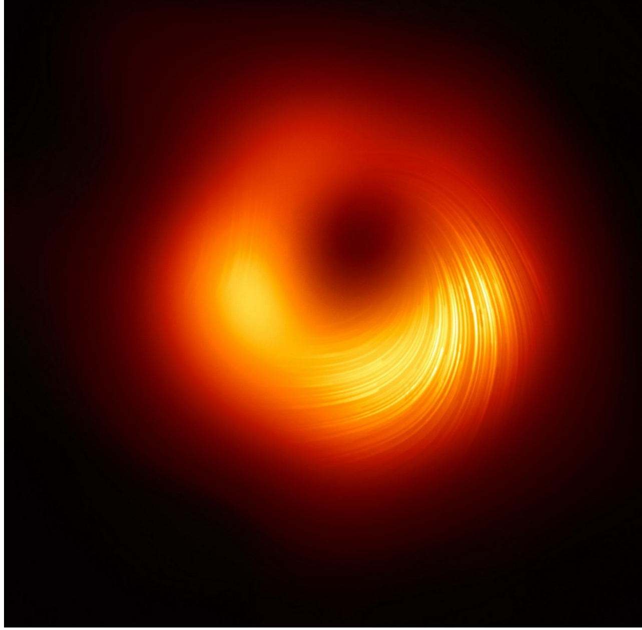
How to lower the entry barrier to your scientific software

Gabriele Bozzola, PhD

gbozzola@caltech.edu

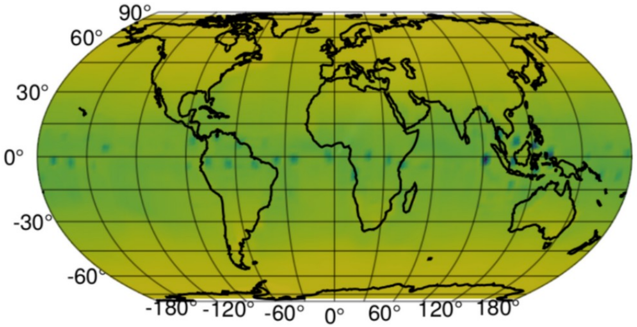
(Views are my own)

I am a (Scientific) Software Engineer



CliMA

CLIMATE MODELING ALLIANCE



An open-source climate model in Julia

Ask me more about any of these!

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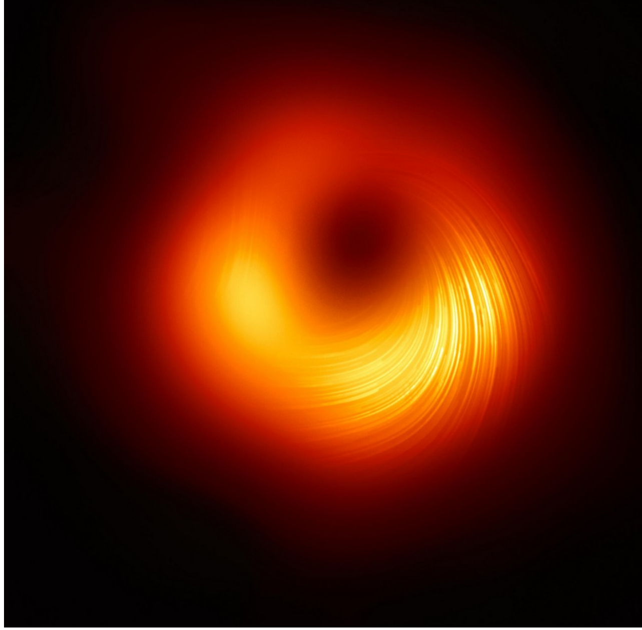

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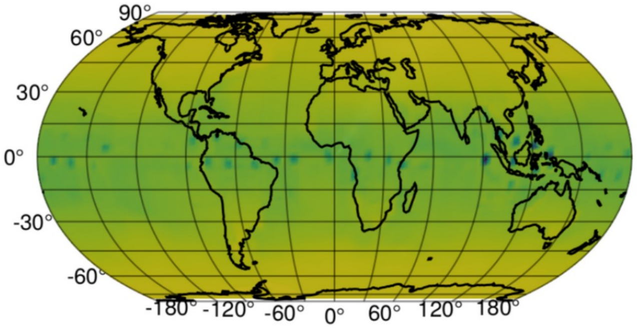

An open-source climate model in Julia

I also review scientific open-source software

JOSS
The Journal of Open Source Software

Ask me more about any of these!

This talk in one slide

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Scientific software has fundamentally unique characteristics and needs …

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Scientific software has fundamentally unique characteristics and needs …

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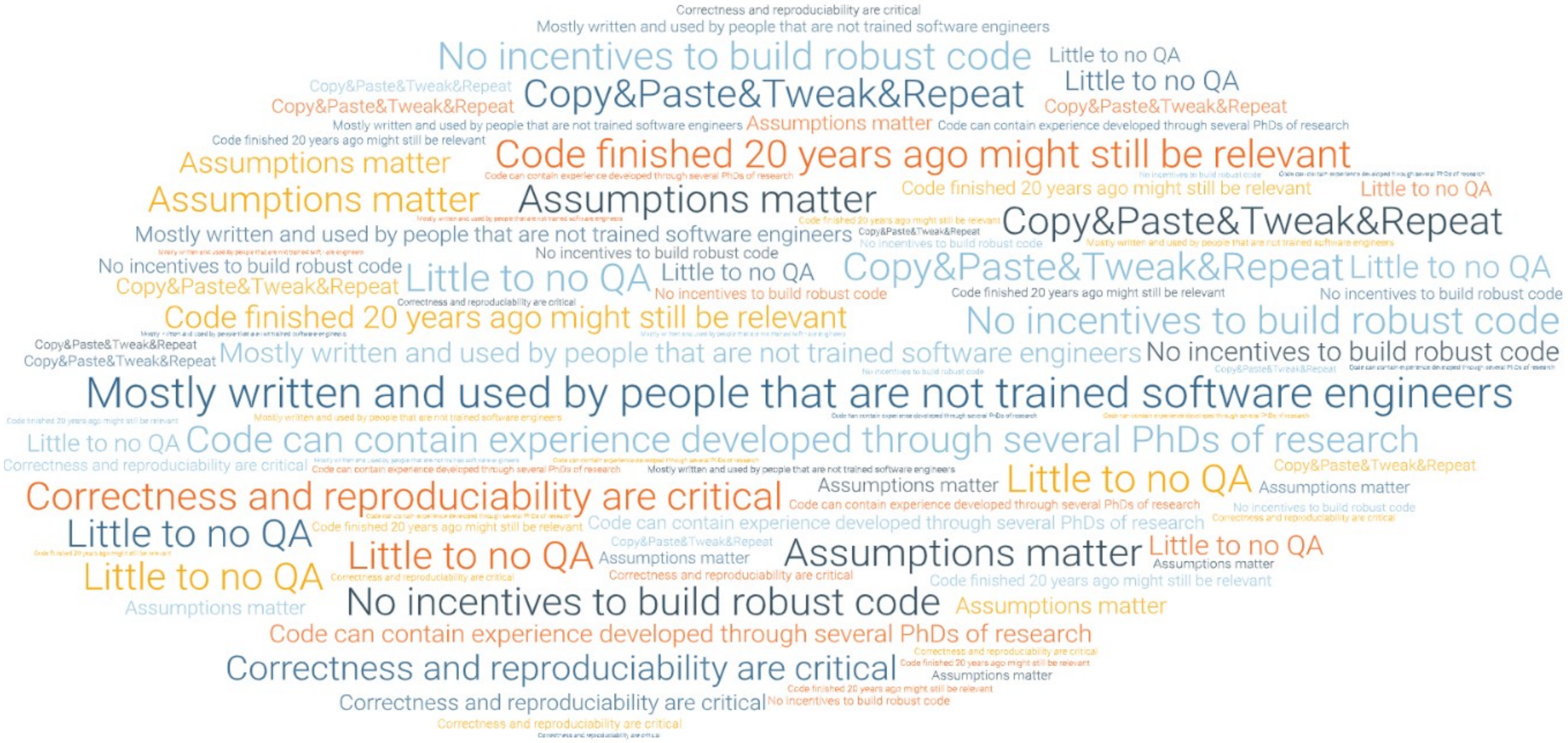
… that we can start addressing with a user/dev/scientist centered approach to documentation …

