Scientific Workflows & the Informatics of Model-Data Fusion

Lecture 04

Synopsis

*Forecasts must be **transparent** and accountable, and generally they must **repeated** and updated regularly. In keeping with the theme of 'best practices', before diving into the statistics of model-data fusion we set the stage with the informatics of model-data fusion by describing new tools that make science more transparent, repeatable, and automated. These tools are not isolated to forecasting – they should become part of all aspects of science -- but they are an essential part of a forecaster's toolkit*

Climategate

- East Anglia University's Climate Research Unit (CRU) hacked 11/17/09
- 1000+ emails, 2000+ docs, source code
- Science out of context

The Aftermath

"...that climate scientists should take steps to make available all the data that support their work (including raw data) and full methodological workings (including the computer codes)."

House of Commons Science and Technology Committee, 2010

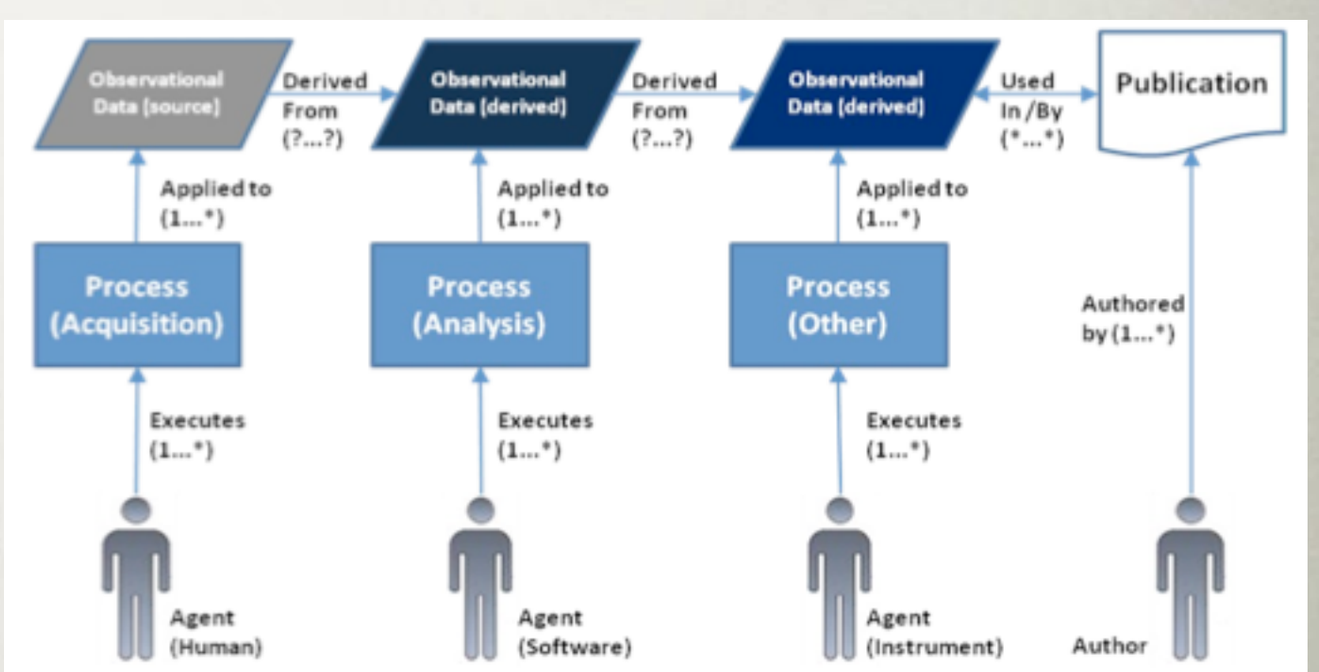


Figure 1. CRU dataset workflows

- Transparency
- Repeatability
- Provenance

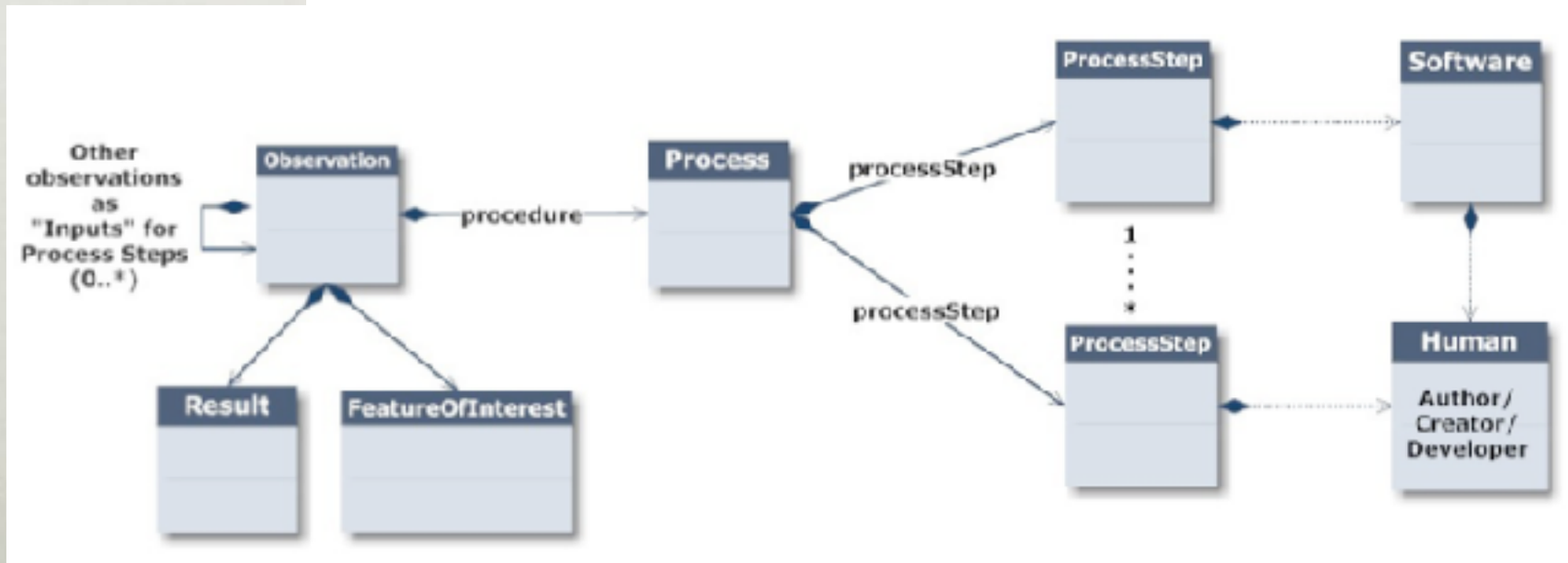


Figure 2. An overview of the ACRID provenance model.

