

Supported by:



Reproducible workflows with R and GitHub

Ceres Barros

July 12th, 2023
2023 MacroBrum
Birmingham UK

Outline

1. The importance of repeatability, reproducibility, reusability and transparency – R³T
2. General guidelines
3. A working example in R and GitHub

Outline

1. The importance of repeatability, reproducibility, reusability and transparency – R³T
2. General guidelines
3. A working example in R and GitHub

Repeatability, reproducibility, reusability and transparency

R³T

What?

Repeatability ≠ Reproducibility ≠ Reusability

Repeatability, reproducibility, reusability and transparency

R³T

What?

Repeatability ≠ Reproducibility ≠ Reusability

agreement of results obtained by
the same individual using same
methods

Repeatability, reproducibility, reusability and transparency

R³T

What?

Repeatability ≠ Reproducibility ≠ Reusability

agreement of results obtained by
the same individual using same
methods

agreement of results obtained by
two individuals/groups using
same methods

Repeatability, reproducibility, reusability and transparency

R³T

What?

Repeatability ≠ Reproducibility ≠ Reusability

agreement of results obtained by
the same individual using same
methods

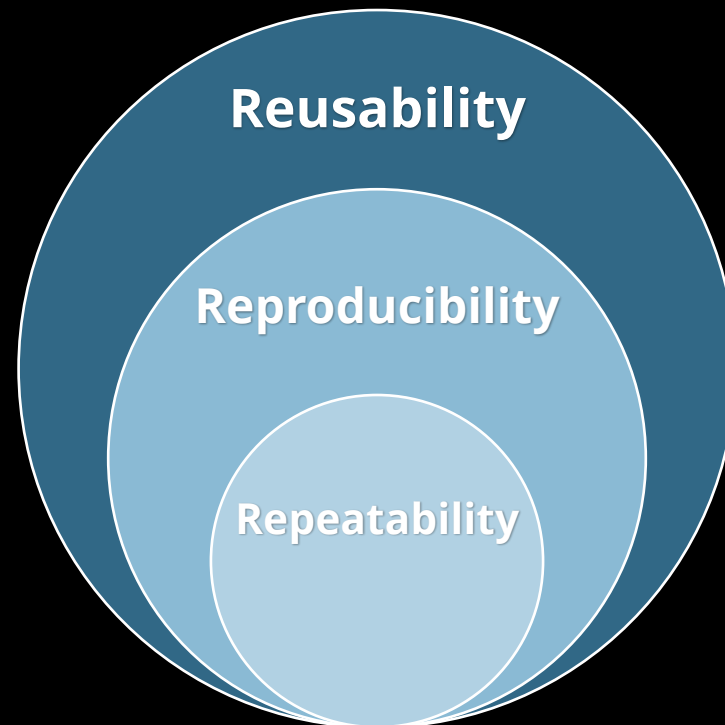
ability to re-use the same methods
in a different context
(e.g. new study area)

agreement of results obtained by
two individuals/groups using
same methods

Repeatability, reproducibility, reusability and transparency

R³T

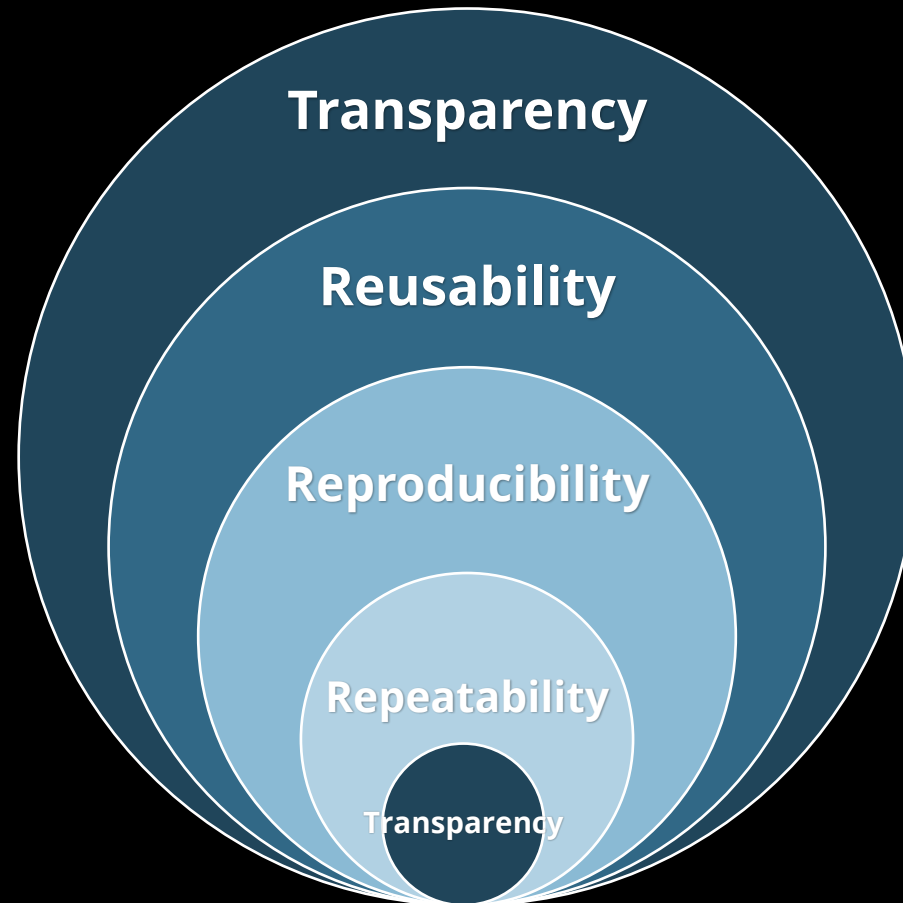
What?



Repeatability, reproducibility, reusability and transparency

R³T

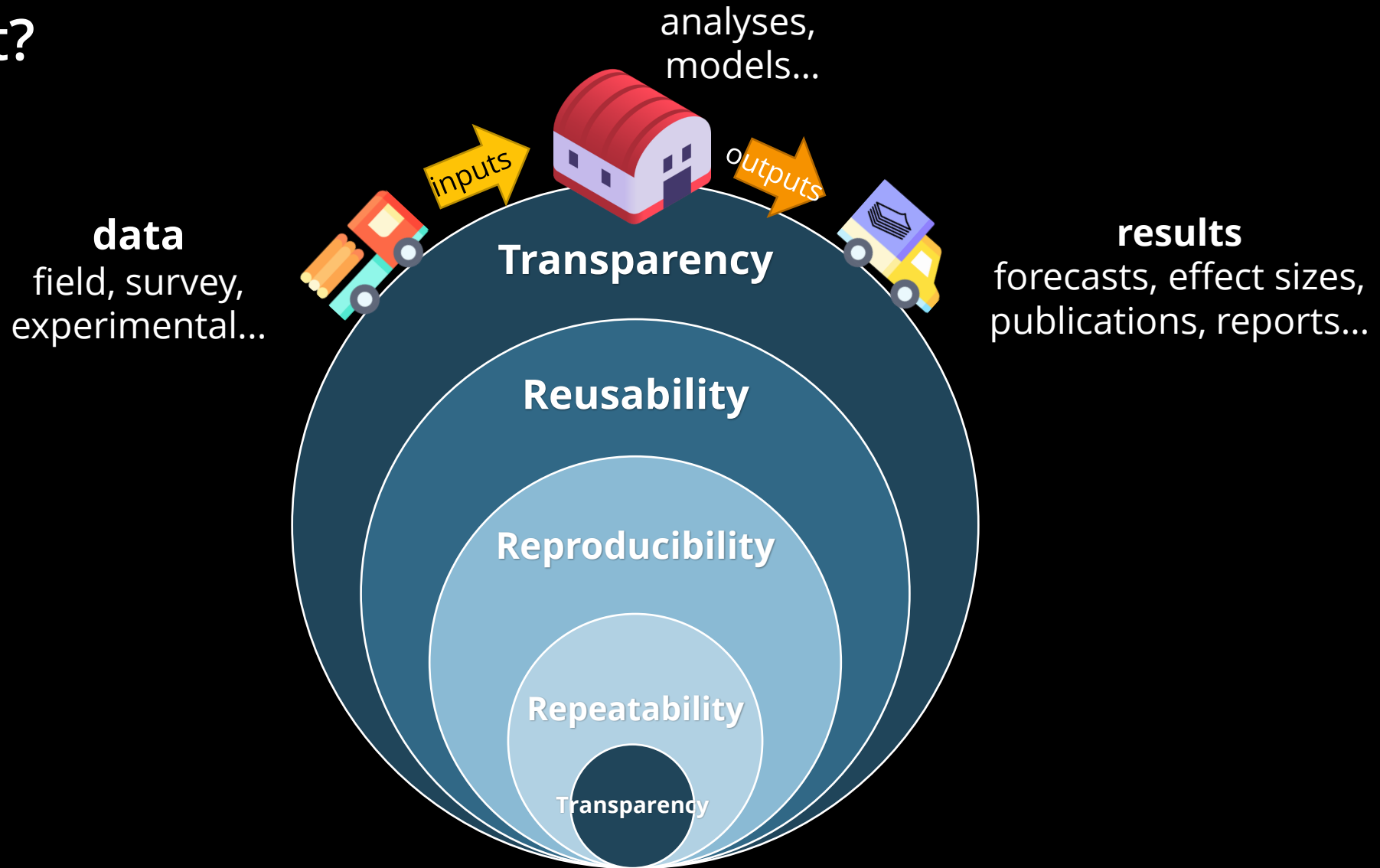
What?



