

# Lab Notebooks for Computational Mathematics, Sciences, & Engineering

*Presented by*

**COLABS: Collaboration for Better Software for Science**

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*In collaboration with*



*With prior support from*



Software Productivity and Sustainability track @ Argonne Training Program on Extreme-Scale Computing summer school

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Additional thanks to: Juan Pablo Haddad, Akash Dhruv, Steve Fickas, Carlo Graziani, Boyana Norris



See slide 2 for  
license details

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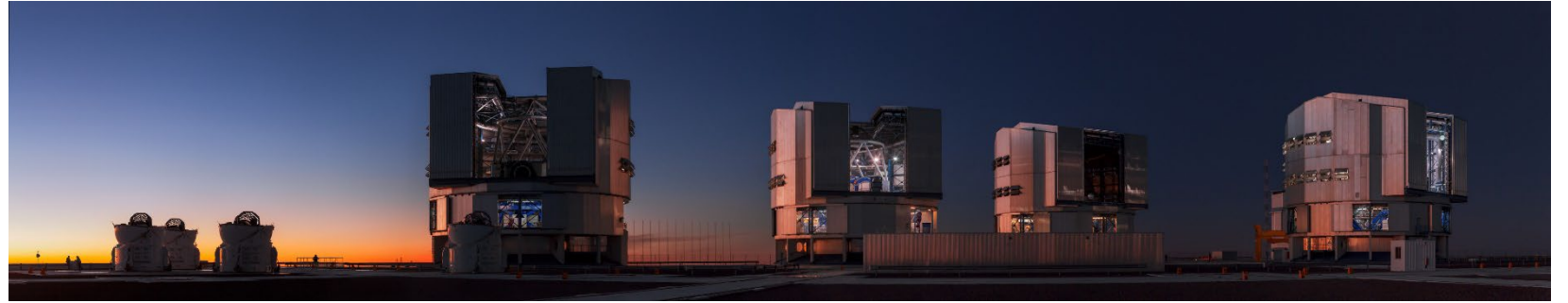
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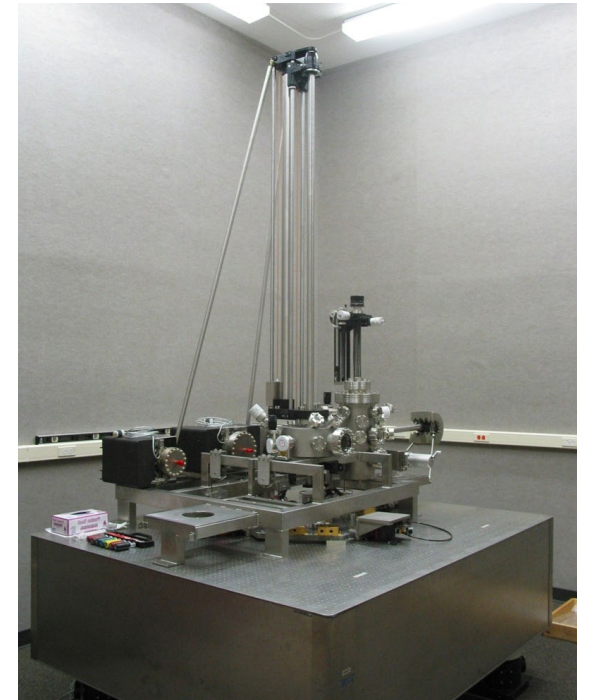
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# My background



Credit: ESO/B. Tafreshi (<http://twanight.org/>)

- Experimental condensed matter physics background
  - Low-energy positron diffraction
  - Low-temperature, ultra-high-vacuum scanning tunneling microscopy
- Professional experience in observational science environment
  - European Southern Observatory's Paranal Observatory
  - Instrumentation & systems engineer specialized in adaptive optics
- Scientific software developer
  - Primarily focused on applications



Always working on **scientific instrumentation**

# Why discuss experimental sciences at ATPESC?

Scientific HPC is several young fields that “on close examination, have not really stabilized or optimized their collaborative processes in a manner analogous to that of more mature, ‘classical’ sciences. As a consequence, valuable science is often needlessly lost, or left uncollected.”