Shaon et al 2012

Transparency & Repeatability

- Reproducibility is one of the fundamental tenants of science
- Analyses getting more and more sophisticated
- “Methods” section rarely provides enough information
- Proprietary, unverifiable tools

TABLE 1. Analytical methods used in the syntheses of the species richness–productivity relationship.

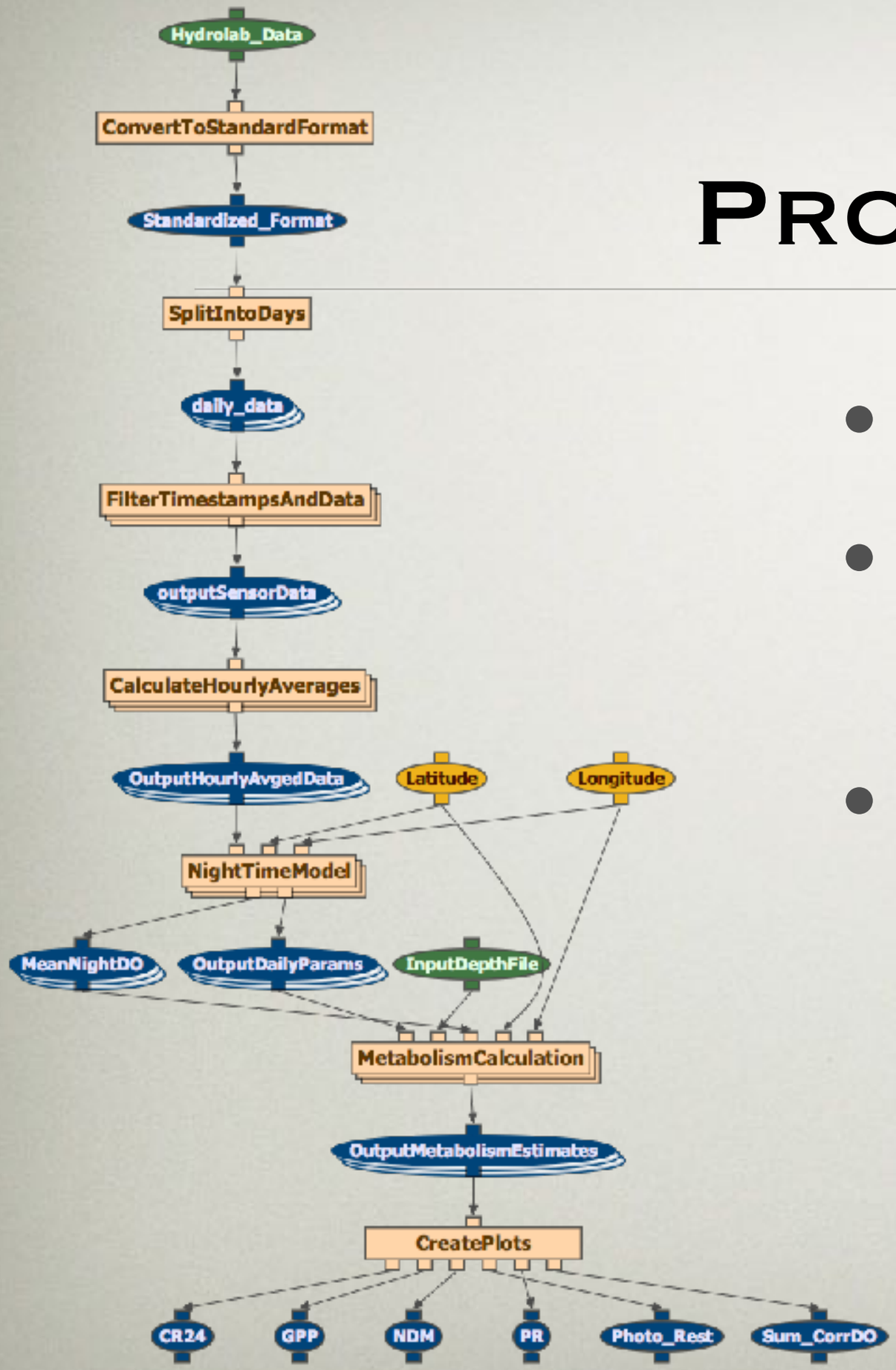
Author	Analytical method(s) used	Analytical tool(s) used	Comments
Waide et al. (1999)	linear and quadratic regressions	none specified	not repeatable
Mittelbach et al. (2001)	ordinary least-squares regression	SYSTAT 8.0	possibly repeatable; current available version is 12.0
	Poisson regression	NAG statistical add-in for Excel	not repeatable; software discontinued
	"Mitchell-Olds and Shaw test" (Mitchell-Olds and Shaw 1987)	none specified	not repeatable; software unavailable (but algorithm available); which of three tests proposed by Mitchell-Olds and Shaw was also not specified
	chi-square exact test	StatXact	possibly repeatable; no version given
	meta-analysis using mixed-effects model	MetaWin 2.0	repeatable; commercial software version still available
Whittaker and Heergard (2003)	Poisson regression	not specified	not repeatable
Gillman and Wright (2006)	ordinary least-squares regression on "some" data sets of Mittelbach et al. (2001)	software not specified; data sets reanalyzed not specified	not repeatable
Pärtel et al. (2007)	multinomial logit regression	Statistica 6.1	possibly repeatable; current release is 8.0
Laanisto et al. (2008)	Fisher exact tests	not specified	possibly repeatable using available algorithms
	general linear model	Statistica 6.1	possibly repeatable; current release is 8.0

Note: Manufacturers of software are: SYSTAT 8.0, Systat Software, Inc., Chicago, Illinois, USA; NAG statistical add-in for Excel, Numerical Algorithms Group, Oxford, UK; StatXact, Cytel, Inc., Cambridge, Massachusetts, USA; MetaWin 2.0, Sunderland Associates, Inc., Sunderland, Massachusetts, USA; Statistica 6.1, StatSoft, Inc., Tulsa, Oklahoma, USA.

Ellison 2010 "Repeatability and transparency in ecological research" Ecology 91: 2536-9

Repeatability and reproducibility of ecological synthesis requires full disclosure not only of hypotheses and predictions, but also of the raw data, methods used to produce derived data sets, choices made as to which data or data sets were included in, and which were excluded from, the derived data sets, and tools and techniques used to analyze the derived data sets.