Repeatability, reproducibility, reusability and transparency

R³T

What?

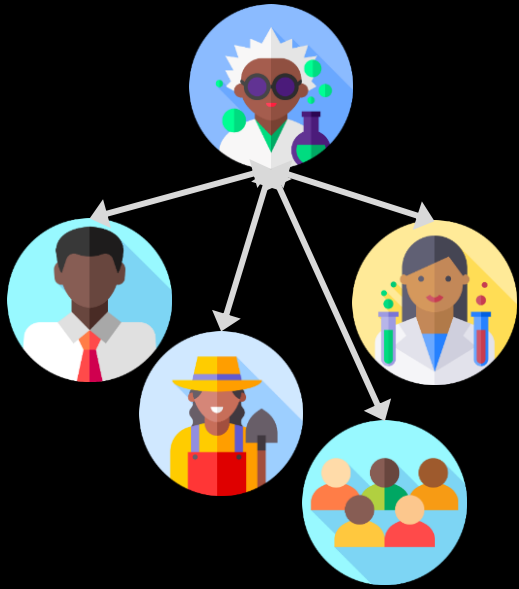


Repeatability, reproducibility, reusability and transparency

R³T

Why?

Trust



Repeatability, reproducibility, reusability and transparency

R³T

Why?

Trust



Benchmarking & meta-analyses

★	▲	●
✓	-	✓
✓	✓	-
-	-	✓

Repeatability, reproducibility, reusability and transparency

R³T

Why?

Trust



Benchmarking & meta-analyses



Building-on & improving analyses/models/workflows



Repeatability, reproducibility, reusability and transparency

R³T

How?

Depends on **context**

- Project type and size
- Purpose
- Audience

Repeatability, reproducibility, reusability and transparency

R³T

How?

Depends on **context**

- Project type and size
- Purpose
- Audience

Data (both input and output) types
Input and output management
Suitable workflow

Repeatability, reproducibility, reusability and transparency

R³T

How?

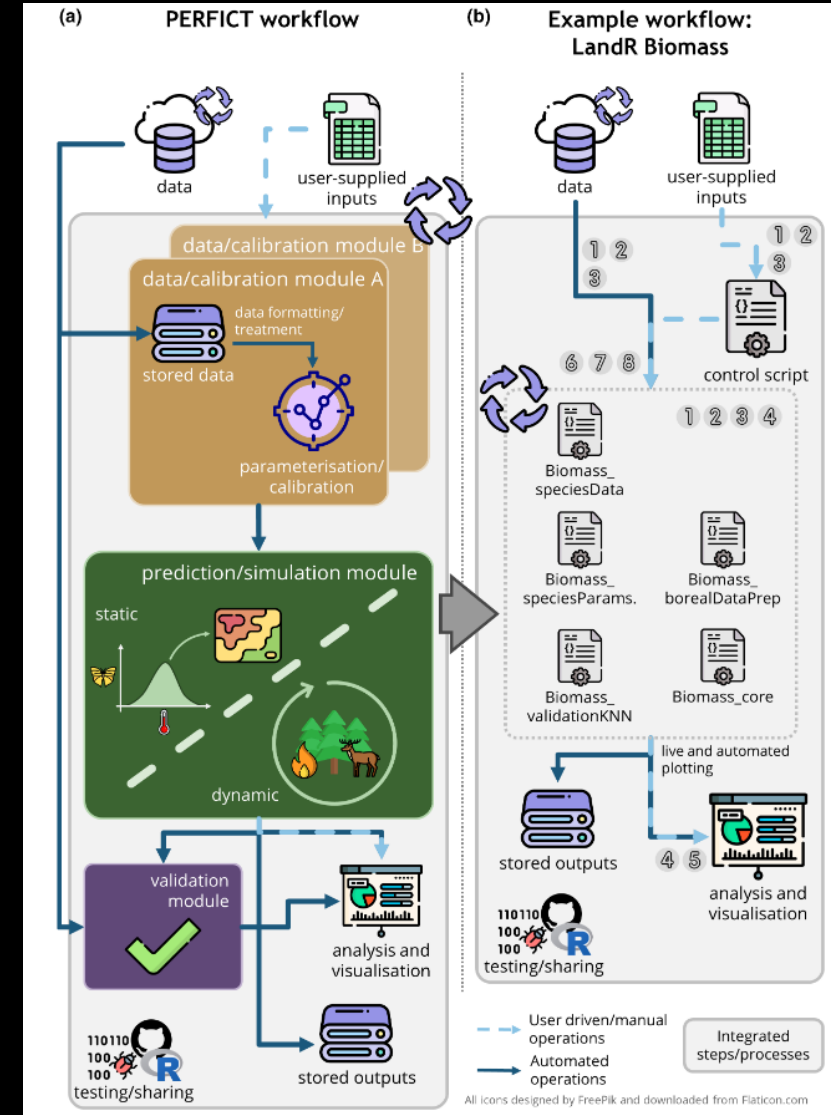
RESEARCH ARTICLE

Realising the Promise of Large Data and Complex Models

Methods in Ecology and Evolution

Empowering ecological modellers with a PERFICT workflow: Seamlessly linking data, parameterisation, prediction, validation and visualisation

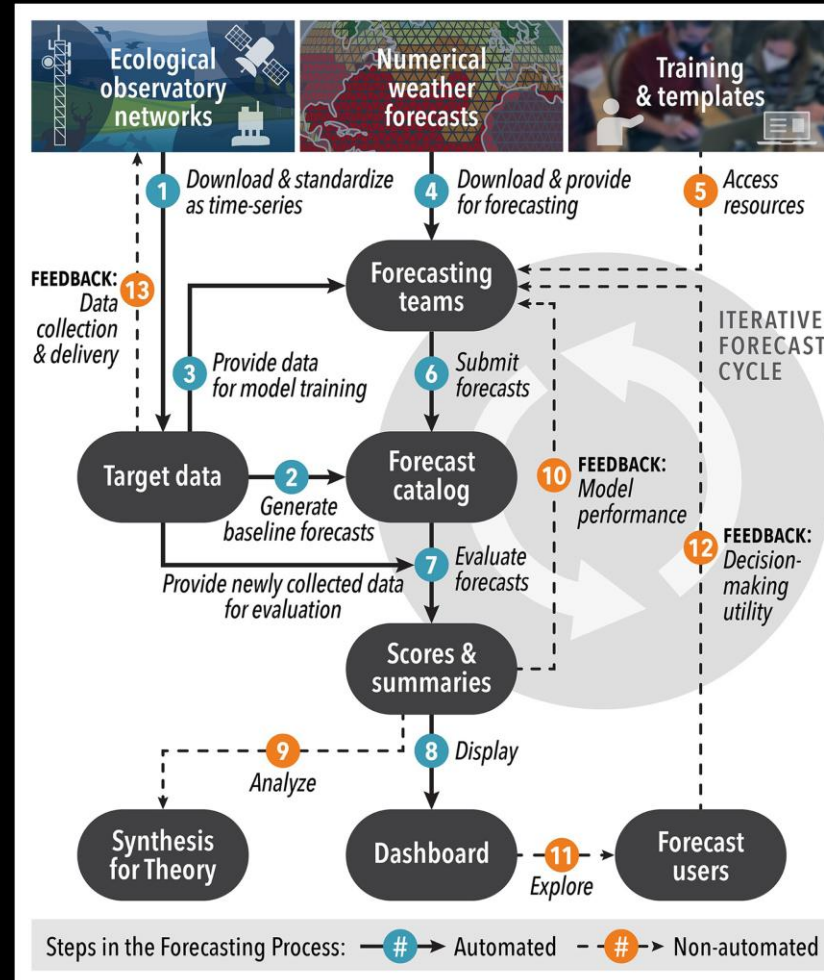
Ceres Barros¹ | Yong Luo^{1,2,3} | Alex M. Chubaty⁴ | Ian M. S. Eddy² |
 Tatiane Micheletti¹ | Céline Boisvenue^{1,2} | David W. Andison⁵ |
 Steven G. Cumming⁶ | Eliot J. B. McIntire^{1,2}



Repeatability, reproducibility, reusability and transparency

R³T

How?



