

## Reproducible Computational Environments with Binder Sarah Gibson She/her she/her





#### Hello, 👋 My name is Sarah Gibson

I'm an **open source infrastructure engineer** at 2i2c.

My research background is Astrophysics

I am a JupyterHub team member and support the infrastructure that powers mybinder.org

I am also a core team member of *The Turing*Way and hold a fellowship from the Software Sustainability Institute, advocating for best software practices in research



Irreproducible research wastes time!





#### What does Reproducibility mean?

		Data			
		Same	Different		
ysis	Same	Reproducible	Replicable		
Analysis	Different	Robust	Generalisable		

Kirstie Whitaker's talk at PyData LDN: https://youtu.be/IG3PcZ6EhiU https://the-turing-way.netlify.app/reproducible-research/overview/overview-definitions



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#### Academic errors have real world effects

0	В	С		J	K	L	M
2	1.20	100000		Real GD	P growth		
3	0.17			Debt	/GDP		
4	Country	Coverage	30 or less	30 to 60	60 to 90	90 or above 3	0 or less
26			3.7	3.0	3.5	1.7	5.5
27	Minimum		1.6	0.3	1.3	-1.8	0.8
28	Maximum		5.4	4.9	10.2	3.6	13.3
29			7				
30	US	1946-2009	n.a.	3.4	3.3	-2.0	n.a.
31	UK	1946-2009	n.a.	2.4	2.5	2.4	n.a.
32	Sweden	1946-2009	3.6	2.9	2.7	n.a.	6.3
33	Spain	1946-2009	1.5	3.4	4.2	n.a.	9.9
34	Portugal	1952-2009	4.8	2.5	0.3	n.a.	7.9
35	New Zealand	1948-2009	2.5	2.9	3.9	-7.9	2.6
36	Netherlands	1956-2009	4.1	2.7	1.1	n.a.	6.4
37	Norway	1947-2009	3.4	5.1	n.a.	n.a.	5.4
38	Japan	1946-2009	7.0	4.0	1.0	0.7	7.0
39	Italy	1951-2009	5.4	2.1	1.8	1.0	5.6
40	Ireland	1948-2009	4.4	4.5	4.0	2.4	2.9
41	Greece	1970-2009	4.0	0.3	2.7	2.9	13.3
42	Germany	1946-2009	3.9	0.9	n.a.	n.a.	3.2
43	France	1949-2009	4.9	2.7	3.0	n.a.	5.2
44	Finland	1946-2009	3.8	2.4	5.5	n.a.	7.0
45	Denmark	1950-2009	3.5	1.7	2.4	n.a.	5.6
46	Canada	1951-2009	1.9	3.6	4.1	n.a.	2.2
47	Belgium	1947-2009	n.a.	4.2	3.1	2.6	n.a.
48	Austria	1948-2009	5.2	3.3	-3.8	n.a.	5.7
49	Australia	1951-2009	3.2	4.9	4.0	n.a.	5.9
50							-0.770
51			4.1	2.8	2.8	=AVERAGE	(L30:L44

https://statmodeling.stat.columbia.edu/2013/04/16/memo-to-reinhart-a nd-rogoff-i-think-its-best-to-admit-your-errors-and-go-on-from-there https://www.bbc.co.uk/news/magazine-22223190



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**Humans** are the hardest part of reproducibility





Is not considered for promotion

Held to higher standards than others

Publication bias towards novel findings

Requires additional skills

# Barriers to reproducible research

Plead the 5th

Support additional users

Takes time



What actually goes into reproducible research?





- Version control
  - Snapshots in time



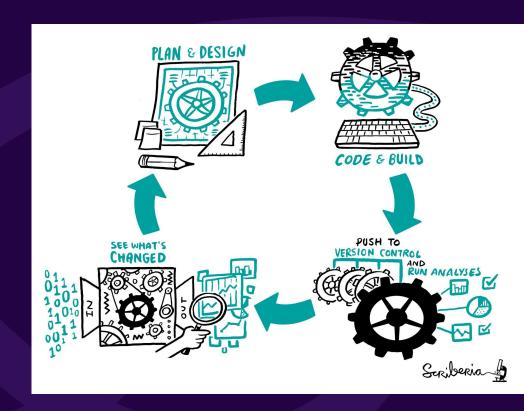


- Version control
  - Snapshots in time
- Testing
  - What's changed?



