Code Review for Scientific Software

experiences building an online tutorial

Helen Kershaw
DAReS, NSF NCAR

Terminology

BSSwF Better Scientific Software Fellowship

NSF National Science Foundation
NCAR National Center for Atmospheric Research

UCAR University Corporation for Atmospheric Research

SEA Software Engineering Assembly (UCAR/NCAR)

DART Data assimilation Research Testbed

DAReS Data Assimilation Research Section

AMS American Meteorological Society

Goals

- Tell you about my BSSwF project
- Share my experience building the tutorial
- Share practice and experience with code review from UCAR SEA

Goals

- Tell you about my BSSwF project
- Share my experience building the tutorial
- Share practice and experience with code review from UCAR SEA

- Get you to think about code review

Goals

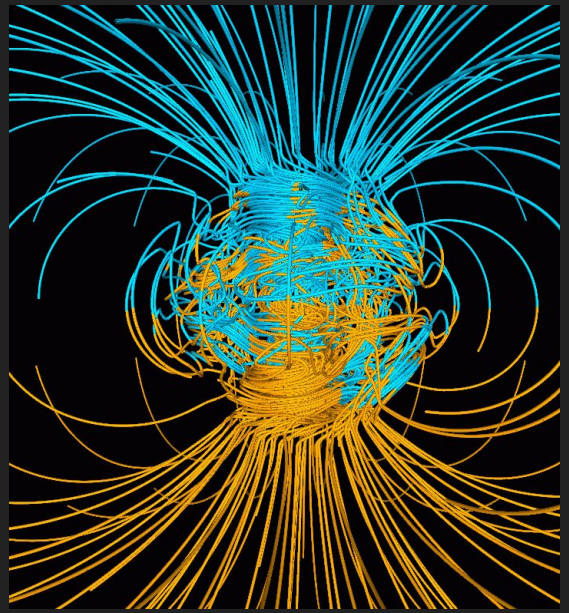
- Tell you about my BSSwF project
- Share my experience building the tutorial
- Share practice and experience with code review from UCAR SEA

- Get you to think about code review
- And the joy of open source software

About me

hkershaw@ucar.edu

About me



The Core ›

2003 · 2h 15min · PG-13

Action · Adventure · Sci-Fi

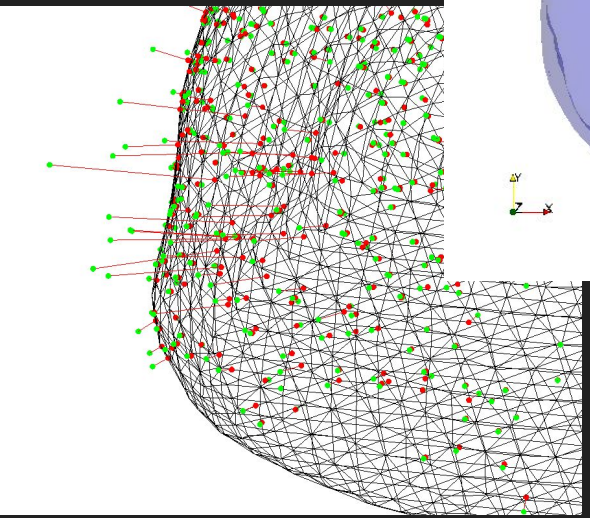
★ 5.5/10 ☆Rate

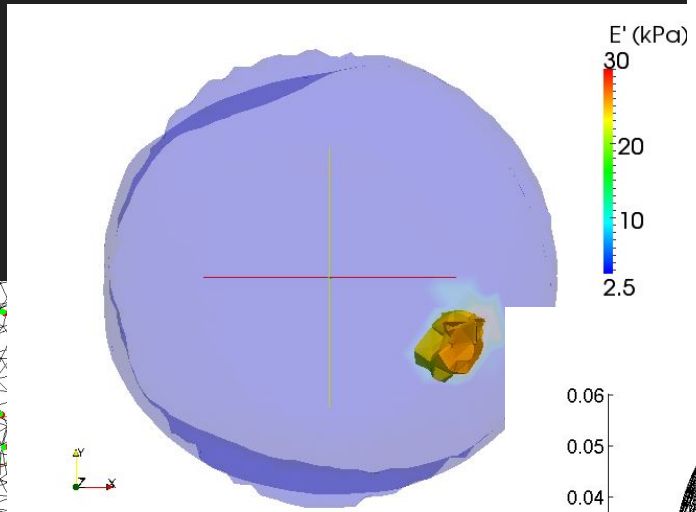
The only way to save Earth from catastrophe is to drill down to the core and set it spinning again.

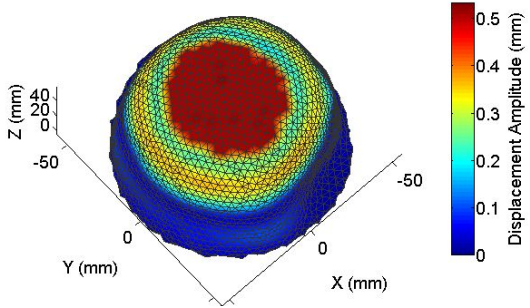
Jonathan Mound's credits: Additional Crew (as Dr. Jonathan Mound)

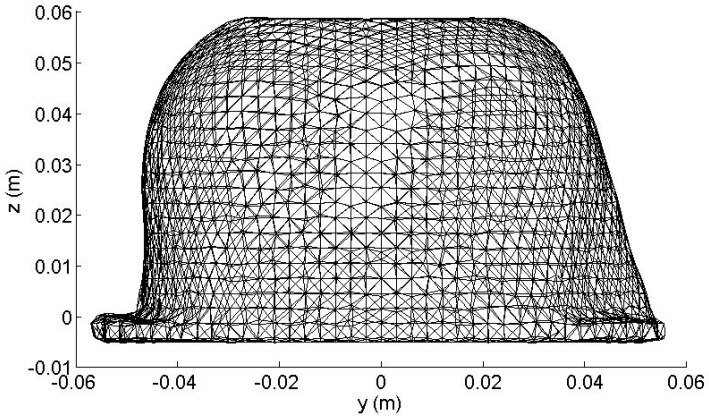
▶ Trailer + Watchlist

About me

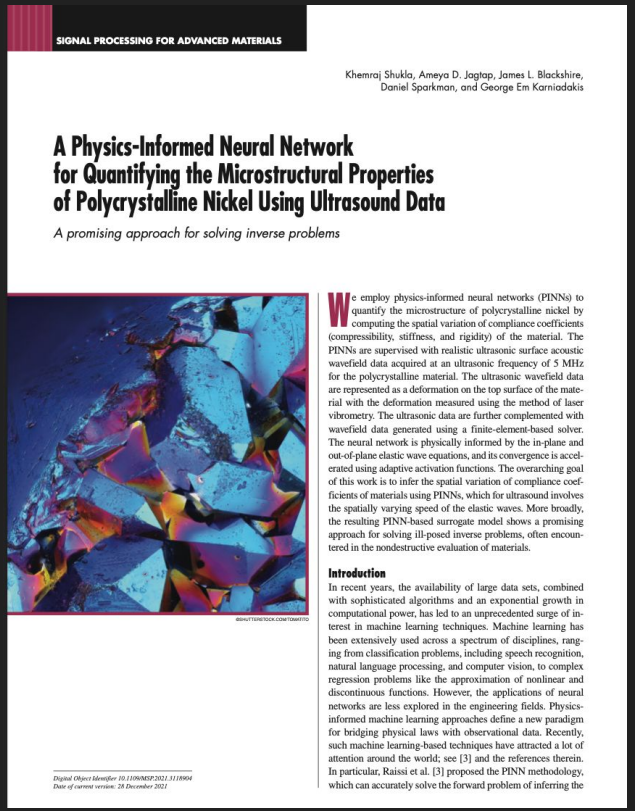



E' (kPa)
30
20
10
2.5


Z (mm)
40
20
0
-50
0
Y (mm)
-50
0
X (mm)
0.5
0.4
0.3
0.2
0.1
0
Displacement Amplitude (mm)


0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
z (m)
-0.06
-0.04
-0.02
0
0.02
0.04
0.06
y (m)

About me



SIGNAL PROCESSING FOR ADVANCED MATERIALS

Khemraj Shukla, Ameya D. Jagtap, James L. Blackshire, Daniel Sparkman, and George Em Karniadakis

A Physics-Informed Neural Network for Quantifying the Microstructural Properties of Polycrystalline Nickel Using Ultrasound Data

A promising approach for solving inverse problems

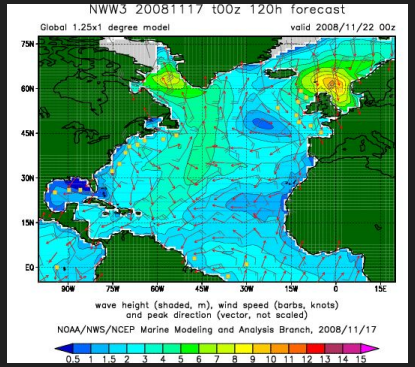
We employ physics-informed neural networks (PINNs) to quantify the microstructure of polycrystalline nickel by computing the spatial variation of compliance coefficients (compressibility, stiffness, and rigidity) of the material. The PINNs are supervised with realistic ultrasonic surface acoustic wavefield data acquired at an ultrasonic frequency of 5 MHz for the polycrystalline material. The ultrasonic wavefield data are represented as a deformation on the top surface of the material with the deformation measured using the method of laser vibrometry. The ultrasonic data are further complemented with wavefield data generated using a finite-element-based solver. The neural network is physically informed by the in-plane and out-of-plane elastic wave equations, and its convergence is accelerated using adaptive activation functions. The overarching goal of this work is to infer the spatial variation of compliance coefficients of materials using PINNs, which for ultrasound involves the spatially varying speed of the elastic waves. More broadly, the resulting PINN-based surrogate model shows a promising approach for solving ill-posed inverse problems, often encountered in the nondestructive evaluation of materials.

Introduction

In recent years, the availability of large data sets, combined with sophisticated algorithms and an exponential growth in computational power, has led to an unprecedented surge of interest in machine learning techniques. Machine learning has been extensively used across a spectrum of disciplines, ranging from classification problems, including speech recognition, natural language processing, and computer vision, to complex regression problems like the approximation of nonlinear and discontinuous functions. However, the applications of neural networks are less explored in the engineering fields. Physics-informed machine learning approaches define a new paradigm for bridging physical laws with observational data. Recently, such machine learning-based techniques have attracted a lot of attention around the world; see [3] and the references therein. In particular, Raissi et al. [3] proposed the PINN methodology, which can accurately solve the forward problem of inferring the

Digital Object Identifier 10.1109/MSP.2021.3118904
Date of current version: 28 December 2021

US RSE



A zebrafish model for calcineurin-dependent brain function

Sara Tucker Edmister [1], Rahma Ibrahim [1], Rohit Kakodkar [2], Jill A Kreiling [1], Robbert Creton [3]

Affiliations + expand

PMID: 34425181 PMCID: PMC8903086 DOI: 10.1016/j.bbr.2021.113544

Free PMC article

Full text links Cite

DART

Data Assimilation Research Testbed

Cross-lab

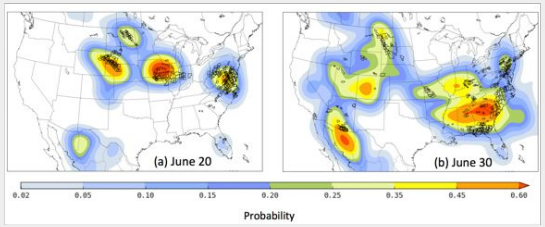
Cross-institution

Cross-country

Cross-world

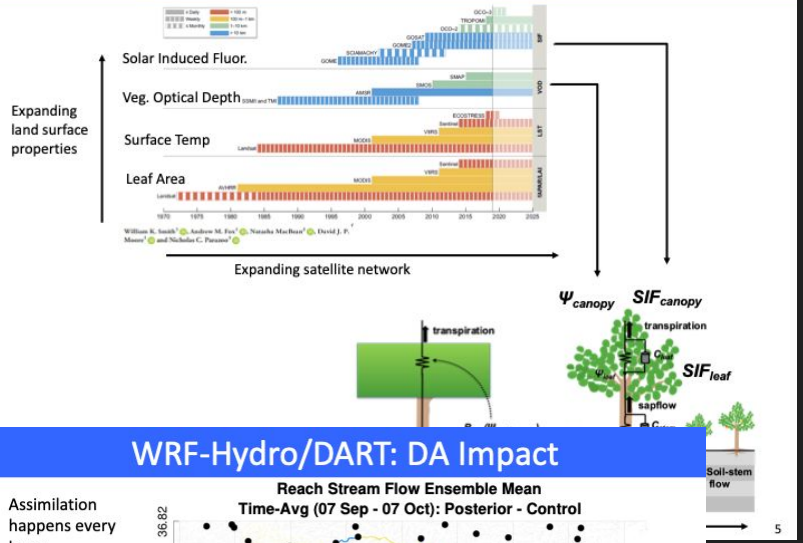
NCAR Real-time ensemble prediction system