- Carlo Graziani, Computational Scientist at ANL, [\*HPC and the Lab Manager\*](#)

“... practicing the scientific method properly requires good software practices. This is understood in the experimental community...The computational science side has had a historic problem with it. As we can see, it’s getting better.”

- Katherine Riley, Director of Science at ALCF, [\*ATPESC 2019\*](#)

# A minimal definition of a lab notebook

A goal of keeping a lab notebook is "...to write with enough detail and clarity that another scientist could pick up the notebook at some time in the future, repeat the work based on the written descriptions, and make the same observations that were originally recorded. If this guideline is followed, even the original author will be able to understand the notes when looking back on them after considerable time has passed!"

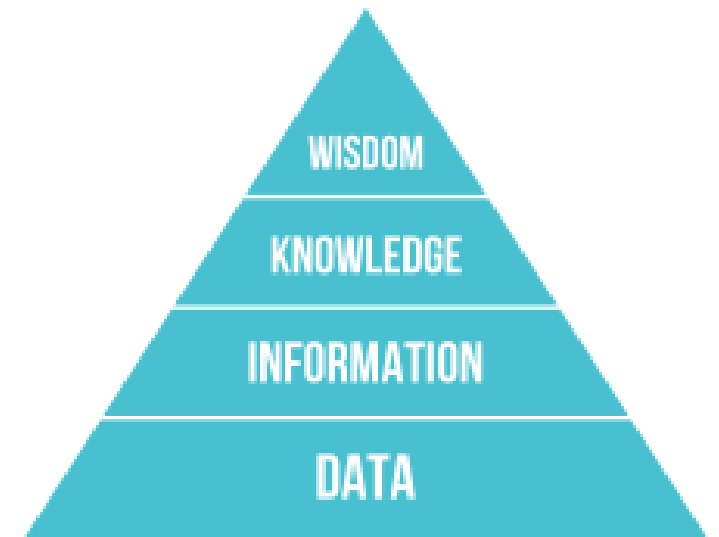
- Howard Kanare, *Writing the Laboratory Notebook*

# DIKUW

## Data, Information, Knowledge, Understanding, Wisdom

A classification scheme that overloads everyday words so that we can use the same language and understand each other.

We will build on this to understand & appreciate documentation & lab notebooks.



[DIKW pyramid](#) (unaltered) – Wikipedia/Longlivetheux

# Data & Information

- Data

- Collection of numbers, symbols, text, *etc.*
- It has value only because it was recorded and exists.
- **Example:** Timeseries representation of temperature, relative humidity, and precipitation.

- Information

- Facts gleaned from data.
- Answers questions such as who, what, when, how much, how long, *etc.*
- **Example:** Starting at 2pm the temperature dropped by 5°F over 15 minutes. At 2:05 pm it started to rain and 0.25” of rain was accumulated over the next 30 minutes.

# Knowledge & Understanding

- Knowledge
  - Derived from information, experience, and **understanding**.
  - **Example**: When relative humidity levels are high and the temperature drops substantially, there is an increased probability of precipitation.
- Understanding
  - A deep theoretical background in and practical experience with the system whose data was acquired and studied?
  - The ability to explain why?
  - “Understanding is a kind of ecstasy” – Carl Sagan
  - **Example**: A meteorologist could explain at different levels of detail how the atmosphere works to substantiate the knowledge.



## Obligatory Einstein quote

“Any fool can know. The point is to understand.”

- Albert Einstein

- Is understanding always the ultimate goal?
- Are there times when mere knowledge is sufficient?
  - I don't need to understand atmospheric science or weather prediction. I just need basic knowledge to determine if I should take an umbrella with me.
- Data, information, and knowledge are key ingredients in developing understanding.
  - Need to manage all, appropriately.

# Sometimes we just want “good enough”

- Not every developer needs to be an expert in git
- We want the people designing the rules of how we use and interact through git to have **understanding** so that collaborating *via* git requires minimal git **knowledge**
  - git workflow should protect code so that we can't do damage
  - Focus on the development/testing and not on git
  - Low barrier for newcomers

# Knowledge Management

- DIKUW is related to knowledge management
- We want to
  - **Recognize** when we generate knowledge
  - **Capture** and **preserve** that knowledge
  - **Communicate** that knowledge
- Scientific work can benefit from knowledge management

Is knowledge communication only about communicating to others?

