## Roots for Resilience in the Year of **Open** Science: Lessons Learned

### Tomasz Wlodarczyk 11/25/2023





THE UNIVERSITY OF ARIZONA RESEARCH, INNOVATION & IMPACT Arizona Institutes for Resilience



RESEARCH, INNOVATION & IMPACT Data Science Institute

https://nasa.github.io/Transform-to-Open-Science/year-of-open-science/

## Roots for Resilience & Foundational Open Science Skills









### Foundational Open Science Skills

CyVerse's 8-week virtual workshop teaches you the principles, practices, and how-tos for doing collaborative open science using cutting-edge, open source cyberinfrastructure, in a collaborative, hands-on setting. To see how our FOSS workshop can support your work, check out the curriculum.

### https://foss.cyverse.org/00\_basics/

The Roots for Resilience Program provides training and support to select graduate students on open, reproducible science and computational infrastructure to enhance research focused on resiliency in the environment.

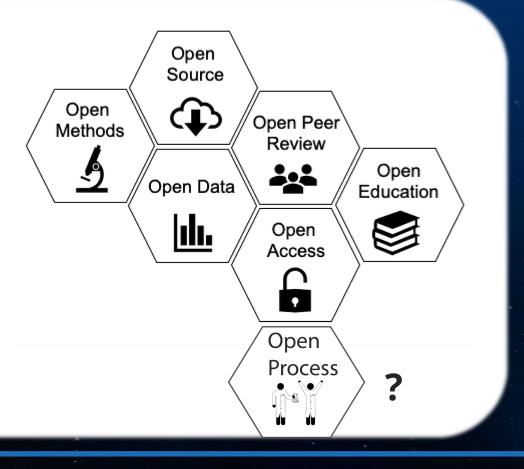
## **Open-Science**

"Open Science is the movement to make scientific research (including publications, data, physical samples, and software) and its dissemination accessible to all levels of society, amateur or professional..." (Wikipedia)

OriginalAwesome List:https://github.com/sindresorhus/awesomeConsolidated

https://tyson-swetnam.github.io/awesome-open-science/

## **Open, FAIR and CARE Science**



DOI Raw Data Archived Open Protocols Reproducible Codes Clear Licensing Open Collaboration FAIR







Findable A

Accessible Interoperable

 $\bowtie$ 

Reusable

Collective Authority Responsibility Ethics

# **Open Process** – In response to Reproducibility Crisis

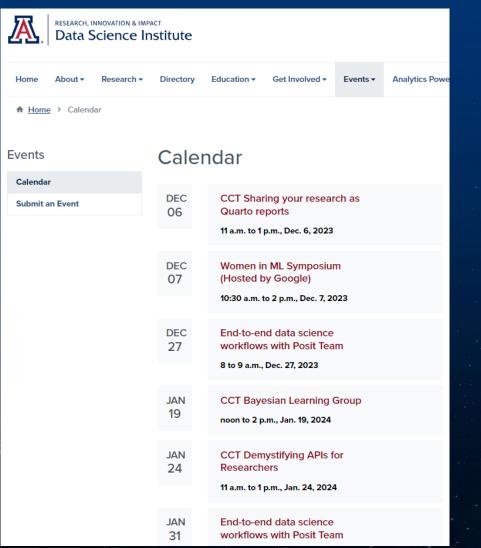
### **Preregistration**

- Prevents HARKing (Hypothesizing After the Results are Known)
- Separates hypothesis-generating from hypothesistesting (because the same data can't be used to generate and test hypothesis)
  - Mitigates **p-hacking** (manipulation of p-value)