Severe weather forecast for *two* days compared to NWS warnings

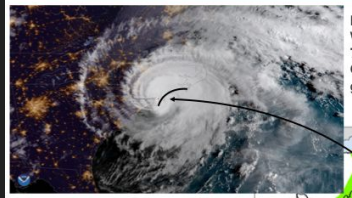


- WRF, 10 member ensemble, GFS for boundary conditions
- Continuous operation from April 2015 to December 2017
- 48 hour forecasts at 3km resolution
- First continuously cycling ensemble system for CONUS
- CISL Dedicated Queues and Computing Support were Vital

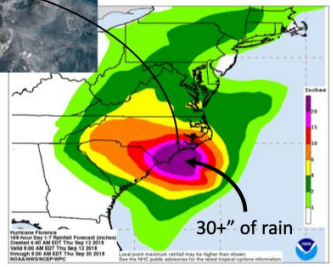
Advancing models & observations together



WRF-Hydro/DART: Florence 2018



Hurricane Florence made landfall near Wrightsville Beach, North Carolina at **7:15 a.m. ET September 14**. The GOES East satellite captured this geocolor image at 7:45 a.m. ET

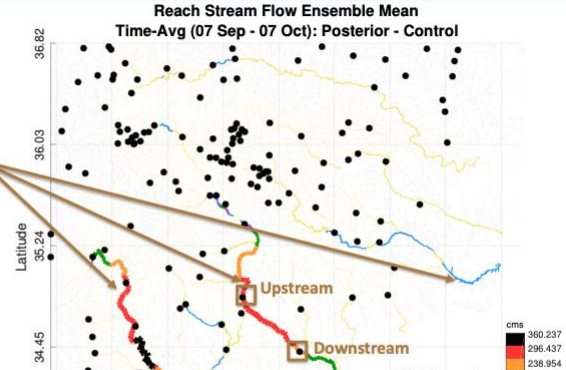


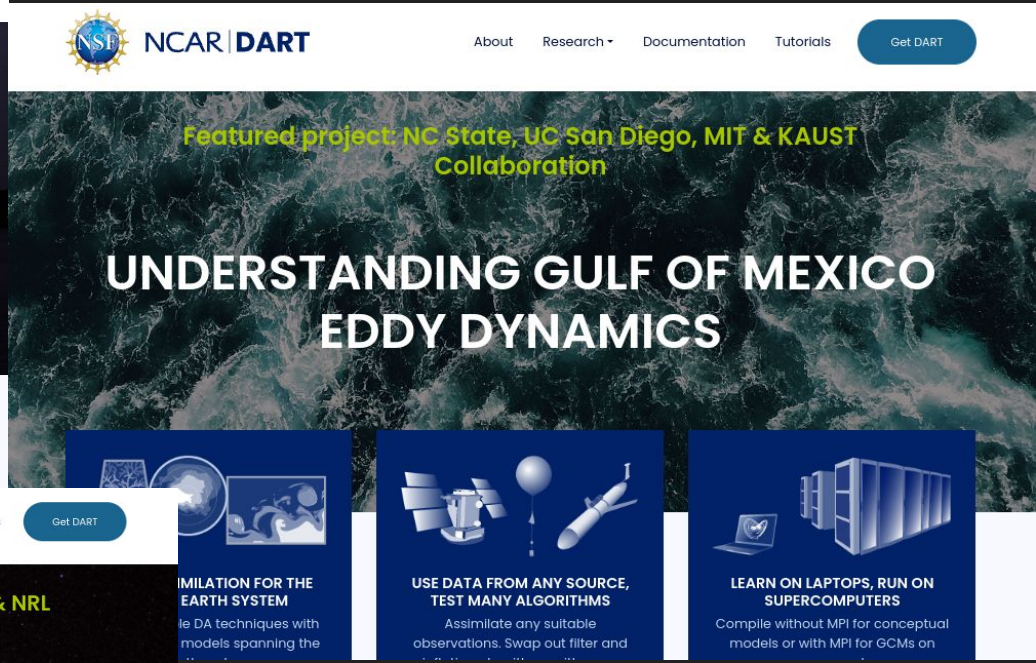
Winds up to 150 mph (240 km/hr)
Damage: $24.23 billion
NOAA/NWS/NCEP/WPC

WRF-Hydro/DART: DA Impact

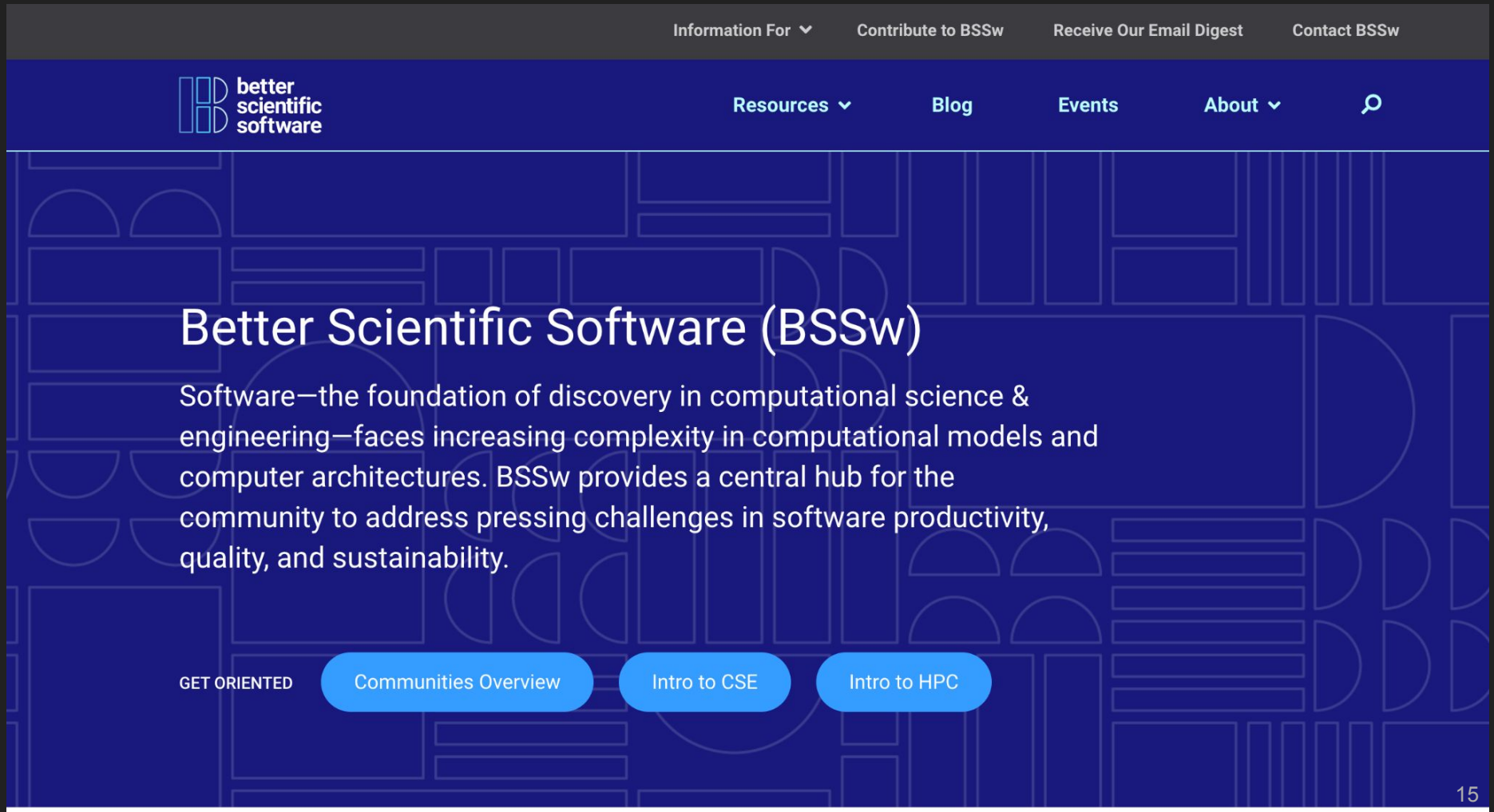
Assimilation happens every hour

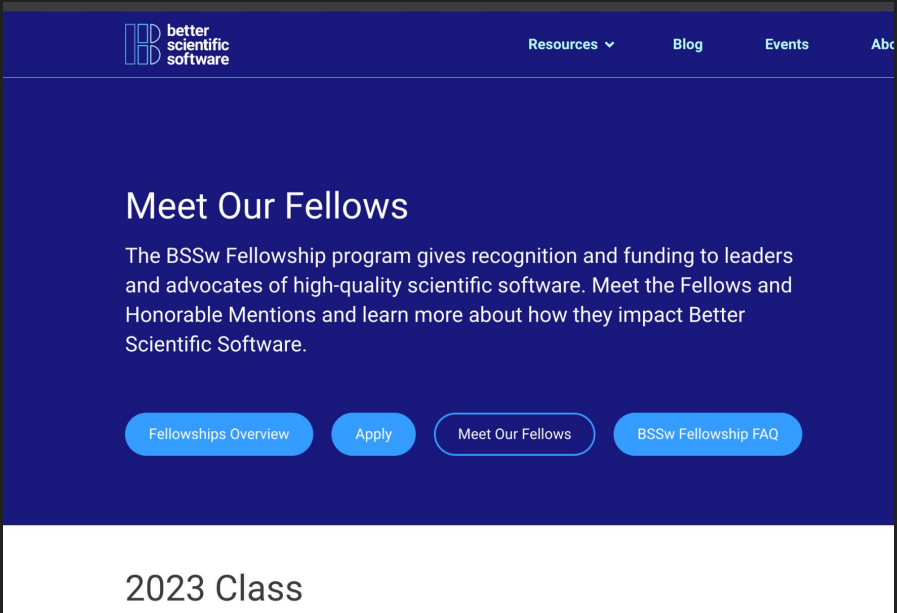
Correction along major reaches. DA is adding water to the stream channels.

