



Lab Notebooks for Computational Mathematics, Sciences, & Engineering

One ex-experimentalist's perspective



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

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Thanks to: Akash Dhruv, Anshu Dubey, Steve Fickas, Carlo Graziani, Tom Klosterman, & Boyana Norris



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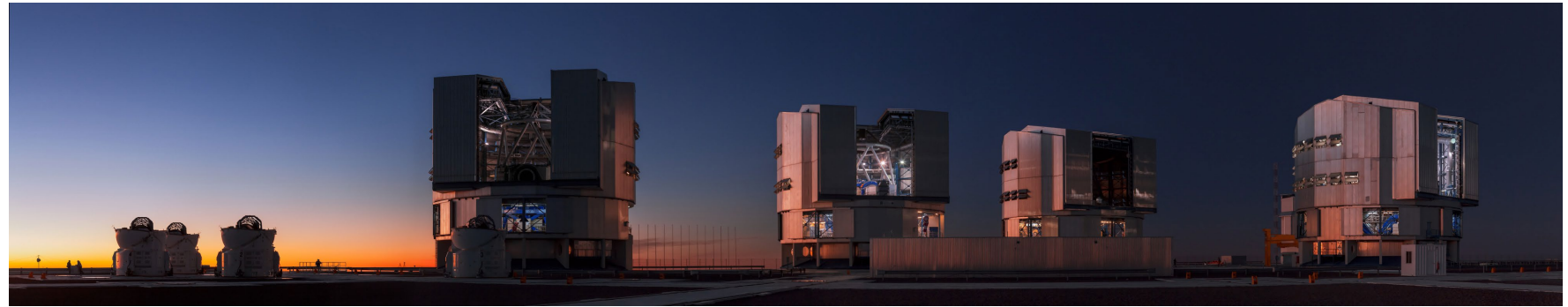
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- **The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Todd Gamblin, Jared O’Neal, and Boyana R. Norris, Software Productivity and Sustainability track, in Argonne Training Program on Extreme-Scale Computing, St. Charles, Illinois, 2022. DOI: [10.6084/m9.figshare.20416215](https://doi.org/10.6084/m9.figshare.20416215).**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial, ISC, 2022 ...

Acknowledgements

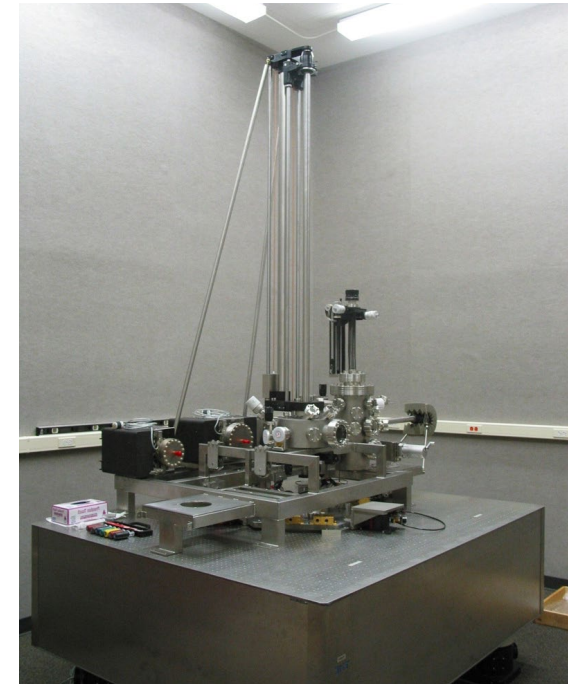
- This work was supported by the U.S. Department of Energy Office of Science, Office of Advanced Scientific Computing Research (ASCR), and by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.
- This work was performed in part at the Argonne National Laboratory, which is managed by UChicago Argonne, LLC for the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.
- This work was performed in part at the Lawrence Livermore National Laboratory, which is managed by Lawrence Livermore National Security, LLC for the U.S. Department of Energy under Contract No. DE-AC52-07NA27344.
- This work was performed in part at the Los Alamos National Laboratory, which is managed by Triad National Security, LLC for the U.S. Department of Energy under Contract No.89233218CNA000001
- This work was performed in part at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.
- This work was performed in part at Sandia National Laboratories. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.
- This work was performed in part at University of Oregon through a subcontract with Argonne National Laboratory.