NEON Forecasting
Challenge workflow
Thomas et al. (2023)

Ecological (iterative) forecasting
(continuous and integrated)
workflow based on monitoring
data

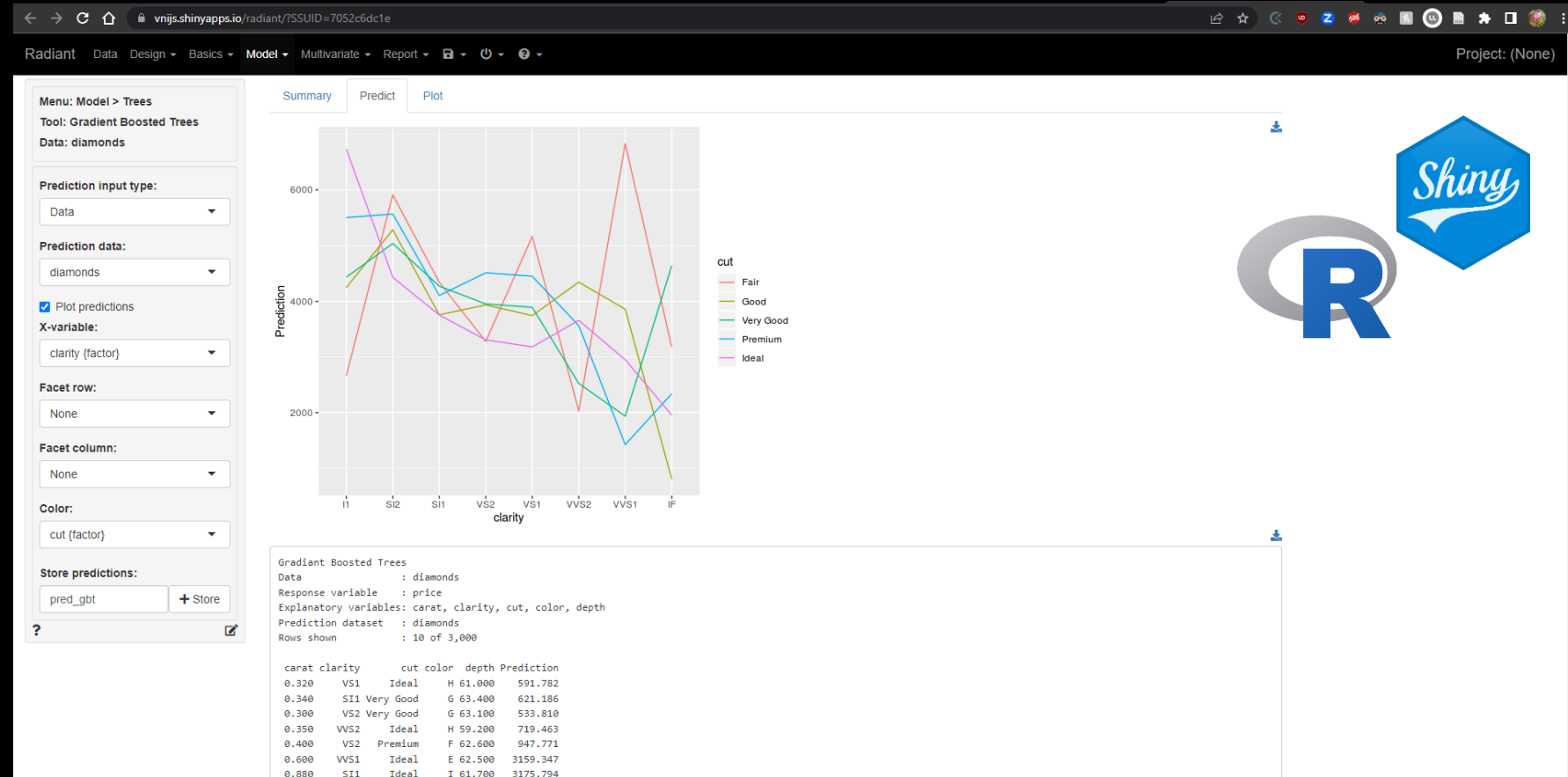
Repeatability, reproducibility, reusability and transparency

R³T

How?

engagement/education
point of view

R-shiny apps can be useful
for education, engaging
stakeholders/public and
delivering an interactive
product to end-users



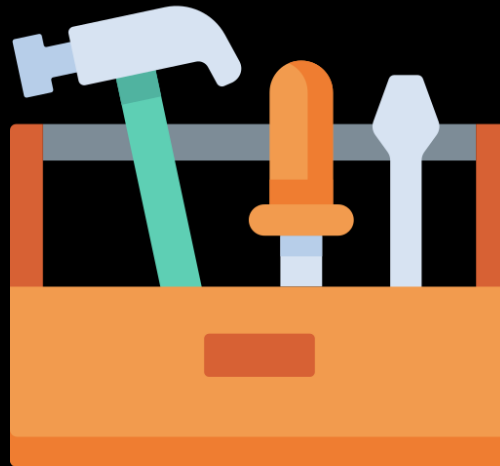
<https://vnijs.shinyapps.io/radiant/?SSUID=03eddd27f4>

Repeatability, reproducibility, reusability and transparency

R³T

How?

Most ecological research likely benefits from using a R³T approach, but the tools used to accomplish it can be varied

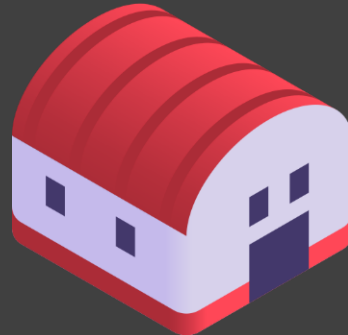


Repeatability, reproducibility, reusability and transparency

R³T

How?

All steps, from processing *raw data* to producing *final figures* are integrated and automated*



Data is FAIR
(Wilkinson *et al.* 2016)

Final outputs can be repeated and are integrated in the reporting**

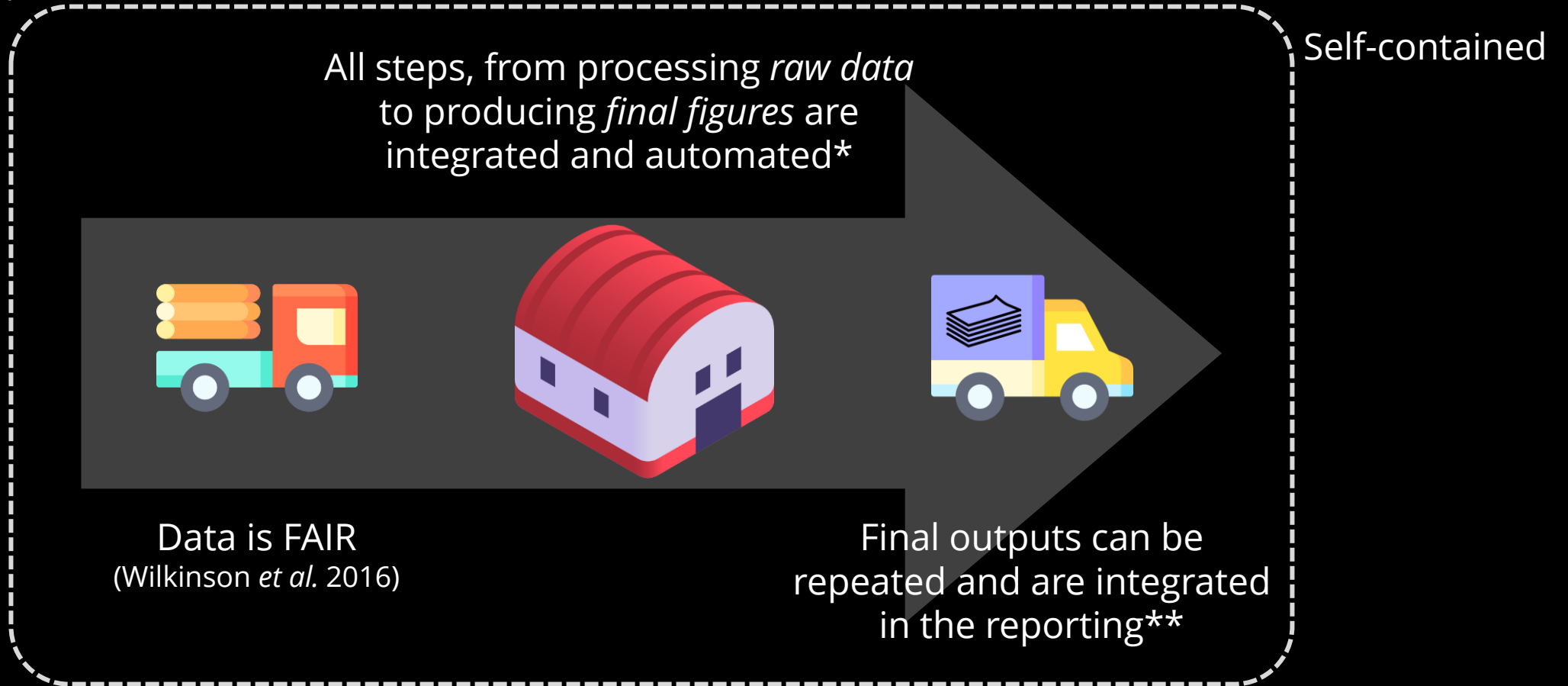
*as much as possible

**directly, or indirectly via links

Repeatability, reproducibility, reusability and transparency

R³T

How?



*as much as possible

**directly, or indirectly via links

Outline

1. The importance of repeatability, reproducibility, reusability and transparency – R3T
2. General guidelines
3. A working example in R and GitHub

General guidelines

1. Scripting/executing the workflow

1.1. Script, script, script

- **Goal:** no “secret handshakes” + record all steps of an analysis
- ALL steps – this includes package/library installation/loading and sourcing data

DOComment your
code



Adapted from EFI

<https://ecoforecast.org/reproducible-forecasting-workflows/>

General guidelines

1. Scripting/executing the workflow

1.1. Script, script, script

1.2. Minimise software/languages used

- **Goal:** increase workflow robustness - fewer “moving parts”, fewer “secret handshakes”, fewer manual operations
- Interpreted languages (real-time user interaction)
R, Julia, Python...
- Compiled languages (pre-compiled programs)
C, C++, C#, Fortran,... Do you really need this?

Adapted from EFI

<https://ecoforecast.org/reproducible-forecasting-workflows/>

General guidelines

1. Scripting/executing the workflow

1.1. Script, script, script

1.2. Minimise software/languages used

1.3. Modularise and “functionise” (!)

- **Goal:** code organisation/readability; easier propagation of code updates/changes
- Avoid looooooong scripts
- Break scripts into logical pieces
- Encapsulate code into functions, *especially* when used multiple times/in multiple places
- Consider “packaging” your functions.

