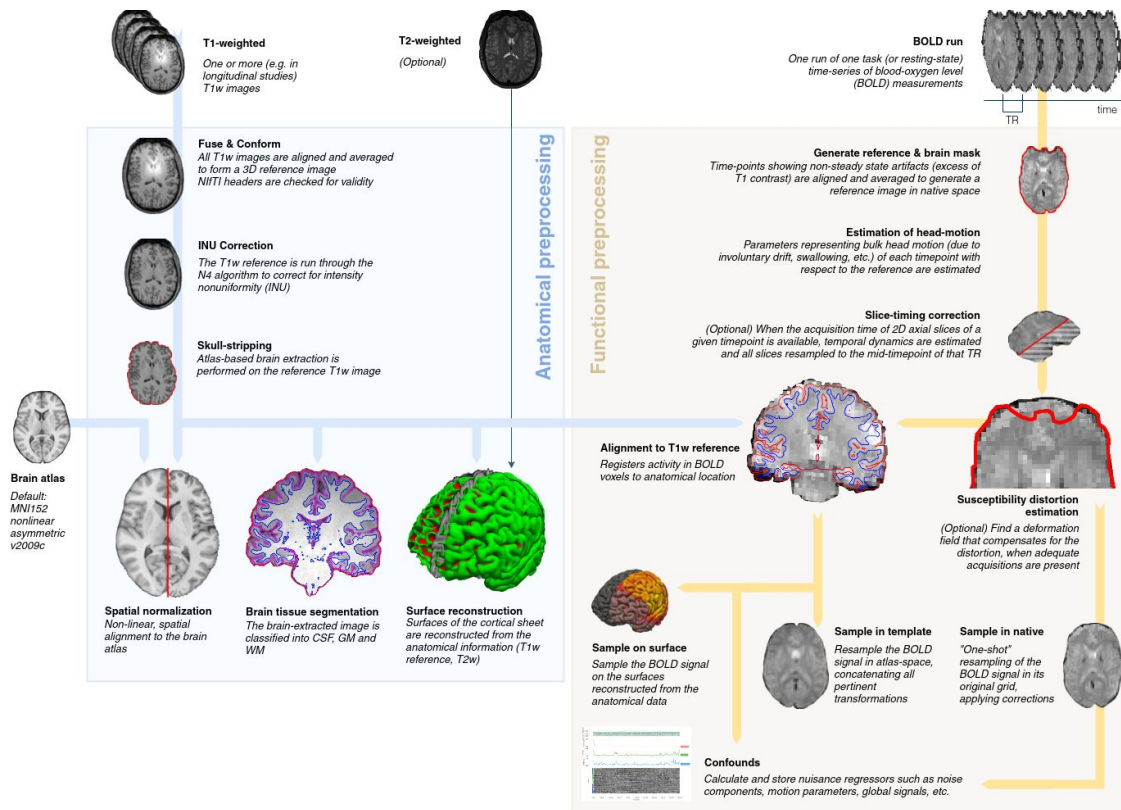
Analysis code

Currently 26 supported BIDS Apps. Wrap your own software with the example app.



THIS IS WHAT A PROGRAMMER
LOOKS LIKE.

One example: fMRIPrep



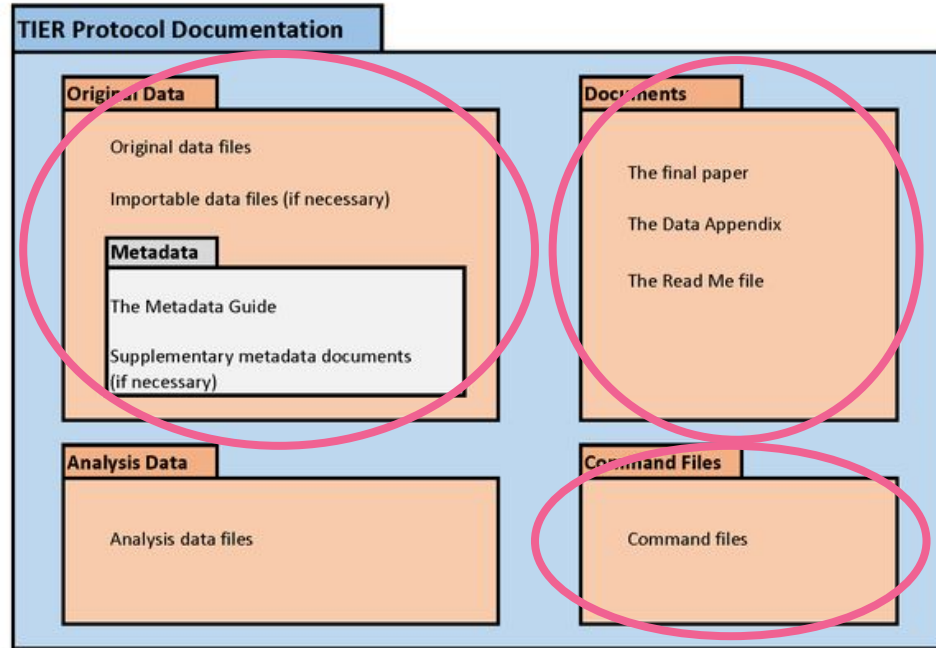
```
>> fmriprep \
    data/ out/ \
    participant \
    -w work/
```