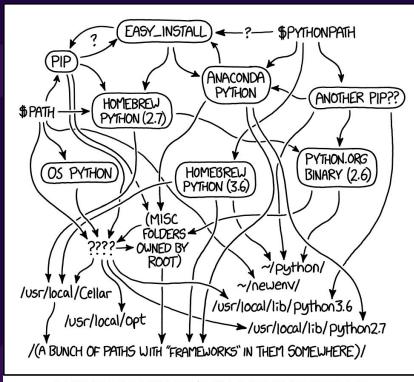


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  - Automatically test each change as you make it
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- Version control
  - Snapshots in time
- Testing
  - O What's changed?
- Continuous Integration
  - Automatically test each change as you make it
  - Be explicit about what's changed!
- Software environment management



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

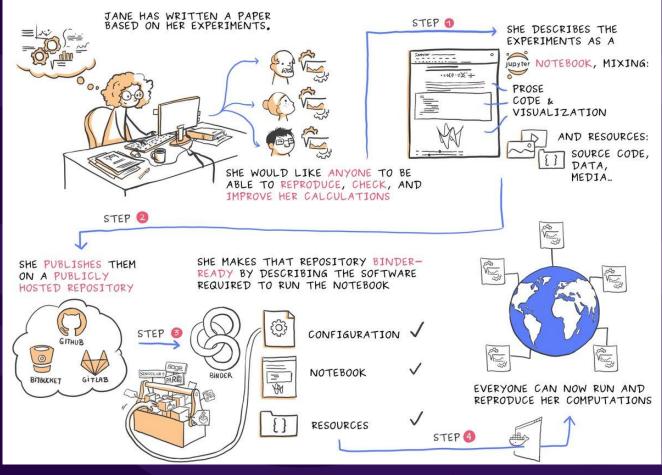