My background



Credit: ESO/B. Tafreshi (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

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!"

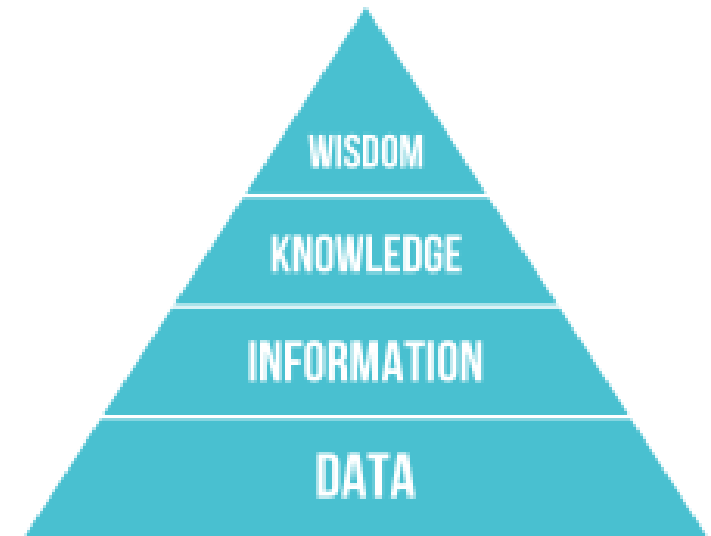
- Howard Kanare, *Writing the Laboratory Notebook*

DIKUW

Data, Information, Knowledge, Understanding, Wisdom

A classification scheme that overloads every day 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.

You can share knowledge, can you share understanding?

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.

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?