… that we can elevate code from just a tool to a self-contained contribution …

… to accelerate science!

Scientific software has unique characteristics and needs


Correctness and reproduciability are critical
Mostly written and used by people that are not trained software engineers
No incentives to build robust code
Little to no QA
Copy&Paste&Tweak&Repeat
Assumptions matter
Code can contain experience developed through several PhDs of research
Code finished 20 years ago might still be relevant

POV: You are an average piece of scientific software

- You have been developed by a graduate student over 5 years (or their advisor 25 years ago)
- People learn how to use you through oral tradition
- You have no automated tests
- You lead to reproducible results only on even days
- You are required to be correct

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- You were used to drive new science and publish papers
- You contain lots of lessons learned
- You could be used for future projects
- You have lots of potential!

Problem:
There is a lot of unrealized scientific potential!

Science killers:

- Time spent understanding the code
- Duplication of efforts
- Incorrect code/usage
- Unknown mismatch in assumptions
- …

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Opportunity:
Code as a self-contained scientific contribution

Science enabler:

- Openness
- Ease of use and extension
- No hidden knowledge
- Sharing the “lessons learned”
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Documentation mitigates risks and contributes to elevating status of code from **tool to scientific contribution**

A practical framework for effective technical documentation

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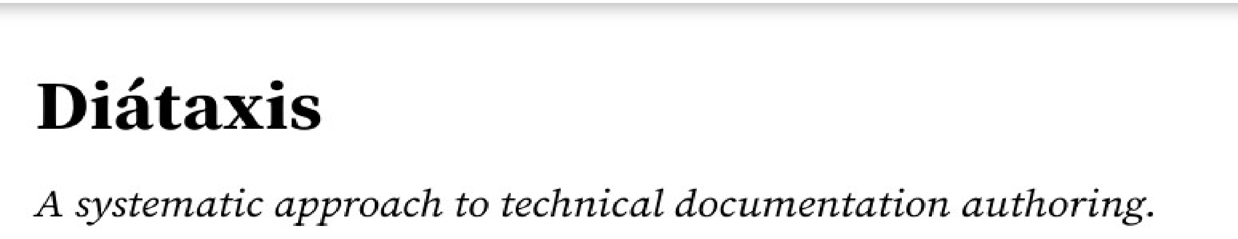
Extending Daniele Procida’s diataxis.fr for scientific code



Diátaxis

A systematic approach to technical documentation authoring.

Two core principles:

Explicitly address **users/developers/maintainers/scientists needs**

Explicitly address **how people learn and seek information**

Doc Braun's lab is studying time travel

The lab is developing `TheLorean.jl`:
A Julia code to compute flux capacitance

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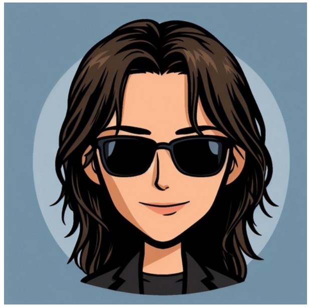

Tera Connor

Postdoc
User and developer

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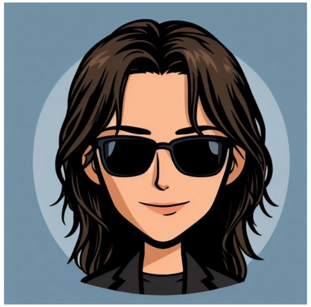

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Interested in methods and capabilities

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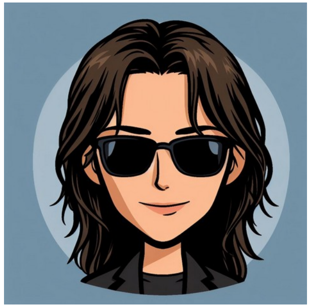

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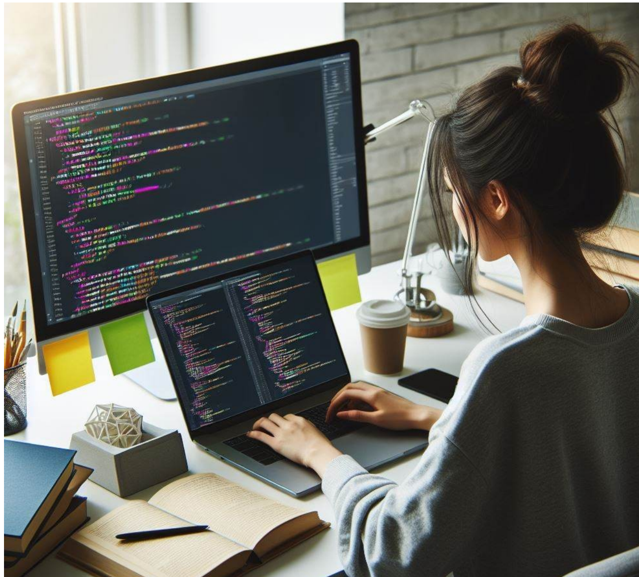
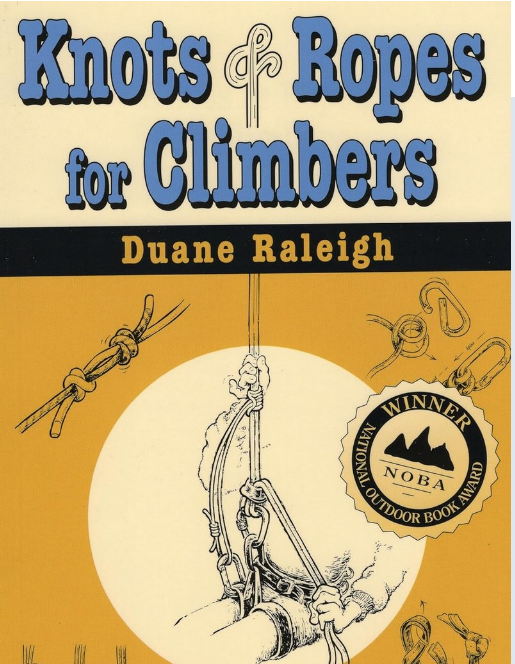
To **use**, to **extend**, to **learn from**