#### **Project Binder**

provides a computational environment without the toil of installing packages

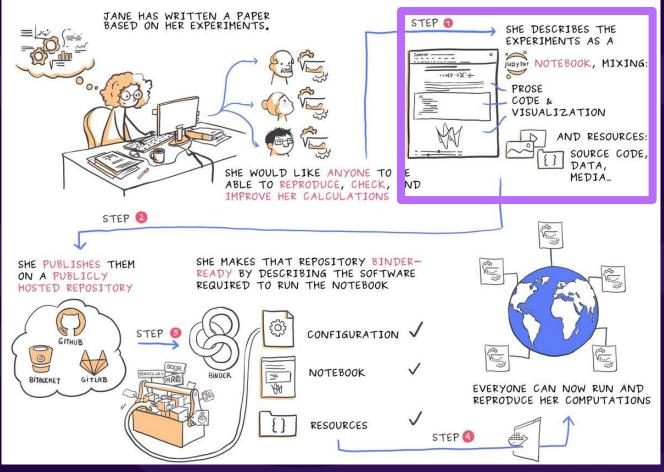






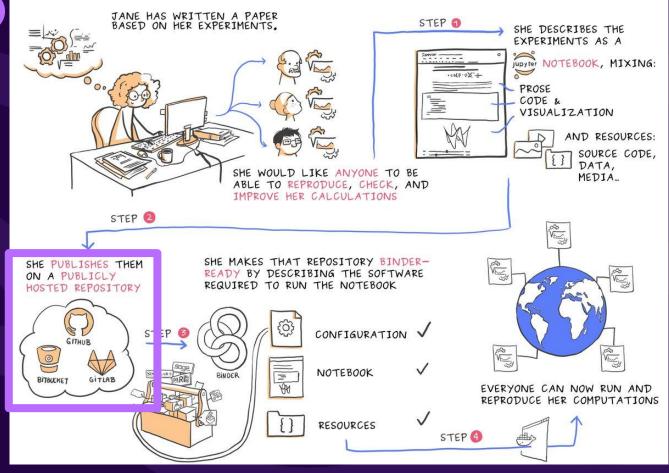






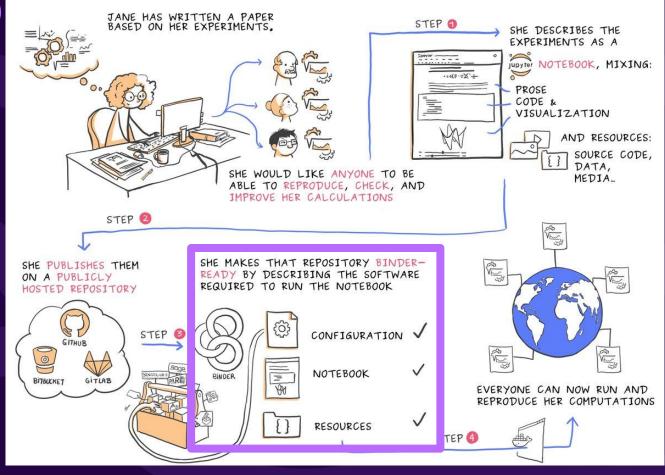




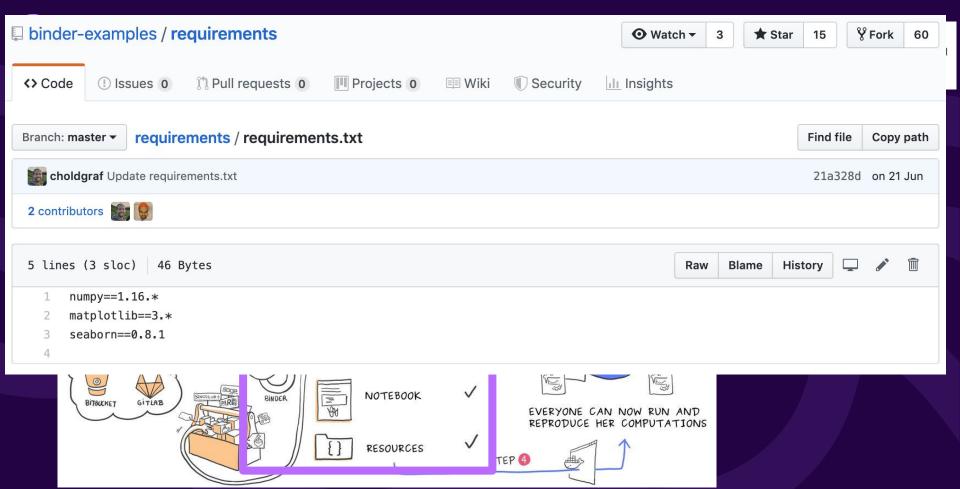








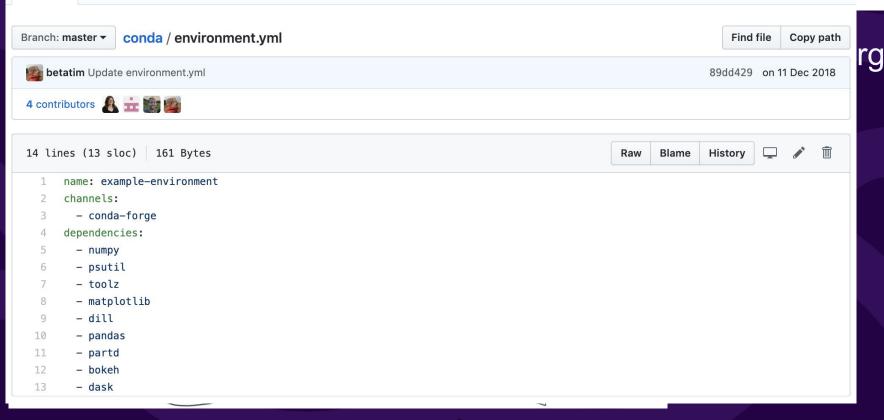




II Insights

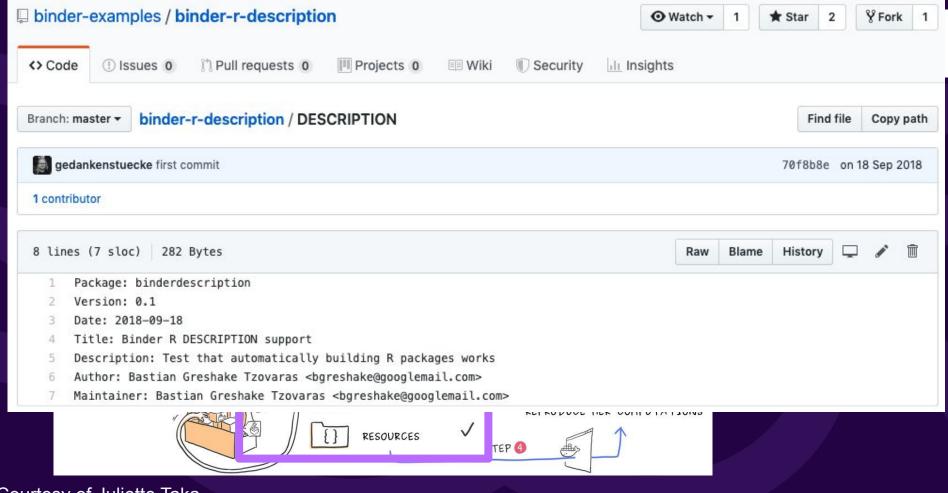
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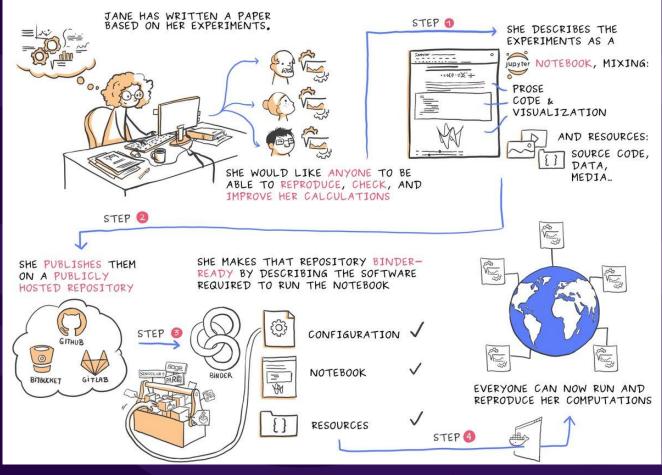
Security