Ellison 2010

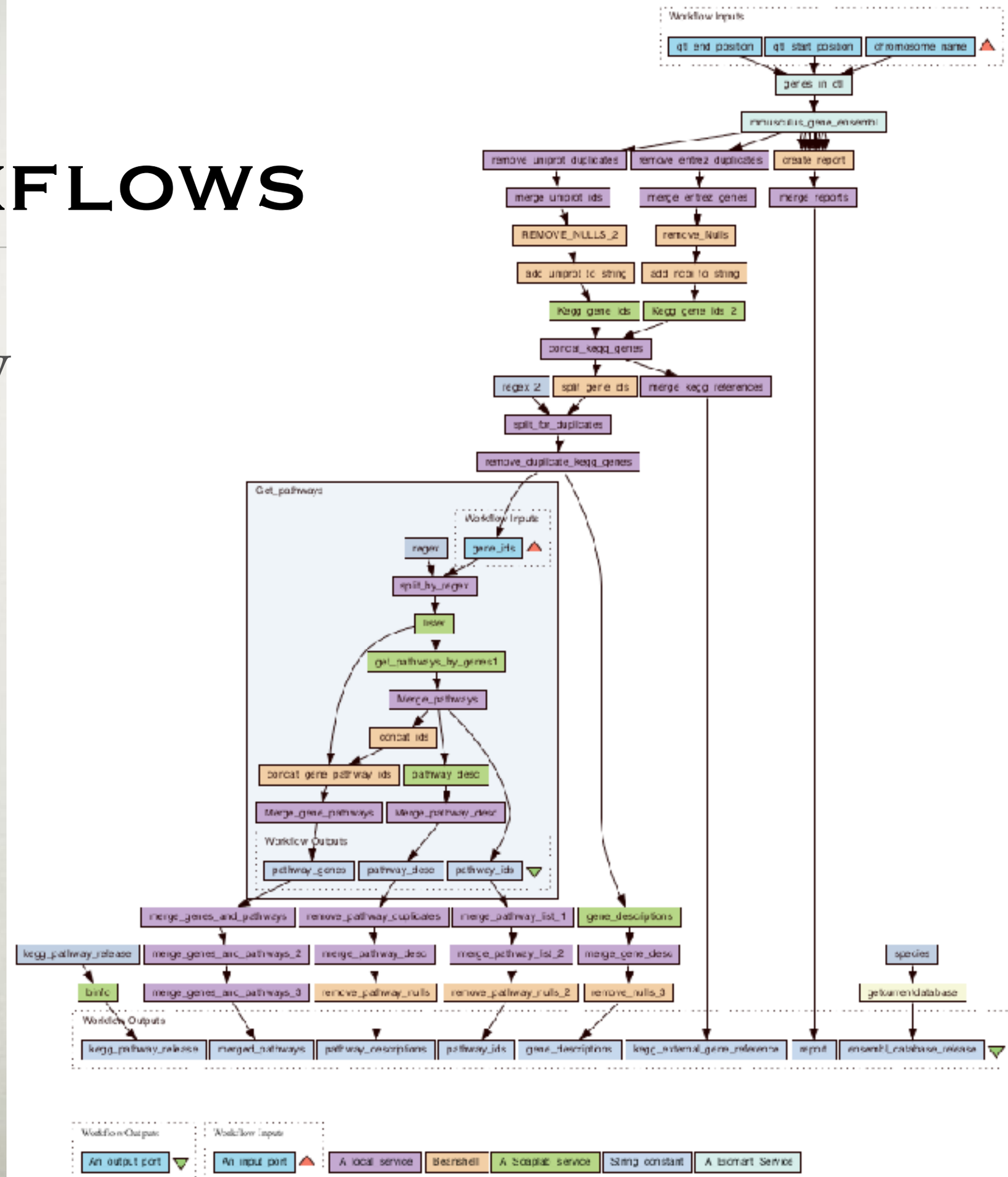


Provenance

- "Chain of custody"
- Metadata about analysis and modeling
- Pre & post-processing: transformation, interpolation, gap-filling, filtering, summarizing, exclusion, visualization, ..

Workflows

- Control the flow of information
- More intuitive than raw code
- Modular
- Heterogeneous
- Reusable
- Sharing

