

Scientific Computing – Best Practices

Software Engineering principles to improve your HPC

Fernando Garzon, August 2025

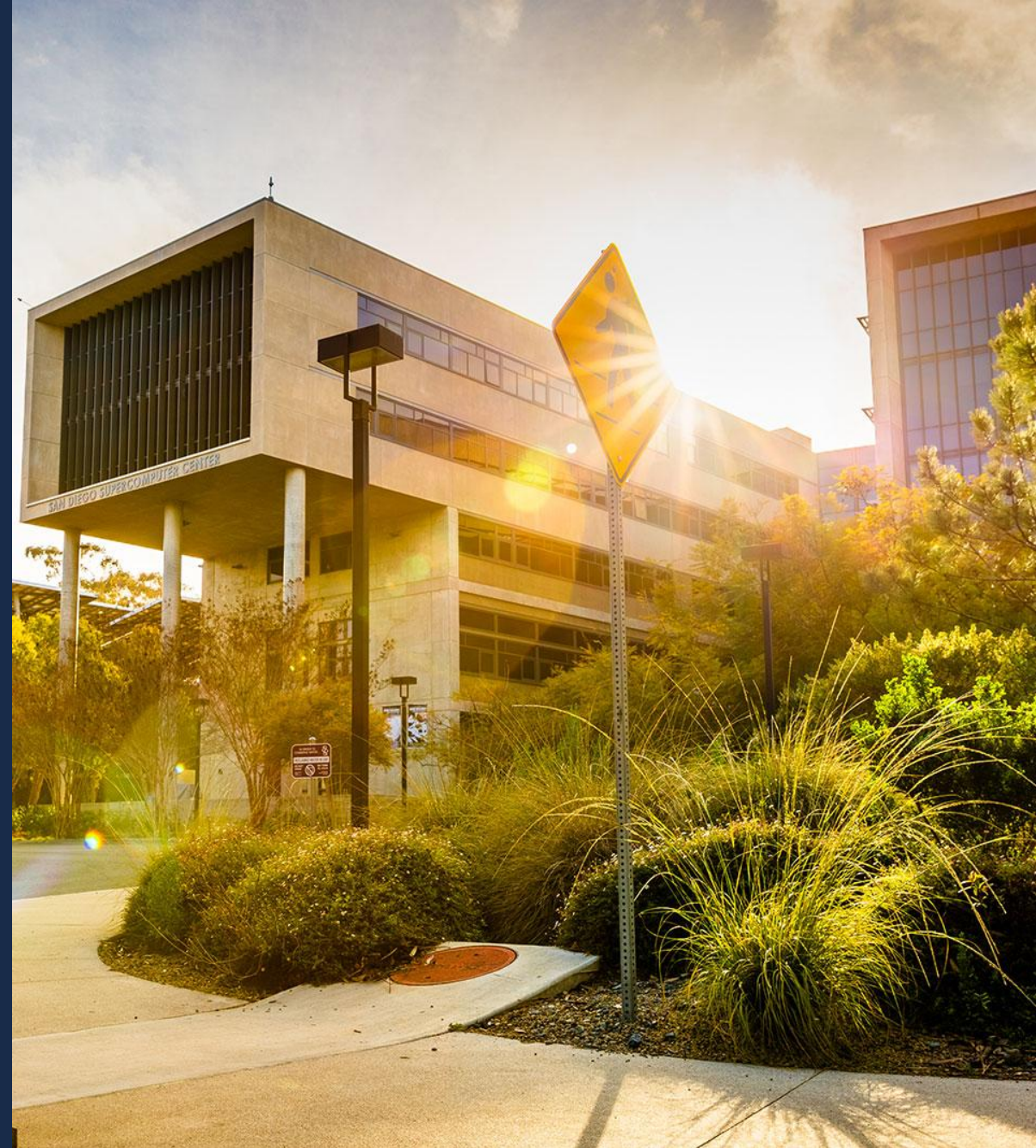
[linkedin.com/in/fgarzonm](https://www.linkedin.com/in/fgarzonm) - github.com/ofgarzon2662

SDSC
SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego

Who's Fernando Garzon

- Software Engineer
- Computational & Data Scientist Research Specialist at SDSC
- Work on User Support for TSCC.
- Also work in Software Dev (SWD) projects within SDSC.
- Passionate about SWD, DevOps, Automation, Cloud Architecture, IaC and more.
- Automation Enthusiast.