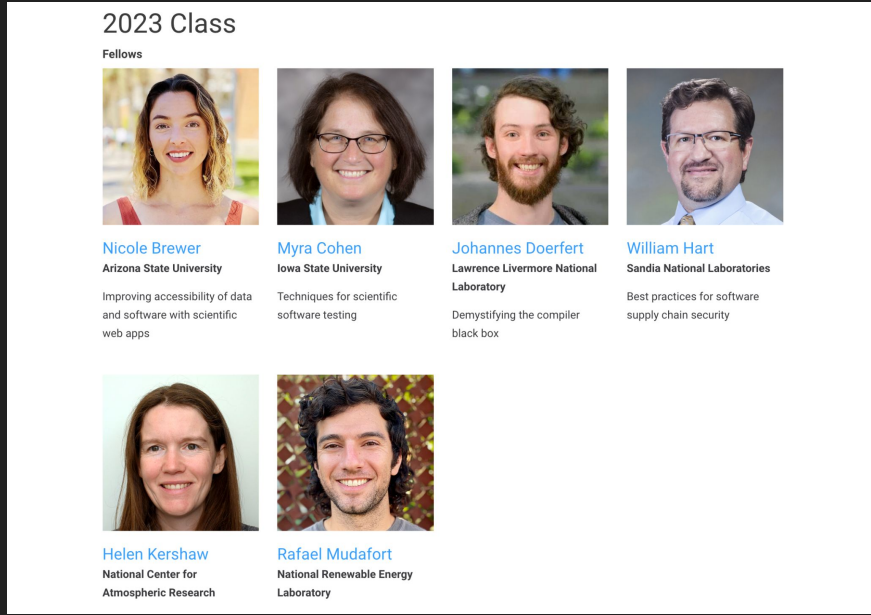




dart.ucar.edu

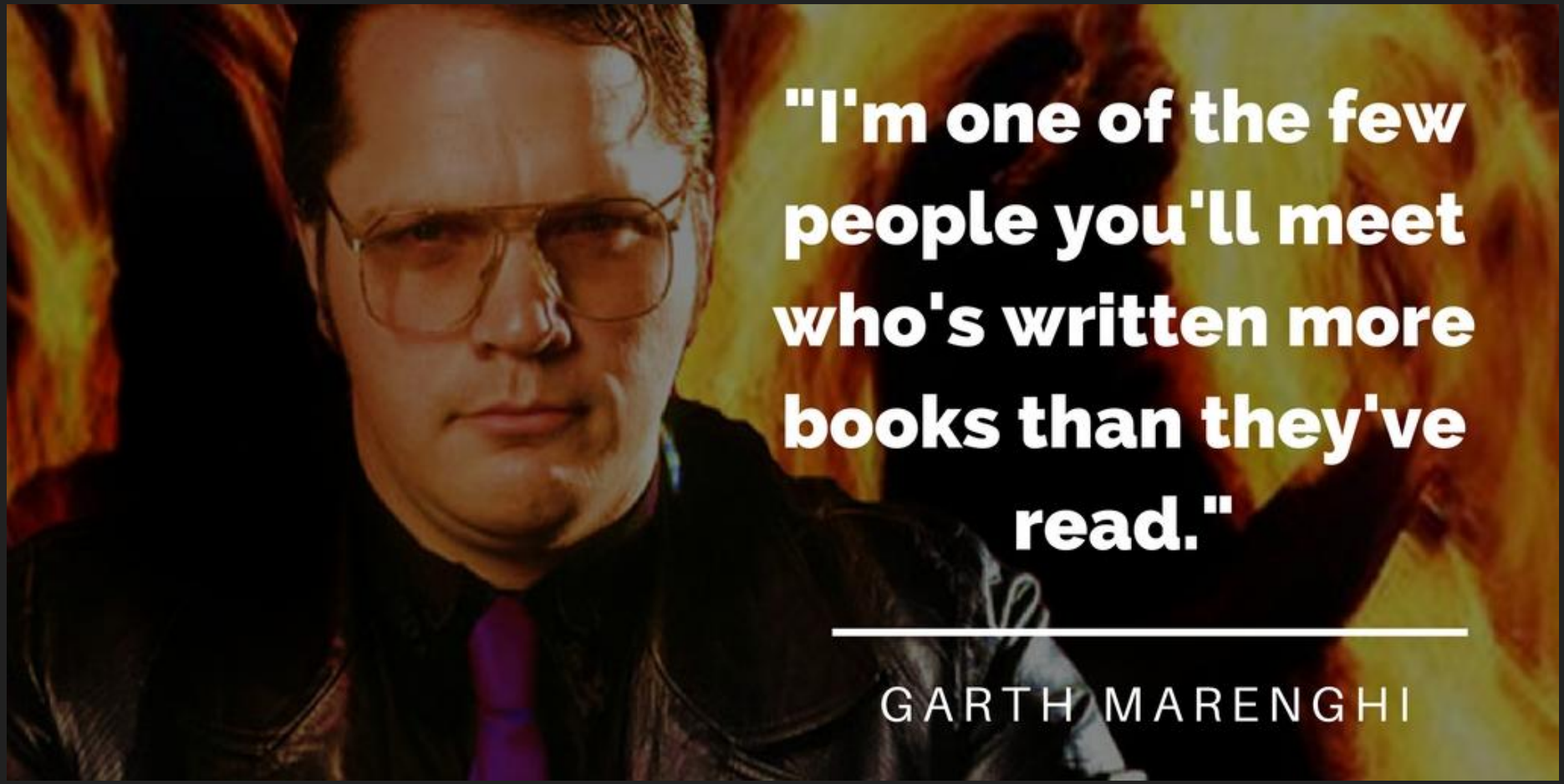

Information For
Contribute to BSSw
Receive Our Email Digest
Contact BSSw
better scientific software
Resources
Blog
Events
About
Better Scientific Software (BSSw)
Software—the foundation of discovery in computational science & engineering—faces increasing complexity in computational models and computer architectures. BSSw provides a central hub for the community to address pressing challenges in software productivity, quality, and sustainability.
GET ORIENTED
Communities Overview
Intro to CSE
Intro to HPC





https://bssw.io/pages/meet-our-fellows

What problem am I trying to solve?



https://www.channel4.com/programmes/garth-marenghis-darkplace 2004

code-review.org

What outcomes would I like to see?

Outcomes

- People reviewing early and often
- People reviewing each others code
- Comfortable with napkin explanations of code
- Become a better reviewer
- Better code
- Take a look inside
- More open source contributors!

Outcomes

- People reviewing early and often
- People reviewing each others code
- Comfortable with napkin explanations of code
- Become a better reviewer
- Better code
- Take a look inside
- More open source contributors! *Ulterior Motive*

Onboard new contributors to DART

Onboard new contributors to DART

But not be specific to DART

Code review is a skill

Learning several things at once

- The mechanics of git and GitHub
- A new programming language
- New science
- Culture of new team

Learning several things at once

- The mechanics of git and GitHub
- A new programming language
- New science
- Culture of new team

Seasoned professional

Early career

Learning several things at once

- The mechanics of git and GitHub
- A new programming language
- New science
- Culture of new team
- And code review

Seasoned professional

Early career

The Tutorial

code-review.org

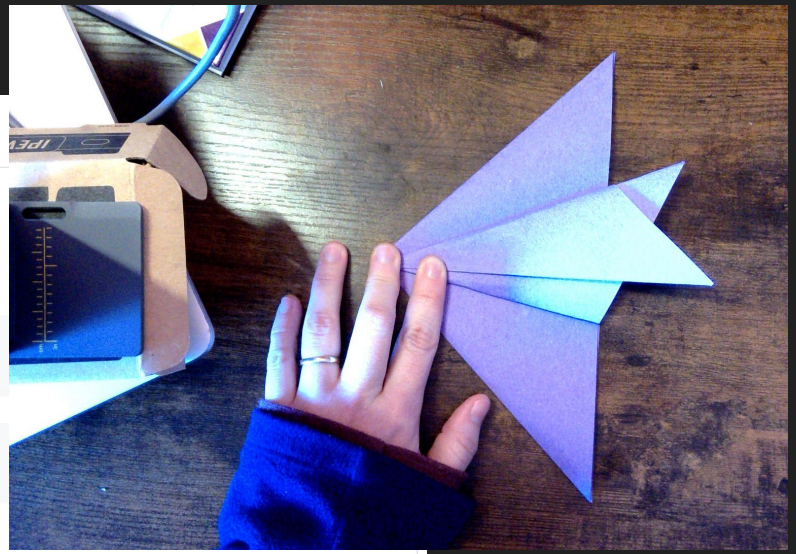
The Tutorial

Three sets of exercises

- No code
- Python
- Fortran

No code exercises

- Cake recipe
- Article on the women's world cup
- Origami instructions to make a fish



Text Exercise 1: Cake recipe

People have reported several problems with a recipe

Some examples of user feedback:

```
Worst Chocolate Cake ever! Not even chocolatey
```

```
Yuk! salty
```

Take a look at the recipe cake.md.

- Are there any problems?

The Tutorial

Three sets of exercises

- No code
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- Fortran

The Tutorial

Three sets of exercises

- No code
- Python
- Fortran

The Tutorial

Three sets of exercises

- No code
- Python
- Fortran

- Issue + prompts
- Pull request + prompts

Setting up the tutorial on GitHub

Code Review Tutorial Blog Get Involved Search docs... Ctrl + /

WELCOME
SETUP THE TUTORIAL
Set up the Tutorial on GitHub
Create the Exercises
EXERCISES
REVIEWING TIPS
HELP

Set up the Tutorial on GitHub

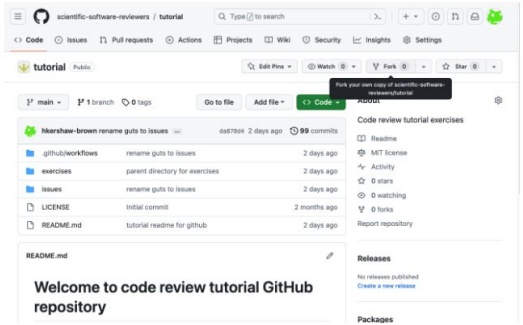
To do the tutorial exercises interactively you will need a GitHub account.

If you are not ready to setup a GitHub account and run workflows, a 'take-a-look' repository with the exercise issues and pull requests is available at take-a-look. You can follow along with the tutorial and read the issues and pull requests without having to run your own GitHub actions. Skip head to the exercises.

For those working through the exercises, this setup guide will take you though forking the tutorial, enabling issues, setting read and write permissions for workflows, and switching on workflows.

Fork the tutorial repository

The tutorial repository is github.com/scientific-software-reviewers/tutorial

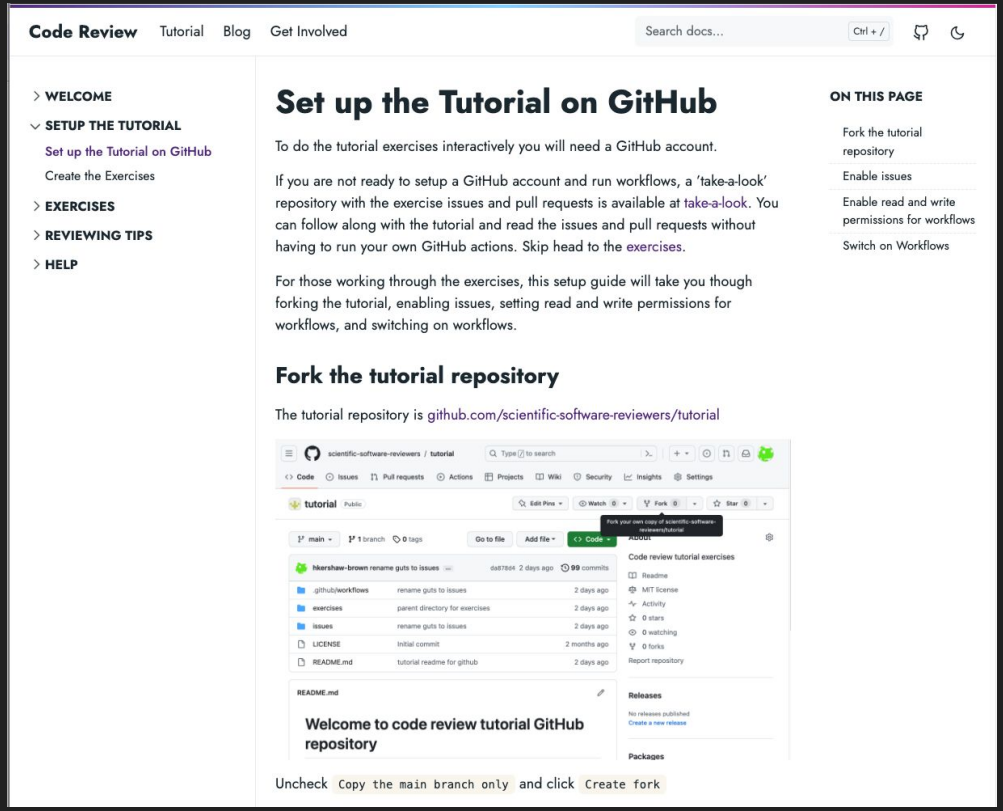


Uncheck `Copy the main branch only` and click `Create fork`

ON THIS PAGE

- Fork the tutorial repository
- Enable issues
- Enable read and write permissions for workflows
- Switch on Workflows

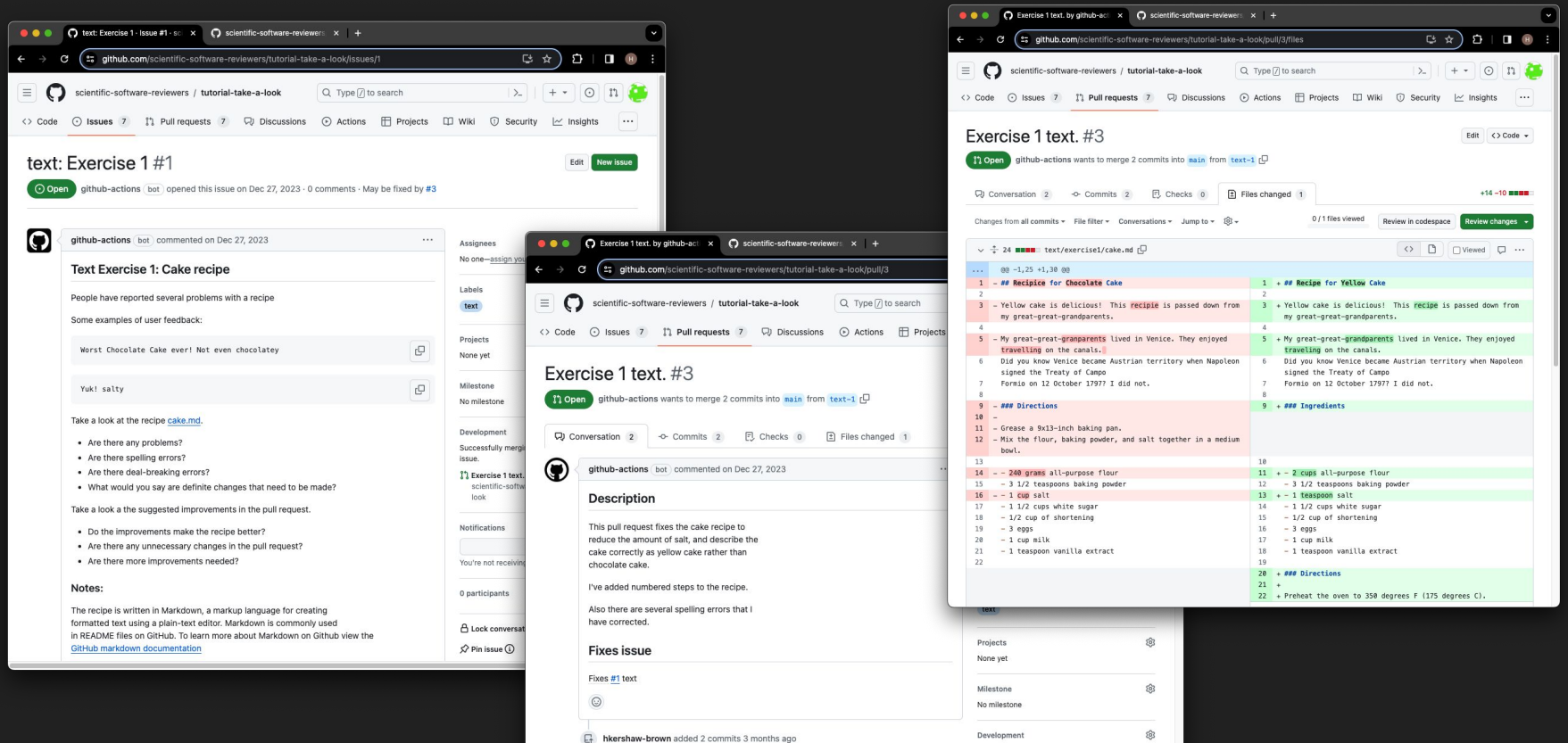
- Fork
- All branches
- Enable workflows
- …