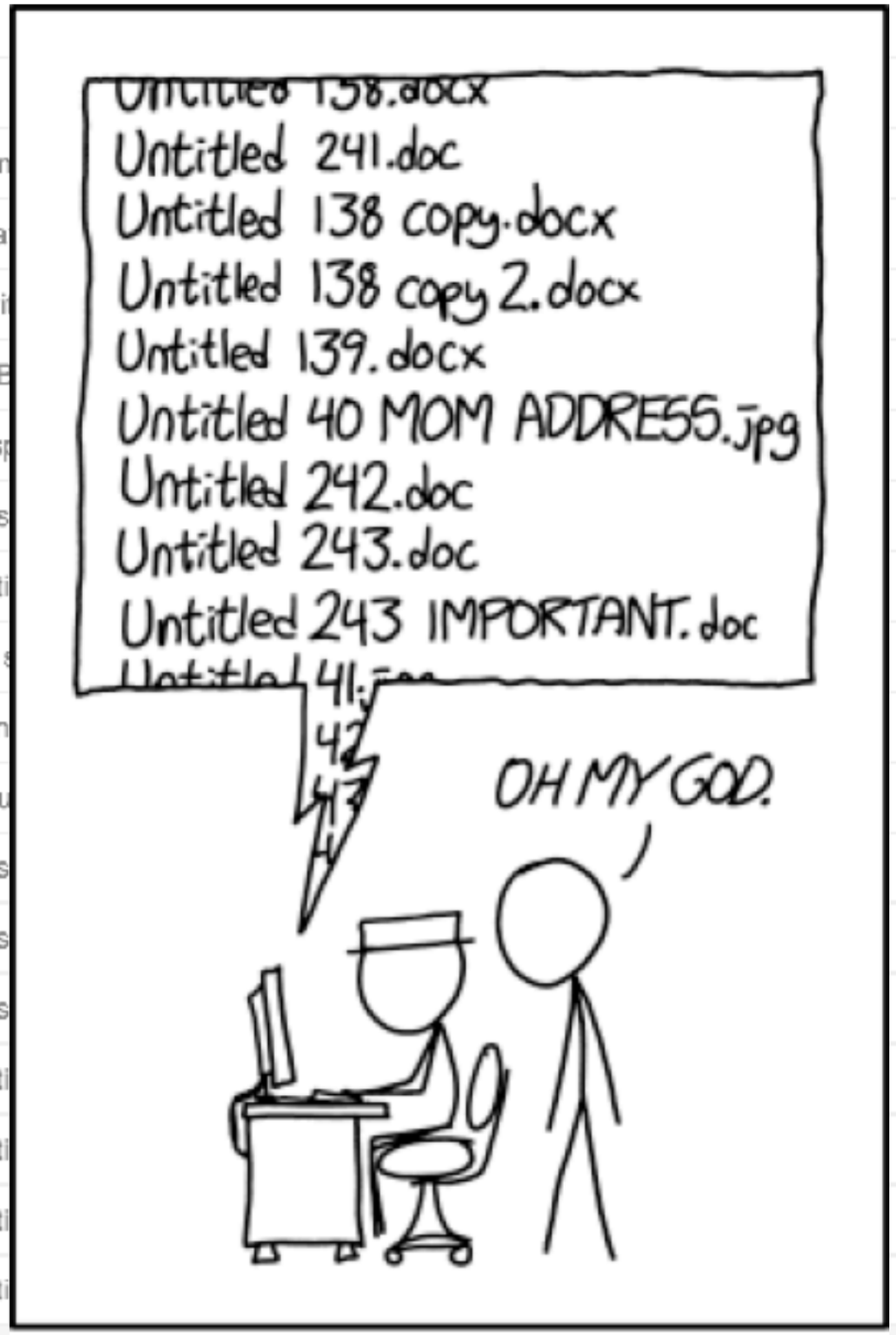


Branch: **master** ▾ **Temporal-Scaling-MS** / **R** /

New file | **Find file** | **History**

crollinson get rid of PFT-specific intercept ··· Latest commit `9e08268` 2 days ago

..		
Exploratory	File Cleanup	7 months ago
Exploratory2	Initial push of fin	3 months ago
0_Calculate_GAMM_Posteriors.R	more flexible da	2 days ago
0_Calculate_GAMM_Weights.R	allow models wi	13 days ago
0_GAMM_Plots.R	Generalize RGB	6 months ago
0_calculate.sensitivity_TPC.R	get rid of PFT-sp	2 days ago
0_process.gamm.R	Modify GAMM s	16 days ago
1_format_metdrivers.R	File reorganizati	20 days ago
2_format_models.R	Update GAMM s	14 days ago
3a_format_treerings_RWI.R	Finish calculatin	20 days ago
3b_format_treerings_NPP.R	All GAMs run su	19 days ago
4_GAMMs_Baseline.R	Modified GAM s	2 days ago
5_GAMMs_TemporalExtent.R	Modified GAM s	2 days ago
6_GAMMs_Composition.R	Modified GAM s	2 days ago
7_analysis_response_baseline_ensembles.R	File reorganizati	9 days ago
7a_graph_ensembles_rgb_AllSites.R	File reorganizati	9 days ago
7b_graph_ensembles_rgb_byModel.R	File reorganizati	9 days ago
8_analysis_sensitivity_TemporalExtent.R	File reorganizati	9 days ago
8a_graph_ensembles_rgb_AllModels.R	File reorganizati	9 days ago
9_analysis_sensitivity_biogeography.R	GAM conceptua	4 days ago



Best Practices for Scientific Computing

Software Engineering is a >$400B industry

Don't Reinvent the Wheel!

Ecologists write Crappy Code

What Ecologists Think Good Code Looks Like:

```
void* Realocate(void*buf, int os, int ns)
{
     void*temp;
     temp = malloc(os);
     memcpy((void*)temp, (void*)buf, os);
     free(buf);
     buf = malloc(ns);
     memset(buf, 0, ns);
     memcpy((void*)buf, (void*)temp, ns);
     return buf;
}
```

- Highly optimized
- Not Human Readable
  - Meaningless variable names
  - Undocumented
- Hard to maintain

Ecologists write Crappy Code

What Good Code Looks Like:

```
/* compute displacement with Newton's equation x = v₀t + ½at² */
const float gravitationalForce = 9.81;
float timeInSeconds = 5;
float displacement = (1 / 2) * gravitationalForce * (timeInSeconds ^ 2)
```

- Written to be human readable
- Self-documenting variables
- Documents WHY something is done not HOW
- Define constants for re-use

Start with a Plan

Flowchart/Outline → Pseudocode

```
## Define settings, load required libraries

## Read and organize data

## Define priors and initial conditions

## Enter MCMC loop

        ## propose new parameter value
        ## run model
        ## evaluate Likelihood and prior
        ## accept or reject proposed value

## Statistical diagnostics

## Visualize outputs
```

Done with documentation before code!

Start with a Plan

Modular Design
(functions, objects, etc)

```
##' Convert NARR files to CF files
##' @name met2CF.NARR
##' @title met2CF.NARR
##' @export
##'
##' @param in.path
##' @param in.prefix
##' @param outfolder
##' @param start_date the start date of the data to be downloaded (will only use the year part of the date)
##' @param end_date the end date of the data to be downloaded (will only use the year part of the date)
##' @param overwrite should existing files be overwritten
##' @param verbose should ouput of function be extra verbose
##' @author Elizabeth Cowdery, Rob Kooper
##'
met2CF.NARR <- function(in.path, in.prefix, outfolder, start_date, end_date, overwrite=FALSE, verbose=FALSE, ...){
```

- Isolates tasks
- Allows reuse (don't cut-and-paste)
- Only have to change in one place
- Separates purpose (inputs -> output) from implementation

Version Control

- **Update** working copy to include the latest changes in the repository (pull)
- **Merge** these changes into their working copy and resolve any conflicts
- **Edit** their working copy to add new features and fix bugs
- **Commit** these changes and communicate them back to the central repository (push, pull request)

Owner

Collaborator

Github

clone

push

Local

git add project.txt
git commit -m “Start project”

project.txt

1) Assemble project team

Owner

Collaborator

Github

Fork

github.com/me/foo

github.com/you/foo

New pull request

clone

push

clone

push

Local

foo

foo

git add project.txt
git commit -m “Plan project”