Professor Smith (circa 2030)



With thanks to [Chris Gorgolewski](#)

ReproIn



RMarkdown,
Jupyter

Cookiecutter

The TIER Specification



Making Your Code Citable

🕒 10 minute read

[Digital Object Identifiers](#) (DOI) are the backbone of the academic reference and metrics system. If you're a researcher writing software, this guide will show you how to make the work you share on GitHub citable by archiving one of your GitHub repositories and assigning a DOI with the data archiving tool [Zenodo](#).

Intro

[Choosing Your Repo](#)

[Login to Zenodo](#)

[Check Repo Settings](#)

Zenodo GitHub integration

Acknowledgements

- Stefan Appelhoff 📖💬😞💡🖥️👁️⚠️📢
- Tibor Auer 💬📖💡🔧📢
- Sylvain Baillet 📖🔍
- Elizabeth Bock 📖💡
- Eric Bridgeford 📖🔧
- Teon L. Brooks 📖🖥️⚠️💬👁️😞🔧💡📢
- Suyash Bhogawar 📖💡⚠️🔧💬
- Vince D. Calhoun 📖
- Alexander L. Cohen 📖🖥️💬
- R. Cameron Craddock 📖📢
- Samir Das 📖
- Alejandro de la Vega 📖🖥️⚠️
- Arnaud Delorme 📖💡
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- Franklin W. Feingold 📖🔍📝✓
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- Katja Heuer 📖🔧
- Chris Holdgraf 📖😞
- Jean-Christophe Houde 📖
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- Mainak Jas 📖🖥️
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- Laura and John Arnold Foundation 📖📖
- Xiangrui Li 📖🖥️

Acknowledgements

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- Zachary Michael 📖

- Ezequiel Mikulan 📖💻

- Michael P. Milham 💡🔍

- Henk Mutsaerts 📖

- National Institute of Mental Health 🇺🇸🇬🇧

- B. Nolan Nichols 📖

- Thomas E. Nichols 📖🔊🔧

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- Robert Oostenveld 📖🔧🔊💡✔️⚠️😞

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- Gaël Varoquaux 📖

- Tal Yarkoni 💻📖😞🔍🔌👁️🔊🐛🎨

A vertical stack of several old, thick books with worn spines, positioned on the left side of the slide. The books are slightly out of focus, with the top ones being more visible than the bottom ones.

Take-home ideas

- **Project management** is for everyone
- **Community-driven standards** enable new kinds of science



[@emdupre](https://twitter.com/emdupre)

An outline for this morning

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- A practical introduction to pyBIDS
- Authoring for collaboration
- A practical introduction to Jupyter Notebooks and JupyterLab