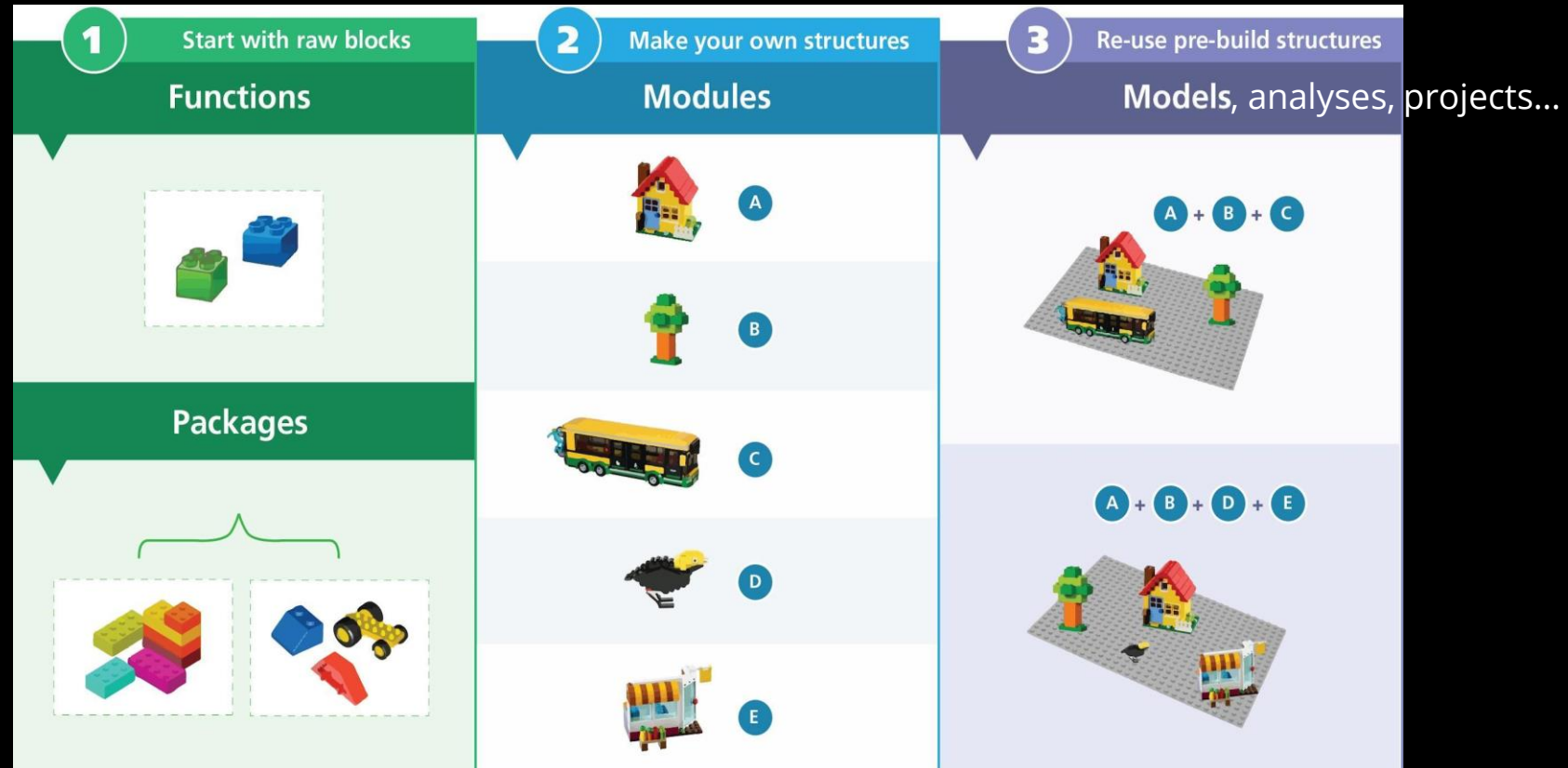


Adapted from EFI

<https://ecoforecast.org/reproducible-forecasting-workflows/>

General guidelines

1. Scripting/executing the workflow



Functions and modules as key tools for R³T, but also for building integrated and continuous workflows
McIntire *et al.* (2022)

General guidelines

1. Scripting/executing the workflow

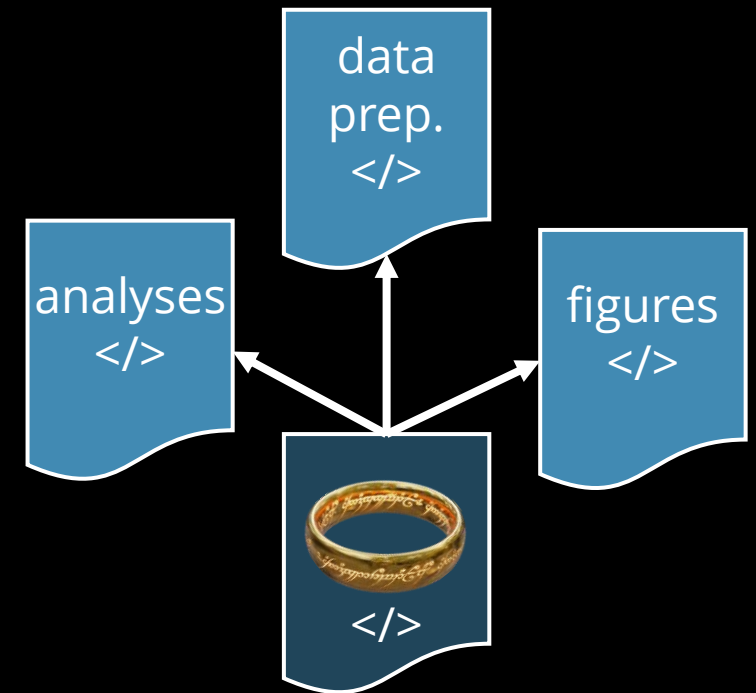
1.1. Script, script, script

1.2. Minimise software/languages used

1.3. Modularise and “functionise” (!)

1.4. Centralise workflow in a single script

- **Goal:** no “secret handshakes” - all scripts are utilised in correct way/sequence
- Call/execute scripts/steps from central (“control”) script



Adapted from EFI

<https://ecoforecast.org/reproducible-forecasting-workflows/>

General guidelines

2. Project structure

2.1. Project-oriented workflows

- **Goal:** the entirely workflow can be re-run easily, and without changing code or files
- Choose a structure that is self-explanatory
- Relative paths vs. absolute paths
- Project-libraries

```
Legend: folder, file, comment
10_data
  out      discharge.tsv # built from get_discharge.R
  raw      sites.txt # site list emailed from collaborators
           README.md # notes on email date, source for sites.txt
  src      get_discharge.R # downloads data from web
15_process_climate
  cfg      climate_variables.yml
  out      climate_2.tsv, climate_2.st
  src      process_climate.R
20_clean
  out      calibration_data.Rds
           estimation_data.Rds
  src      combine_CQ.R
40_forecast
  cfg      model_parameters.yml # no need for job_dir when models are reliable, simple
  out      model_01.Rds
           model_02.Rds
           ...
           model_68.Rds
  src      flux_model.R # makefile runs this 68 times
           helpers-flux_model.R
60_visualize
  out      fig_annual_flux_forecast.png
  src      plot_fluxes.R
90_model_archive
  cfg      metadata_parent.yml
  out      models_posted.st
  src      create_metadata.R, package_models.R, post_models.R # creating metadata for forecasts
95_report
  cfg      limnology-and-oceanography.csl, style.docx # journal-specific formatting
  fig      map.png, droughts.png, regression.png
  tbl      model_stats.Rmd
  txt      manuscript.Rmd, supplement_1.Rmd
  out      manuscript.docx, supplement_1.docx
build
  Makefile, 1_dat_spatial.mak, 1_dat_timeseries.mak, 2_process_climate.mak, ..., 9_report.mak
explore
  170802_check_boundaries      [...files...]
  170807_compare_climate_data_sources      [...files...] # Analyses to determine which drivers to use
lib
  download_helpers.R # functions for downloading data from web
  process_helpers.R
README.md
```