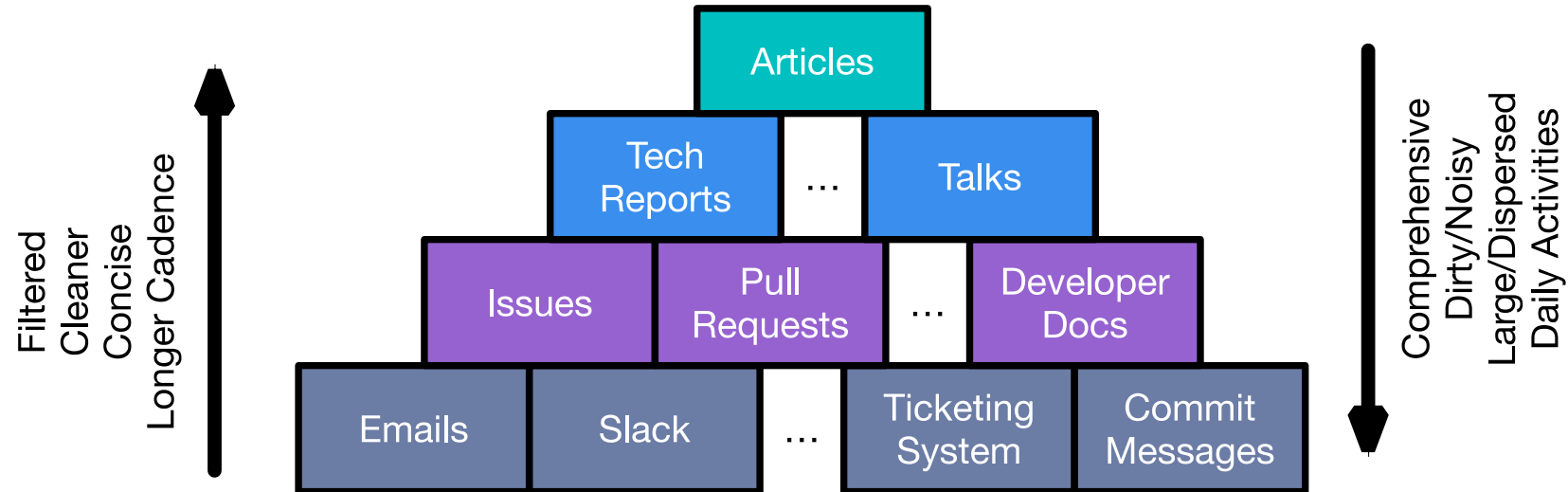
# Example: Lessons learned

- After we live through an experience, we want to derive lessons learned
  - Experience is valuable, more so if we reflect and are thoughtful
  - Generate/capture knowledge to grow, improve, and avoid difficulties/mistakes
  - Hope to improve understanding
- We get more if we derive lessons learned together
  - Create more or higher quality knowledge
  - Communicate the knowledge implicitly

Should we communicate lessons learned to others?

# Which leads us to documentation

Documentation is knowledge communication & can build understanding



- Data at the bottom. Knowledge as we move up?
- Some documents frozen at creation. Others are living.
- Does this capture how hard it is to do documentation in a distributed, digital world?

# And finally, we reach our destination

Lab notebooks are

- A fundamental part of communication as well as rigorous, reproducible science in a lab,
- A common-place or required part of an experimental laboratory,
- Populating a scientific “lab notebook” was an “automated” process at the observatory,
- A tool for preventing scientific fraud, and
- Record of invention and defending against allegations of fraud.

Lab notebooks

- Should be used regularly,
- Should be comprehensive and never filtered,
- Don't need perfect grammar and full sentences,
- Content is frozen at creation, and
- Hopefully contains more than just data (*e.g.*, motivation, reasoning, conclusions).

They aren't good at communicating knowledge, **but** people interact, evolve, and grow by collaborating through the notebook.

# Example notebook entries

A bad example

**Monday July 25, 2022**

9:05 am - Do study ABC

8:47 pm - Lot's of interesting data!  
- Results are in GCE

A better example

**Monday July 25, 2022** (Jared)

9:05 am - Continuing work for study ABC. (See July 7)  
- I presently believe that if A happens, then B must also happen.