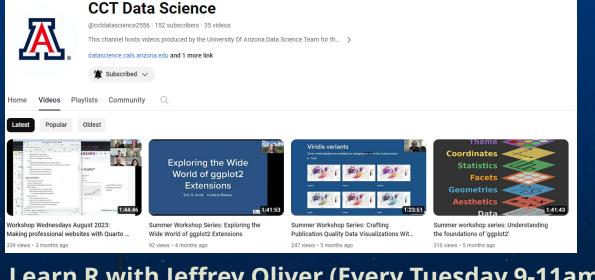
https://www.cos.io/initiatives/prereg

### **Check Data Science Institute's events**



### https://datascience.arizona.edu/calendar

### **CCT Data Science YouTube Channel**



Learn R with Jeffrey Oliver (Every Tuesday 9-11am) Sign up for the UA Data Science Slack workspace

https://jcoliver.github.io/uadatascience-slack/

**Contact your Data Science Ambassador** 

https://datascience.arizona.edu/dsa



Popular

**Kelsev** Gonzalez

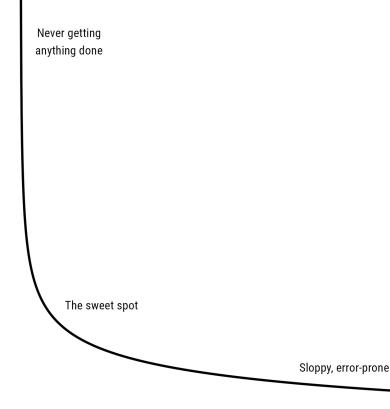
@KelseyGonzalez · 994 subscribers · 12 videos https://kelseygonzalez.github.io/ >

🁚 Subscribed 🗸

Playlists Community Home Videos Oldest

## **Project Management**

"The best time to organize is at the start, the 2nd best is right now"



Time spent finding stuff

- 1. Add README file to your project
- 2. Create consistent folder structure for each project
- 3. Keep raw data raw
- 4. Avoid manual (point-and-click) steps as much as possible
- 5. Create collaborative workspace
- 6. Backup your data (multiple locations)
- 7. Use AGILE

Time spent organizing

## **Project Structure**

## **Option 1:** Create a bash script to automate the process.

File Edit Format View Help  mkdir "\$1" cd "\$1"    exit		
cd "\$1"    exit		
echo "# \$1" >> README.md		
mkdir data		
mkdir data/raw		
mkdir data/cleaned		
mkdir scripts		
mkdir images		
mkdir reports		
I     Image: Structure       File     Home       Share     View		
$\leftarrow$ $\rightarrow$ $\checkmark$ $\uparrow$ $\bigcirc$ CNR	S + Synch > Cy	/Verse > Folder Structure
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😞 Creative Cloud	C	11/25/2023 2:57 PM
scripts	C	11/25/2023 2:57 PM
	2	11/25/2023 2:57 PM
OneDrive - Un     Image: Construction - Un     Attachments     Structure.sh	C	11/25/2023 2:55 PM

### **Option 2: Use CookieCutter**



### https://drivendata.github.io/cookiecutter-data-science/

LICENSE	0
└── Makefile	<- Makefile with commands like `make data` or `make train`
README.md	<- The top-level README for developers using this project.
├── data	····· ··· ··· ····
⊨ external	<- Data from third party sources.
→ interim	<- Intermediate data that has been transformed.
processed	<- The final, canonical data sets for modeling.
L raw	<- The original, immutable data dump.
	- The or egenacy climatable adea dampt
- docs	<- A default Sphinx project; see sphinx-doc.org for details
⊢ models	<- Trained and serialized models, model predictions, or model summaries
├── notebooks	<- Jupyter notebooks. Naming convention is a number (for ordering), the creator's initials, and a short `-` delimited description, e.g. `1.0-jqp-initial-data-exploration`.
   references	<- Data dictionaries, manuals, and all other explanatory materials.
- reports	<- Generated analysis as HTML, PDF, LaTeX, etc.
L— figures	<- Generated graphics and figures to be used in reporting
l cgui cs	· · · · · · · · · · · · · · · · · · ·
├── requirements.txt	<- The requirements file for reproducing the analysis environment, e.g. generated with `pip freeze > requirements.txt`
∣ ├── setup.py	<- Make this project pip installable with `pip install -e`
⊢ src	<- Source code for use in this project.
	<- Makes src a Python module
1 1py	< Hakes she a hyeron modale
	<- Scripts to download or generate data
L make datas	
⊢ features	<- Scripts to turn raw data into features for modeling
L— build_feat	
	<- Scripts to train models and then use trained models to make
i i i	predictions
predict_mo	odel.py
L- train_mode	
│ └── visualization │ └── visualize.	<- Scripts to create exploratory and results oriented visualizations py
∣ └── tox.ini	<- tox file with settings for running tox; see tox.readthedocs.io