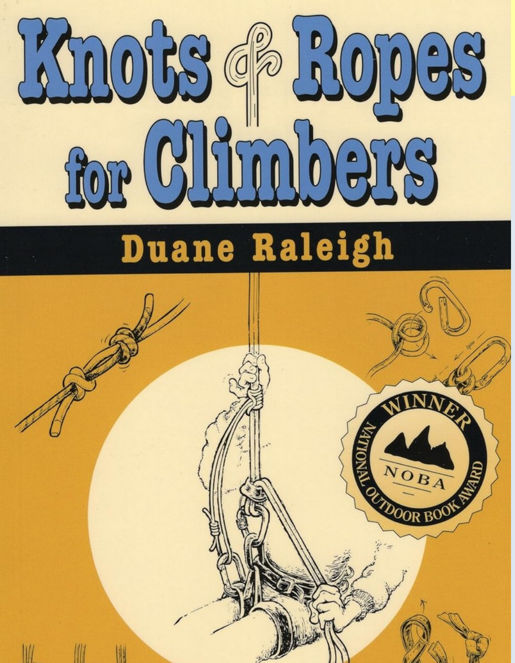
So, you decided you want to learn to <insert craft>





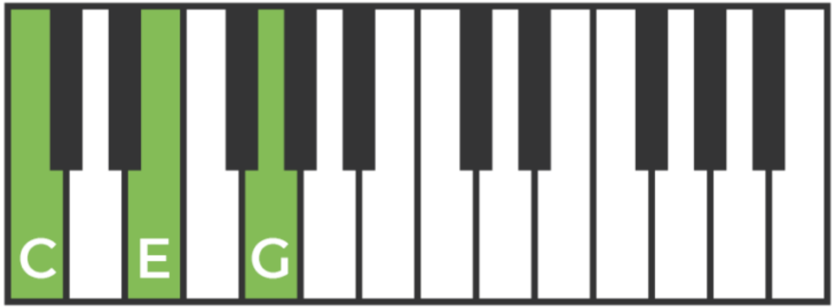
THEORETICAL KNOWLEDGE

PRACTICAL SKILL

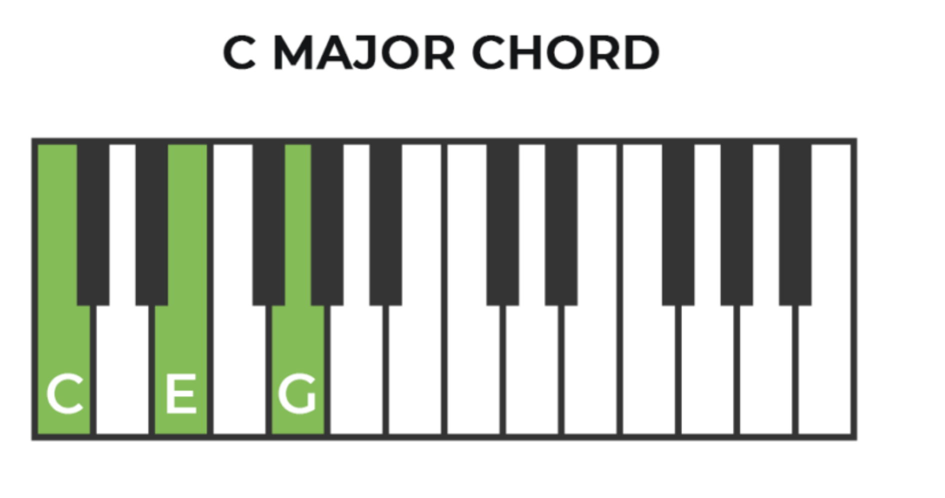


THEORETICAL KNOWLEDGE

C MAJOR CHORD

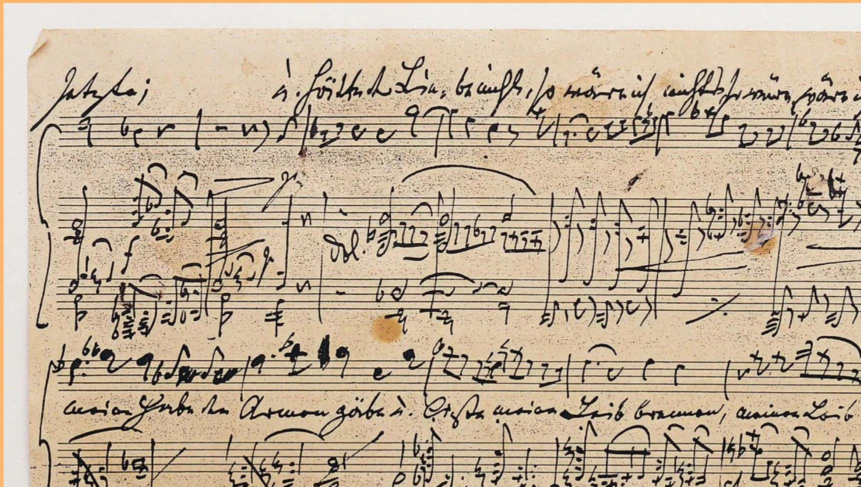


WHILE LEARNING



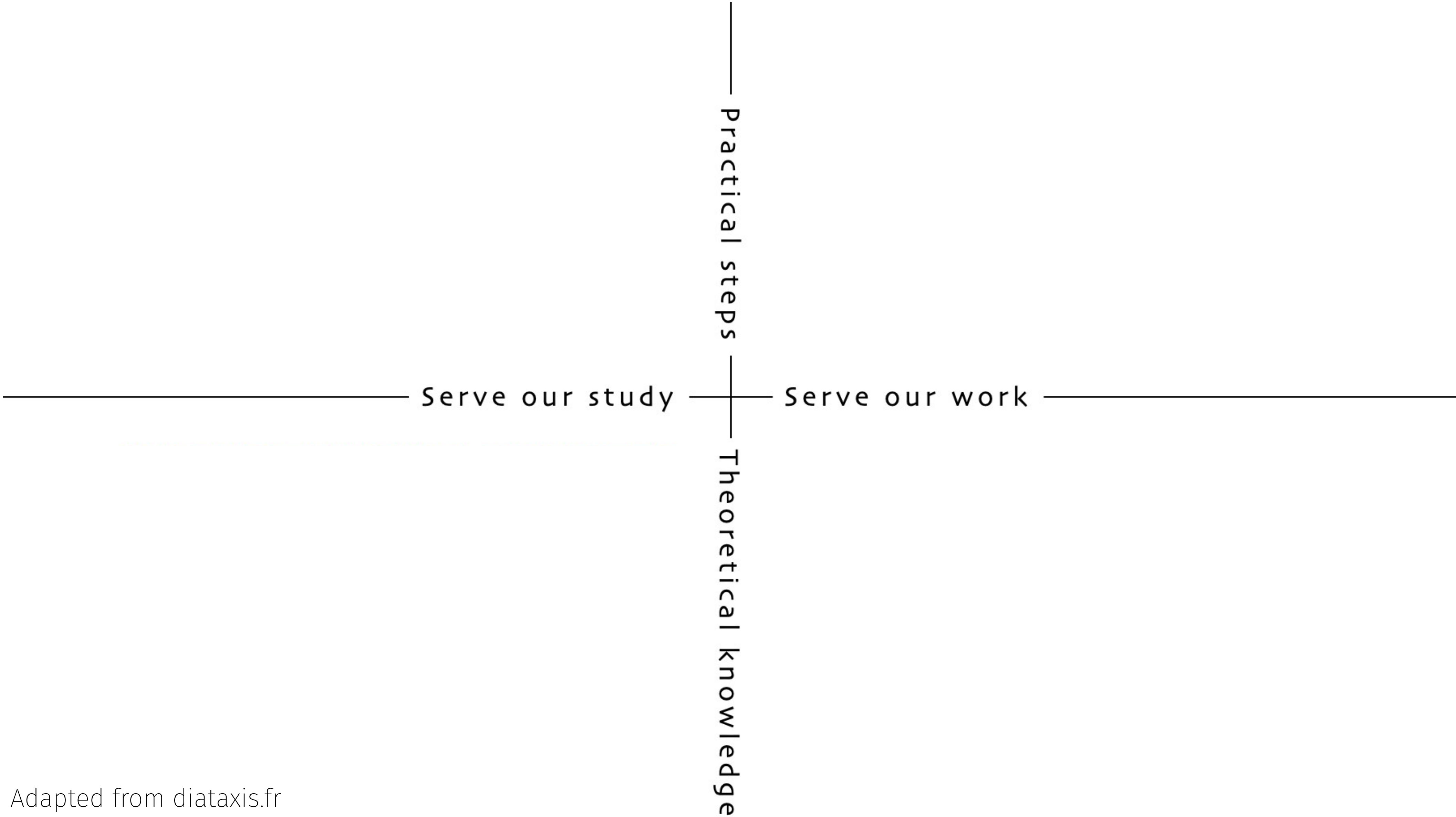
WHILE LEARNING

WHILE DOING



The key idea:

DOCUMENTATION IS NOT ONE THING, AND IS NOT FOR ONE PERSON



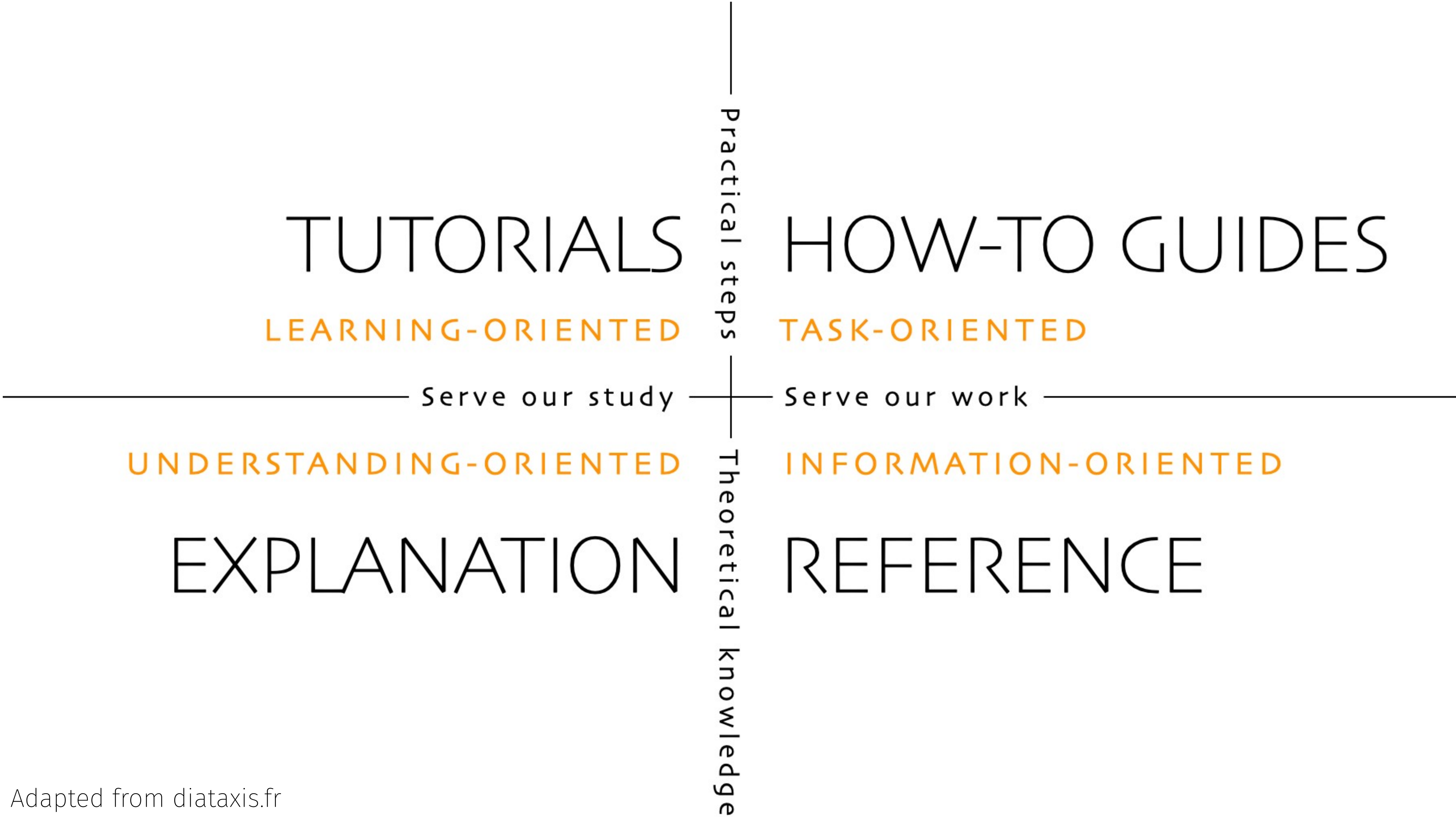
Practical steps

Serve our study

Serve our work

Theoretical knowledge

Adapted from diataxis.fr



Practical steps

TUTORIALS

LEARNING-ORIENTED

HOW-TO GUIDES

TASK-ORIENTED

Serve our study

Serve our work

UNDERSTANDING-ORIENTED

EXPLANATION

INFORMATION-ORIENTED

REFERENCE

Theoretical knowledge

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Practical steps

TO USE

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TO EXTEND

INFORMATION-ORIENTED

REFERENCE

TO USE