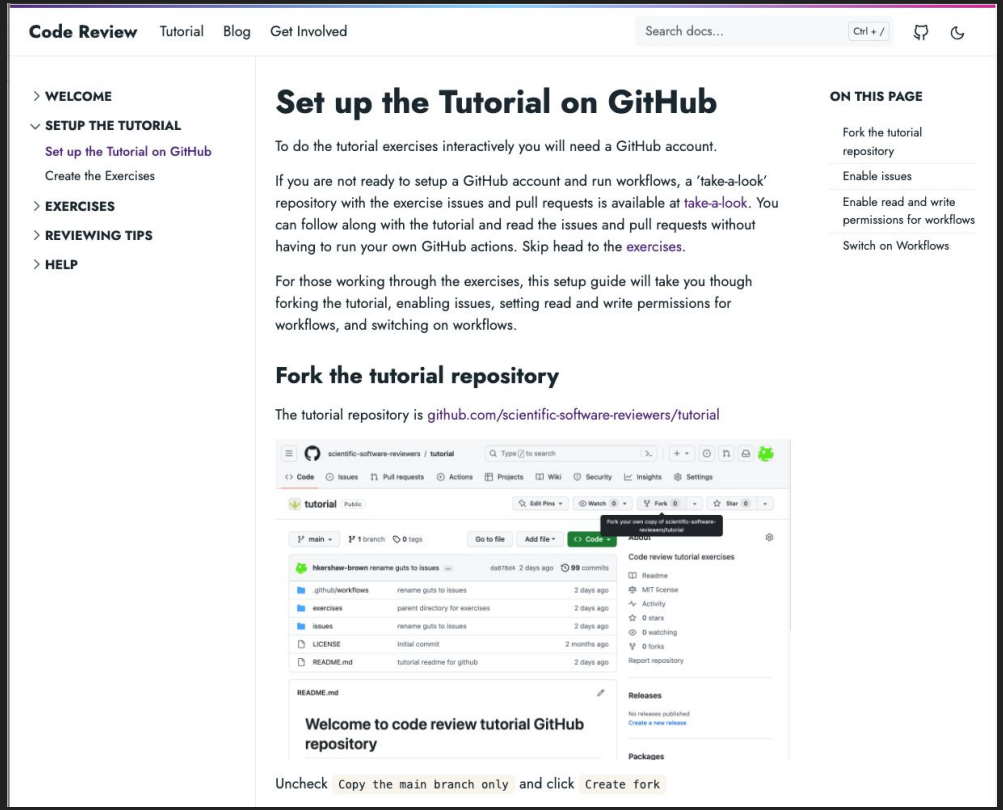
- Fork
- All branches
- Enable workflows
- …

Barrier before I've started

take-a-look repository

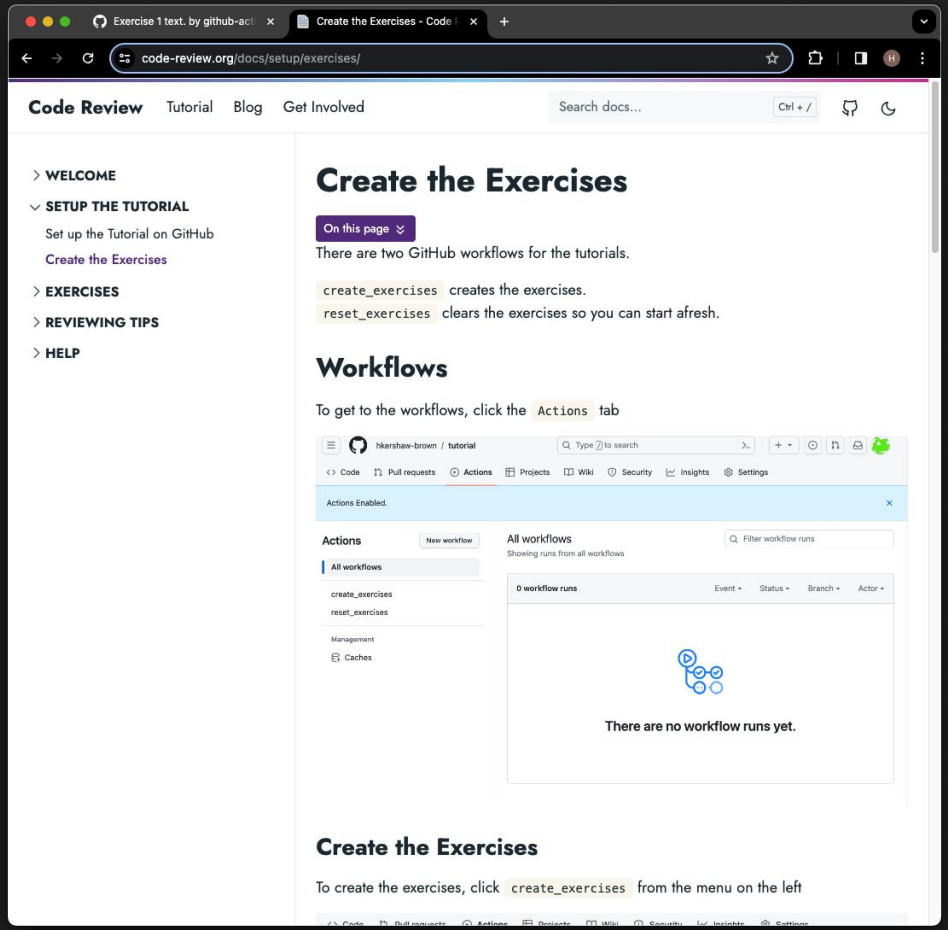


Setting up the tutorial on GitHub



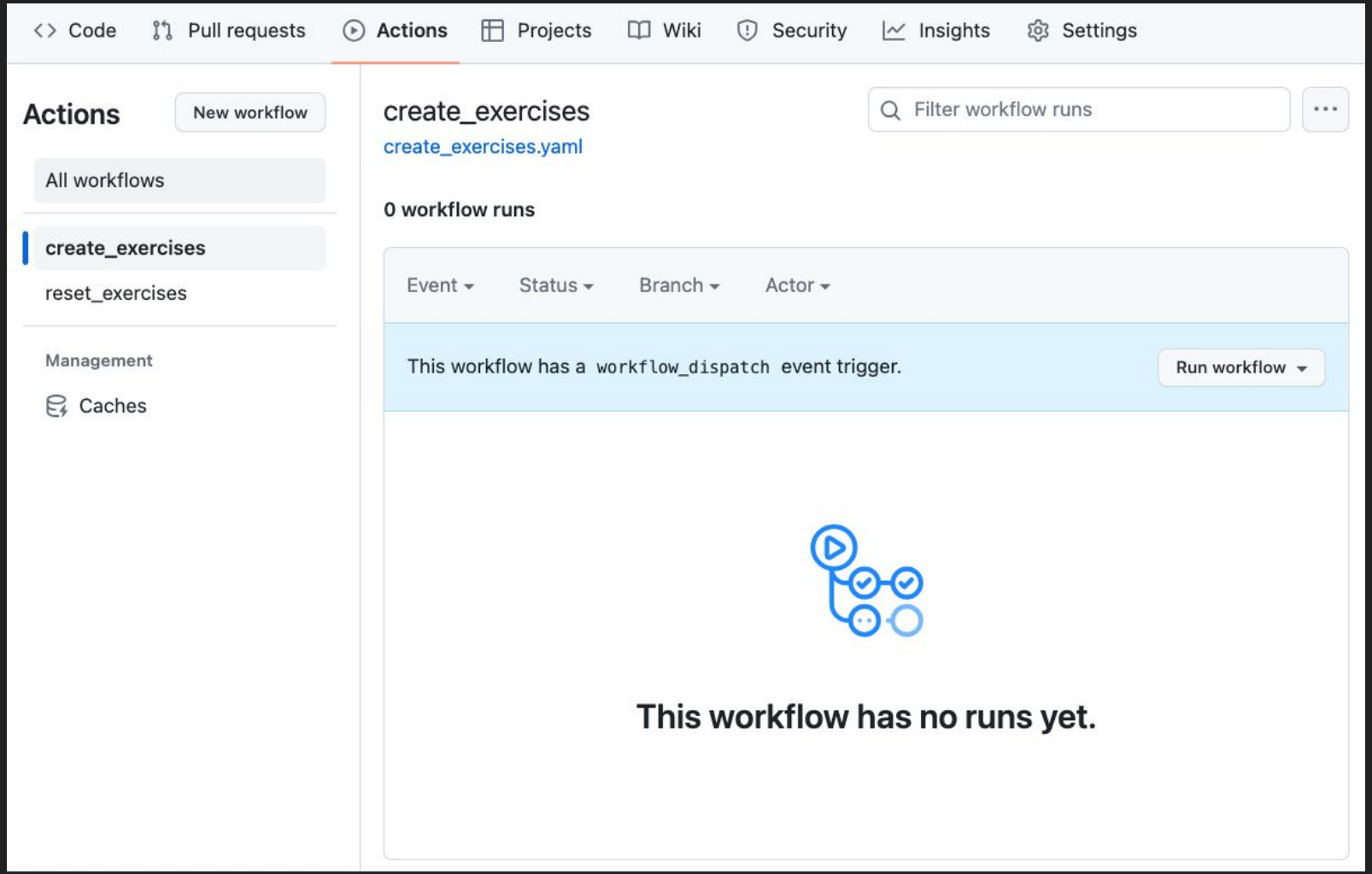
- Fork
- All branches
- Enable workflows
- Run workflows