## **Project Governance**

Project Governance is the set of rules, procedures and policies that determine how projects are managed and overseen

### GenoPhenoEnvo Governance and Operations Manual

Munoz-Torres, Monica C 1 💿; Bartelme, Ryan P 2 🔞; Behrisch, Michael 3; Cain, Emily J 2 🔞; Chang, Remco 4 🎯; Debnath, Ishita 5;
Heidorn, Bryan² 🔞 ; 🛛 Jaiswal, Pankaj¹ 🄞 ; 🛛 LeBauer, David S² 💿 ; Mosca, Ab⁴ 💿 ; Ross, Arun⁵ 💿 ; Swetnam, Tyson L² 💿 ;
Thessen, Anne <sup>1</sup> 🔞

This Governance and Operations Manual (GOM) defines standard operating procedures and various policies created to clarify, support, and further the goals of the Genomics Phenotypes, and Environment (GenoPhenoEnvo) Research Team.

#### Files

GenoPhenoEnvo Governance -	SUBMITTED - 20200521.pdf		*
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### GenoPhenoEnvo Governance and Operations Manual

This is a living document. Changes are expected throughout the life of the project.

Introduction	1
Primary Office	2
Mission	2
Vision	2
Goals	2
Participation and Roles	2
Our Team	3
Organizational Structure	5
Operations	5
Communications	5
Work Procedures	6
Scientific and Technical Decision making	7
Community Practices	7
Our Commitment to Open Science	7
Diversity Statement	7
Code of Conduct	8
Conflict resolution	9
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Attribution, Authorship, and Ownership	9
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### Introduction

Show affiliations

This Governance and Operations Manual (GOM) defines standard operating procedures and various policies created to clarify, support, and further the goals of the Genomics Phenotypes and Environment (GenoPhenoEnvo) Research Team.

https://zenodo.org/records/383912



## Work management - Kanban

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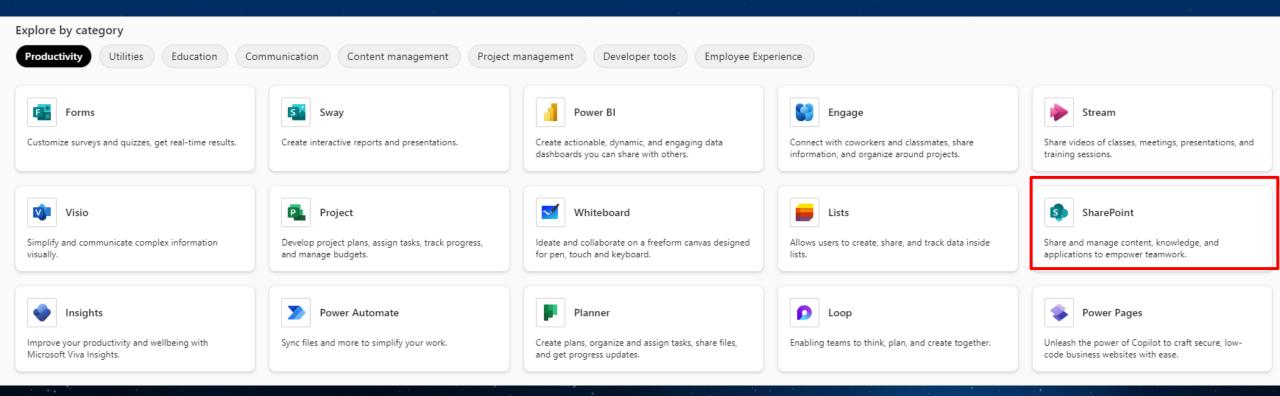
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## **Microsoft Office 365**