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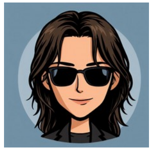
TO LEARN FROM



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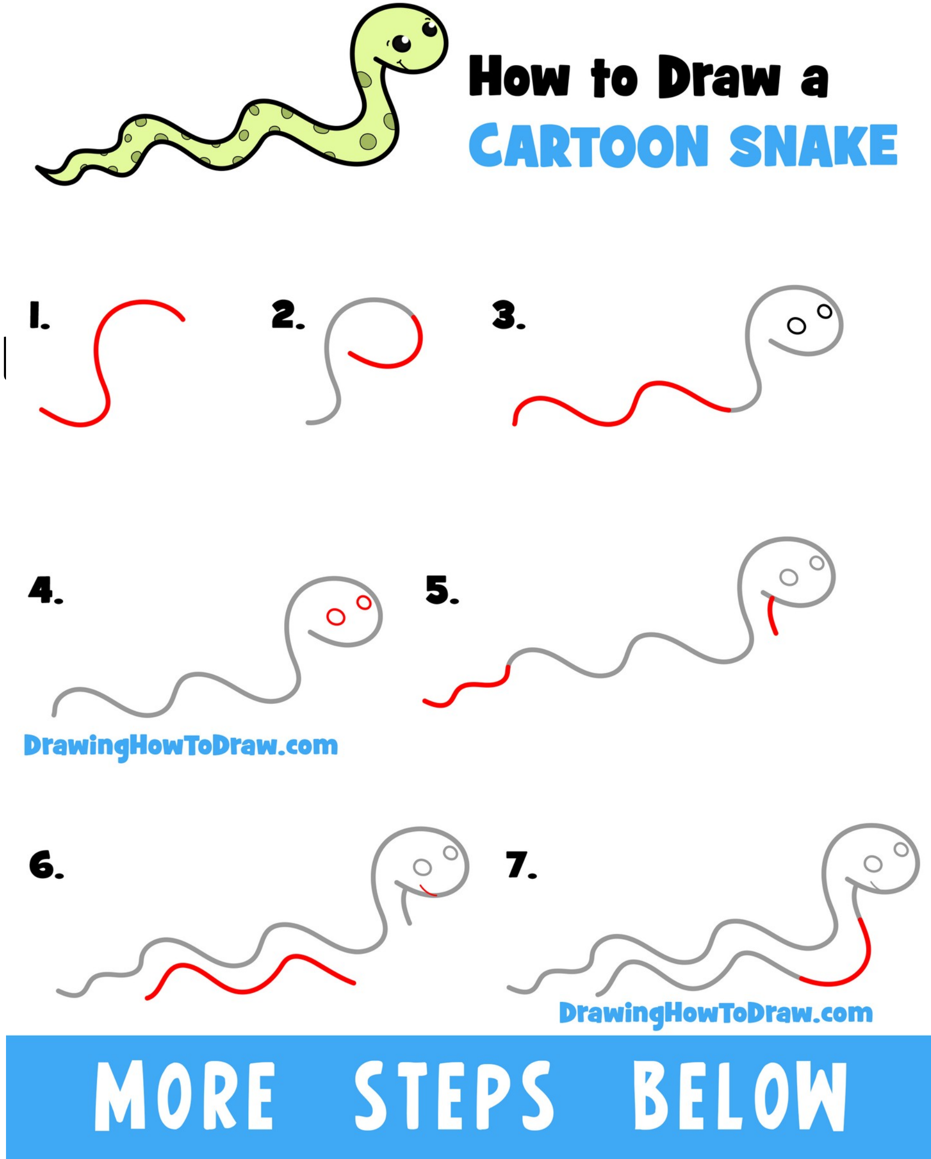
TUTORIALS

GOAL: Get the user started,
provide familiarity with the vocabul

- Provide a complete picture before they start
- Ensure the user sees results immediately
- Describe concrete steps, not abstract concepts
- Offer only minimum, necessary, explanation
- Ignore options and alternatives

Tutorials are learning-oriented



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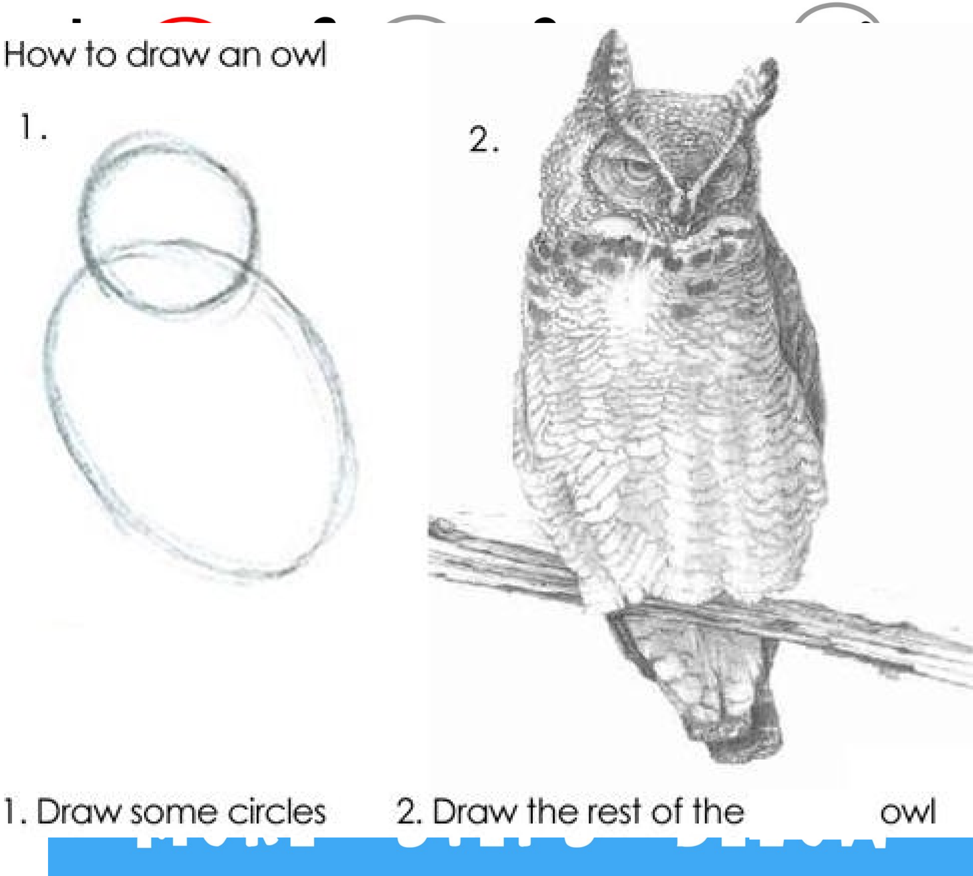