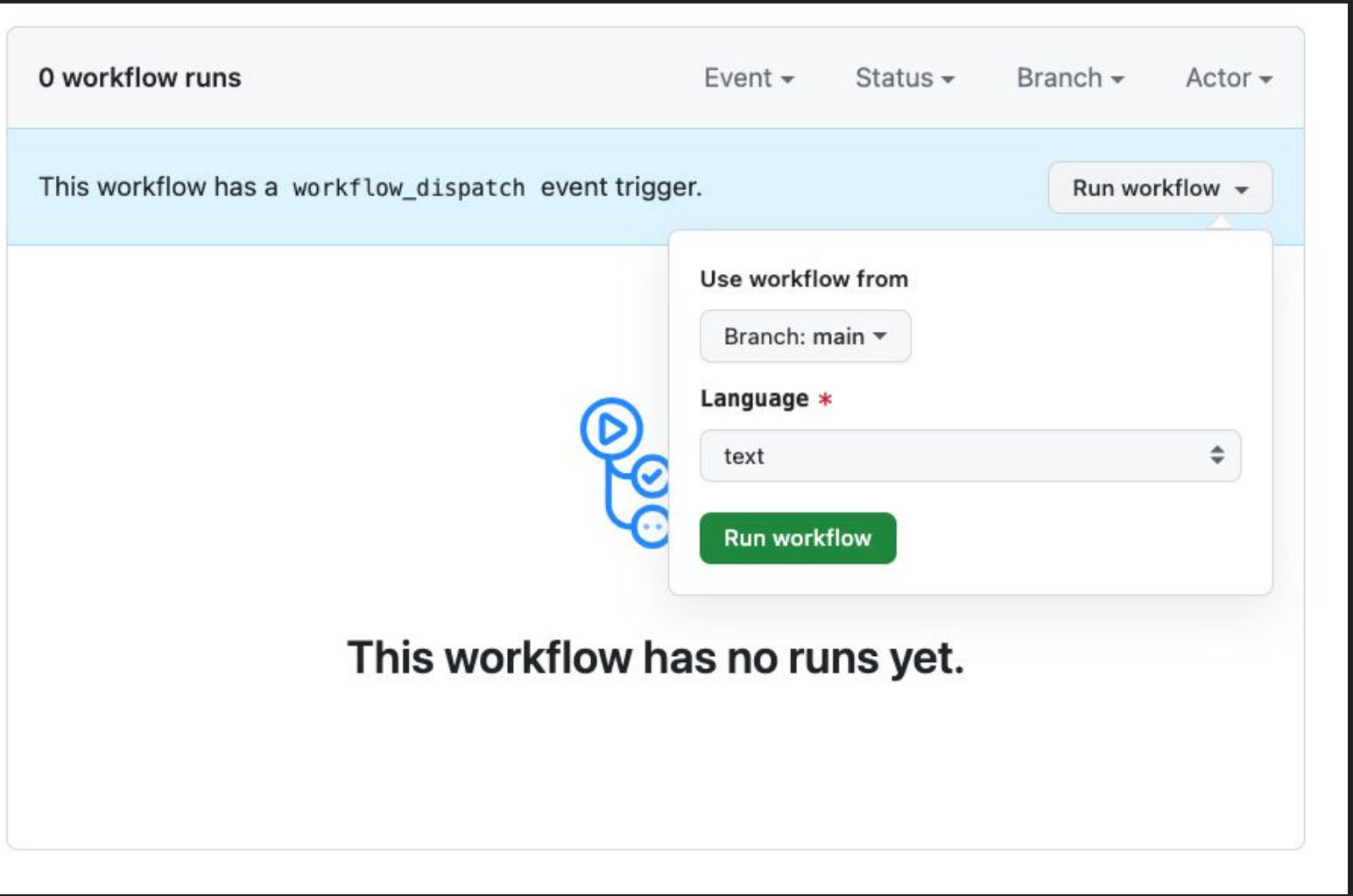
Setting up the tutorial on GitHub

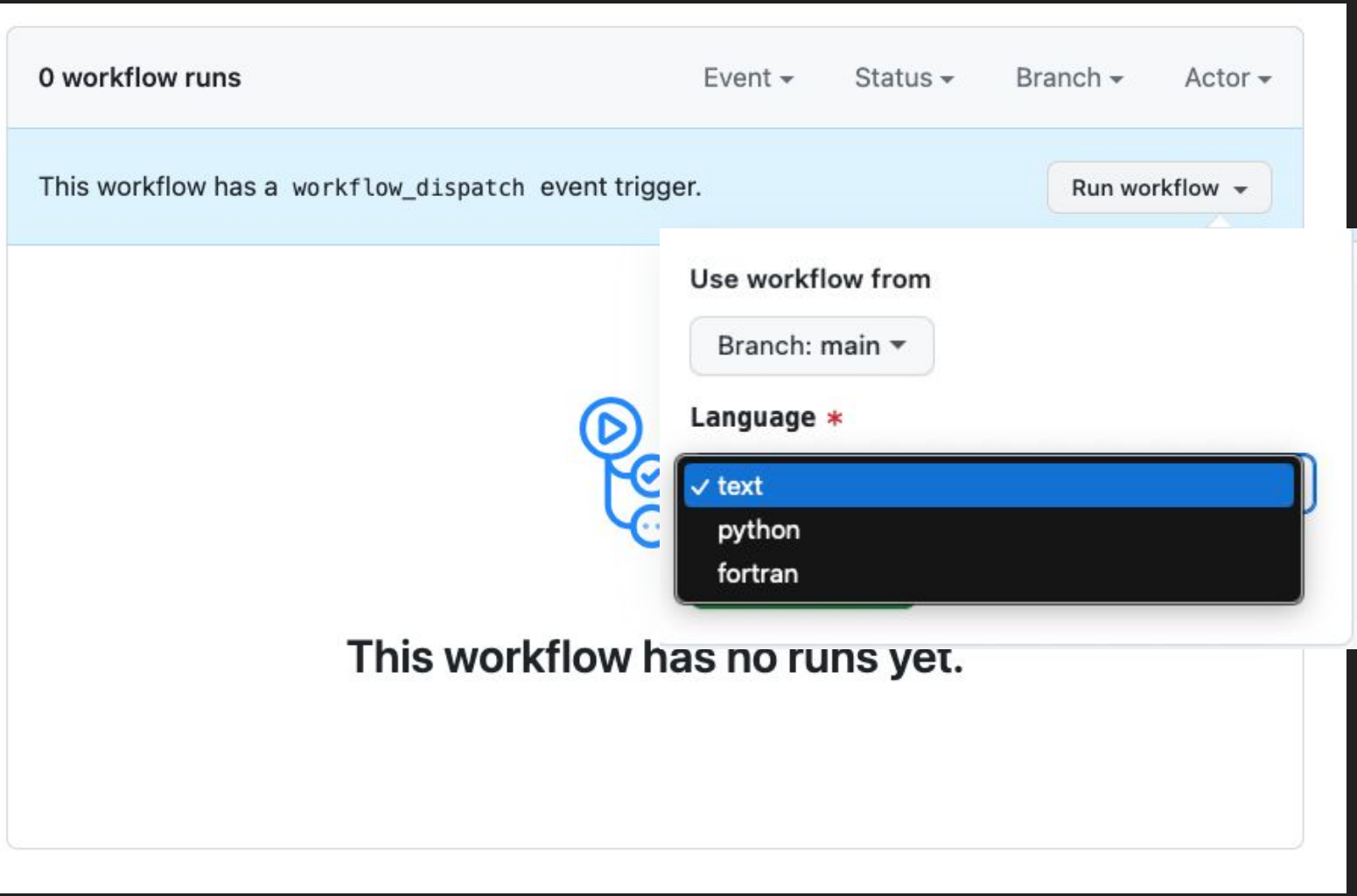


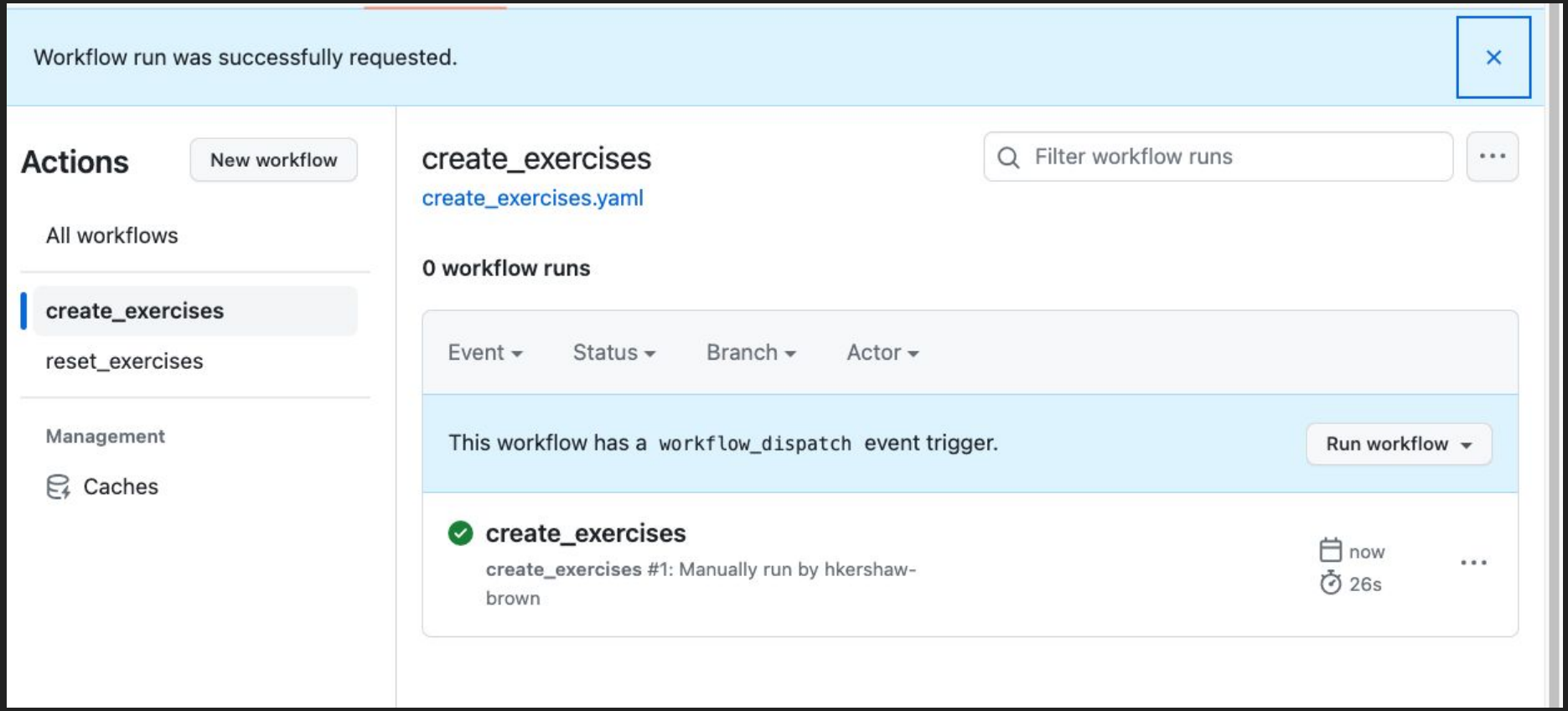
- Fork
- All branches
- Enable workflows
- Run workflows

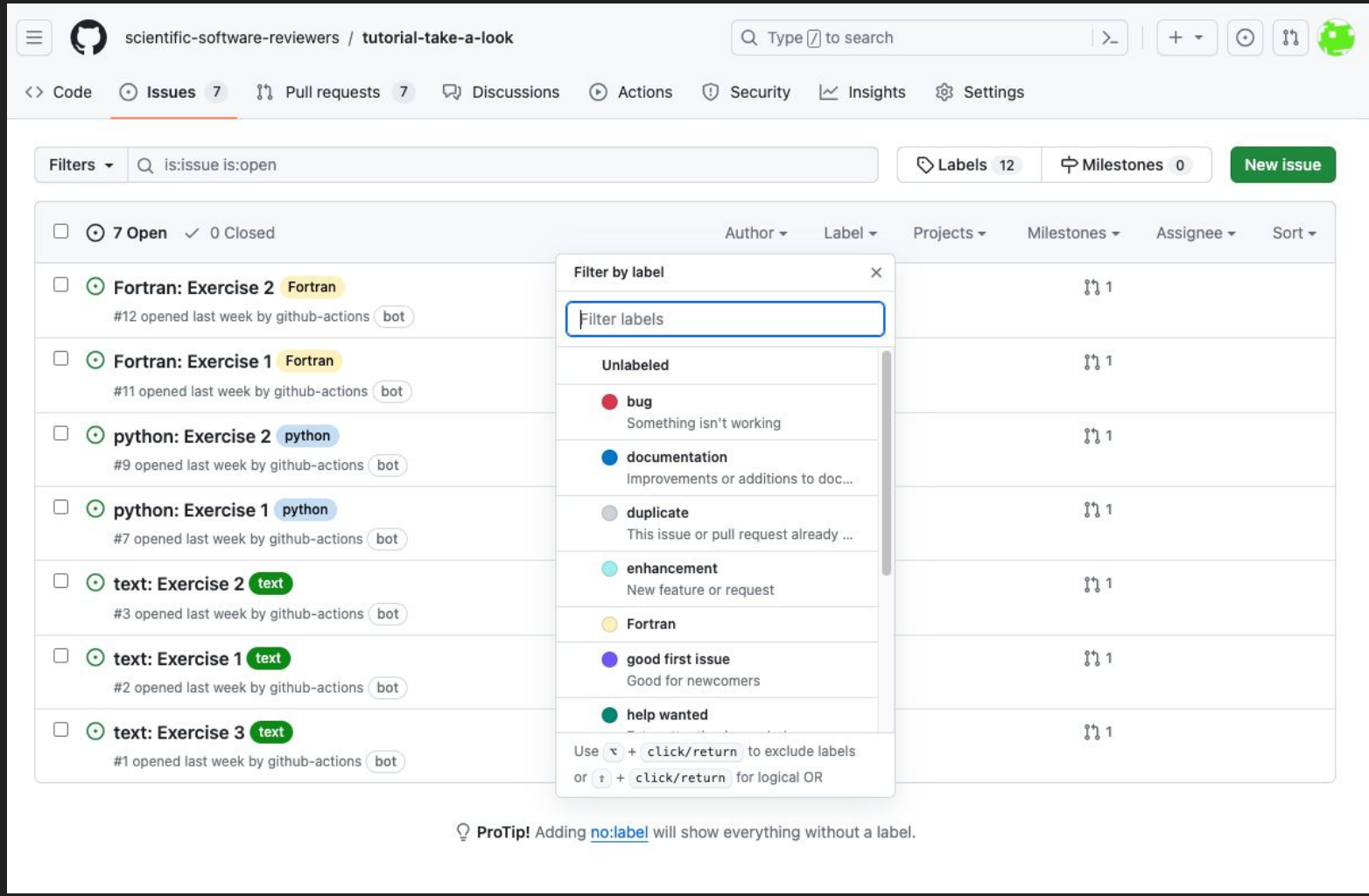
Create the exercises


Code
Pull requests
Actions
Projects
Wiki
Security
Insights
Settings
Actions
New workflow
All workflows
create_exercises
reset_exercises
Management
Caches
create_exercises
create_exercises.yaml
Filter workflow runs
0 workflow runs
Event
Status
Branch
Actor
This workflow has a workflow_dispatch event trigger.
Run workflow
This workflow has no runs yet.