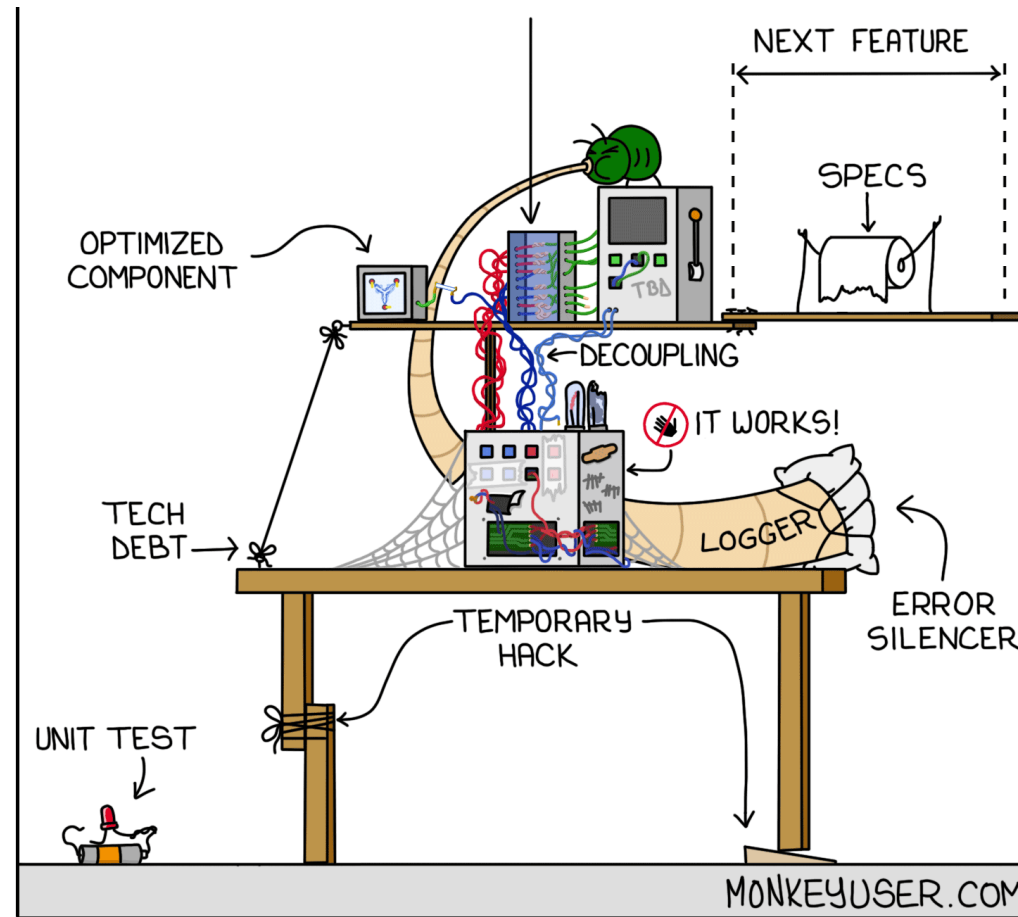




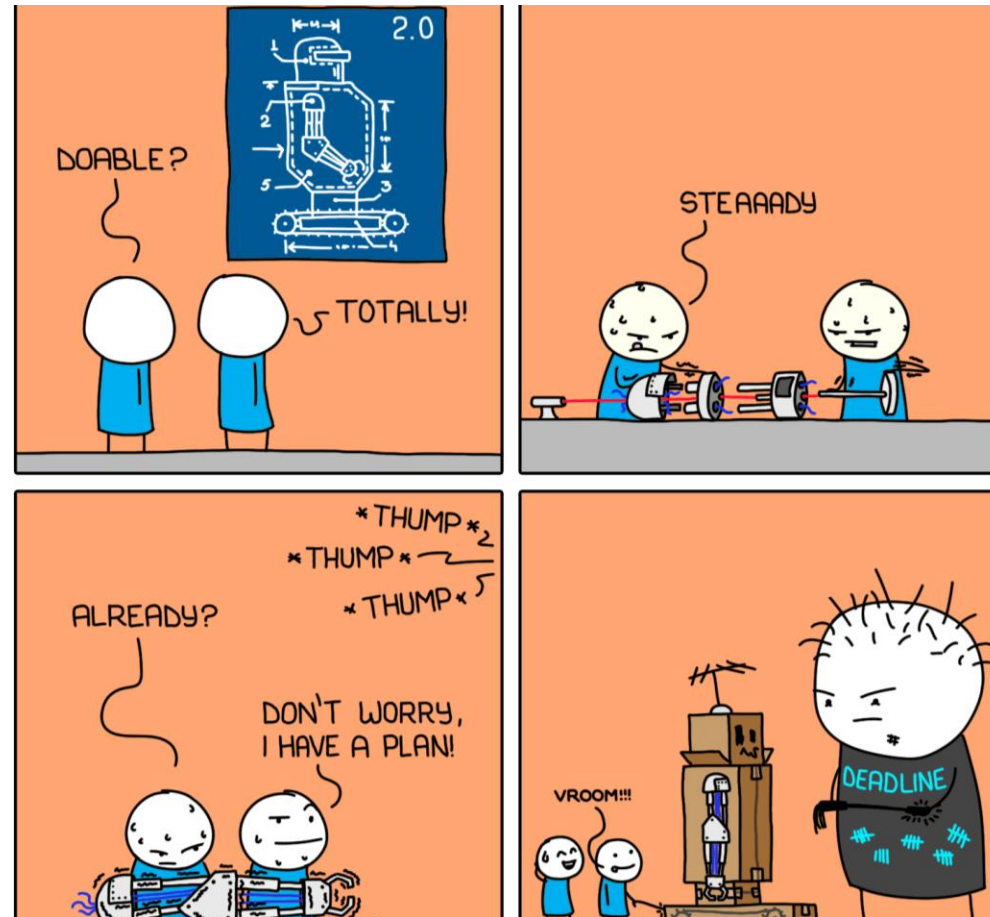
Outline

1. Intro: The un-reproducibility horror
2. Notebooks Don't Scale. Packages Do.
3. Let's Prod this.
4. Lights, Camera, GitHub Actions!
5. MLOps – Turning your Notebook into a Money-Printing Machine.
6. Final remarks