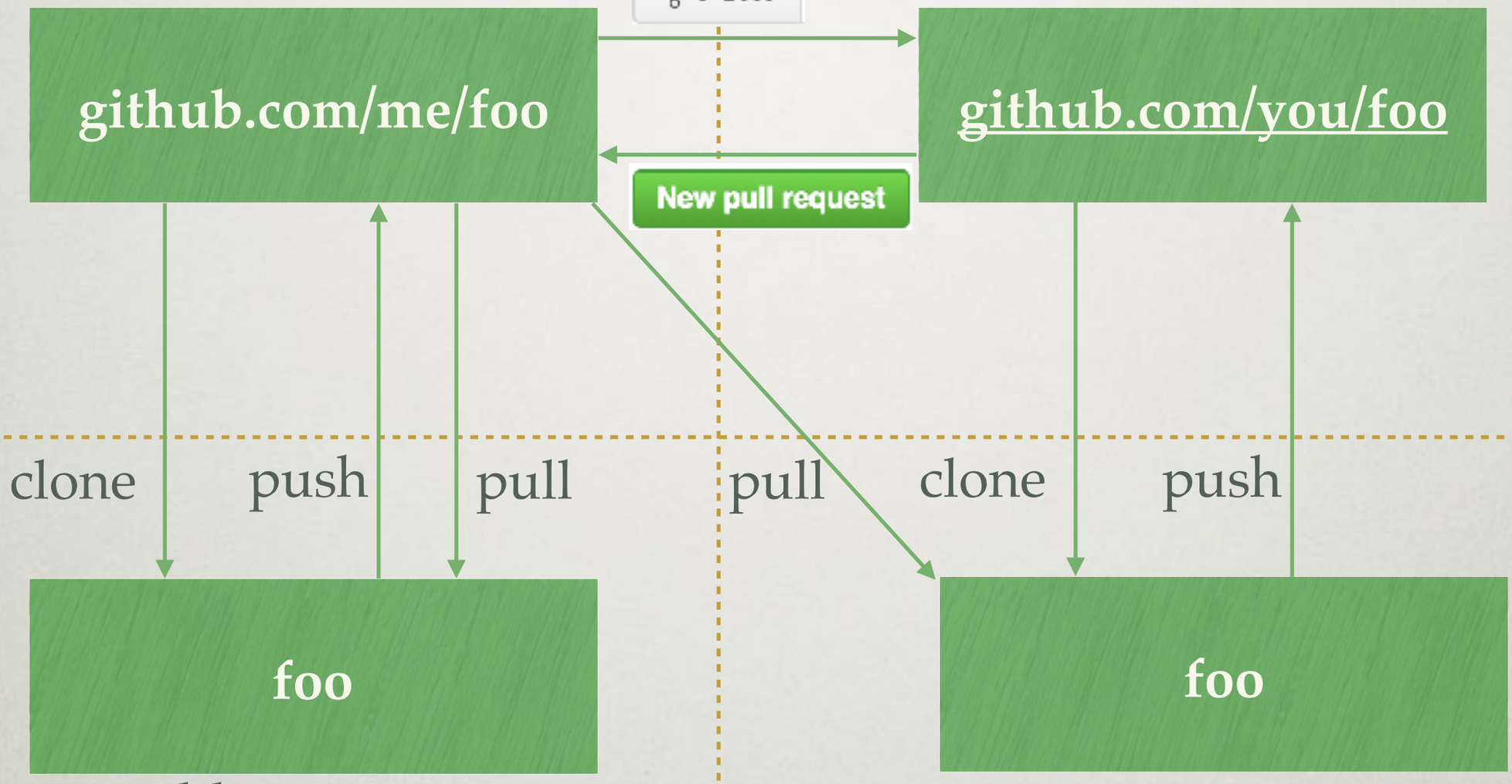
project.txt

1) Assemble project team
2) Flowchart / outline

Owner

Collaborator

Github



Local

git add project.txt
git commit -m “Modules”

project.txt

1) Assemble project team
2) Flowchart / outline
3) Module Design

Owner

Collaborator

Github

github.com/me/foo

github.com/you/foo

New pull request

push

pull

pull

push

Local

foo

foo

Make Incremental Updates

Commit often!!!!
Automate Tests
Continuous Integration

https://travis-ci.org/EcoForecast/EF_Activities

Travis CI Blog Status Help Michael Dietze MD

EcoForecast / EF_Activities

Current Branches Build History Pull Requests Settings

✓ **Pull Request #9** Answers to exercise #2

#30 passed

Commit 17258f1

#9: Answers to exercise #2

Elapsed time 6 min 7 sec

2 days ago

parevalo authored and committed

This job ran on our new platform for Precise builds. Please read our blog post for more information.

Remove log Raw log

```
  1 Worker information                                              worker_info
  6 Build system information                                        system_info
 95
 96 $ git clone --depth=50 https://github.com/EcoForecast/EF_Activities.git   git.checkout   1.08s
115
116 Setting environment variables from .travis.yml
117 $ export BOOTSTRAP_LATEX="1"
118
119 $ export CC=gcc
120 $ gcc --version
121 gcc (Ubuntu/Linaro 4.6.3-1ubuntu5) 4.6.3
122 Copyright (C) 2011 Free Software Foundation, Inc.
```

Document!

```
##' Convert NARR files to CF files
##' @name met2CF.NARR
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##' @export
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##' @param verbose should ouput of function be extra verbose
##' @author Elizabeth Cowdery, Rob Kooper
##'
met2CF.NARR <- function(in.path, in.prefix, outfolder, start_d
```

met2CF.NARR {PEcAn.data.atmosphere} R Documentation

met2CF.NARR

Description

Convert NARR files to CF files

Usage

```
met2CF.NARR(in.path, in.prefix, outfolder, start_date, end_date,
  overwrite = FALSE, verbose = FALSE, ...)
```

Arguments

in.path	
in.prefix	
outfolder	
start_date	the start date of the data to be downloaded (will only use the year part of the date)
end_date	the end date of the data to be downloaded (will only use the year part of the date)
overwrite	should existing files be overwritten
verbose	should ouput of function be extra verbose

Author(s)

Elizabeth Cowdery, Rob Kooper

[Package *PEcAn.data.atmosphere* version 1.4.4 Index]

Done is better than perfect.

Sheryl Sandberg

Wilson et al 2014

Best Practices for Scientific Computing

1. **Write programs for people, not computers.**
    1. A program should not require its readers to hold more than a handful of facts in memory at once.
    2. Names should be consistent, distinctive, and meaningful.
    3. Code style and formatting should be consistent.
    4. All aspects of software development should be broken down into tasks roughly an hour long.