0 workflow runs
Event
Status
Branch
Actor
This workflow has a workflow_dispatch event trigger.
Run workflow
Use workflow from
Branch: main
Language *
text
Run workflow
This workflow has no runs yet.


0 workflow runs
Event
Status
Branch
Actor
This workflow has a workflow_dispatch event trigger.
Run workflow
Use workflow from
Branch: main
Language *
text
python
fortran
This workflow has no runs yet.


Workflow run was successfully requested.
Actions
New workflow
All workflows
create_exercises
reset_exercises
Management
Caches
create_exercises
create_exercises.yaml
Filter workflow runs
0 workflow runs
Event
Status
Branch
Actor
This workflow has a workflow_dispatch event trigger.
Run workflow
create_exercises
create_exercises #1: Manually run by hkershaw-brown
now
26s


scientific-software-reviewers / tutorial-take-a-look
Type / to search
Code
Issues 7
Pull requests 7
Discussions
Actions
Security
Insights
Settings
Filters
is:issue is:open
Labels 12
Milestones 0
New issue
7 Open
0 Closed
Author
Label
Projects
Milestones
Assignee
Sort
Fortran: Exercise 2 Fortran
#12 opened last week by github-actions bot
Fortran: Exercise 1 Fortran
#11 opened last week by github-actions bot
python: Exercise 2 python
#9 opened last week by github-actions bot
python: Exercise 1 python
#7 opened last week by github-actions bot
text: Exercise 2 text
#3 opened last week by github-actions bot
text: Exercise 1 text
#2 opened last week by github-actions bot
text: Exercise 3 text
#1 opened last week by github-actions bot
Filter by label
Filter labels
Unlabeled
bug
Something isn't working
documentation
Improvements or additions to doc...
duplicate
This issue or pull request already ...
enhancement
New feature or request
Fortran
good first issue
Good for newcomers
help wanted
Use ⌥ + click/return to exclude labels
or ⇧ + click/return for logical OR
ProTip! Adding no:label will show everything without a label.

Navigating the exercises

Issues

Pull Requests

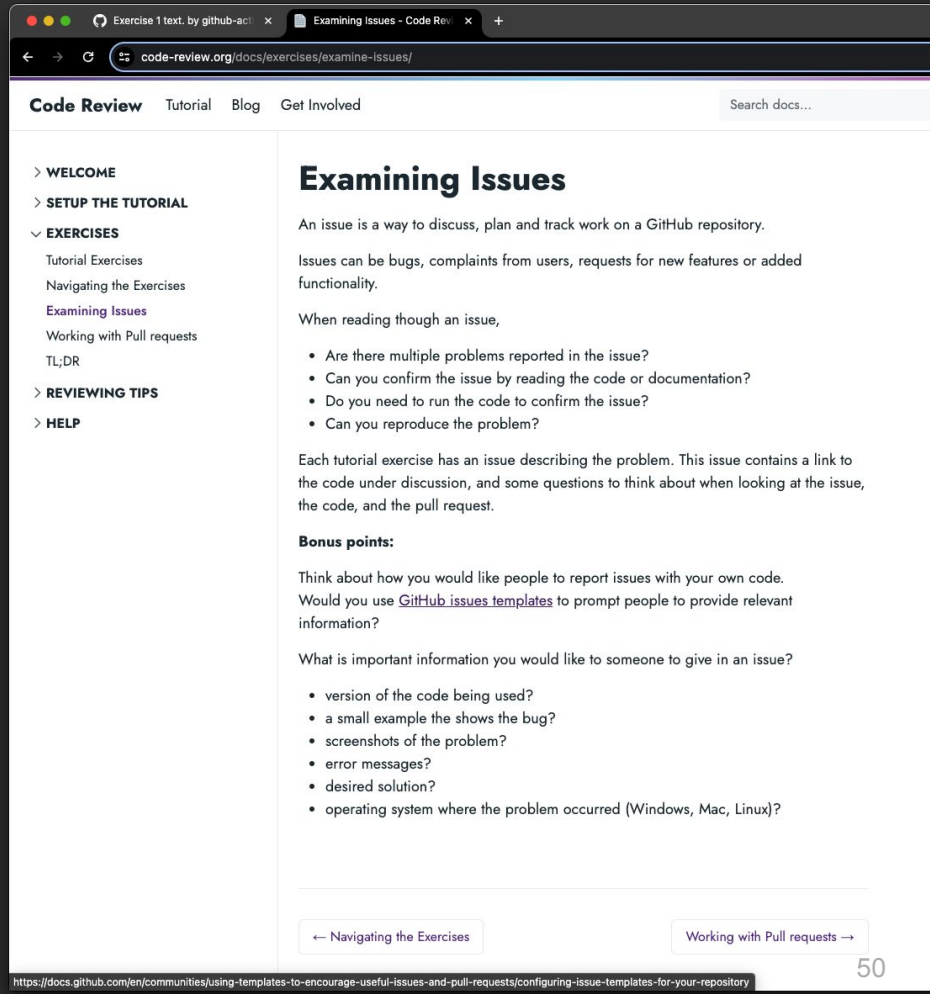
Issues

Problem

Pull Requests

Solution

Issues


Exercise 1 text. by github-act
Examining Issues - Code Rev
code-review.org/docs/exercises/examine-issues/
Code Review
Tutorial
Blog
Get Involved
Search docs...
WELCOME
SETUP THE TUTORIAL
EXERCISES
Tutorial Exercises
Navigating the Exercises
Examining Issues
Working with Pull requests
TL;DR
REVIEWING TIPS
HELP
Examining Issues
An issue is a way to discuss, plan and track work on a GitHub repository.
Issues can be bugs, complaints from users, requests for new features or added functionality.
When reading though an issue,
Are there multiple problems reported in the issue?
Can you confirm the issue by reading the code or documentation?
Do you need to run the code to confirm the issue?
Can you reproduce the problem?
Each tutorial exercise has an issue describing the problem. This issue contains a link to the code under discussion, and some questions to think about when looking at the issue, the code, and the pull request.
Bonus points:
Think about how you would like people to report issues with your own code. Would you use GitHub issues templates to prompt people to provide relevant information?
What is important information you would like to someone to give in an issue?
version of the code being used?
a small example the shows the bug?
screenshots of the problem?
error messages?
desired solution?
operating system where the problem occurred (Windows, Mac, Linux)?
← Navigating the Exercises
Working with Pull requests →
https://docs.github.com/en/communities/using-templates-to-encourage-useful-issues-and-pull-requests/configuring-issue-templates-for-your-repository

Pull Requests

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- WELCOME
- SETUP THE TUTORIAL
- EXERCISES
  - Tutorial Exercises
  - Navigating the Exercises
  - Examining Issues
  - Working with Pull requests
  - TL;DR
- REVIEWING TIPS
- HELP

Working with Pull requests

A pull request is a proposed change. A review is feedback on the change.

When you are reviewing, you'll need to assess the scope and size of the pull request. This will give you some idea of how much work will be involved in the review, and what feedback you need to give.

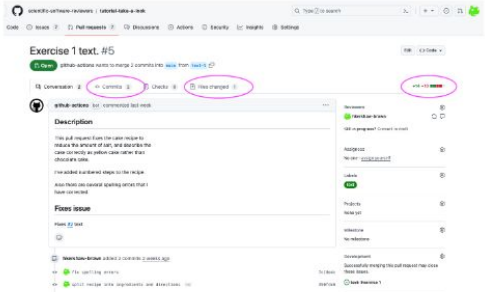
Read the pull request description. Ideally this will give you the scope:

- What's changed.
- Why the changes were made.
- What the person is looking for from the review. They may have code ready to release, they may have an urgent bug fix, they may have a draft that they want you to look at before they do any more work.

Small code changes can have big impacts, so lines of code changed does not necessarily correlate with how difficult, important, or necessary a change is. But you can use GitHub to see:

- How many lines of code have been added or removed.
- How many files have been changed.
- How many commits were made.

These are circled below in pink, and will give you an idea of how big the pull request is.



The lines of code changed is show by the green/red +/-. In this case 14 new lines, 10 lines removed:

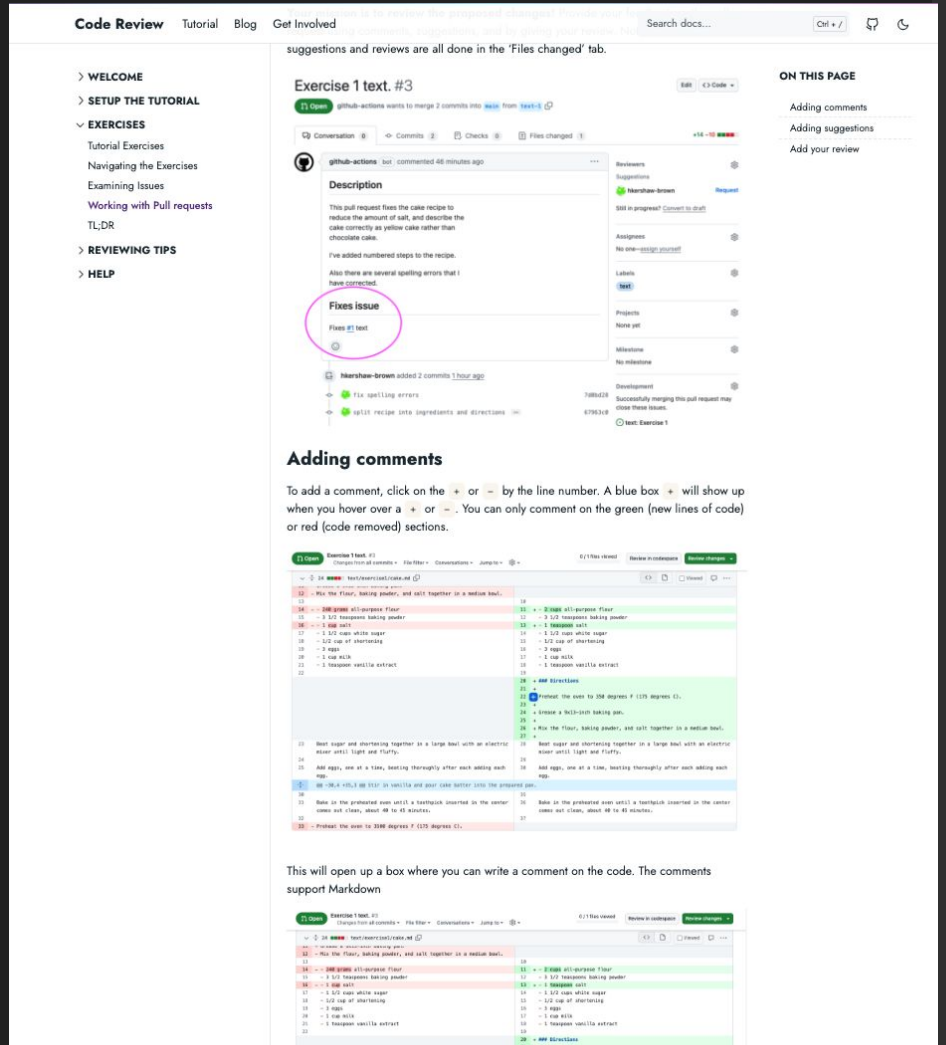
Click on 'Files changed' to see what changes are proposed in this pull request.

Each exercise has a pull request which proposes a change to the existing code. You can read about the reasons for the change in the issue linked from the pull request description. The issues contain questions to think about during review.