An outline for this morning

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Jupyter

*Authoring the next generation
article*

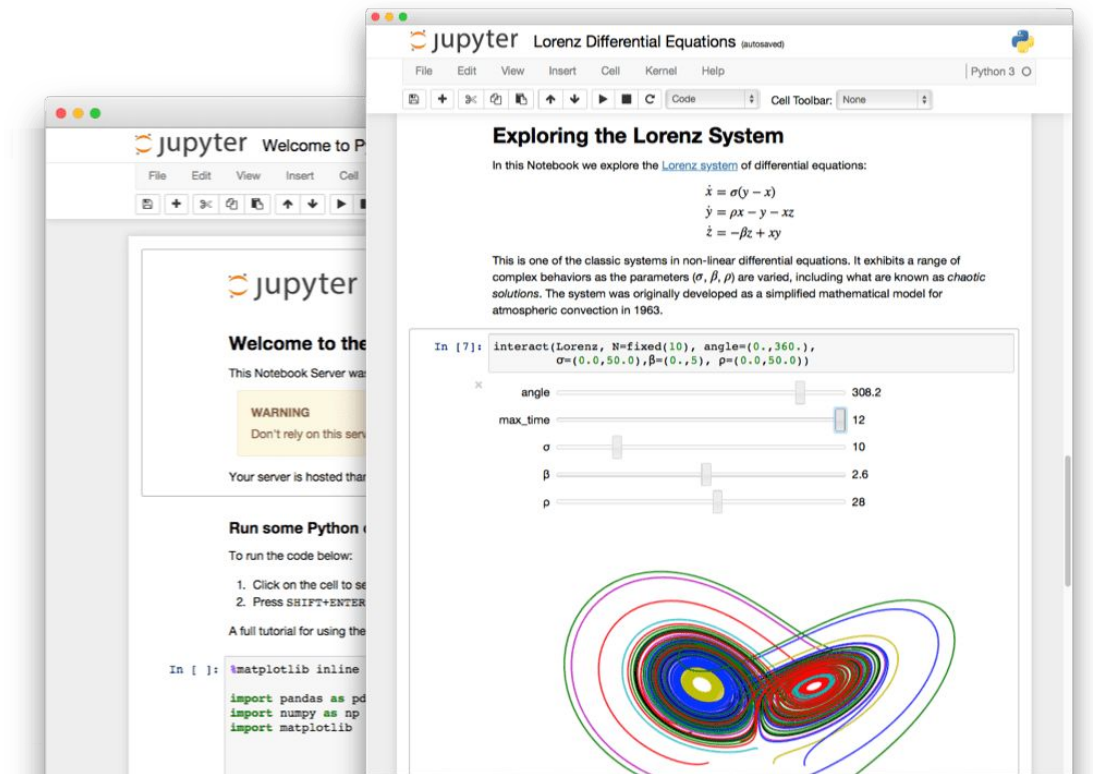


An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the **complete software development environment** and the **complete set of instructions** which generated the figures.

-- Buckheit and Donoho
WaveLab and Reproducible Research, 1995



For example: the Jupyter Notebook





a *community* of people and an *ecosystem* of open tools and standards for interactive computing

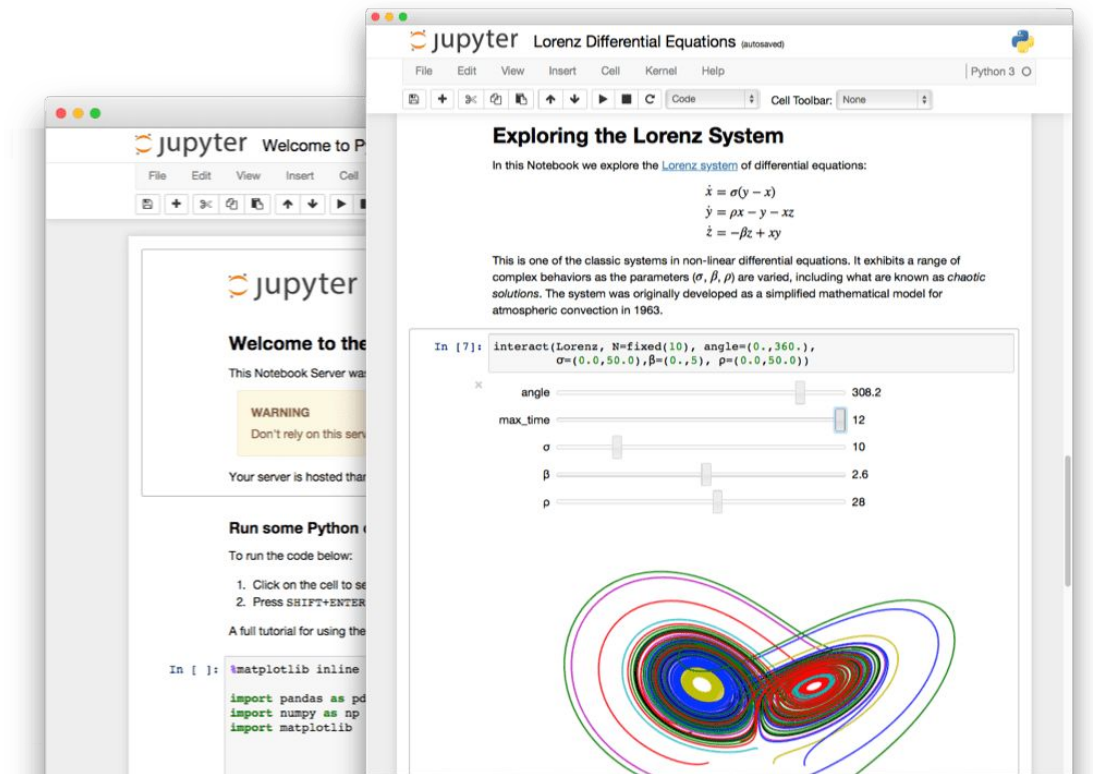
With thanks to [Chris Holdgraf](#)