Intro: The un-reproducibility horror

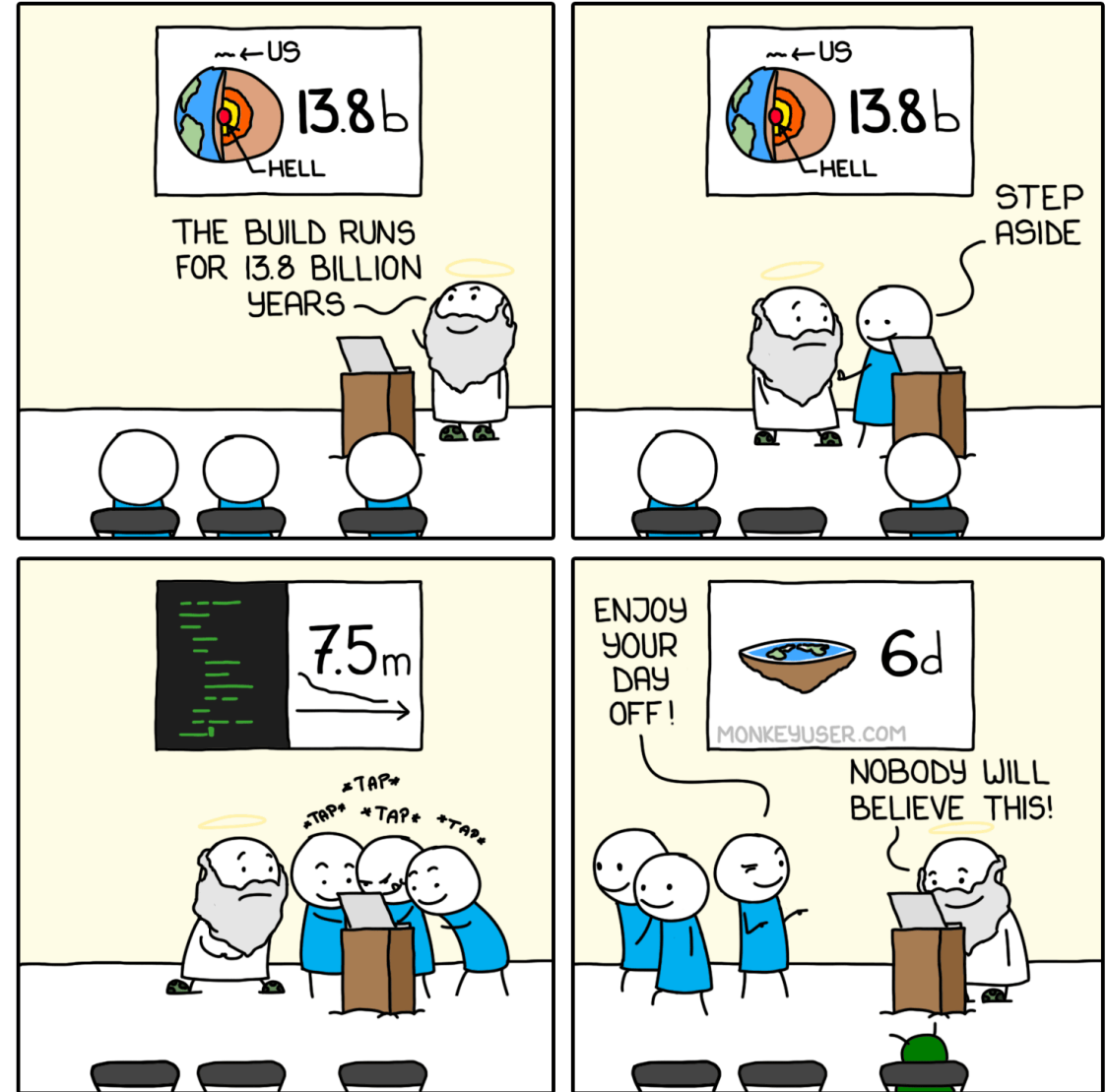


Notebooks Don't Scale. Packages Do.



Let's Prod this

NEW WORLD



Lights, Camera, GitHub Actions!