2. **Automate repetitive tasks.**
    1. Rely on the computer to repeat tasks.
    2. Save recent commands in a file for re-use.
    3. Use a build tool to automate their scientific workflows.
3. **Use the computer to record history.**
    1. Software tools should be used to track computational work automatically.
4. **Make incremental changes.**
    1. Work in small steps with frequent feedback and course correction.

5. **Use version control.**
    1. Use a version control system.
    2. Everything that has been created manually should be put in version control.
6. **Don't repeat yourself (or others).**
    1. Every piece of data must have a single authoritative representation in the system.
    2. Code should be modularized rather than copied and pasted.
    3. Re-use code instead of rewriting it.

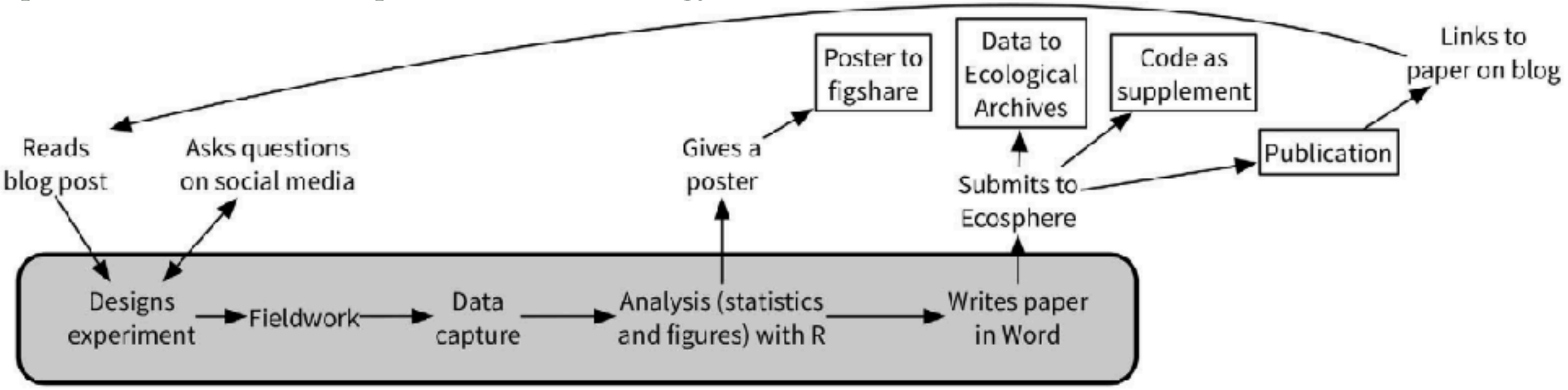
7. **Plan for mistakes.**
    1. Add assertions to programs to check their operation.
    2. Use an off-the-shelf unit testing library.
    3. Turn bugs into test cases.
    4. Use a symbolic debugger.
8. **Optimize software only after it works correctly.**
    1. Use a profiler to identify bottlenecks.
    2. Write code in the highest-level language possible.

9. **Document the design and purpose of code rather than its mechanics.**
    1. Document interfaces and reasons, not implementations.
    2. Refactor code instead of explaining how it works.
    3. Embed the documentation for a piece of software in that software.
10. **Conduct code reviews.**
    1. Use code review and pair programming when bringing someone new up to speed and when tackling particularly tricky design, coding, and debugging problems.
    2. Use an issue tracking tool.

Open source code and community models

- Open Source
  - free as in freedom
  - free as in no (direct) cost
  - public license (e.g. GNU GPL, CC)
- Community tools & models
  - Rules and mechanisms for contribution, evolution

Hampton et al 2015 “Tao of Open Science for Ecology”



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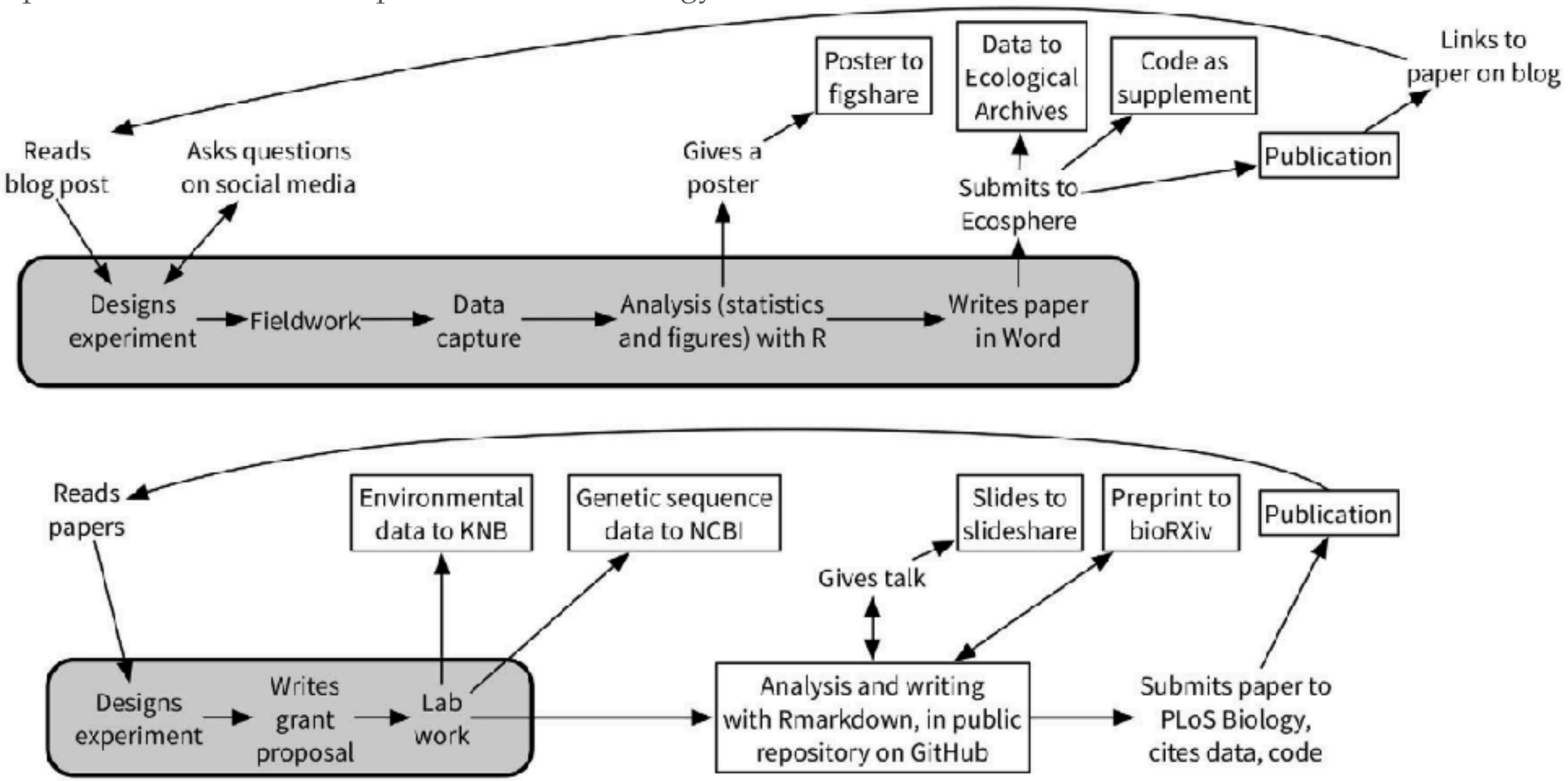