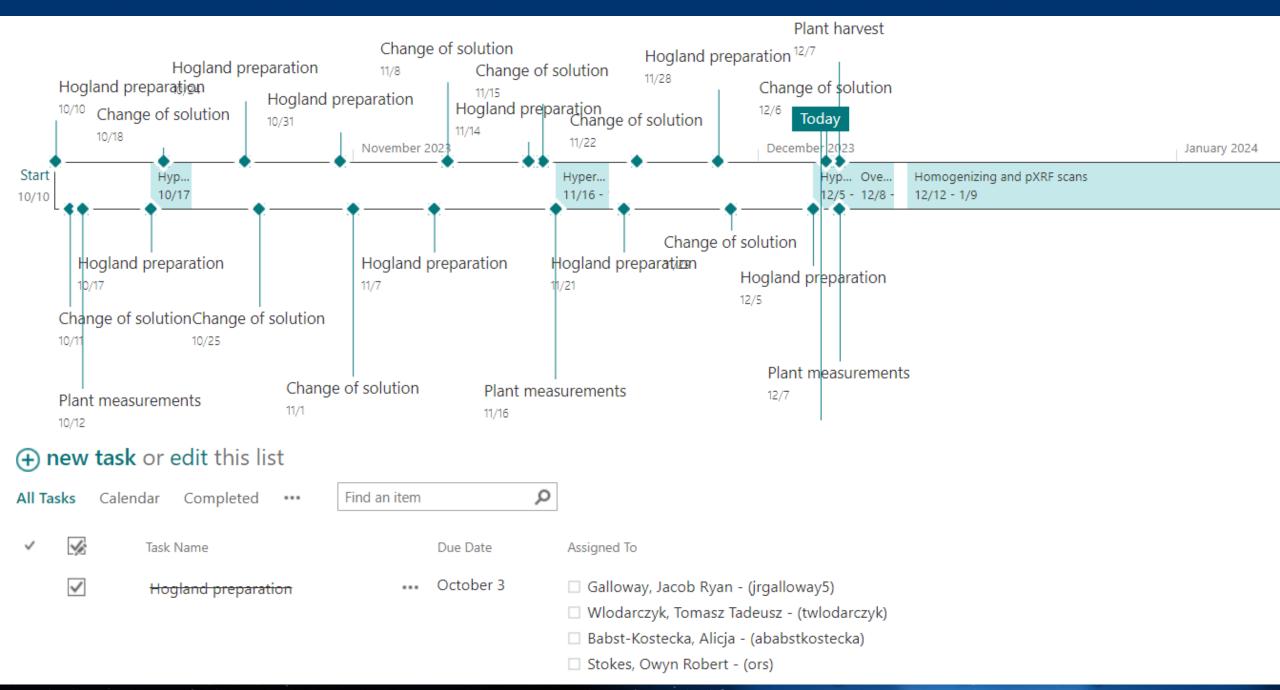
### https://www.office.com/





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		Solitude_Measurement Table_and_Control.x July 28 Wlodarczyk, Tomasz Tadeu	
		Week Time Table .xlsx August 26, 2022 Wlodarczyk, Tomasz Tadeu	

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## Version Control – Git and GitHub

<b>ø</b> git	GitHub
1. It is a software	1. It is a service
2. It is installed locally on the system	2. It is hosted on Web
3. It is a command line tool	3. It provides a graphical interface
4. It is a tool to manage different versions of edits, made to files in a git repository	4. It is a space to upload a copy of the <b>Git</b> repository
5. It provides functionalities like Version Control System Source Code Management	5. It provides functionalities of Git like VCS, Source Code Management as well as adding few of its own features