- To verify this, I intend to

- ...
- \*\*\*

9:30 am - Started executing this experiment on Bebop.

- Built debug version of binary with Intel 20.4
- Based on clean commit 5a43b21c
- Build log saved to `my_test_2022.log`
- No errors or warnings emitted
- Used job script `run_my_test` with configuration 24 (Job ID 123456)
- Stdout/err & results saved in folder ABC

10:07 am - Analysis run with script

`analyze_my_test.py` and results saved in same folder.

- Since no peak seen around 1.5 MeV, I was wrong. But based on this, I now *believe* that if A happens, then C must also happen.

# Conversations with Carlo

Carlo Graziani is a Computational Scientist at ANL  
BSSw blog article [\*HPC and the Lab Manager\*](#)

- As researchers' careers progress
  - The problems become more complex and larger
  - Previous informal techniques for executing a study start to fail
  - The researchers sense that something is missing
  - They invent processes and tools to compensate

This happened to Carlo and at some point, he realized that  
**“I had re-invented the lab notebook!”**





# Not all lab notebooks are alike

- Lab notebooks to record work done on instrument
- Lab notebooks to record acquisition of data
- Pull Request as **filtered** lab notebook – higher up the hierarchy
  - PR allows for additional content that's distinct from the individual commits
  - Flash-X PR #247 is example
  - Record process to verify correctness of changes
  - 2-2.5 days effort carried out over a week
  - Copy/pasted from previous PR and adapted first (designed process)
  - Improved as I carried out process – converging on a quasi-procedure
  - Filtered so that reviewers aren't overwhelmed
  - Helped me organize effort & design good tests
  - Senior reviewers provide feedback & suggest improvements
  - Junior reviewers exposed to work habits of other people



jared321 commented on Aug 18 · edited ▾

Author 😊 ⋮

Working on GCE/compute-012 with

Currently Loaded Modules:

```
1) intel/20.4  2) mpich/3.4.2-intel  3) hdf5/1.12.1-mpich-3.4.2-parallel-fortran
```

- All tests will be built in debug mode using the Intel/20.4 + MPICH + HDF5 stack loaded via GCE modules.
- The same pseudo-UG-only testing was carried out identically for the 2D/Sedov/simpleUnsplit and 3D/Sedov/Unsplit simulations with Paramesh, AMReX, and Milhoja. These two simulations were chosen as they will hopefully become official Milhoja Comparison tests in the GCE test suite.
- All 2D tests ran in 304 steps with 6 checkpoint files including the initial conditions; 3D, 61 steps and 2 checkpoint files.
- Ran the 2D tests with 4 MPI processes; the 3D, with 8 MPI processes. These are the number of processes presently used for Sedov tests in the GCE test suite.
- Confirmed with `sfocu` that the Paramesh and AMReX final checkpoints are identical and that the Paramesh and Milhoja final checkpoints are identical.
- Confirmed that the integrated quantities were conserved in each case up to a reasonable level and that the initial values were consistent across all associated runs to at least 12 decimal digits.
  - standard deviation of 2D conserved quantities less than  $2.5e-14$
  - standard deviation of 3D conserved quantities less than  $3.25e-14$
  - Confirmed that the initial values of the [xyz]-momenta were all exactly zero and that the z-momenta was exactly zero for each all time steps in the 2D simulations.
- Confirmed in Milhoja 2D case that we get, as expected, the identical final checkpoints if we run with 4 and 8 MPI processes.
- Where possible, the `milhoja.log` files were reviewed to confirm correct configuration and execution.
- Viewed the Milhoja final checkpoints in Visit to qualitatively confirm reasonable results for all variables and correct mesh overlays. 3D data was viewed with a slice at 50%.

## Example: Flash-X PR #247

# No one likes writing lab notes...

We love to consume documentation; write it, not so much.

## Optimistic

- Lack of experience
- Lack of training
- Lack of appreciation
- Lack of incentives

## Cynical

- We want and appreciate when others share knowledge with us.
- We don't want to take the time to capture, preserve, and communicate knowledge we generate.

## One aspect of productivity

One person decreases their short-term efficiency so that many (and the team) achieve long-term efficiency and quality.