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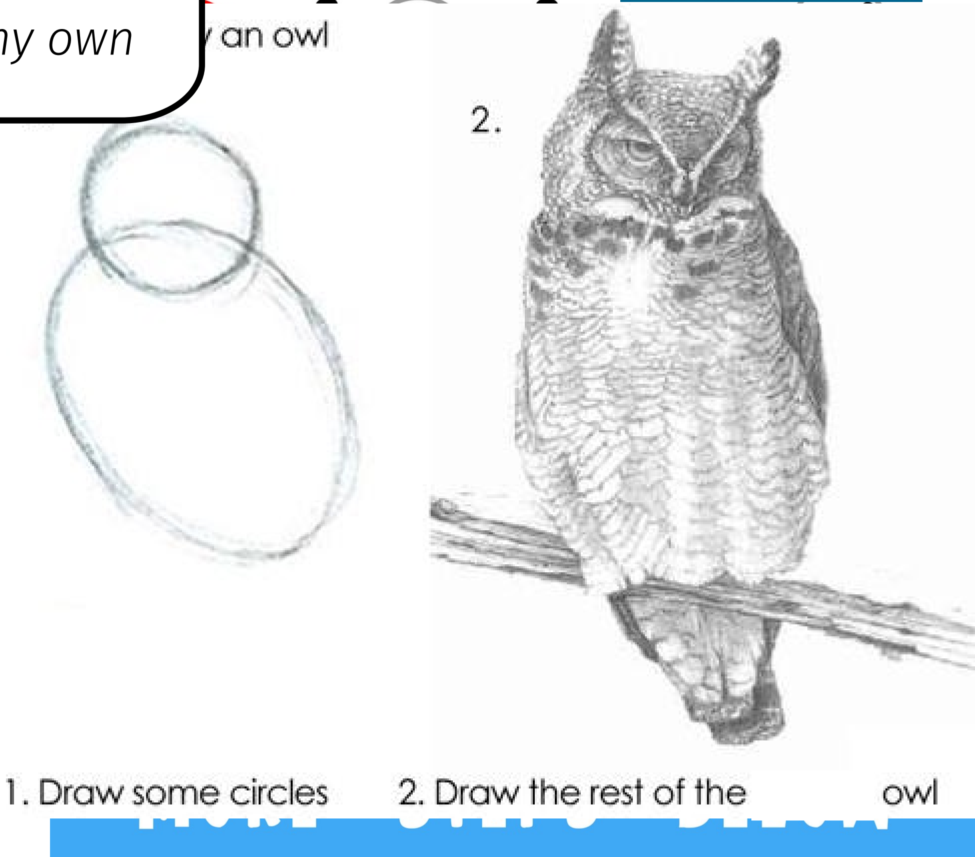
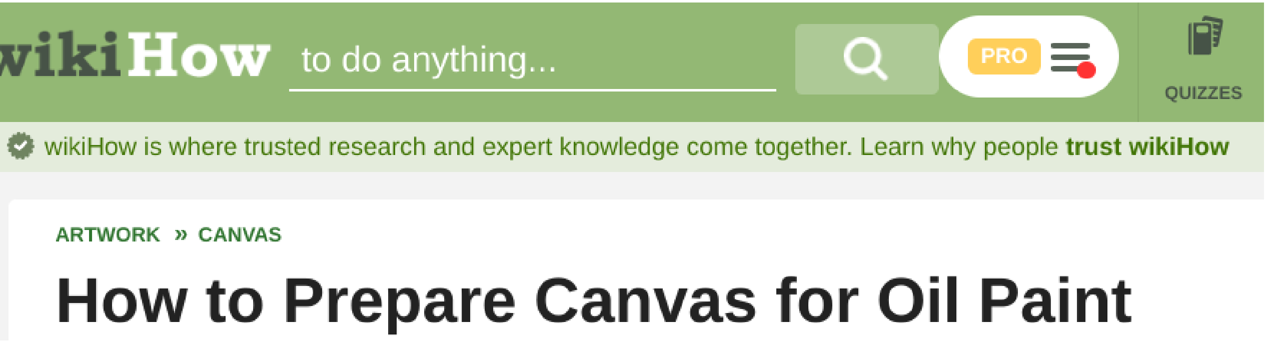
Tutorials are learning-oriented

I like this because it allows me to get familiar with the code on my own



HOW-TO GUIDE



wikiHow is where trusted research and expert knowledge come together. Learn why people **trust wikiHow**

ARTWORK » CANVAS

How to Prepare Canvas for Oil Paint

How to Tie a Tie
1
2
3
4
5
6
7

GOAL: Provide steps to accomplish something

- Describe a sequence of actions
- Solve a problem
- Don’t explain concepts
- Be flexible
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How-to guides are goal oriented

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do anything...
PRO
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ARTWORK » CANVAS
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I like this because I want to use this code for specific scientific applications
1
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HOW-TO GUIDE

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How-to guides are goal oriented

A tool to bridge learning-doing bridge: EXAMPLES

GOAL: Demonstrate real-life usage

- Showcase and provide idiomatic implementations
- Be starting point for typical use cases
- Maintain a pedagogical spirit
- Can be small or large
- Must-have in scientific software