create things that are **language-agnostic** and **modular**.
Empower people to use **other open tools**.

With thanks to [Chris Holdgraf](#)

For example: the Jupyter Notebook



complete set of instructions

open-source languages are the raw material



python™



complete set of instructions

capture the steps

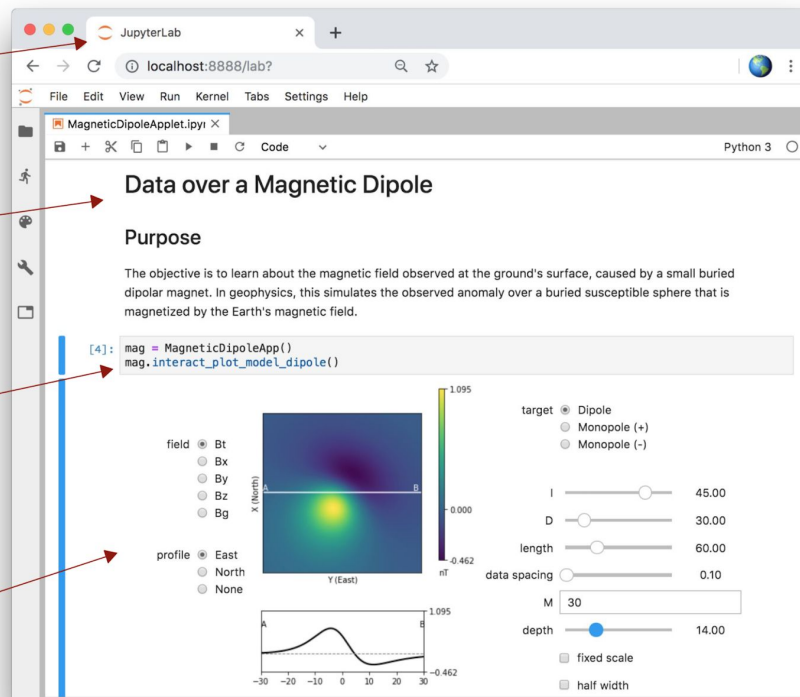


Runs in web browser

Text, comments, equations

Lines of code
(Python, Julia, R, Matlab, ...)

Output: values, images, plots,
tables, interactive widgets



complete set of instructions

maintenance and sharing



- version control
- issue tracking
- licensing
- integrations with
 - testing services
 - documentation hosting
 - ...

What can we do with it ?

- Interleave explanatory text, code, and generated figures
- Add in additional kernels
- Create outputs in a variety of formats (HTML, PDF, Markdown)



Magic !