ON THIS PAGE

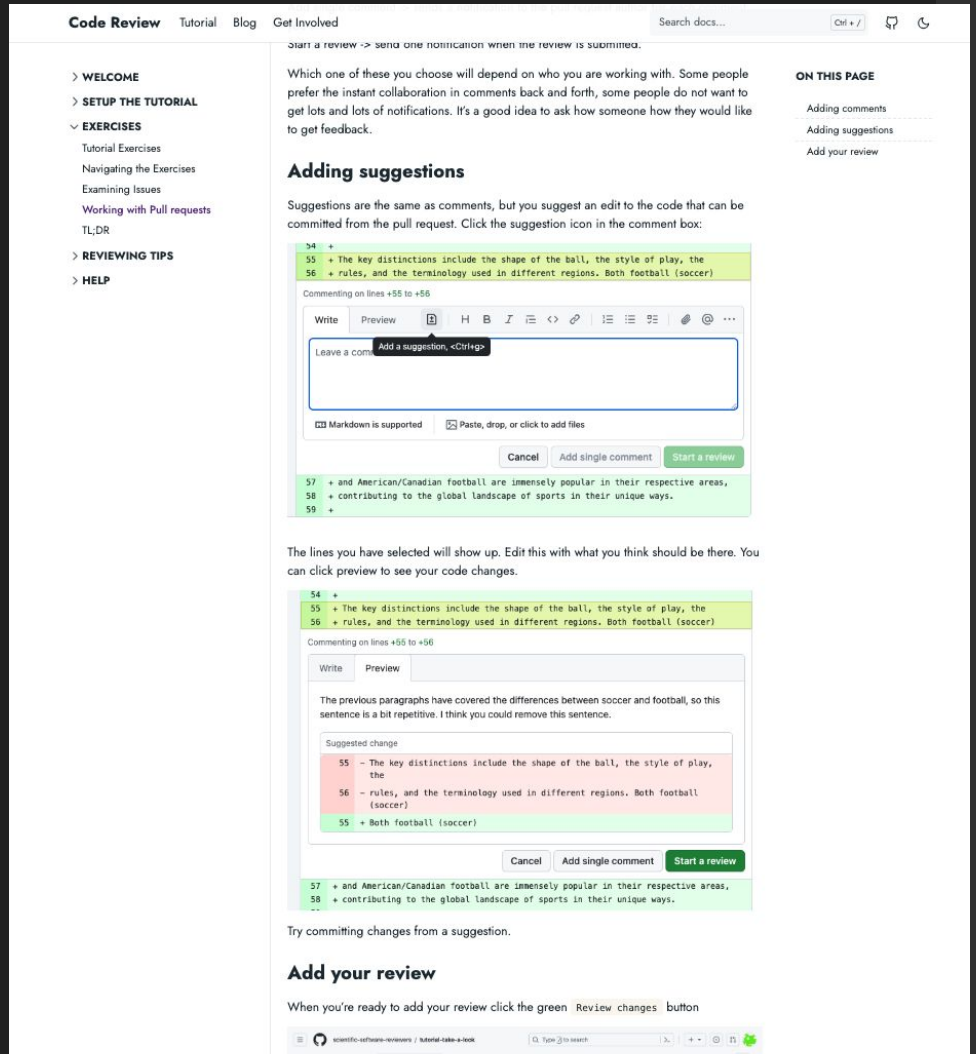
- Adding comments
- Adding suggestions
- Add your review

Pull Requests

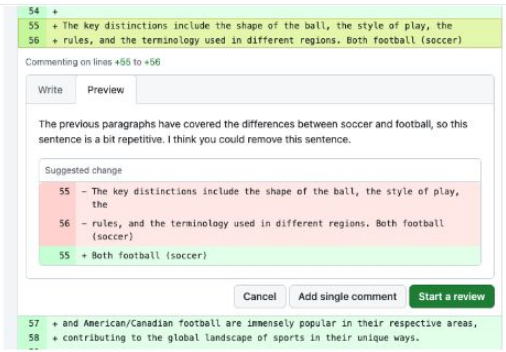


Navigating Pull Requests

size and scope



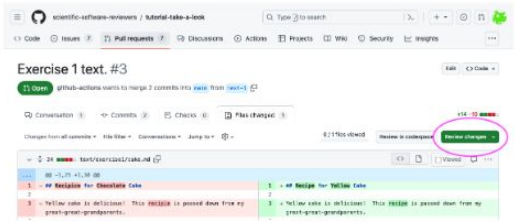
Adding suggestions



Try committing changes from a suggestion.

Add your review

When you're ready to add your review click the green `Review changes` button



You're choices are:

- Comment
- Approve
- Request changes

Bonus points:

- What makes a pull request easy to review?
- What makes a pull request difficult to review?

← Examining Issues
TL;DR →

Adding your review

Reviewing

Reviewing

Being reviewed

Reviewing

Does the pull request address the issue?

Are there any deal breakers that would stop you accepting the changes?

Can you suggest any improvements?

What is a good way to phrase your suggested improvements?

Is the solution overly complicated? Are the comments up to date, necessary, helpful?

Would you accept the pull request as it is now? Are your suggested changes must-do? nice-to-have? nitpicks? How would you communicate this?

Do you spend a lot of time reviewing the code style? Is it worth having a style guide for contributors? Can you make use of an existing style guide? Or a linter?

Being reviewed

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Being reviewed

When putting in a pull request, how can you make it easy for a reviewer to understand what you have done?

What makes a good pull request, what makes a bad pull request?

Can you commit code in a way that lets someone review your code more easily? Should you separate functional changes from style changes?

Would you use a tool such as commitizen to prompt yourself at commit time? Why? Why not?

Mechanics of the tutorial

Adding exercises

Adding exercises

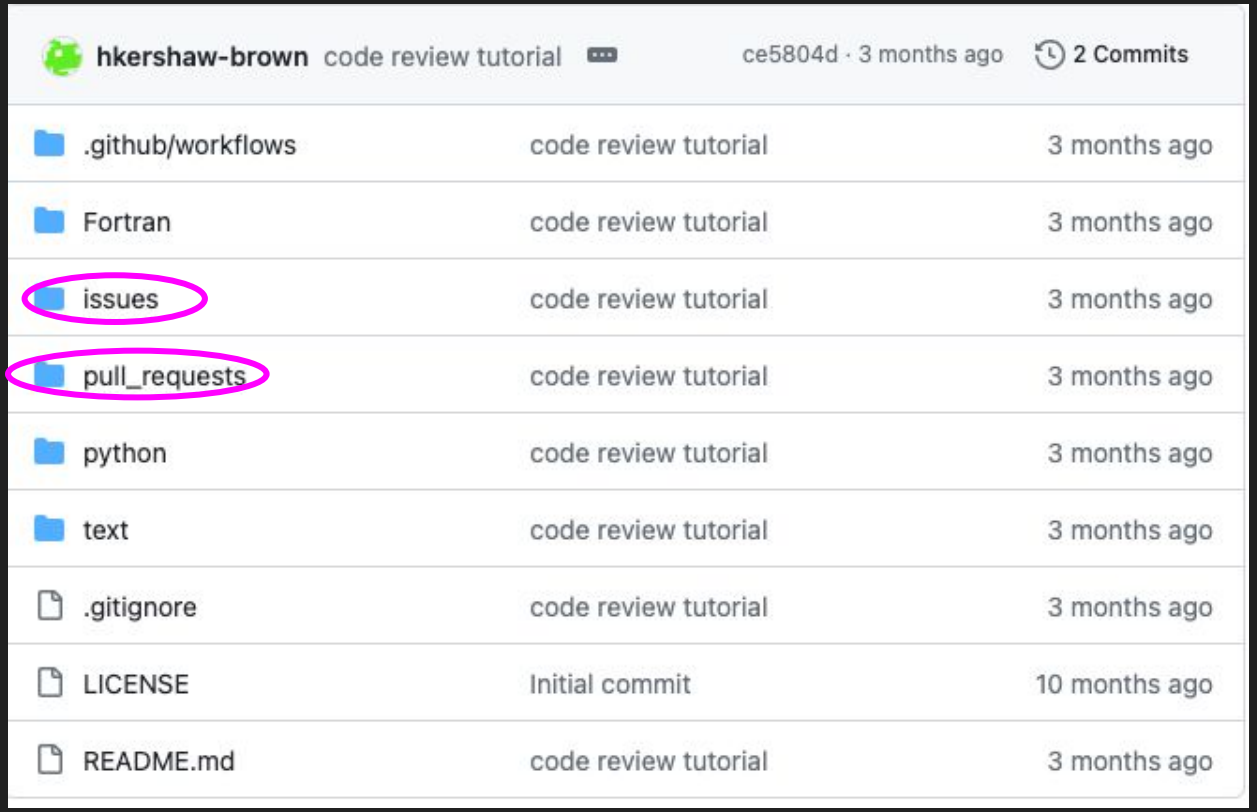
Two GitHub workflows:

create_exercises create_exercises.yaml

reset_exercises close_issues_and_pulls.yaml

https://github.com/scientific-software-reviewers/tutorial

Adding exercises



Adding exercises

issues/{Language}-ex{#}-issue.md

pull_requests/{Language}-ex{#}-pull_body.md

Branch: {Language}-{#}

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.github/workflows/create_exercises.yaml is the action that takes ‘Language’, and for each exercise {1..n}:

Adding exercises

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Adding exercises

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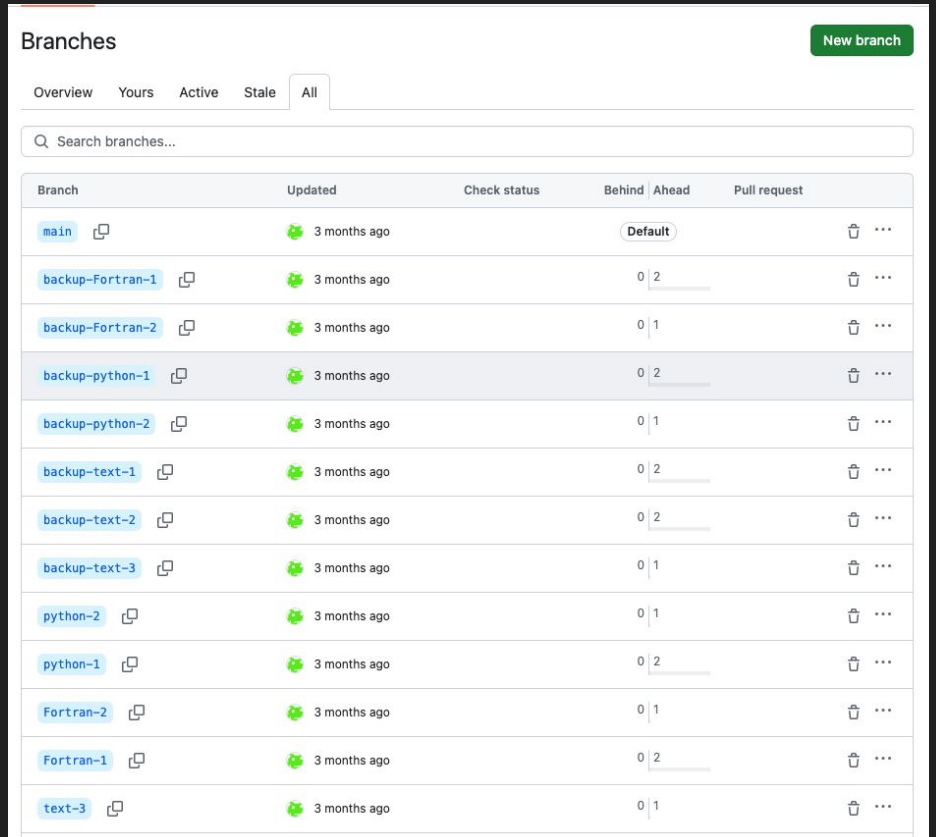
Code is in the directories:

{Language}/exercise{#}

Adding exercises



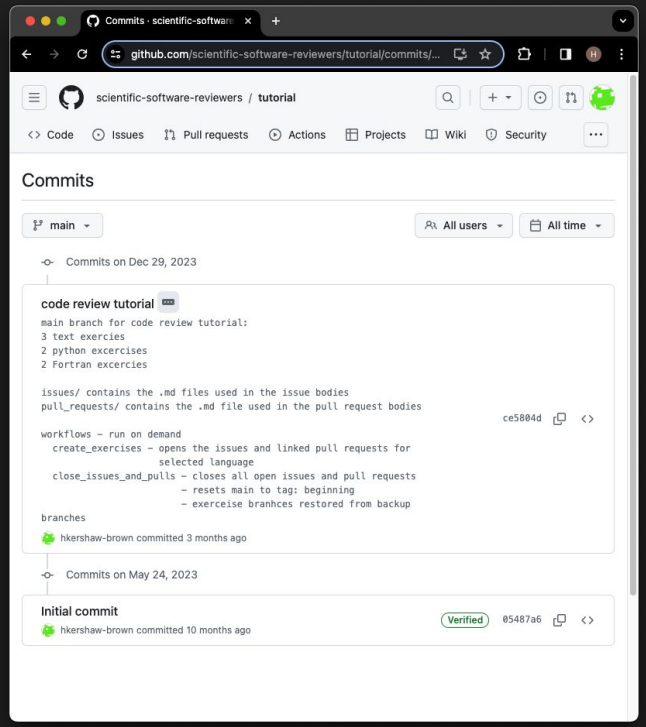
.github/workflows/close_issues_and_pulls.yaml

Resets the exercises:

Roll back the repo with git reset hard

Restores the {Language}-{#} branch from a corresponding backup-{Language}-{#} branch