© Arduino

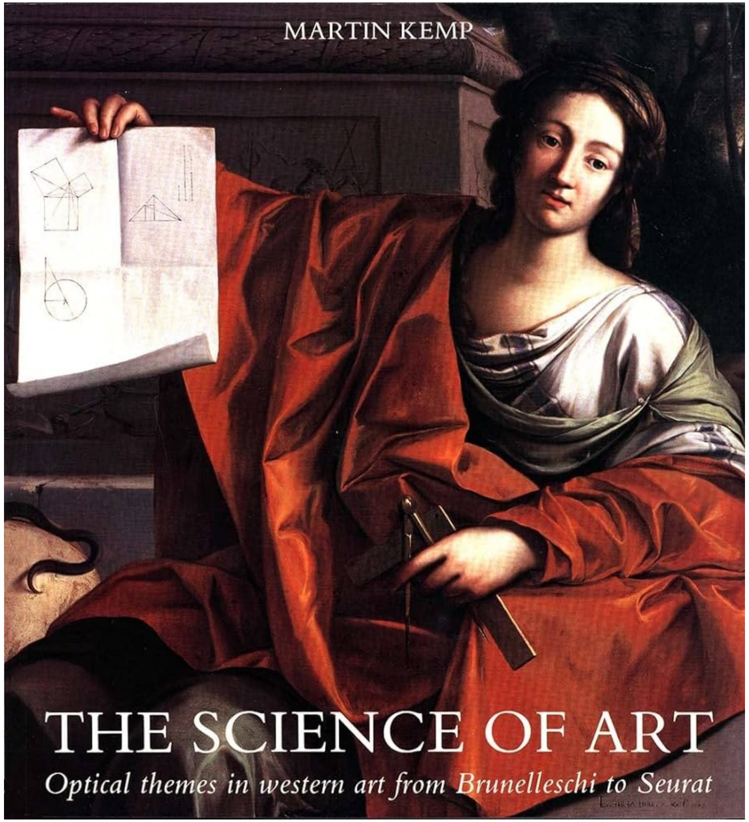
Examples bridge learning and doing

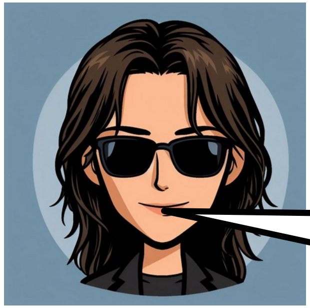
EXPLANATION

GOAL: Provide holistic understanding, Clarify the Whys

- Make connections
- Provide context
- Talk about the subject
- Discuss alternatives and opinions
- Don’t instruct

Explanation is understanding oriented





I like this because it gives me confidence to make large changes

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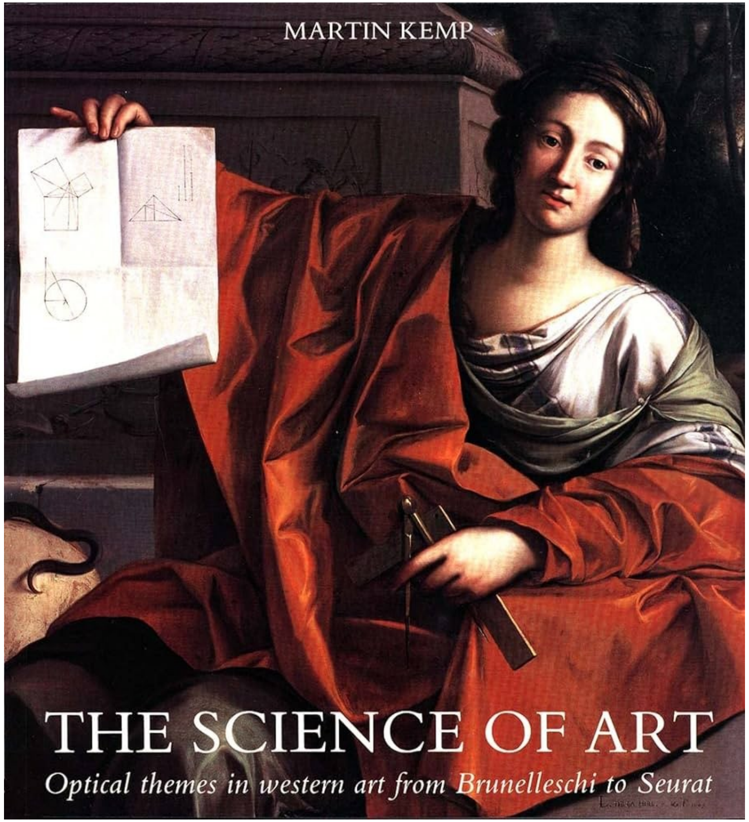
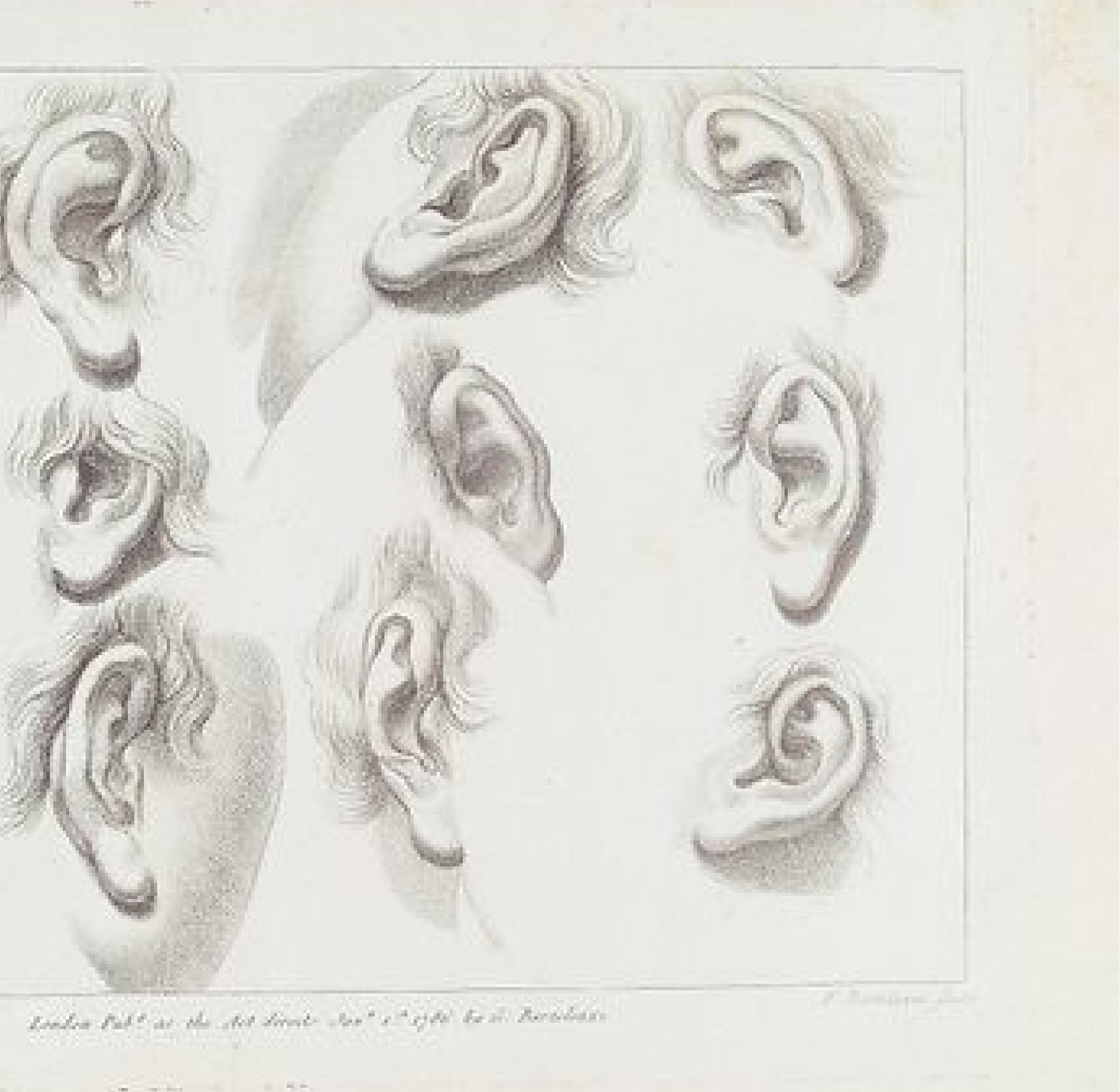