- `%matplotlib`
- `%timeit`
- `%load`
- `%history`



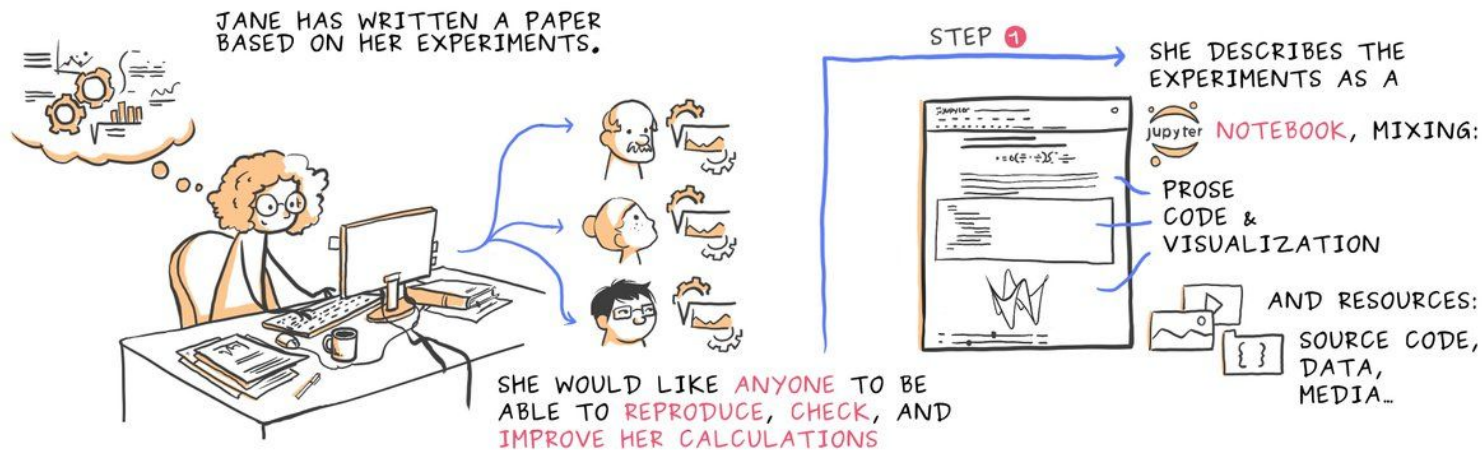


Here's one workflow for
collaborative authoring



With thanks to Chris Holdgraf





With thanks to [Chris Holdgraf](#)