## Version Control – Git

### Commit, Push, Pull, Clone, Fork

```
Cu \ll ggplot(dt_selected, aes(x = reorder(Scientific_Name, Predicted_Cu_ICP, FUN = median),
1117
1118
                                    y = Predicted_Cu_ICP, Sceintific_Name = Scientific_Name)) +
        geom_boxplot(linewidth=0.3) +
1119
        geom_point(aes(shape = Plot), size = 2.5) + # Adjust the size parameter here
1120
        scale_shape_manual(values = c(21, 21, 21, 4)) +
1121
        geom_hline(yintercept = 70, linetype = "dashed", color = "#9a9a9a", size = 0.4) +
1122
        geom_hline(yintercept = 300, linetype = "dotdash", color = "#454545", size = 0.4) +
1123
        scale_y_continuous(limits = c(0, 900), breaks = seq(0, 900, by = 150)) +
1124
        coord_flip() +
1125
        theme_classic()+
1126
        theme(panel.grid.major = element_blank(), panel.grid.minor = element_blank(),
1127
              axis.text.x = element_text(size=12),
1128
              axis.title.x = element_text(size = 15),
1129
              axis.text.y = element_text(size=12, face="italic"),
1130
1131
              axis.title.y = element_blank(),
              legend.key.size = unit(1, "lines"),
1132
              legend.text = element_text(size = 13).
1133
              legend.title = element_text(size=14, face = "bold"))+
1134
        guides(color = guide_legend(override.aes = list(size = 3.5)),
1135
               shape = guide_legend(override.aes = list(size = 3.5))) +
1136
        ylab("Cu (mg kg-1)")
1137
1138
     Cu
```





### Git

**Create** Git repository: git init **Add** files to track versions: git add. **Checking** the status of the file: *git status* git –m "…" **Committing** after modifying: **Pushing** changes to GitHub: git push

### https://www.youtube.com/watch?v=tRZGeaHPoaw&ab\_ channel=KevinStratvert

MINGW64:/c/Users/twlodarczyk

#### twlodarczyk@CALS-ENVS21-03 MINGW64 ~ \$ git

usage: git [-v | --version] [-h | --help] [-C <path>] [-c <name>=<value>] [--exec-path[=<path>]] [--html-path] [--man-path] [--info-path] [-p | --paginate | -P | --no-pager] [--no-replace-objects] [--bare] [--git-dir=<path>] [--work-tree=<path>] [--namespace=<name>] [--super-prefix=<path>] [--config-env=<name>=<envvar>] <command> [<args>]

These are common Git commands used in various situations:

	ing area (see also: git help tutorial) Clone a repository into a new directory
init	Create an empty Git repository or reinitialize an existing one
work on the	current change (see also: git help everyday)
add	Add file contents to the index
mv	Move or rename a file, a directory, or a symlink
restore	Restore working tree files
rm	Remove files from the working tree and from the index
	Listen and state free alone ait hale envisions?
	history and state (see also: git help revisions)
hisect	Use binary search to find the commit that introduced a bug

bisect	Use binary	search to	find the	commit	that	introduced	a bug
1	Charles and a second	- <b>b</b> - <b>b</b>				and the second second	_

- Print lines matching a pattern grep
- Show commit logs log
- Show various types of objects show
- Show the working tree status status

grow, mark and tweak your common history

- List, create, or delete branches branch
- commit Record changes to the repository
- Join two or more development histories together merge
- Reapply commits on top of another base tip rebase
- Reset current HEAD to the specified state reset
- switch Switch branches
- Create, list, delete or verify a tag object signed with GPG tag

collaborate (see also: git help workflows)

- Download objects and refs from another repository fetch
- pull Fetch from and integrate with another repository or a local branch
- push Update remote refs along with associated objects

'git help -a' and 'git help -g' list available subcommands and some concept guides. See 'git help <command>' or 'git help <concept>' to read about a specific subcommand or concept. See 'git help git' for an overview of the system.