MARTIN KEMP

THE SCIENCE OF ART

Optical themes in western art from Brunelleschi to Seurat

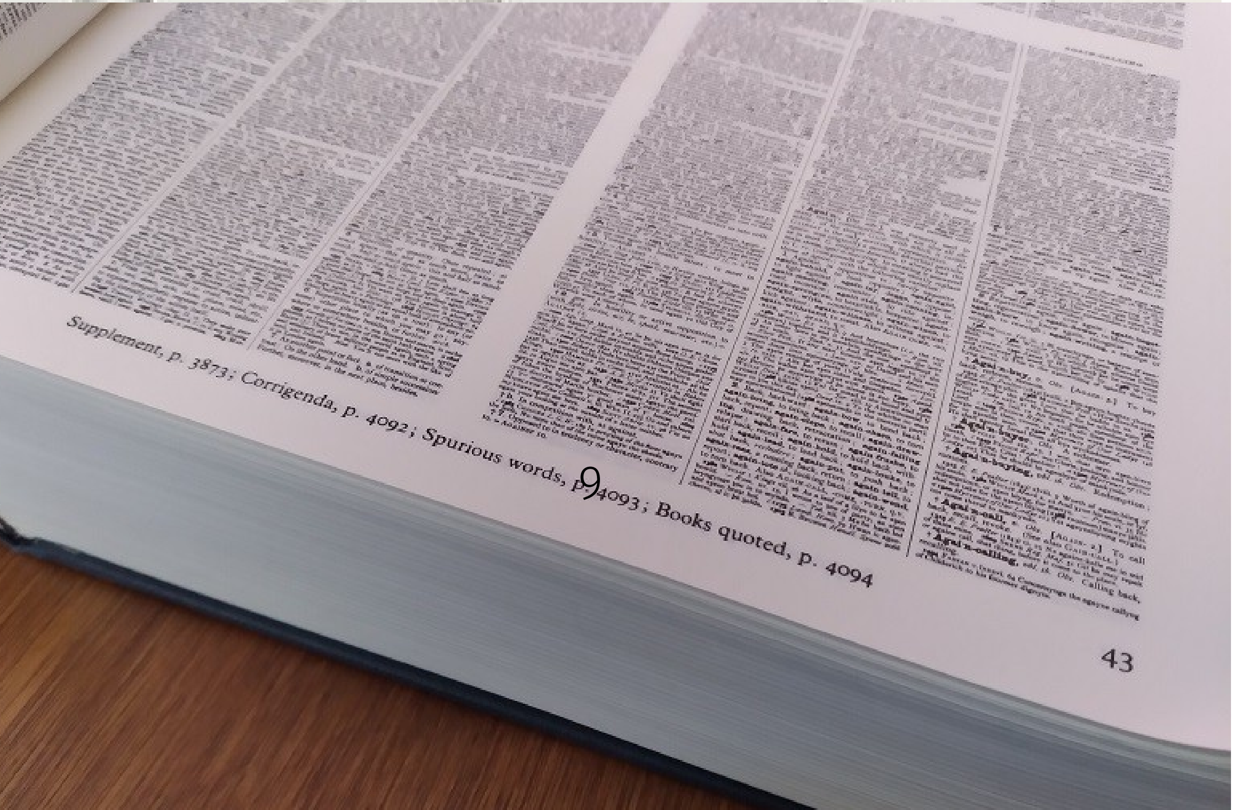


REFERENCE

GOAL: Provide authoritative information on how things are and work

- Do nothing but describe
- Be consistent
- Be accurate

Reference is consultation oriented



Supplement, p. 3873; Corrigenda, p. 4092; Spurious words, p. 4093; Books quoted, p. 4094

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- Function signatures
- Public APIs
- System architecture
- Object hierarchy
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+

REFERENCE for scientific software

- Spell out assumptions, methods, formalism, equations
- Define acronyms
- List and link relevant papers
- List all the working features (in one place)

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I like this because it allows me to get a high-level view on the science

The documentation matrix

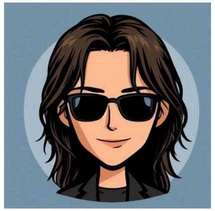
	TUTORIALS	HOW-TO GUIDES	EXPLANATION	REFERENCE
GOAL	Get started, Become familiar	Accomplish a specific task	Build understanding	Describe
ORIENTED TO	Learning	Tasks	Grokking	Consultation
TARGETING	New users	Users	Advanced users/developers	Everyone (+ scientific community)

EXAMPLES

Adapted from diataxis.fr

How to lower the entry barrier to your scientific software

This framework provide natural entry points for **everyone** at **any stage**



Important: This is not the final word!

Frequently Asked Questions

> I only want to spend 15 minutes on documentation, what should I prioritize?

One paragraph where you explain what your code is supposed to accomplish, what input it expects, and what outputs it produces.

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A **features** page/section

- Immediately useful to everyone that is not you
- Clearly identifies what features are supposed to work

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A **features** page/section

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- Clearly identifies what features are supposed to work

> I want to write the best documentation ever, what should I do?

I don't know. Think about the core principles. :)

Assess your project with these at-home tests

The survivability test:

Would someone with reasonable experience be able to independently use and extend my code?

Assess your project with these at-home tests

The survivability test:

Would someone with reasonable experience be able to independently use and extend my code?

The accessibility test:

Would a beginner graduate student be able to use and extend my code with proper guidance?

My call for action

Think of scientific software as a standalone scientific contribution

Design your documentation by keeping in mind that documentation is not one thing and not for one person

Get in touch with me:
gbozzola@caltech.edu
Linkedin: gabrielebozzola