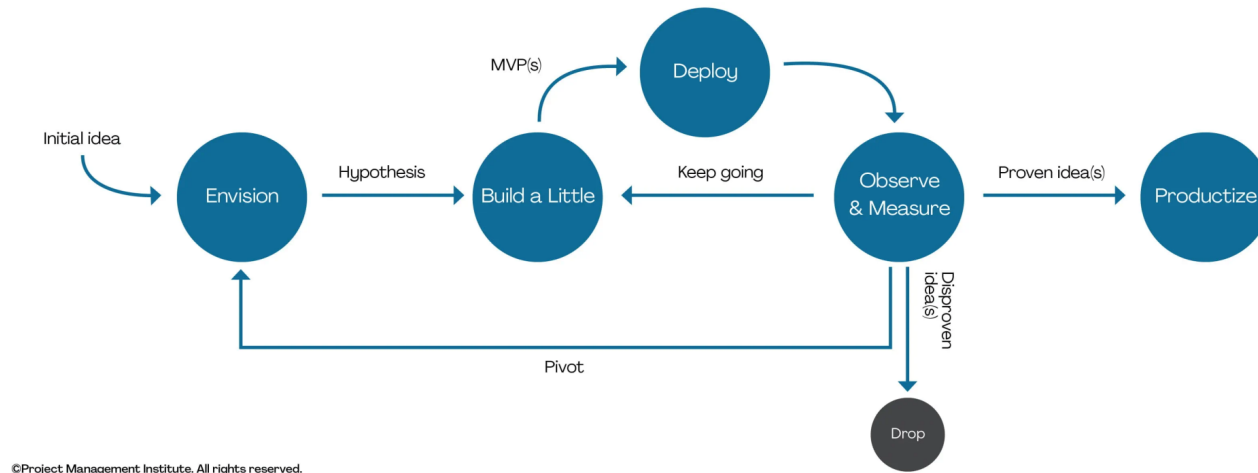
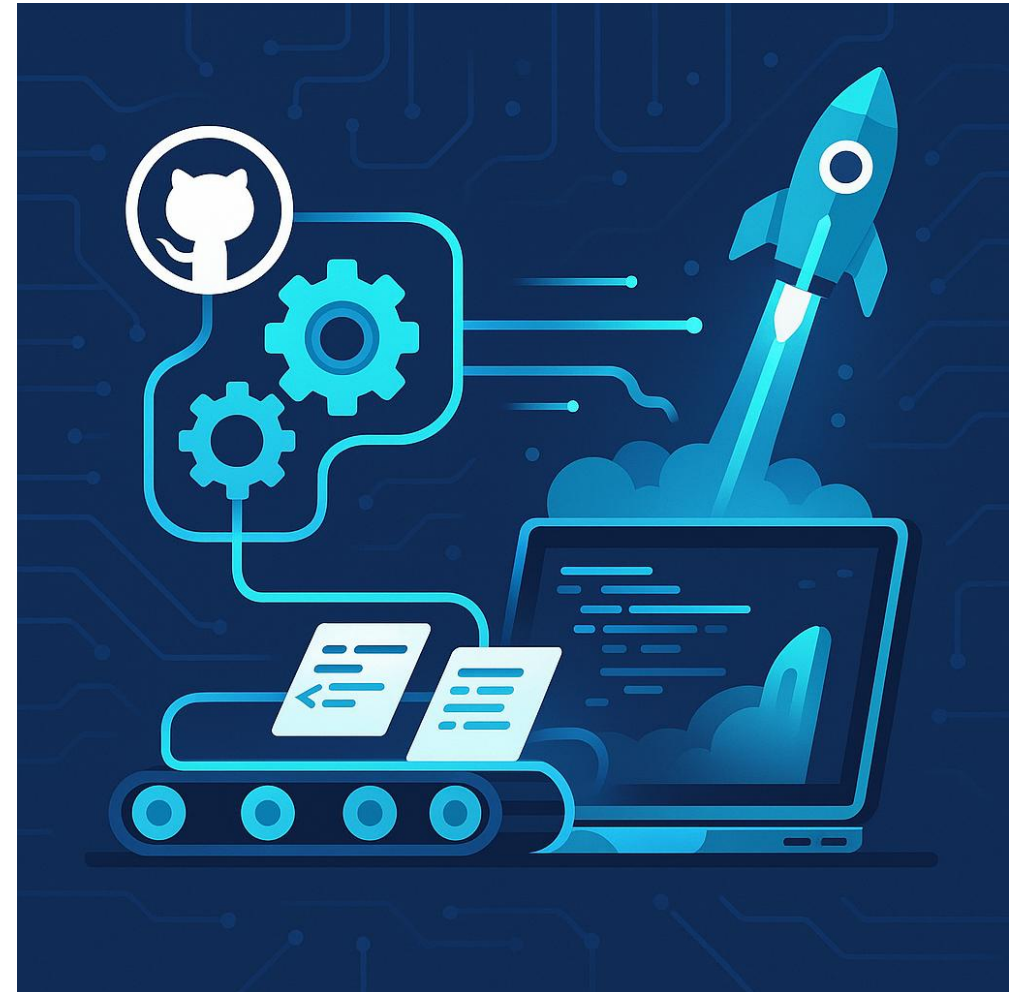
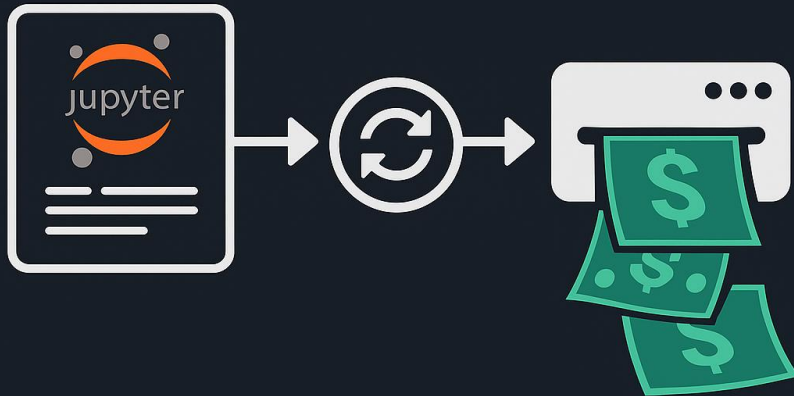