Source: <https://ecoforecast.org/reproducible-forecasting-workflows/>

Adapted from EFI
<https://ecoforecast.org/reproducible-forecasting-workflows/>

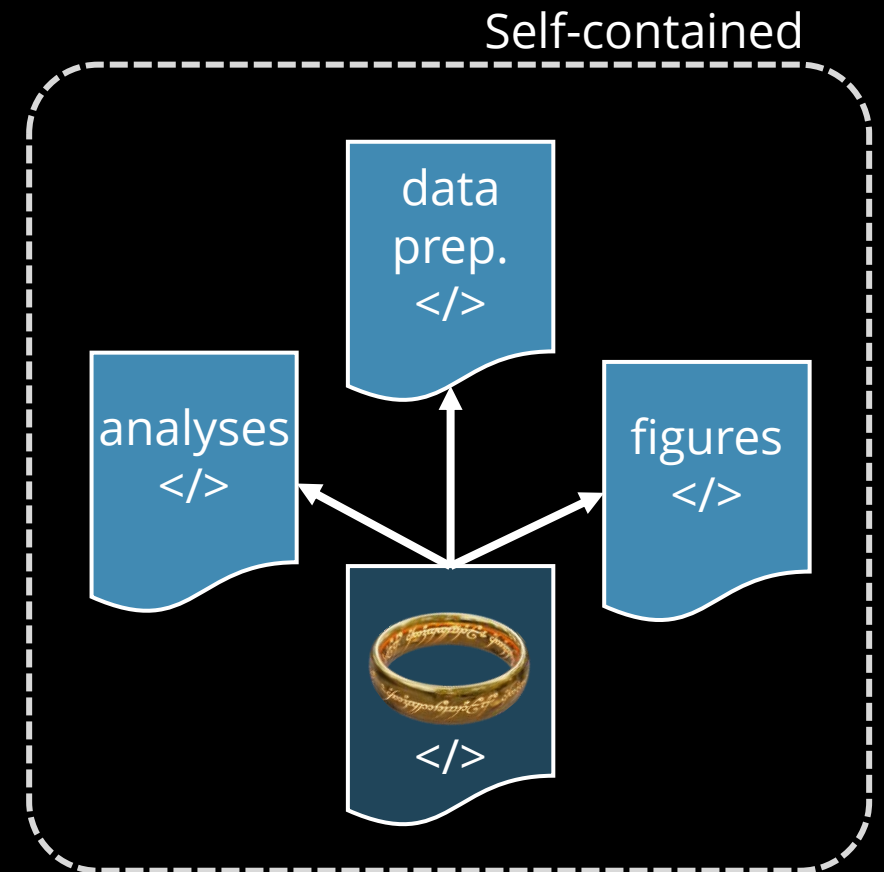
General guidelines

2. Project structure

2.1. Project-oriented workflows

2.2. Self-contained workflows

- **Goal:** ensure reproducibility
- E.g. RStudio-projects
- Containerisation – encapsulates the whole system (even OS) – e.g. Docker



Adapted from EFI

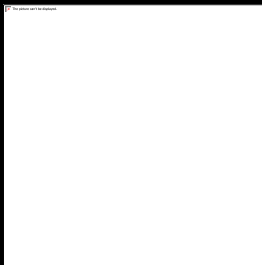
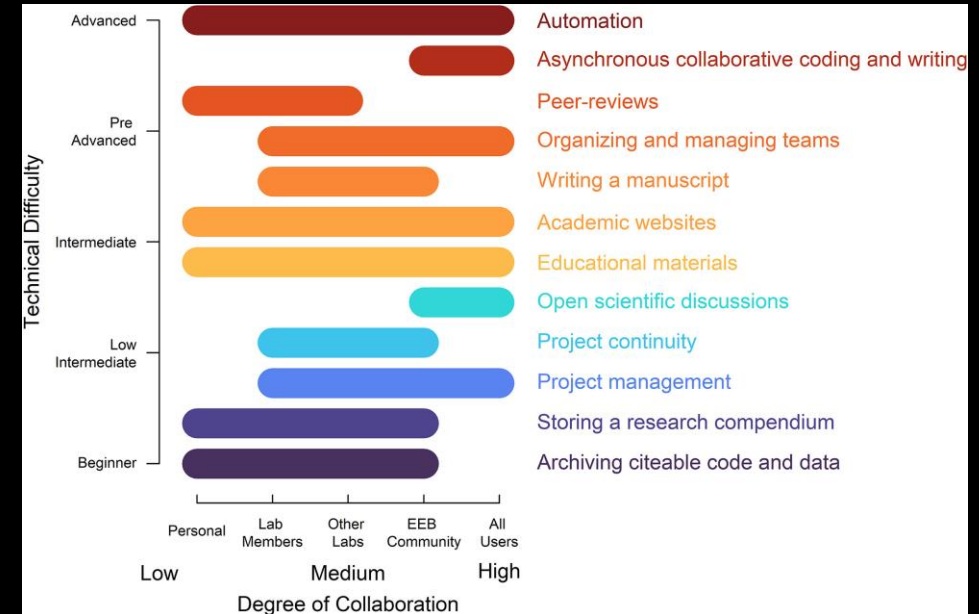
<https://ecoforecast.org/reproducible-forecasting-workflows/>

General guidelines

3. Project management

3.1. Version control

- **Goal:** change tracking in code/files + continuous and collaborative development
- Keeps a formal record of all changes
- Allows recovering old versions
- Allows keeping/working on multiple versions of the same code/project
- E.g. Git, CVS, SVN, ...



We'll come back to this!



GitHub is a multifaceted tool that can be appropriate to manage, track and collaborate on projects for various purposes and at various levels of complexity.
(Braga *et al.* 2023)

General guidelines

3. Project management

3.1. Version control

3.2. Integrated testing

- **Goal:** enhance code robustness and longevity
- Not always necessary, but always a good idea ;)
- Integration tests vs unit tests vs assertions
- Manual vs automated execution
- E.g.
 - testthat in R (unit tests)
 - simple code/object checks (assertions)
 - GitHub Actions and Travis CI for automated testing – all types.

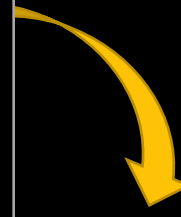
General guidelines

4. Literate programming

4.1. Integrate code and reporting/publication

- **Goal:** establishing explicit links between report/publication, data and analyses
- Integrates code and text in a single file
- Enhances transparency/reproducibility of reported outputs.
- E.g.
 - RMarkdown, Quarto – static or interactive; multiple languages in a single file
 - Jupyter – interactive; single language at a time (Julia, R or Python)

```
##
## output:
## pdf_document:
##   citation_package: natbib
##   keep_tex: true
##   fig_caption: true
##   latex_engine: pdflatex
##   template: ../sw-latex-no.tex
## bibliography: master.bib
## header-includes:
##   - \usepackage{hyperref}
##   - \usepackage{array}
##   - \usepackage{caption}
##   - \usepackage{graphics}
##   - \usepackage{units}
##   - \usepackage[table]{xcolor}
##   - \usepackage{multicol}
##   - \usepackage{nltxline}
##   - \usepackage{calc}
##   - \usepackage{suburl}
##   - \usepackage{fontawesome}
##   - \usepackage{paraonline,flushleft}[threeparttable]
## bibliography: app
## title: "A Pandoc Markdown Article Starter and Template"
## author: "Steven V. Miller"
## affiliation: "Clemson University"
## abstract: "This document provides an introduction to R Markdown, argues for its benefits, and presents a sample manuscript template intended for an academic audience. It includes basic syntax for R Markdown and a minimal working example of how the analysis itself can be conducted within R with the 'knitr' package."
## keywords: "pandoc, r markdown, knitr"
## doi: "r-forrest.github.io/2018/04/01/"
## geometry: margin-left=1cm,margin-right=1cm
## fontfamily: libertine
## fontsize: 11pt
## spacing: double
## monotel: no
## ---
## [r_setup, include=FALSE]
## # Introduction
## Academic workflow, certainly in political science, is at a crossroads. The "American Journal of Political Science"
## (AJPS) announced a (my words) "show your work"
## initiative (https://ajps.soc.2018/01/26/the-ajps-replication-policy-innovations-and-revisions/) in which authors who are
## tentatively accepted for publication at the journal must hand over the raw code and data that produced the results
## shown in the manuscript. The editorial team at "AJPS" then reproduces the code from the manuscript. Pending successful
## replication, the manuscript moves toward publication. The "show your work" initiative might be at the fore of this movement, and it could be
## the most aggressive among political science journals, but other journals in our field have signed the
## Access to Research Transparency (https://www.dartcenter.org) (DART) initiative. This, at a bare minimum,
## uploading code from quantitatively-oriented publisher articles to in-house directories hosted by the
## services like (DataVerse) (https://dataverse.org/).
## The implications for workflow are fairly substantial. Authors can rather quickly display the code they
## analyses in the document itself (likely in the appendix), so such there's little guesswork for reviewers
## in understanding what the author did in the analyses reported in the manuscript.
## It doesn't end there. In fact, here's what happens when 'eval=FALSE' is omitted or changed to 'eval=TRUE'
## code runs within R. Observe.
## [r_evalTRUE, tidy = TRUE, cache=FALSE, fig.cap="A Coefficient Plot", message=F, warning=F]
## library(stevemisc)
## data(unionsdensity)
## library(tidyverse)
## unionsdensity %>%
##   mutate(z_left = r2sd(left),
##          z_size = r2sd(size),
##          z_concen = r2sd(concen)) -> unionsdensity
## M1 <- lm(union ~ z_left + z_size + z_concen, data=unionsdensity)
## library(arm)
## arm: coefplot(M1)
```



A Pandoc Markdown Article Starter and Template *

Steven V. Miller *Clemson University*

This document provides an introduction to R Markdown, argues for its benefits, and presents a sample manuscript template intended for an academic audience. It includes basic syntax for R Markdown and a minimal working example of how the analysis itself can be conducted within R with the `knitr` package.

Keywords: pandoc, rmarkdown, knitr

Introduction

Academic workflow, certainly in political science, is at a crossroads. The *American Journal of Political Science* (AJPS) announced a (my words) "show your work" initiative in which authors who are tentatively accepted for publication at the journal must hand over the raw code and data that produced the results shown in the manuscript. The editorial team at AJPS then reproduces the code from the manuscript. Pending successful replication, the manuscript moves toward publication. The AJPS might be at the fore of this movement, and it could be the most aggressive among political science journals, but other journals in our field have signed the joint Data Access

The implications for workflow are fairly substantial. Authors can rather quickly display the code they used to run the analyses in the document itself (likely in the appendix). As such, there's little guesswork for reviewers and editors in understanding what the author did in the analyses reported in the manuscript.