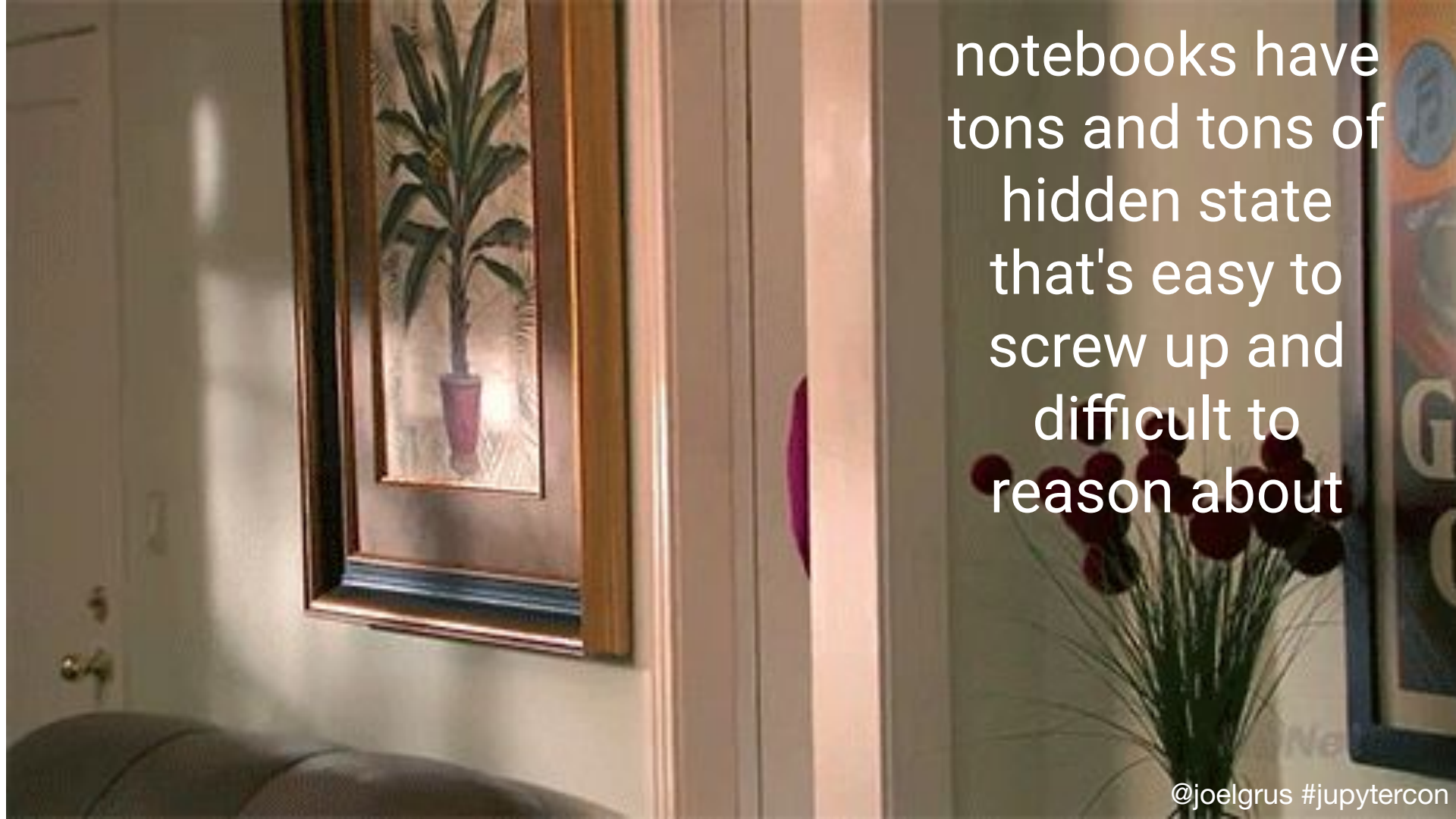
I Don't Like Notebooks



Joel Grus (@joelgrus)

#JupyterCon 2018

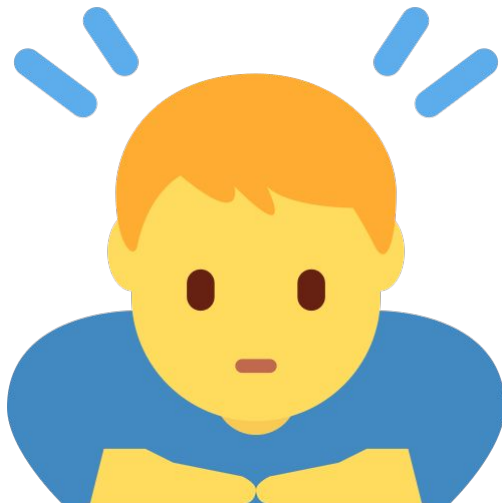
(audience booing)

A photograph of a hallway. On the left wall, there is a framed painting of a plant in a pot. In the foreground on the right, there is a vase with red flowers. The text is overlaid on the right side of the image.

notebooks have
tons and tons of
hidden state
that's easy to
screw up and
difficult to
reason about

We can respect statefulness

- `Kernel restart and run-all`
- Think about using tools beyond just the Notebook



JupyterLab

The next generation Jupyter interface



`jupyterlab.readthedocs.io`

A complete software development environment

File Edit View Run Kernel Tabs Settings Help

Files

- + notebooks
- home > notebooks
- Name Last Modified
- Data.ipynb an hour ago
- Fasta.ipynb a day ago
- Julia.ipynb a day ago
- Lorenz.ipynb seconds ago**
- R.ipynb a day ago
- iris.csv a day ago
- lightning.json 9 days ago
- lorenz.py 3 minutes ago

Running

Commands

Cell Tools

Output View

sigma 10.00

beta 2.67

rho 28.00

lorenz.py

In this Notebook we explore the Lorenz system of differential equations:

$$\begin{aligned}\dot{x} &= \sigma(y - x) \\ \dot{y} &= \rho x - y - xz \\ \dot{z} &= -\beta z + xy\end{aligned}$$