# Nothing beats good ol' pen and paper

“Since at least the 1990s, articles on technology have predicted the imminent, widespread adoption of electronic laboratory notebooks (ELNs) by researchers. It has yet to happen — but more and more scientists are taking the plunge.”

- Roberta Kwok, [\*How to pick an electronic laboratory notebook\*](#), Nature

## Pen & Paper Pros

- Most can use paper and pen in any situation
- Open format can allow for creativity and easier annotation
- Concentrate on the work rather than tooling
- Good if notetaking slows down progress
- Notebook is stored **publicly** next to where it is used

## Electronic Woes

- Tied to technology that could fail
- Overwhelming variety of possible solutions with different pros and cons
- Uncertainty about future of tool, increased costs, inability to export
- Does funding restrict where and how digital notes can be stored?

# Criteria for lab notebooks for computing?

- **Paper won't work.** We work anywhere and sometimes in distributed way.
- Should notebooks be public and how to do that?
- How many different types of notebooks do we need?
- Do we use a single ELN or distribute notes across a suite of tools?
- How can we use automation appropriately to overcome difficulties and increase productivity?

We likely need many streams of lab notes

# Different streams of lab notes

- Lab notebook for changes to scientific instrument
  - Changes in code repo necessary for study
  - Changes to SW environments
  - Changes to build/job files and build systems
- Lab notebook for data analysis tools
- Lab notebook to detail how experiment was designed and executed
- Right tool for the job
  - We don't want a single 10,000-line README

# Git lab notes stream

Keep lab notes for your software as close to the “instrument” as possible

```
Date: Mon Jun 27 10:42:22 2022 -0500
```

```
(Issue #215) Added in Milhoja Init unit test. I have tried to structure this in accord with the unitTest architecture in the User Manual. One main consequence of this is that it uses the generic Grid unitTest evolveAll routine, which writes a unitTest output file. Since this test also uses the ut_testDriverMod framework, I had to simplify that so that it doesn't attempt to write the same file. This change will likely affect the AMReX unit tests.
```

```
I have run this successfully in 1D, 2D, and 3D on GCE/compute-12 with Intel. The test correctly creates a unitTest_XXXX output file and adds in a success line only if the test was 100% successful. I temporarily dumped the ICs and final solution to AMReX-format files and manually confirmed correct content.
```

Details not obvious from commit diff:  
Motivation, reasoning, consequences

Testing notes

\*This message is missing a title as the first line.

Use Pull Request to capture final verification streams

# README lab notes streams

- High-level road maps with motivation, documented decisions, and conclusions
- Concise living docs that function as executive summaries
  - Higher up in documentation hierarchy
- Low-level notes such as managing software stack
  - Traceability of SW environment & therefore verification
  - Can be turned into procedures



# High-level README

## My Study Executive Summary

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This repository encapsulates the computational laboratory environment constructed and used for our 2022 My Study scientific research. Not only does it contain all tools needed to setup and use the environment, but it also contains the metadata and context needed to understand how data was acquired and how to use it for analysis and drawing conclusions.

## Study Goals

---

Our motivation for this study is ...

We believe that ...

We intend to use our software to ...

To accomplish our goals we require that ...

We understand that our software is limited and therefore that our study is limited in the sense that ...

Some optional goals are ...

Ideally, we would like to publish our results in the Journal ZYX with a submission target date of ...

## Organization

---

ABC will be the PI and will ...

XYZ is responsible for ...

# Low-level README

## AMReX Installation History

---

### 5 March 2020 - FlashFluxRegister b1dd083

- Using changes from FlashFluxRegister branch by Weiqun.
- Need for improved flux handling across all branches.
- Built 1D/2D/3D libraries for both gfortran and Intel at this commit.
- These were tested with the Staged/Staged-Intel/Master compute00x test suites with no other changes made. All tests passed.

### 6 November 2019 – master – 93fb085d

- Austin encountered an AMReX based bug and reported it in Issue #643. He reports that AMReX fixed that bug at commit - 23f943f.
- New install location is /nfs/proj-flash5/ a shared group at MCS, we are no longer going to use the /sandbox/flash/ versions on compute00[123]
- Built 1D/2D/3D libraries for both gfortran and Intel at this commit.
- These were tested with the Staged/Staged-Intel/Master compute00x test suites with no other changes made. All tests passed.