It doesn't end there. In fact, here's what happens when `eval=FALSE` is omitted or changed to `eval=TRUE`. Now, the code runs within R. Observe.

```
library(stevemisc)
data(unionsdensity)

M1 <- lm(union ~ left + size + concen, data = unionsdensity)

library(arm)
coefplot(M1)
```

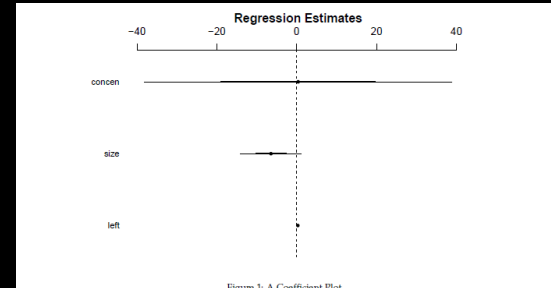


Figure 1: A Coefficient Plot

Outline

1. The importance of repeatability, reproducibility, reusability and transparency – R3T
2. General guidelines
3. A working example in R + RStudio + GitHub

Shall we try this?

What we will cover:

Project structure and management

- Version control – using GitHub and GitKraken
- Self-contained workflows – using R and Rstudio

Scripting/executing the workflow

- Script, script, script
- Modularise and “functionise” (!)
- Centralise workflow in a single script

Adapted from EFI

<https://ecoforecast.org/reproducible-forecasting-workflows/>

Shall we try this?

What we will cover:

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- Self-contained workflows – using R and Rstudio

Scripting/executing the workflow

- Script, script, script
- Modularise and “functionise” (!)
- Centralise workflow in a single script

The order is variable;
it depends on the stage of the
project and your own preference

Tools used in each step can also vary



*you can do this in...



1. Create a repository for your project

Assuming you already have an account on GitHub.com...

Create a repo

Create a new repository

A repository contains all project files, including the revision history. Already have a project repository elsewhere? [Import a repository.](#)

Required fields are marked with an asterisk (*).

Repository template

No template ▾

Start your repository with a template repository's contents.

Owner *

CeresBarros ▾

Repository name *

reproducible-workflows-e

reproducible-workflows-example is available.

Great repository names are short and memorable. Need inspiration? How about [sturdy-umbrella](#) ?

Description (optional)

Example of a simple reproducible workflow based in R and RStudio projects



Public

Anyone on the internet can see this repository. You choose who can commit.



Private

You choose who can see and commit to this repository.

Initialize this repository with:

Add a README file

This is where you can write a long description for your project. [Learn more about READMEs.](#)

Add .gitignore

.gitignore template: None ▾

Choose which files not to track from a list of templates. [Learn more about ignoring files.](#)

Choose a license

License: Creative Commons Zero v1.0 Universal ▾

A license tells others what they can and can't do with your code. [Learn more about licenses.](#)



1. Create a repository for your project

Assuming you already have an account on GitHub.com...

Or fork someone else's

The screenshot shows the GitHub interface for a repository named `reproducible-workflows-example`. The repository is public and has 0 forks and 0 stars. The `Fork` button is circled in orange. The repository has 1 branch (main) and 0 tags. The commit history shows a commit by CeresBarros with the message "GHA: need Require" 26 minutes ago, and a commit by the repository owner with the message "set seed before kfold" 12 hours ago. The repository description is "Example of a simple reproducible workflow based in R and RStudio projects".

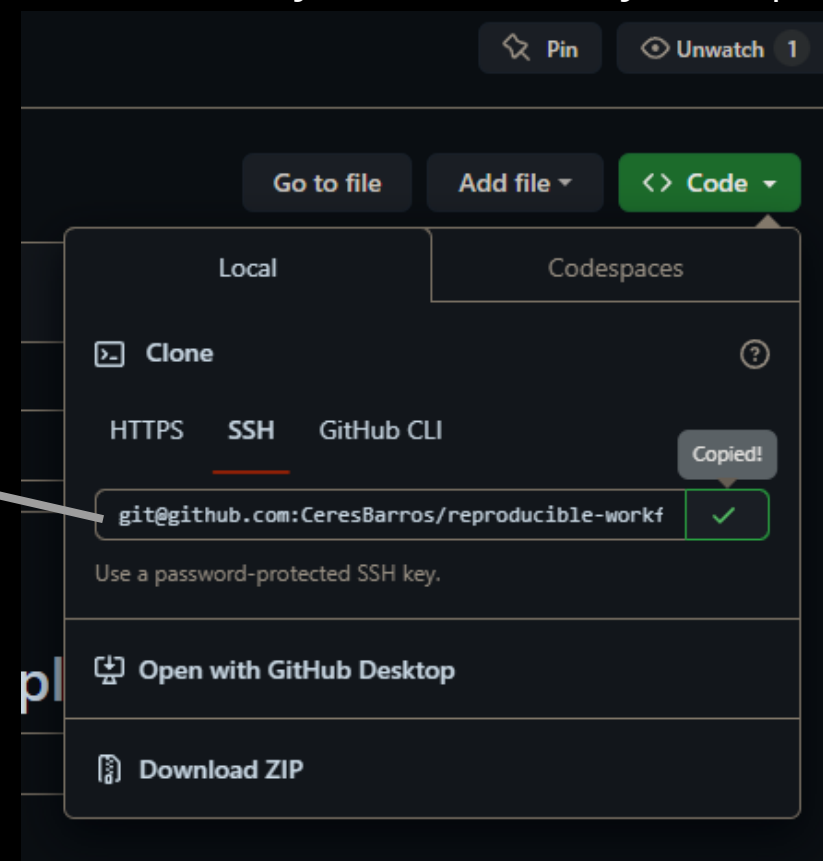
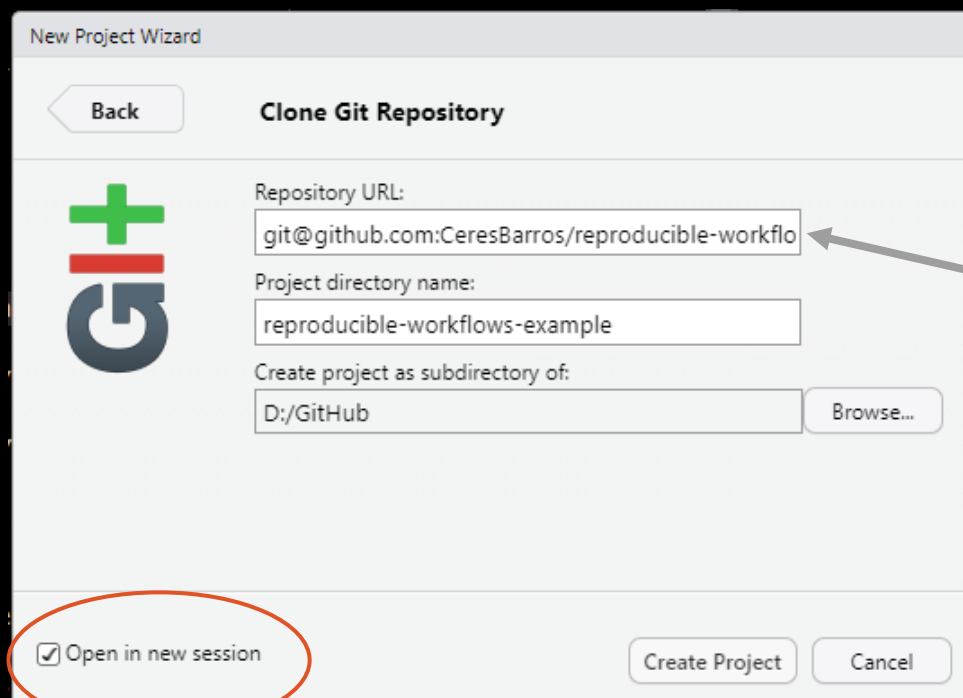
Commit	Message	Time
1e9bf37	GHA: need Require	26 minutes ago
	set seed before kfold	12 hours ago