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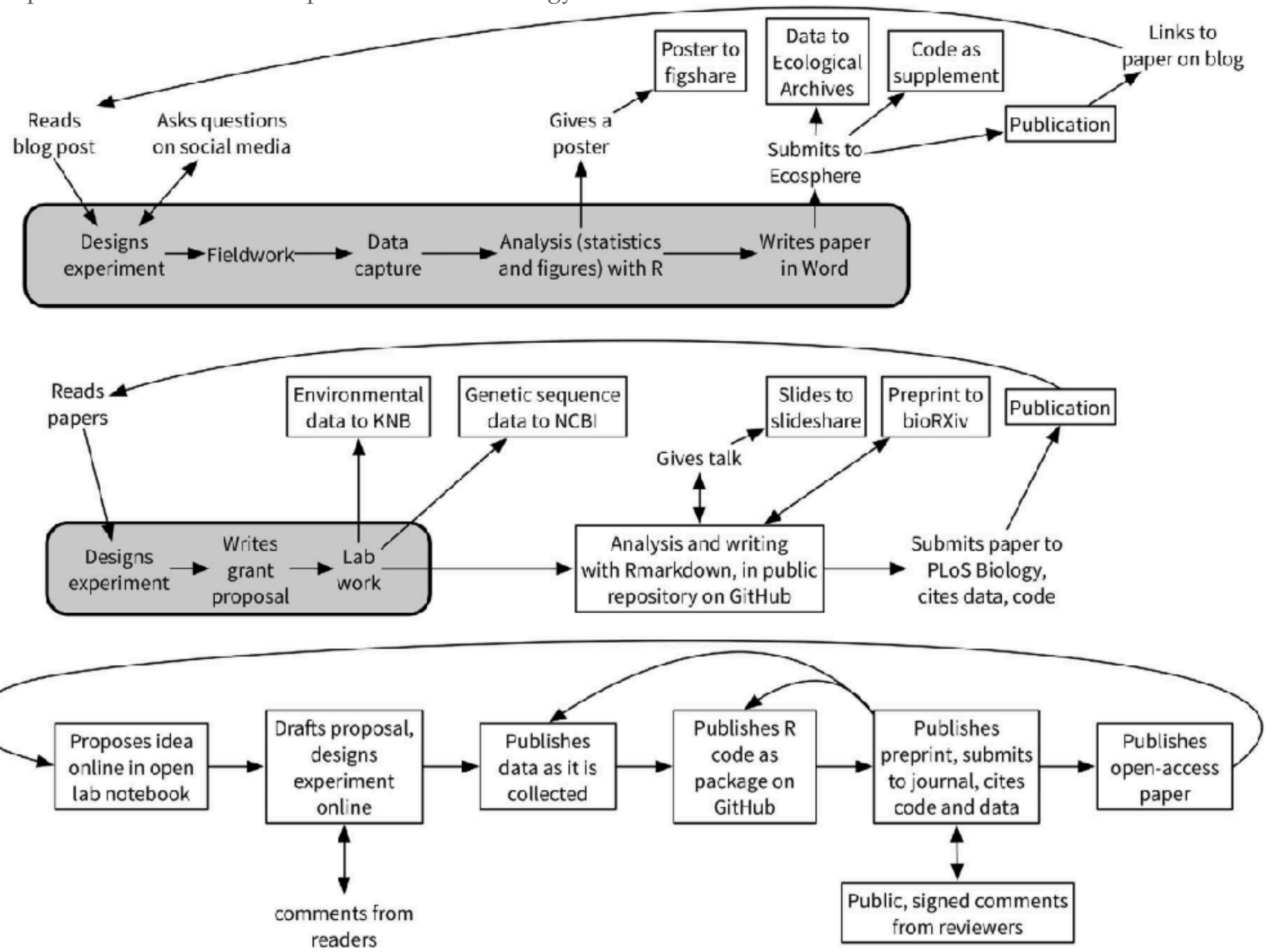
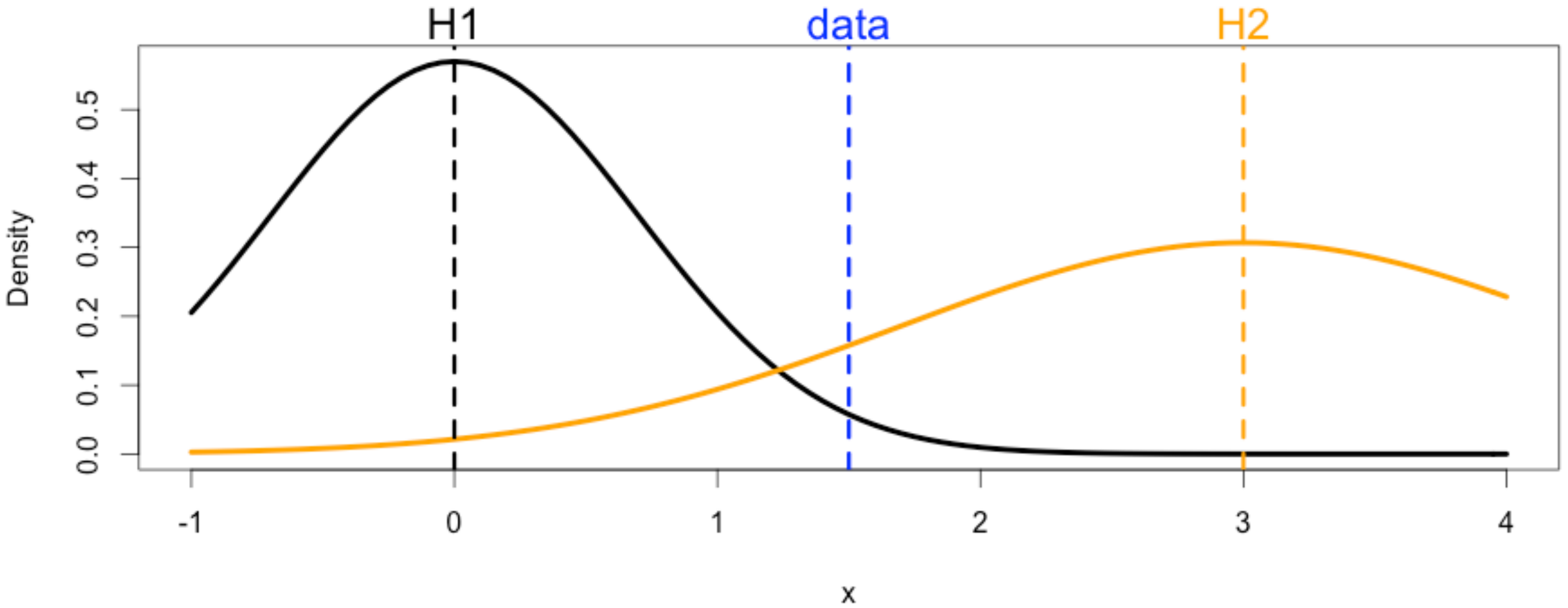