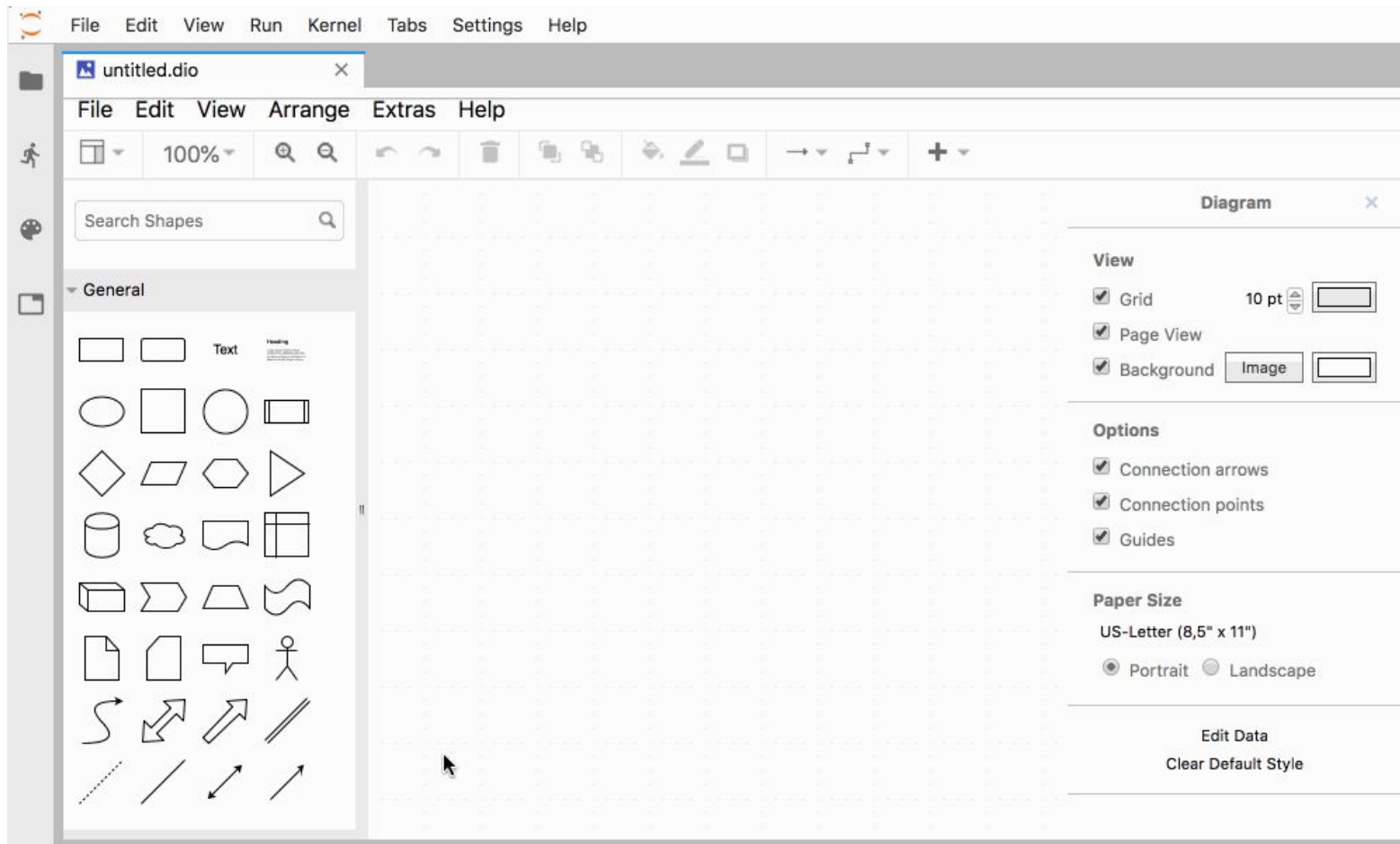
Let's call the function once to view the solutions. For this set of parameters, we see the trajectories swirling around two points, called attractors.

```
In [4]: from lorenz import solve_lorenz
t, x_t = solve_lorenz(N=10)
```