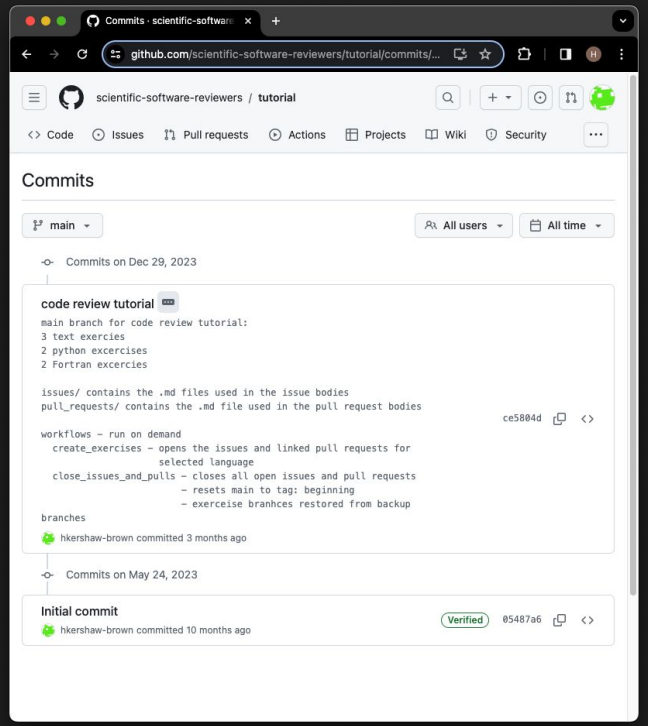
Squashing git history



main branch has only two commits:

- Initial commit
- Code review tutorial

Squashing git history



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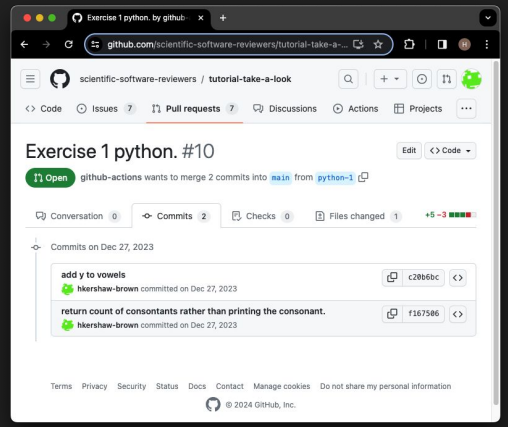
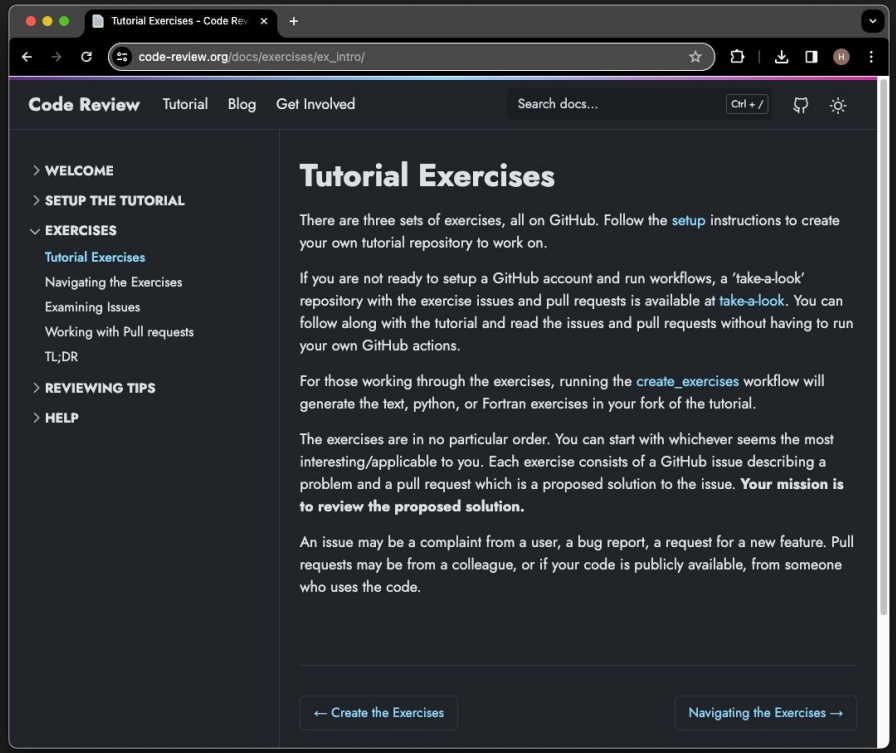


Examine commit history in exercises



code-review.org

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Software Engineering is “programming integrated over time”

Winters, T., Manshreck, T., & Wright, H. (2020). *Software engineering at google: Lessons learned from programming over time*. O'Reilly Media

Experiences from UCAR SEA
Software Engineering Assembly

What is the SEA?

UCAR Software Engineering Assembly

- Foster community for software engineering professionals within UCAR
- Facilitate effective participation
- Advocate for Software Engineers

SEA Improving Scientific Software Conference April 15th-18th
https://sea.ucar.edu/conference/2024

Code Review
Experiences from UCAR SEA
Software Engineering Assembly

Experiences from UCAR SEA

Join the UCAR Software Engineering Assembly for a lightly-moderated discussion on code review across UCAR.

Any discussion topics are welcome, as are all experience levels. We encourage you to share your good and bad experiences with code review.

- Do you use code review in your group? Who does the reviewing? Have you used code review to transfer knowledge between team members?
- Reviewing is hard. Being reviewed can be difficult. How do you give and receive constructive and actionable criticism?
- Do you do in person code reviews? Offline code-reviews? What works, what doesn't?
- Do you spend too much time in review, and have ideas to improve the process?

Experiences from UCAR SEA

Code review feels like someone works with me and we learn from each other

GitHub made it much easier to code review.

When people do not know much about what others do in the code, review gives an opportunity to learn about what is going on in the project

Downside:Back/forth that happens, especially since the code review is not #1 priority. Can slow down the process.

Getting very burned out with code reviews generally
e.g. Do a review, wait ~2 weeks, can feel really negative sometimes
Recently got more negative on it but would love to hear positive experiences about it

Experiences from UCAR SEA

Used to do code reviews in person years ago. Finding bugs and avoiding problems down the line works great. Can't imagine deploying code without reviews. Couldn't maintain the code without reviews.

Experience mostly getting my code being reviewed rather than reviewing others'. Need to coordinate with each other to find the time. Trick is that it'd be helpful to walk the reviewer through the code first.

The objectives can be communicated well beforehand using a pull request template to reduce the overhead of back & forth and expectations for a due date for the pull request can be set.

Communicating what to look at in the code is really important.

Experiences from UCAR SEA

A lot of friction points about code review.
Ethics around code review is not clear.
Code review is a lot of times not equitable,
e.g. more pushback for women's code.

Code style actions, automation could be helpful with the code reviewing process to reduce unwanted reviewing (code styling, etc.)

Systemic Gender Inequities in Who Reviews Code
The Pushback Effects of Race, Ethnicity, Gender, and Age in Code Review – Communications of the ACM
Presentation by Dr. Kelly Blincoe about code review as a socio-technical activity. Includes relevant data and potential policy implications on code review processes and impact.

Pick the most impactful aspects of the code to comment on, no need to mention everything. Impact can include functionality, quality, maintainability, readability, testability.

Experiences from UCAR SEA

Submitting changes without sufficient descriptions is less helpful.

Make it clear about the asynchronous aspect of the PRs. Also use “why would you do that?” for asking the reasoning (?)

Sometimes reviews have a lot of back & forth, and can get political. Try to keep it very non-personal. The thing being reviewed is not the person but the code that will benefit an entire project/organization.

Having been in both scientist and developer perspectives, set expectations and convey what the goals are for each group, collective set of expectations. And, things may differ from person to person, even if they are all one kind (e.g. scientist).

It’s a joint responsibility.

Encourage "the code" and not "your code". We are not our code

Consistency. Type of code you are working on (pure research vs. operational product/deliverable) and how you set expectations is also very important.

Experiences from UCAR SEA

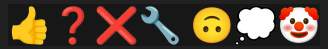
1:1 code review in person is a bit different than remote.

When getting someone new to our code contributions, reach out individually with an email that clarifies some important points about the process.

Code review as an onboarding task

Do onboarding by working side-by-side rather than a remote pull request review process. Some form of pair programming.

How Microsoft do code reviews mentions the use of emojis to describe things like nitpick, thinking out loud, take it or leave it, etc.



Finding Community

Finding Community

- US-RSE. A community of people who make research software happen.
- Society of Research Software Engineering which emerged from the successful grass-roots RSE movement and is the successor to the UK RSE Association.
- Better Scientific Software. A hub for scientific software development resources.
- Campus Champions. Uniting Research Computing Facilitators
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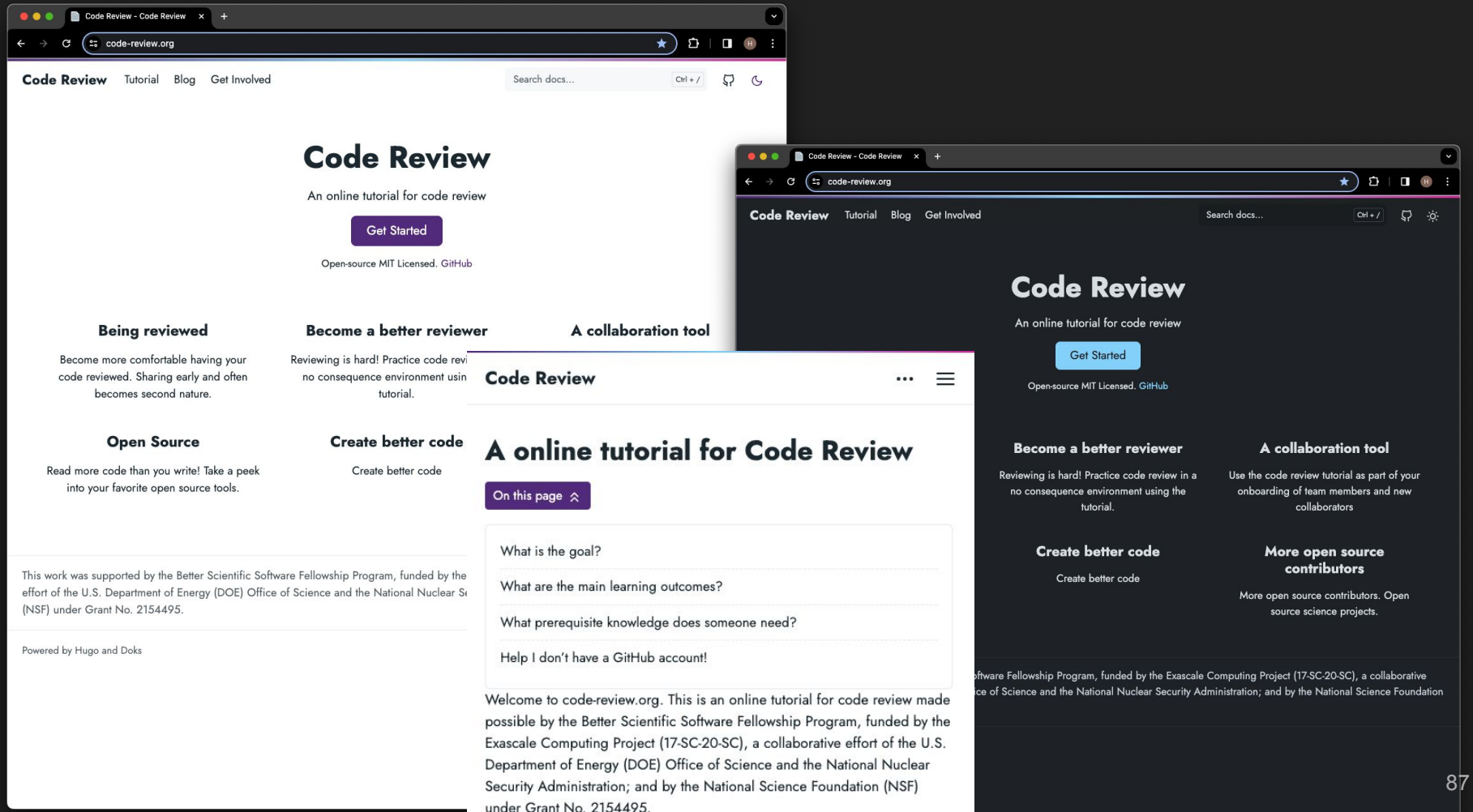
hkershaw@ucar.edu
USRSE slack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Become more comfortable having your code reviewed. Sharing early and often becomes second nature.
Become a better reviewer
Reviewing is hard! Practice code revi
no consequence environment usin
tutorial.
A collaboration tool
Open Source
Read more code than you write! Take a peek into your favorite open source tools.
Create better code
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effort of the U.S. Department of Energy (DOE) Office of Science and the National Nuclear S
(NSF) under Grant No. 2154495.
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Reviewing is hard! Practice code review in a no consequence environment using the tutorial.
A collaboration tool
Use the code review tutorial as part of your onboarding of team members and new collaborators
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More open source contributors
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ftware Fellowship Program, funded by the Exascale Computing Project (17-SC-20-SC), a collaborative
ce of Science and the National Nuclear Security Administration; and by the National Science Foundation
Code Review
A online tutorial for Code Review
On this page
What is the goal?
What are the main learning outcomes?
What prerequisite knowledge does someone need?
Help I don't have a GitHub account!
Welcome to code-review.org. This is an online tutorial for code review made possible by the Better Scientific Software Fellowship Program, funded by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy (DOE) Office of Science and the National Nuclear Security Administration; and by the National Science Foundation (NSF) under Grant No. 2154495.