#### twlodarczyk@CALS-ENVS21-03 MINGW64 ~

## Version Control – Git and Github

### Commit, Push, Pull, Clone, Fork

	Tomasz Add new figures	6db05c6 5 days ag	go 🕚 97 commits
	images	new	8 months ago
Ľ	.gitignore	Dataframe transformation and visualization of all species for individ	9 months ago
Ľ	CESMlogo.jpg	new	8 months ago
Ľ	CESMlogo.png	Add files via upload	7 months ago
Ľ	Dataset_LODs.R	Add new files	6 months ago
Ľ	Figures_CESM.R	qwe	3 months ago
Ľ	Hyperspectral_Test.R	Add new	3 months ago
Ľ	LICENSE	Initial commit	9 months ago
Ľ	Manuscript_Analyses.R	New analysis	2 weeks ago
Ľ	Manuscript_Figures.R	Add kruskal	3 weeks ago
Ľ	Manuscript_Mastefile.R	Add new loops	last week

GitHub





## **Version Control – R Studio**

Cu <- ggplot(dt\_selected, aes(x = reorder(Scientific\_Name, Predicted\_Cu\_ICP, FUN = median), 1117 y = Predicted\_Cu\_ICP, Sceintific\_Name = Scientific\_Name)) + 1118 geom\_boxplot(linewidth=0.3) + geom\_point(aes(shape = Plot), size = 2.5) + # Adjust the size parameter here 1120  $scale_shape_manual(values = c(21, 21, 21, 4)) +$ 1121 geom\_hline(yintercept = 70, linetype = "dashed", color = "#9a9a9a", size = 0.4) + 1122 geom hline(vintercept = 300, linetype = "dotdash", color = "#454545", size = 0.4) + scale\_y\_continuous(limits = c(0, 900), breaks = seq(0, 900, by = 150)) + 1125 coord\_flip() + 1126 theme\_classic()+ theme(panel.grid.major = element\_blank(), panel.grid.minor = element\_blank(), axis.text.x = element\_text(size=12), 1128 axis.title.x = element\_text(size = 15), 1129 axis.text.y = element\_text(size=12, face="italic"), 1130 1131  $axis.title.y = element_blank()$ , legend.key.size = unit(1, "lines"), 1132 legend.text = element\_text(size = 13), legend.title = element\_text(size=14, face = "bold"))+ 1134 guides(color = guide\_legend(override.aes = list(size = 3.5)), shape = guide\_legend(override.aes = list(size = 3.5))) + 1136 ylab("Cu (mg kg-1)") 1137 1138 Cu

Environment His	tory Connections Git Tutorial
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### https://jcoliver.github.io/learn-r//010-github.html



## **GitHub** Pages

#### CyVerse Foundational Open Science Skills 2023

📀 🔍 Search

Home Lessons Capstone Project

#### Lessons

#### 0. The Shell and Git

- 1. Open Science
- 2. Managing Data
- 3. Project Management
- 4. Documentation and Communication
- 5. Version Control
- 6. Reproducibility I: Repeatability
- 7. Reproducibility II: Containers

### The Unix Shell, Git, Github and LLMs: an Introduction

#### Requirements

Command Line Interfaces (CLI) are found throughout all Operating Systems, however we recommend the use of the Unix CLI. If you have a Unix based machine such as Linux/Ubuntu (or other Linux distributions), macOS, you are ready for the next step. If you use a Windows machine, please install the Windows Subsistem for Linux (WSL) as seen in the Before FOSS Starts section.

#### Home CV Gallery Projects Blog



Tomasz Wlodarczyk.

PhD Student in Environmental

• The University of Arizona

• Tucson, AZ, USA

ResearchGate

🖀 Google Scholar

MSc

Science

M Email

💟 Twitter

in LinkedIn

G Github

I am a PhD student pursuing a degree in <u>Environmental Science</u> at the University of Arizona. My research focuses on the identification and study of native plant species that accumulate and tolerate heavy metals. In my PhD program, I am collaborating with researchers from The French National Centre for Scientific Research (CNRS) at the intersection of phytoremediation and green chemistry. I also conduct research within the Center for Environmentally Sustainable Mining at the University of Arizona (<u>CESM</u>).