Image reference: <https://www.pmi.org/disciplined-agile/lifecycle/exploratory-lifecycle>



MLOps: Turning your Notebook into a Money-Printing Machine.

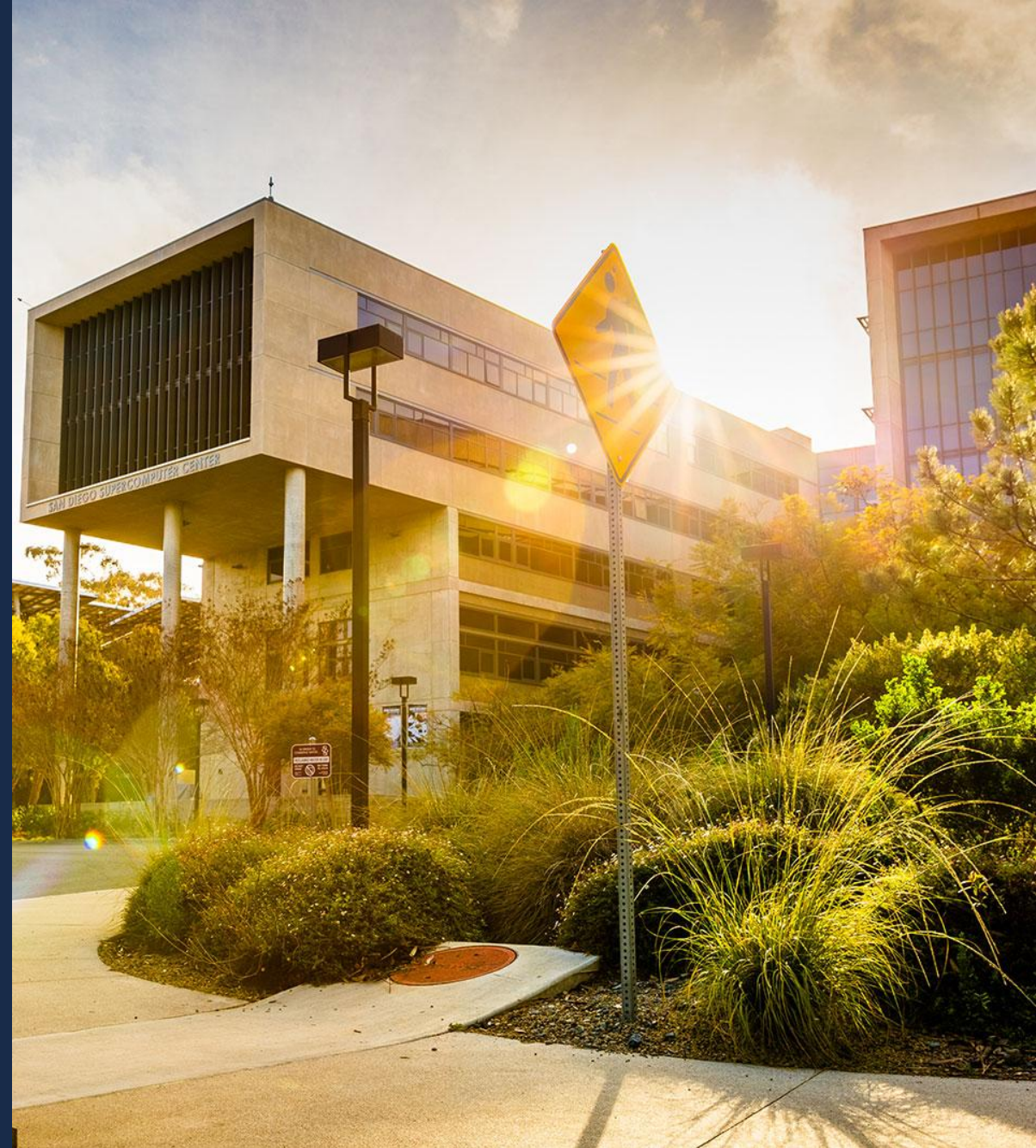
MLOps: Turning your Notebook into a Money-Printing Machine