And now for something completely different....

Absent: beta, binomial, gamma, exponential,
Laplace, Pareto, Bernoulli, geometric,
hypergeometric, Wishart



Which Hypothesis is more Likely to have generated this Data?

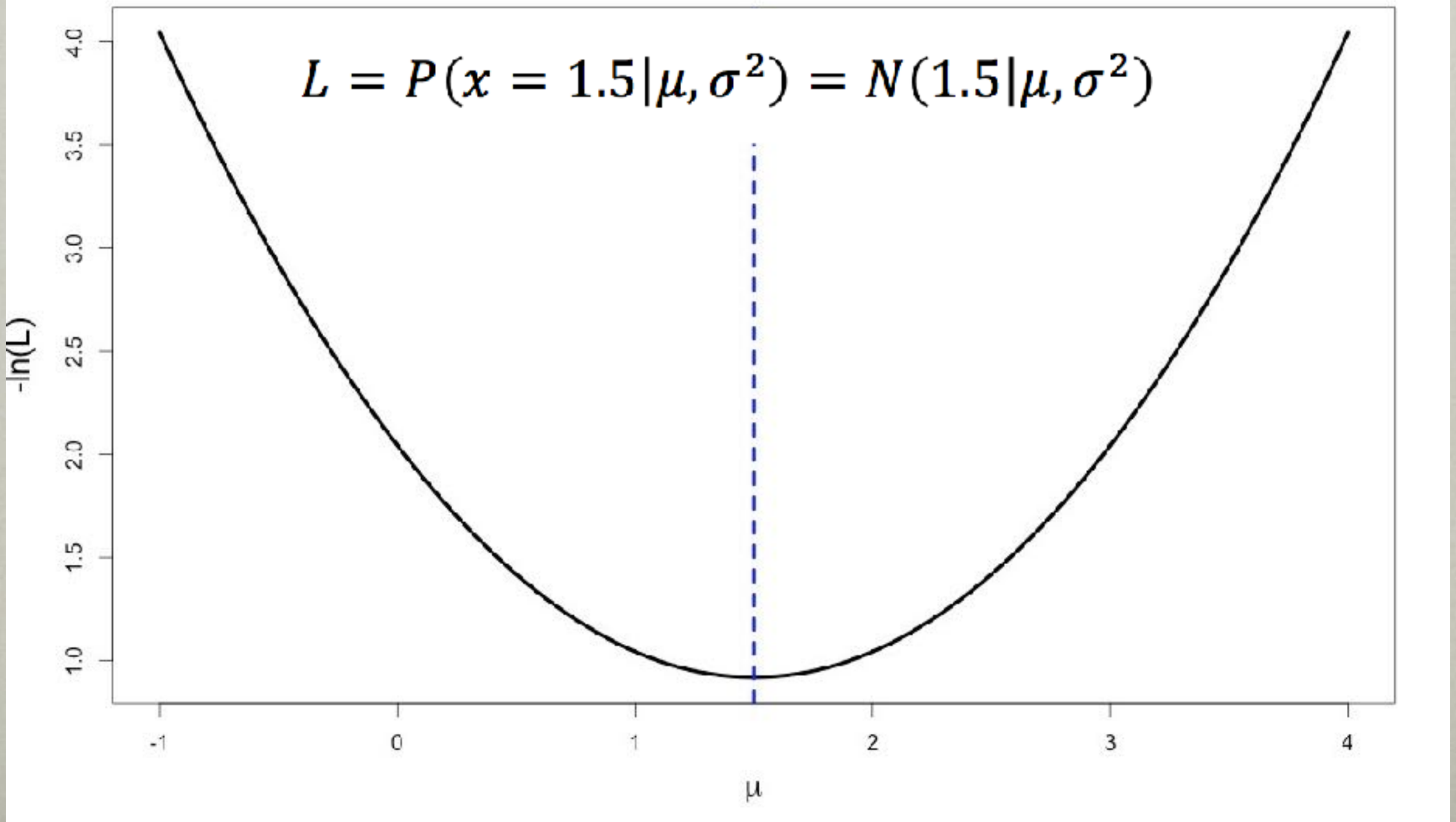
Likelihood

$$L = P(X = x|\theta) = P(data|model)$$

- Probability of observing a given data point x conditional on parameter value Θ

- Likelihood principle: a parameter value is more likely than another if it is the one for which the data are more probable

Likelihood Profile



What μ maximizes L?

$$L = N(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{\sigma^2}}$$

$$-\ln L = \ln 2\pi + 2ln\sigma + \frac{(x-\mu)^2}{\sigma^2}$$

$$-\frac{\partial lnL}{\partial \mu} = -2\frac{(x-\mu)}{\sigma^2} = 0$$

$$\mu_{MLE} = x$$

Maximum Likelihood

1. Write down the Likelihood
2. Take the log
3. Take the derivatives w.r.t. each parameter
4. Set equal to 0 and solve for parameter

Maximum Likelihood Estimate (MLE)