2. Create a self-contained project



In RStudio, go to
File > New Project... > Version Control > Git

Get repo URL from
GitHub.com/your_username/your_repo

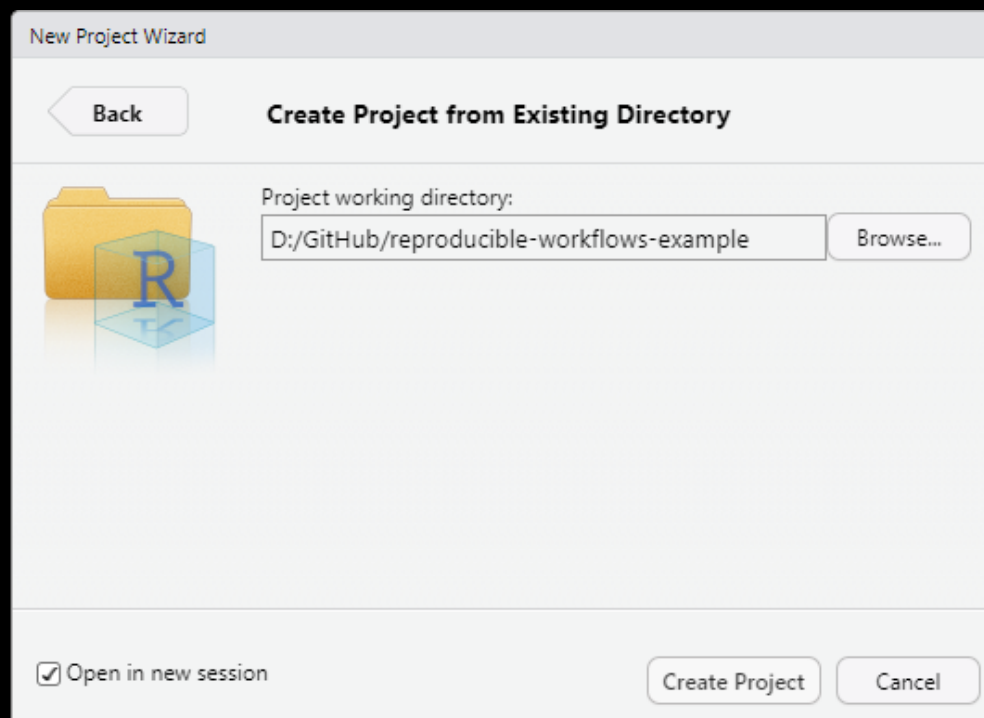


2. Create a self-contained project



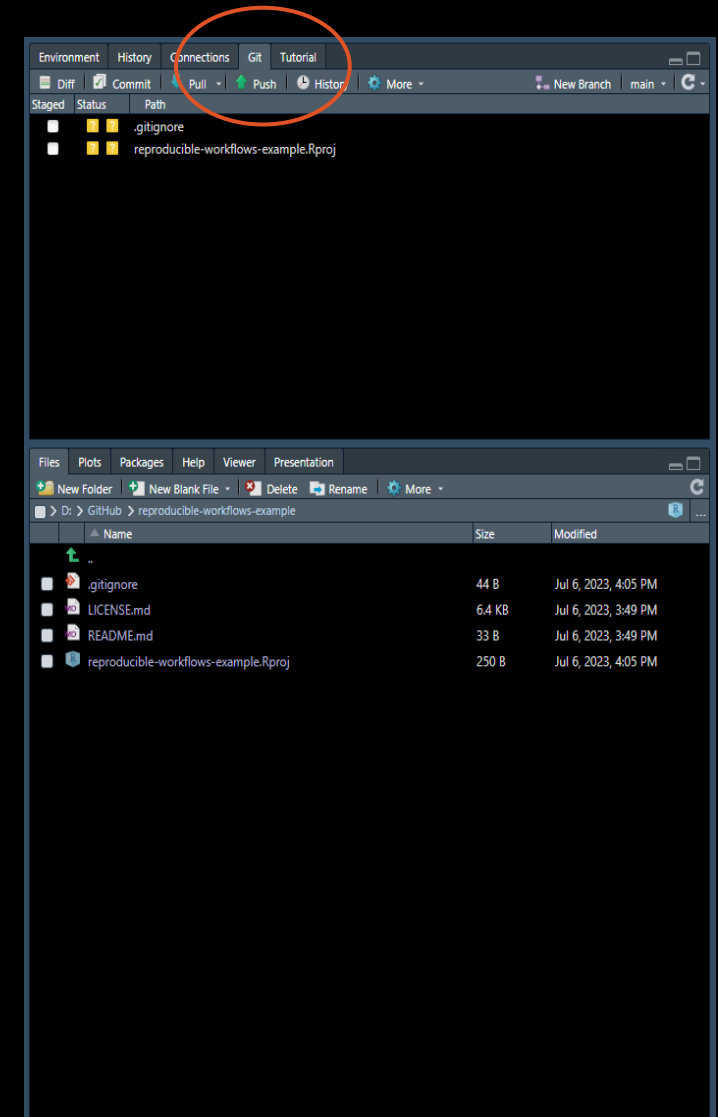
If you already have a project folder (e.g. created by GitKraken, or from an existing project):

In RStudio, go to
File > Existing Directory



2. Create a self-contained project

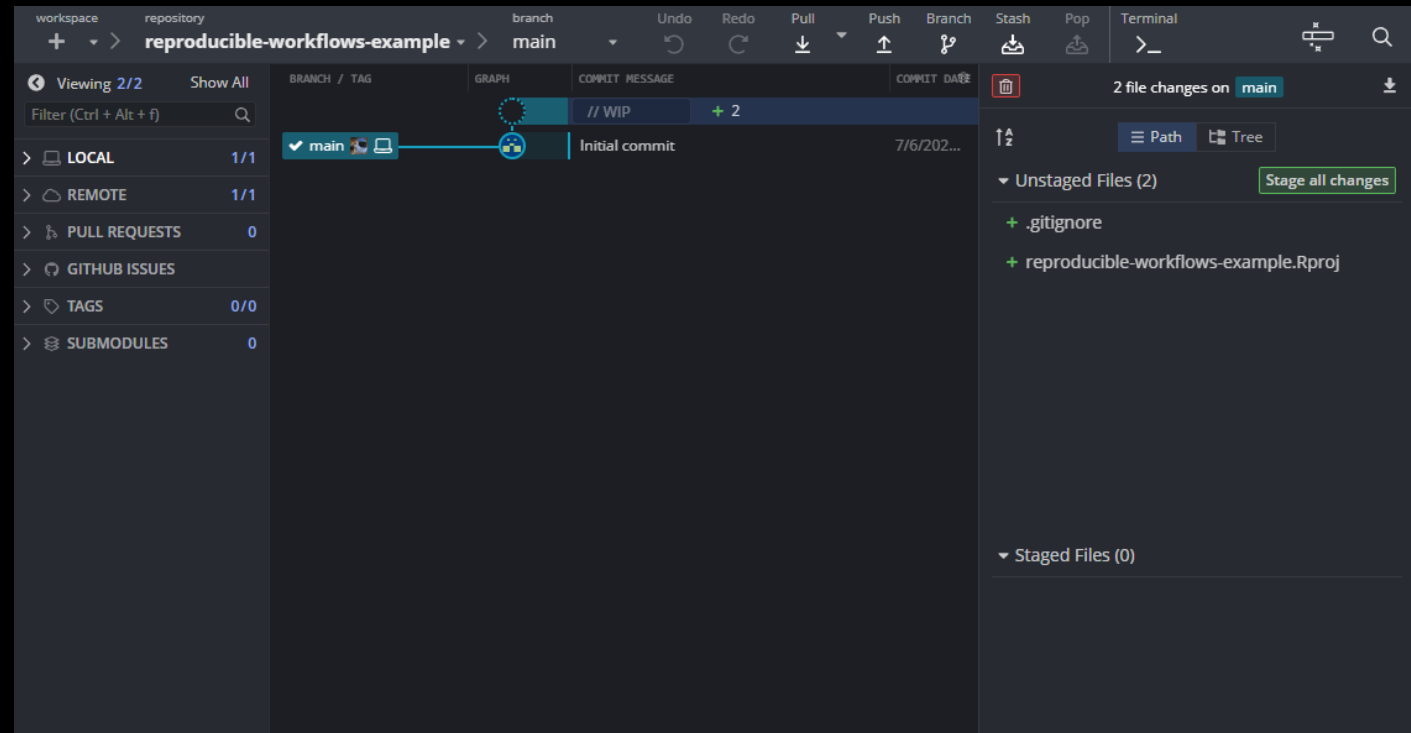
You can now manage your Git repo from RStudio





