### Open Source: Science vs. Software. What's Different? What's the Same?

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• Former nuclear physicist who wrote simulations for nuclear and particle interactions 30+ years as a software engineer • Recently led engineering for the Accelerated Discovery Platform at IBM Research

So, I've lived the "fabulous" life of both a computational scientist and a software engineer

### Why me??





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# Topics



What Does "Open Source" Mean? • The Different Motivations and Goals for OSS and OSSci • What Can OSSci Learn from OSS? What Can OSS Learn from OSS ci?

### **IODICS**







### What Does "Open Source" Mean?





### • Characteristics according to the Open Source Initiative: • Free redistribution Includes the source code • No discrimination - people, institutions, or applications Derived works permitted under the same license 0 License, automatic distribution with software, not product-specific, $\bigcirc$ restrictive of other software, ...

### What Does "Open Source" Mean?





 But opinions and situations differ: • Free redistribution But what about commercial vs. non-commercial use? • Includes the source code But what about data? No discrimination - people, institutions, or applications But what about use in weapons, nuclear plants (e.g., Java...)? 

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### What Does "Open Source" Mean?





### But opinions and situations differ: $\bigcirc$ Derived works permitted under the same license 0 License, .... 0 A major headache is all the license choices.

### What Does "Open Source" Mean?

Gnu General License limits use in proprietary software

Advice: Avoid GPL. Use Apache, MIT, or Berkeley licenses.





• Automobile patents shared in the early 20th century. IBM Mainframe software distributed as source • <u>SHARE</u> (not an acronym) and <u>GUIDE</u> (an acronym) • BSD, then eventually Linux

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## A Little History (Wikipedia)







# • The term "Open Source": • "Free Software" movement o "Open Source" suggested by <u>Christine Peterson</u> o Netscape Navigator

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### A Little History (Wikipedia)

 Eric S. Raymond, et al. started the Open Source Initiative <u>Tim O'Reilly</u>, Open Source Summit (today's version)



Software Engineers (SWEs) want to: • Collaborate with industry peers on common needs Saves effort Yields the best quality Spreads learning Provides personal rewards Achievement recognition Meets desire to interacte with peers who share common interests

 Software Engineers (SWEs) want to: • Evaluate an OSS project: Clone an OSS repo and determine what it does, is it useful, and is the quality sufficiently high Therefore building, installing, and adopting the software has to be as easy and automated as possible

• Clone: Make a local copy of a repo • Repo: "Asset" repository that tracks versions



 Software Engineers (SWEs) want to: etc.

# Expect high quality, reliability, ease of use, maintainability,



Scientists\* want to: • Collaborate with colleagues, for similar reasons... • Enable reproducibility of results

 Scientists\*: Used for brevity. Also research SWEs and other staff.



Scientists usually don't need to:
 Use their software in "production" scenarios
 ... but not always!

 Production: Catch-all term for deploying software for others to use... and rely on.



OSSci is more likely to include data.
OSS is less likely to include data.
But open AI models, which are data and code, and the training data sets used to create them are a very important topic right now!

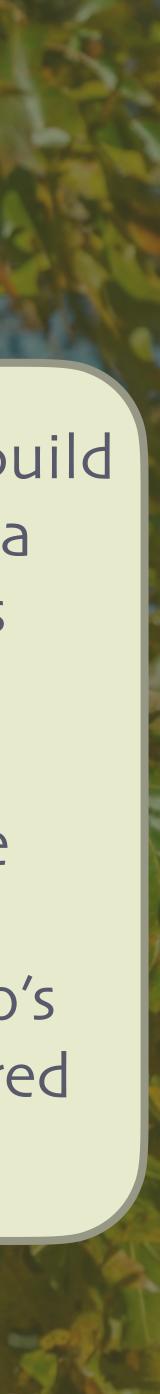
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OSS Excels at Reproducibility
 The relatively new requirement for research reproducibility can be achieved in part with tools long familiar to SWEs.
 You should learn and use the most important techniques they use...



• Asset management in git repos • Share work with collaborators • Asset: code, docs, notebooks, build and deployment tools, and data Enable concurrent work with Git: The dominant tool for this purpose, especially GitHub branches Branch: different sequence of • Track all changes modifications. Branches can be merged when desired Analogous to using a lab • Release: a snapshot of the repo's notebook to record what you "main" branch that can be shared and used by others did, what worked (or didn't) Know what is in every release  $\bigcirc$ 



Verify behavior
Use tests to confirm the software behaves as expected
Rigorous and thorough software test processes exist,
but they aren't used as much as they should be used.
Still, OSS tends to follow to follow better practices than proprietary software projects



Automation
Tests (and build and installation) processes are great,
but tedious and error prone to do by hand
Make all processes automated, on-demand, fast. and robust



Language ecosystem
Pick the language ecosystem that works best...
for your domain,
for the problems that need solving,
for the skill level of the team

• Language ecosystem: Catch-all term for the programming language, libraries, tools for running the code, etc.



Things I've seen scientists overlook
Managing dependencies
Having too many dependent libraries and tools, especially when you require two or more versions of the same library!
Makes your software far less useful



Things I've seen scientists overlook
CVEs ("Common Vulnerabilities and Exposures")
I.e., security holes, risks to you and your users
Keep dependencies up to date; they "patch" CVEs.





 Open Source Code vs. Open Source Data Data has been important for reproducible science for a 0 long time It is sometimes more important than the research code used to analyze it Not previously true for OSS, but suddenly really 0 important for AI

### What Can OSS Learn from OSSci?



 Deterministic vs. Probabilistic and Statistical Results • Science is accustomed to working with P&S results Experiments are never deterministic, even in the classical world (i.e., no Quantum effects) • Al and ML before it have forced SWEs learn and use P&S Lots of active research topics in Generative AI, too 

## What Can OSS Learn from OSSci?



• Scale-out Distributed Computing, e.g., HPC Science has long needed cluster-scale computing for: 0 Drove supercomputer development Data processing from giant experiments, like at Fermilab and CERN Simulations of complex fluid flows, QCD, Others... • Science pioneered HPC for cluster computing, which predate AWS, Hadoop, Kubernetes, etc. Even specialized hardware 

### What Can OSS Learn from OSSci?

• HPC: High performance computing





## Summary



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### Summary

• For science: they use and write to have high quality mandatory Solution: 0 Embrace open source science (OSSci) 

# • More and more, scientific research needs the software • Reproducibility of results and collaboration with peers are

# Leverage OSS software engineering tools and practices



## Summary

• For Software General-purpose software is becoming more probabilistic, less deterministic, driven in large part by Al Large-scale distributed computing is now unavoidable • Solution: Leverage the lessons from scientific research and scientific computing on: Sharing and using data High-performance computing software and hardware





## Questions?

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