### https://squidfunk.github.io/mkdocs-material/

### https://jekyllcodex.org/ https://themes.jekyllrc.org/ https://github.com/TRwlodarczyk/TW-Science



lam

## **Open Data – Where to store?**

## **Private**

**DOX** 

**Public** 





The University of Arizona Report Data Repository



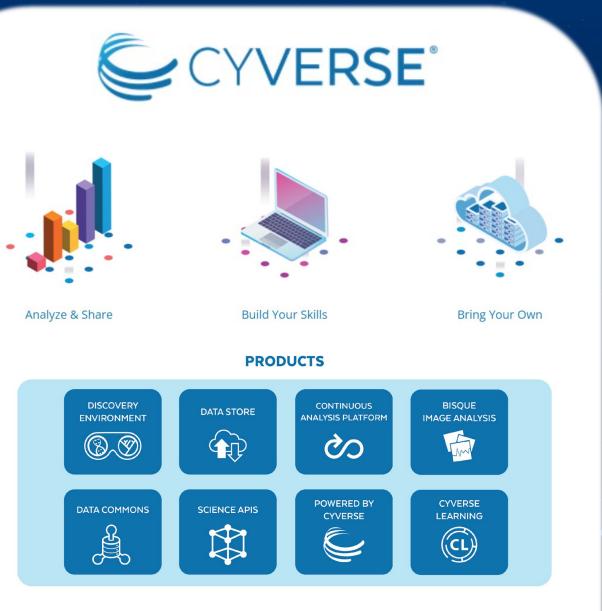
Google Drive

**SharePoint** 





## **CyVerse Platform**



## **CyVerse platform <u>http://www.cyverse.org</u>** provides data management tools such as:

- Data storage (upload 100GB, request 10 TB)
- Cloud-based analysis using VICE (Visual and Interactive Computing Environment)
- Enhances FAIR data principles (DOI request and data publishing directly on CyVerse Data Commons).

## Al tools

## COGNOSYS

Al Knowledge Discovery / Research Assistants

- chatPDF
- Consensus
- Cradle. (Proteins design).
- Elicit
- Genei ٠
- Research Rabbit
- SciSummary
- SciSpace typeset.io
- scite
- Semantic Scholar
- TextLayer
- Wizdom.ai

### **General Writing Assistants**

- Jasper
- Lex
- Notion.so
- Rytr

#### Al Generated Presentation Templates

SlidesPilot

#### Code assistants

- AlphaCode, DeepMind.
- Included in Bard. Google.
- Included in GPT 3.5 | GPT 4.0. OpenAl.
- Included in Claude. Anthropic.
- Code Whisperer, Amazon.
- CoPilot X. Github.
- Ghostwriter. Replit.
- Tabnine

### Popular

#### General AI Chat bots

- Bard. Google.
- Bing Chat. (Use Microsoft Edge).
- GPT 3.5 | GPT 4.0. OpenAl.
- Claude, Anthropic.
- Perplexity.ai. (Try Perplexity Labs to play with different LLM)
- · Poe. (Offers a wide collection of bots).

#### other options

- ٠ glean
- mem
- OpenIndex.ai
- Rewind

#### Chat bots as Chrome Extensions

- WebChatGPT. ChatGPT/Claude/Bard/Bing.
- Google Search Labs Generative

#### Text-to-image

- DALL-E 3.0. OpenAl.
- Deep Dream Generator
- Firefly. Adobe
- Image Creator. (Use Microsoft Edge)
- Leonardo
- Midjourney(via Discord channel)
- StableDiffusion

#### Text-to-video

- Runway
- Fliki
- Wonder

## **Reproducibility - containers**





- Docker is the virtualization software
- Docker does packaging the application with all dependencies, configuration, system tools and runtime into a container
- You no longer have to install exact versions and dependencies to reproduce a code
- Run a container with its own isolated environment
- Focus on the development, instead of on installing and configuring services on your machine

bash docker pull username/my-custom-environment:tag bash

docker run -it username/my-custom-environment:tag



## **Exploratory Data Analysis**

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# Explore, refine and visualize data (no coding)





### **OpenRefine**







*"In the canvas of open science, every stroke of data paints a picture of universal understanding" –* ChatGPT

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### Access Presentation Links: https://trwlodarczyk.github.io/OpenScience/

"In the canvas of open science, every stroke of data paints a picture of universal understanding" – ChatGPT