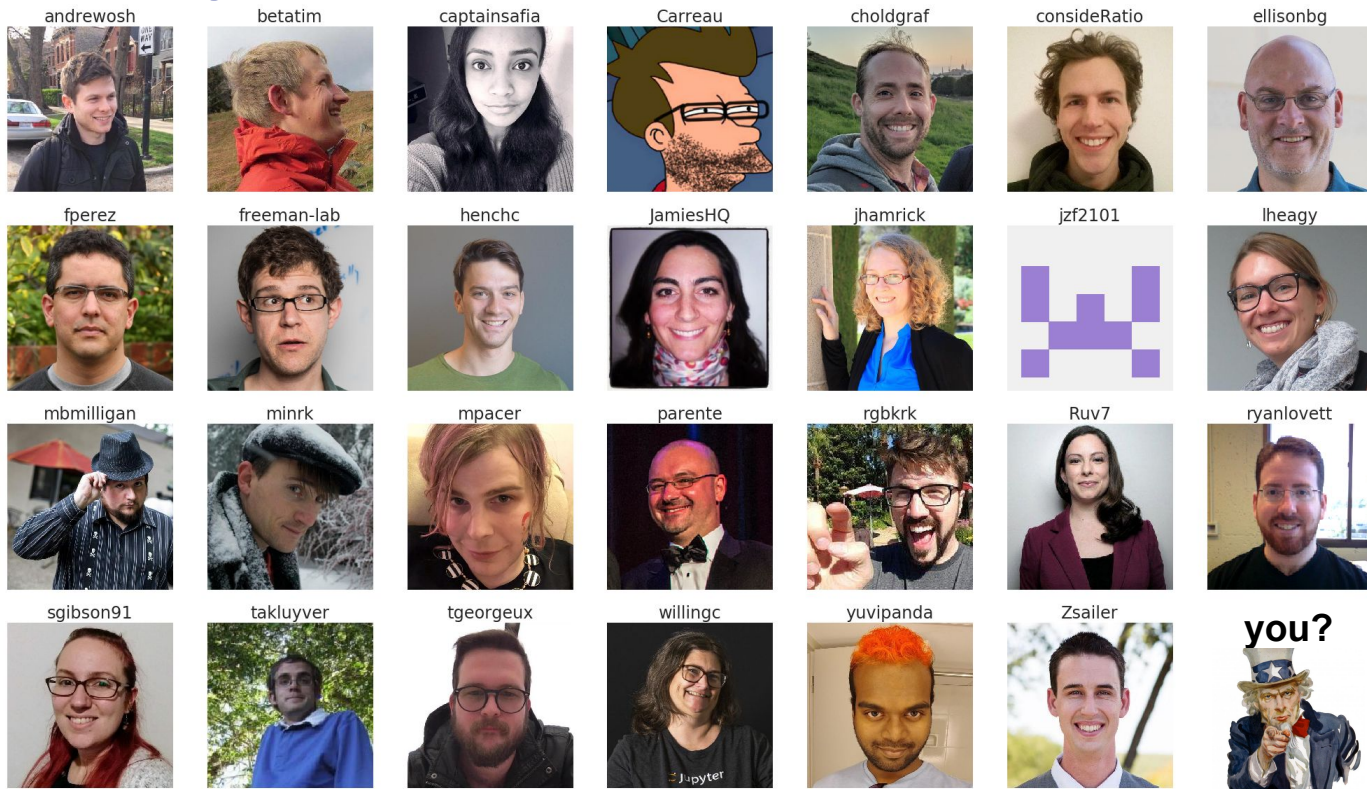
9 def solve_lorenz(N=10, max_time=4.0, sigma=10.0, beta=8./3, rho=28.0):
10 """Plot a solution to the Lorenz differential equations."""
11 fig = plt.figure()
12 ax = fig.add_axes([0, 0, 1, 1], projection='3d')
13 ax.axis('off')
14
15 # prepare the axes limits
16 ax.set_xlim((-25, 25))
17 ax.set_ylim((-35, 35))
18 ax.set_zlim((5, 55))
19
20 def lorenz_deriv(x_y_z, t0, sigma=sigma, beta=beta, rho=rho):
21 """Compute the time-derivative of a Lorenz system."""
22 x, y, z = x_y_z
23 return [sigma * (y - x), x * (rho - z) - y, x * y - beta * z]
24
25 # Choose random starting points, uniformly distributed from -15 to 15
26 np.random.seed(1)
27 x0 = -15 + 30 * np.random.random((N, 3))
28

JupyterLab Extensions





Acknowledgements



With thanks to Chris Holdgraf

A vertical stack of several books, mostly with light-colored spines, some showing signs of wear. The books are stacked on a dark surface.

Take-home ideas

- There's a whole galaxy **beyond the PDF**, and Jupyter can help us get there



[@emdupre](#)

An outline for this morning

- Community-based project management
- A practical introduction to pyBIDS
- Authoring for collaboration
- A practical introduction to Jupyter Notebooks and JupyterLab