1. Amazon: 136k Deps. a day.
2. Google: O(10k) Deps a day.
3. Netflix: 500 Deps. a day.
4. Etsy: 50 Deps. a day.
5. Meta: 1 Dep. a day.

Final Remarks

1. There are bad ML/AI Engineers, and then there are ML/AI Engineers who can deploy their code to prod.
2. Don't commit big resources and time into testing ML/AI models. Use automated Unit Test first.
3. Github Actions are the 1st step in the automation process but there is plenty more you can learn to leverage your computing practices: (CI/CD, DevOps, MLOps).
4. AI won't take your AI Engineering job. Someone who knows how to use DevOps pipelines to streamline the deployment of AI/ML models into production and generates absurd amounts of revenue, that person will.





Questions



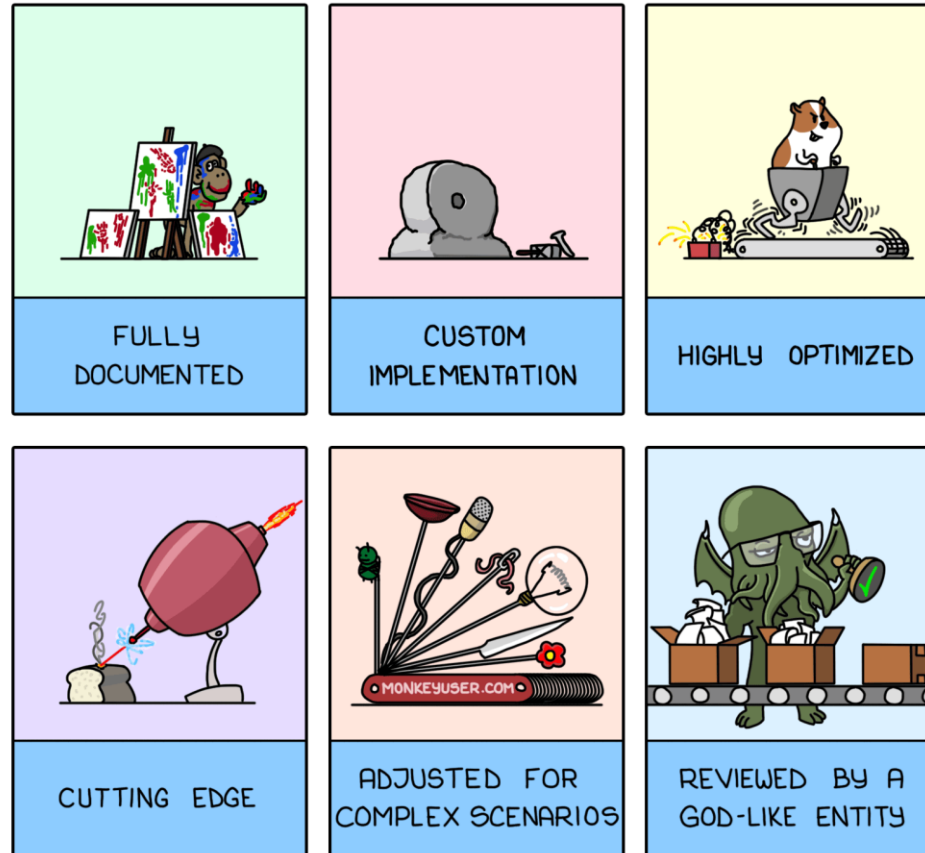
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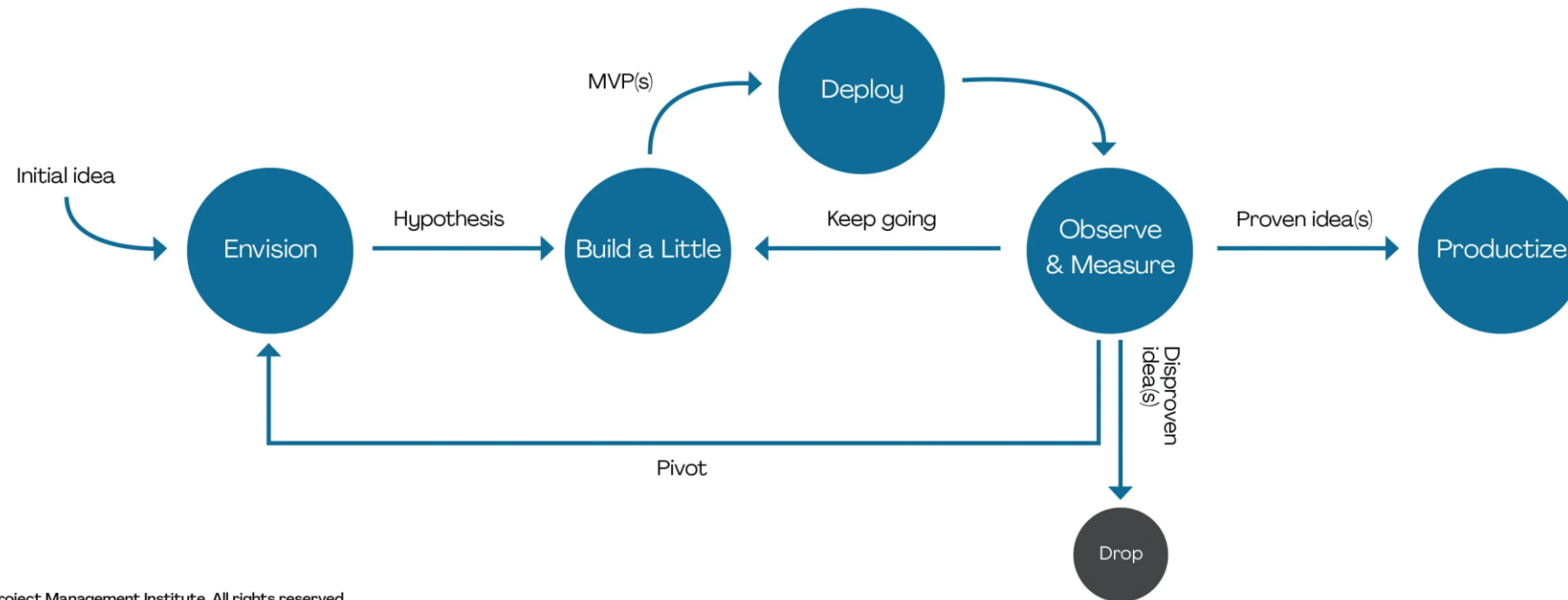
Be Agile: Don't Hit the Nail With the Hammer Handle

PRODUCT DESCRIPTION



Be Agile: Don't Hit the Nail With the Hammer Handle

DAD Exploratory cycle



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Image reference: <https://www.pmi.org/disciplined-agile/lifecycle/exploratory-lifecycle>

Let's Talk GH, Not Jargon



Be Agile: Don't Hit the Nail With the Hammer Handle