Courtesy of Juliette Taka https://twitter.com/mybinderteam/status/1082556317842264064

doi.org/10.5281/zenodo.10075621



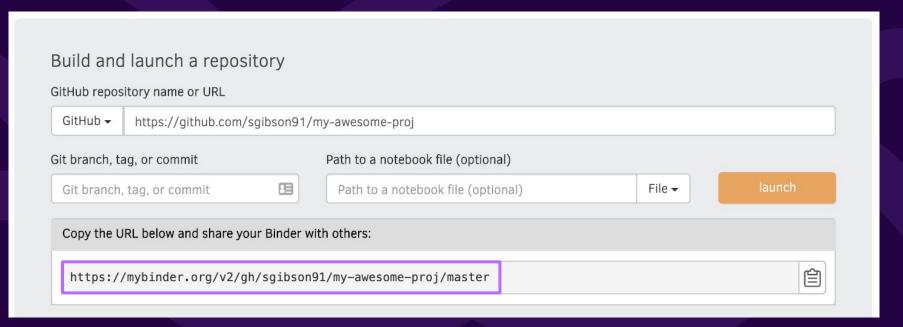






#### Accessing an environment via a URL

- Entire information of the project is encoded in the URL
- Easily accessible, easily shareable





#### **Kirstie Whitaker**

"I like to use Binder when working with my students and collaborators because I can very easily check the analysis on my phone! While feeling fun, Binder also requires version control, the computational environment and a new build for each change.

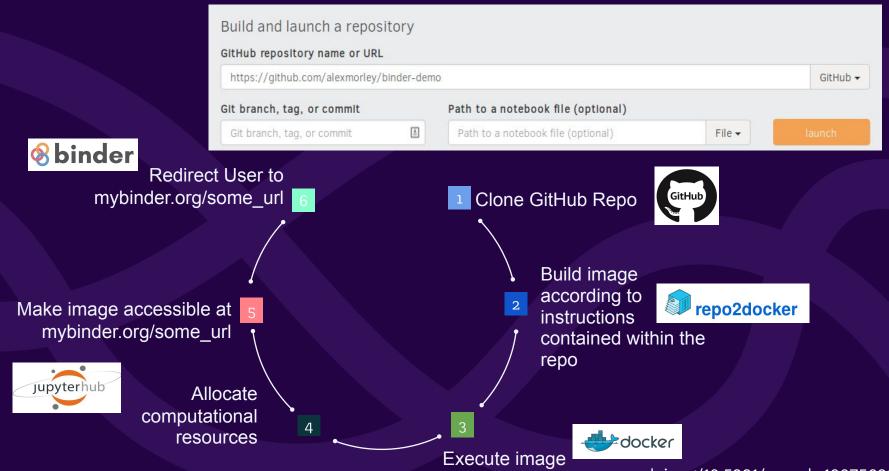
Binder makes it much easier to share responsibility with busy PIs."



https://www.turing.ac.uk/people/researchers/kirstie-whitaker



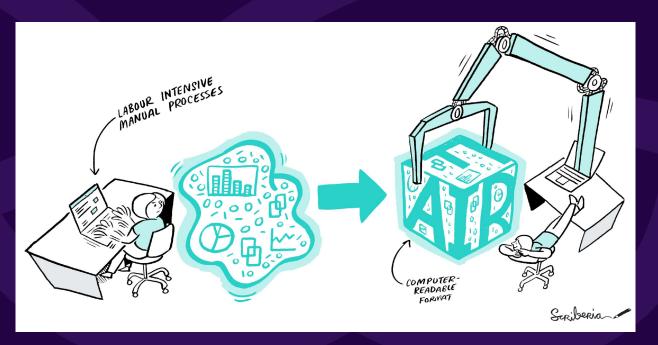
#### **BinderHub**





#### **Containerisation tends towards Portability**

- Modern datasets are big! Need to take the software to the data
- Need to develop the analysis in the current environment
- Move software stacks between systems without costly setup time
- Reduce toil of one-off setups: events, trainings, workshops, etc





#### What next?





- Whether it's HPC centres or cloud datacentres they're all just someone else's computers
- Need to port software stacks across systems
- How can concepts from Binder's API or repo2<container>
   be integrated into HPC operations to assist this?
  - Reducing toil for one-time setups
  - Facilitating ease-of-access to the development environment with all the expected tooling



### Thank You

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