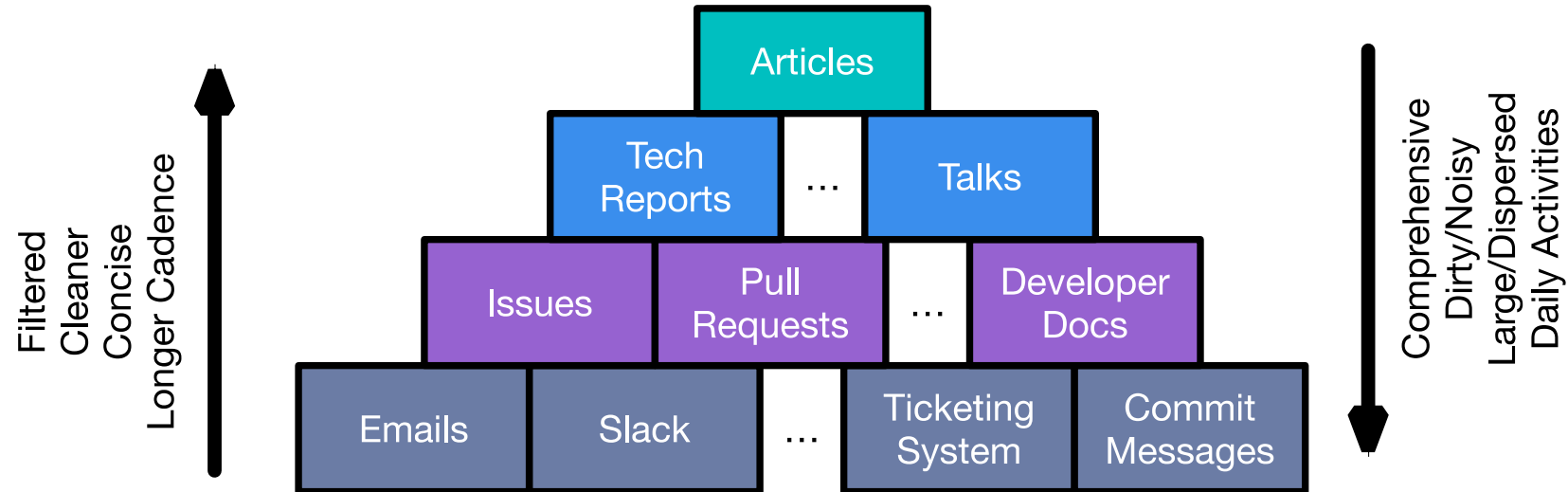
Example: Lessons learned

- 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.

Not all lab notebooks are alike

- Lab notebooks to record work done on instrument
- Lab notebooks to record acquisition of data
- **Filtered** lab notebook for users – higher up the hierarchy

From the [CRIRES+ News \(ESO\)](#) page

Instrument News

- **May 18, 2022:** User Manual for Phase 2 P110 has been released.
- **May 05, 2022:** intervention of the warm part of CRIRES (calibration unit, MACAO) from April 24th until May 7th. ← Hardware team
- **May 04, 2022:** the metrology system is now operational in all wavelength settings.
- **Mar 16, 2022:** a new Exposure Time Calculator version has been published
- **Feb 24, 2022:** the User Manual for Phase 1 P110 has been released.
 - Please note that the current version of the CRIRES ETC has a glitch which concerns polarimetry; a new version of the ETC will be released soon.
 - For P110, **polarimetry and spectro-astrometry** will NOT be offered for Large Programs and Monitoring Programs (see the "ESO Call for Proposals P110" document) as these modes require further characterization
- **Jan 31, 2022:** An updated Exposure Time Calculator including the correct thermal background of the instrument has been released.
- **Jan 18, 2022:** In the Exposure Time Calculator, the thermal background of the instrument was strongly underestimated, thereby affecting the S/N estimates for observations of (faint) targets in the K, L and M bands.
- **Oct 1st, 2021: Start of regular science operations of the upgraded CRIRES.**
- **Sep 27th, 2021:** Public release of the **cr2res pipeline** ← Data analysis team
- **Sep 15th, 2021:** First night of the 4-nights long CRIRES Science Verification. ← Science team

Science team



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 it 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.

Conversations with Carlo

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

My take away from the article and conversations

- 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, and
 - 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!”



Tried-and-true

Nothing will ever beat good ol' pen and paper

- 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
- Quicker to scribble down notes than to use a digital tool
- Good if notetaking slows down progress
- Notebook is stored **publicly** next to where it is used

No really. I'm not joking...

“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

- Some must be purchased to access features and lift resource limits
- Some include templates and collaboration tools
- 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?**

What would a lab notebook look like for us?

- We work anywhere and sometimes in distributed way. **Paper won't work.**
- 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?

```
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



Citations

- Carlo Graziani, *HPC and the Lab Manager*. **Better Scientific Software**. https://bssw.io/blog_posts/hpc-and-the-lab-manager. Nov 17, 2021.
- Katherine Riley, *What All Codes Should Do: Best Practices*. ATPESC 2019 presentation. Retrieved from [YouTube](#). Nov 5, 2019.
- Howard M. Kanare, [*Writing the Laboratory Notebook*](#). American Chemical Society, Washington, D.C., 1985.
- Roberta Kwok, [*How to pick an electronic laboratory notebook*](#). **Nature** 560, pp. 269-270, Aug 6, 2018.
- DIKW pyramid. 2022, August 4. In *Wikipedia*. https://en.wikipedia.org/wiki/DIKW_pyramid.

Meta conclusions

This module

- Was **not** about sharing knowledge, but
- Was about (hopefully) building **understanding**.

We established concepts, pros/cons, difficulties, & questions.
The next talk will address these in concrete way.

From my perspective

- 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

To be continued...