2. Create a project

You can now manage your Git repo from RStudio, GitKraken





2. Create a project

You can now manage your Git repo from RStudio, GitKraken, or even the command-line (e.g., git bash for Windows)

```
MINGW64:/d/GitHub/reproducible-workflows-example
w-VIC-A127584+cbarros@w-VIC-A127584 MINGW64 /d/GitHub/reproducible-workflows-example (main)
$ git status
On branch main
Your branch is up to date with 'origin/main'.

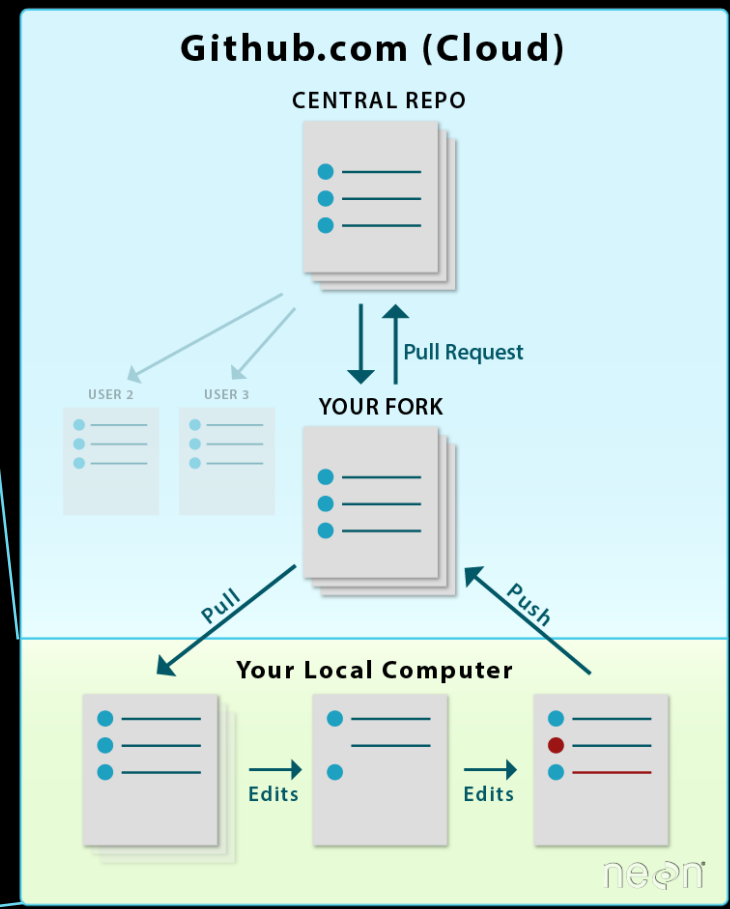
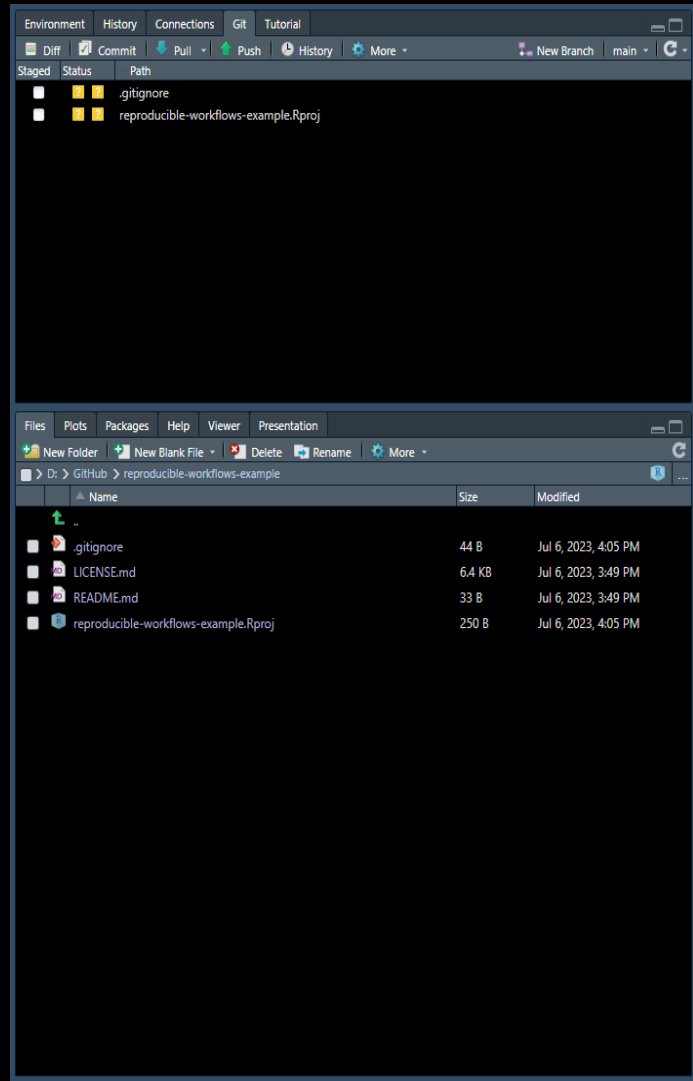
Untracked files:
  (use "git add <file>..." to include in what will be committed)
  .gitignore
  reproducible-workflows-example.Rproj

nothing added to commit but untracked files present (use "git add" to track)
w-VIC-A127584+cbarros@w-VIC-A127584 MINGW64 /d/GitHub/reproducible-workflows-example (main)
$
```



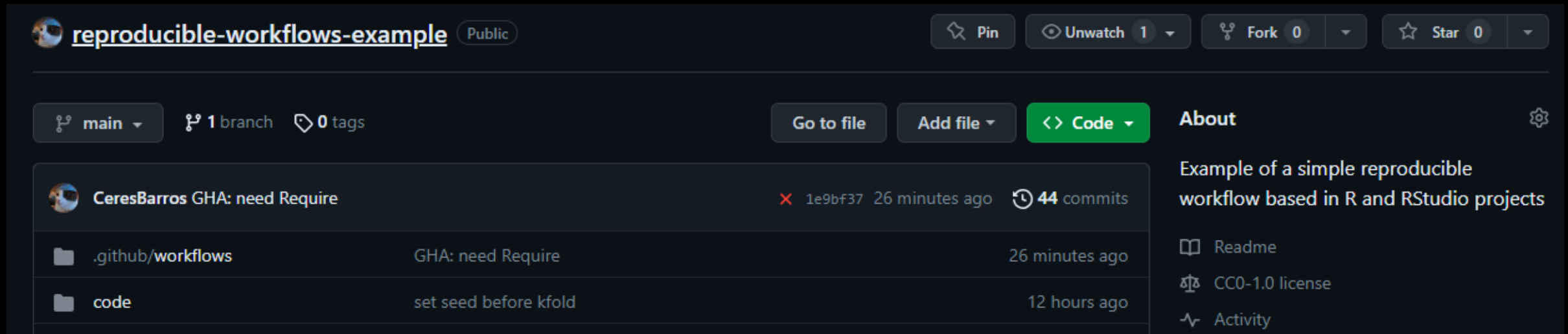
3. Version control

- ✓ keep master/main branch clean; develop in other branches
- ✓ small, incremental, commits
- ✓ **.gitignore sensitive and large files** – think about data storage
- ✓ pull first, push after



Source: <https://www.earthdatascience.org/workshops/intro-version-control-git/pull-request/>

3. Example of a reproducible workflow in R, RStudio and GitHub



The screenshot shows the GitHub interface for the repository 'reproducible-workflows-example' by user 'CeresBarros'. The repository is public and has 0 stars, 0 forks, and 1 unwatch. It features a 'main' branch, 1 other branch, and 0 tags. The repository contains two folders: '.github/workflows' (GHA: need Require, 26 minutes ago) and 'code' (set seed before kfold, 12 hours ago). The repository description is 'Example of a simple reproducible workflow based in R and RStudio projects'. The 'About' section includes links to the README, CC0-1.0 license, and Activity.

reproducible-workflows-example Public

Pin Unwatch 1 Fork 0 Star 0

main 1 branch 0 tags

Go to file Add file Code

CeresBarros GHA: need Require 1e9bf37 26 minutes ago 44 commits

.github/workflows	GHA: need Require	26 minutes ago
code	set seed before kfold	12 hours ago

About

Example of a simple reproducible workflow based in R and RStudio projects

- Readme
- CC0-1.0 license
- Activity

<https://github.com/CeresBarros/reproducible-workflows-example>

Useful resources

Peer-reviewed:

- Barros, C., Luo, Y., Chubaty, A.M., Eddy, I.M.S., Micheletti, T., Boisvenue, C., *et al.* (2023). Empowering ecological modellers with a PERFICT workflow: Seamlessly linking data, parameterisation, prediction, validation and visualisation. *Methods Ecol Evol*, 14, 173–188.
- Braga, P.H.P., Hébert, K., Hudgins, E.J., Scott, E.R., Edwards, B.P.M., Sánchez Reyes, L.L., *et al.* (2023). Not just for programmers: How GitHub can accelerate collaborative and reproducible research in ecology and evolution. *Methods in Ecology and Evolution*, 14, 1364–1380.
- Brousil, M.R., Filazzola, A., Meyer, M.F., Sharma, S. & Hampton, S.E. (2023). Improving ecological data science with workflow management software. *Methods in Ecology and Evolution*, 14, 1381–1388.
- Ellison, A.M. (2010). Repeatability and transparency in ecological research. *Ecology*, 91, 2536–2539.
- McIntire, E.J.B., Chubaty, A., Cumming, S., Andison, D., Barros, C., Boisvenue, C., *et al.* (2022). PERFICT: a Re-imagined Foundation for Predictive Ecology. *Ecology Letters*.
- Thomas, R.Q., Boettiger, C., Carey, C.C., Dietze, M.C., Johnson, L.R., Kenney, M.A., *et al.* (2023). The NEON Ecological Forecasting Challenge. *Frontiers in Ecology and the Environment*, 21, 112–113.
- Wilkinson, M.D., Dumontier, M., Aalbersberg, I.J., Appleton, G., Axton, M., Baak, A., *et al.* (2016). The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data*, 3, 160018.

Reproducible workflows:

- Ecological Forecasting Initiative. (2020). *Reproducible Forecasting Workflows*. Ecological Forecasting Initiative. Available at: <https://ecoforecast.org/reproducible-forecasting-workflows/>. Last accessed 6 July 2023.
- **The Practice of Reproducible Research** (<http://www.practicereproducibleresearch.org/>)
- **R Markdown: The Definite Guide** (<https://bookdown.org/yihui/rmarkdown/>)
- **R Markdown cheat sheets** (<https://www.rstudio.com/wp-content/uploads/2015/02/rmarkdown-cheatsheet.pdf>)
- **GitHub Quickstart** (<https://docs.github.com/en/get-started/quickstart/hello-world>)

Software:

RStudio

R

GitKraken

Git

References

GIFs/Images:

- https://www.reddit.com/r/gifs/comments/4a3exq/cat_typing_a_document_on_laptop/
- https://en.wikipedia.org/wiki/One_Ring#/media/File:One_Ring_Blender_Render.png
- All icons designed by Freepik and downloaded from Flaticon.com

Literature

- Barros, C., Luo, Y., Chubaty, A.M., Eddy, I.M.S., Micheletti, T., Boisvenue, C., *et al.* (2023). Empowering ecological modellers with a PERFICT workflow: Seamlessly linking data, parameterisation, prediction, validation and visualisation. *Methods Ecol Evol*, 14, 173–188.
- Braga, P.H.P., Hébert, K., Hudgins, E.J., Scott, E.R., Edwards, B.P.M., Sánchez Reyes, L.L., *et al.* (2023). Not just for programmers: How GitHub can accelerate collaborative and reproducible research in ecology and evolution. *Methods in Ecology and Evolution*, 14, 1364–1380.
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