### 29 March 2019 – development – 06c6c0e2

- Rebuilt the libraries from a commit that contains the multifab changes implemented manually in the previous libraries. These changes were merged in to AMReX at commit 66392f8d on Tue Mar 26. No code in AMReX needed modifying for this build.
- These libraries were also built with Particles and linear solvers enabled for Saurabh's tests. He showed me that I had to update the automagically updated makefile to get the Particles Fortran interface into the libraries.
- Built 1D/2D/3D libraries for both gfortran and Intel at this commit.
- These were tested with the Staged/Staged-Intel/Master compute00x test suites with no other changes made. All tests passed.

### 20 March 2019 – master – 884d3194 (modified)

- Updated the files AMReX\_multifab\_fi.cpp and AMReX\_multifab\_mod.F90 at commit to incorporate the local tile index in the Fortran interface. These changes had already been tested during development in local repositories.
- Built 1D/2D/3D libraries with both gfortran and intel on compute001. These were then copied over to compute002 and compute003.

# Capturing data context & metadata

- Automate as much as possible
- Build dates, user, system name, git hashes, configuration data in file headers
  - Self-documenting files
- Build & job logs
  - Software environment info (e.g., modules, `ldd` output)
  - git diffs
  - Environment variables

# Jupyter notebooks

## The exception to the rule?

- Jupyter notebook can put context & metadata next to data
  - High-level design & motivation up top
  - Low-level lab notes for acquiring data
  - Load & use data
  - Generate visualizations in place
  - Comment on results
- Where do notebooks fit into the documentation hierarchy?
- Repetitive use of notebook?
  - Limit amount of code in notebook

Jupyter4Science Community Knowledge Base  
2023 BSSw Fellow Nicole Brewer

# How to organize your “virtual” (multi-stream) lab notebook?

- It should be
  - Easy to create and maintain lab notes
  - Easy to concentrate more on executing work & less on documenting it
  - Easy to find what you need
- Each stream should
  - Have a clear identity for what it records
  - Not contain notes contained in other streams
  - Be recorded by using the right tool for the job

This implies the need for a documentation scheme.

I design my lab notebooks into a larger execution environment.

# Experimental laboratory environment

- In an experimental lab,
  - Have all my tools at hand, clean, and ready for use,
  - Know how to use my tools,
  - Fully characterized and configured instrument,
  - Understand broken or underperforming instrument performance, and
  - I want to take comprehensive lab notes quickly and easily.

## The Goal

Concentrate on acquiring data, analyzing the data, drawing conclusions, designing next steps, and recording the work for reproducibility.

# Computational laboratory environments

Use many simple, minimal lab environments

- Tailor formality, complexity, and automation to each use case
- Store context & metadata next to data
- Each code repository has dedicated test environment
- One environment per scientific study
- Each developer can have dedicated development environment (optional)
- Environments are encapsulated
  - Dedicated documentation
  - Dedicated software environments
  - Can be updated and managed independently
  - “Store on a shelf” for later

# Do execution environments work?

- Work in progress (and always will be)
- Used for different types of studies across different projects
- I'm not the only one
  - [BSSw article by Jean Shuler](#)
    - [Popper](#) – 2018 BSSw Fellow [Ivo Jimenez](#)
    - [Code Ocean](#)
    - [Weight & Biases](#) (ML)
  - [Multiphase Simulations](#) – Akash Dhruv (ANL)
  - [FlashKit](#) – Aaron Lentner (George Washington University)

[Computational Lab Execution Environment Example](#)



# Citations

- Carlo Graziani, *HPC and the Lab Manager*. **Better Scientific Software**. [https://bssw.io/blog\\_posts/hpc-and-the-lab-manager](https://bssw.io/blog_posts/hpc-and-the-lab-manager). Nov 17, 2021.
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# Summary

- Software best practices are foundational science & are mandatory
- Knowledge management can improve science & productivity
- Productivity can arise from selflessness
- Not all documents are alike
- Not all lab notebooks are alike
- Lab notebooks are mandatory
- Lab notebooks allow for learning
- Lab notebooks for CMSE are hard
- We want to construct & use execution environments