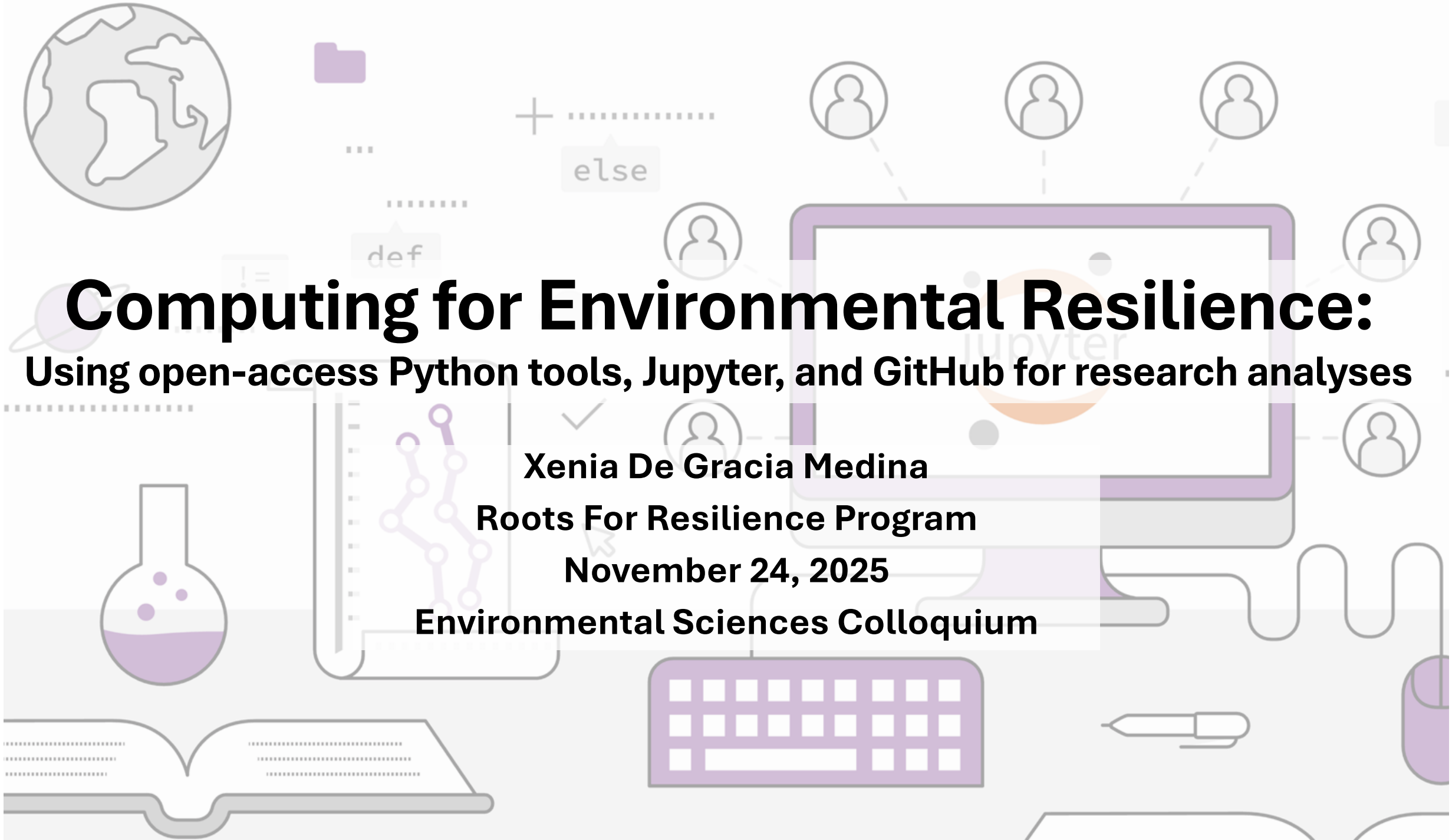


Computing for Environmental Resilience:

Using open-access Python tools, Jupyter, and GitHub for research analyses

Xenia De Gracia Medina

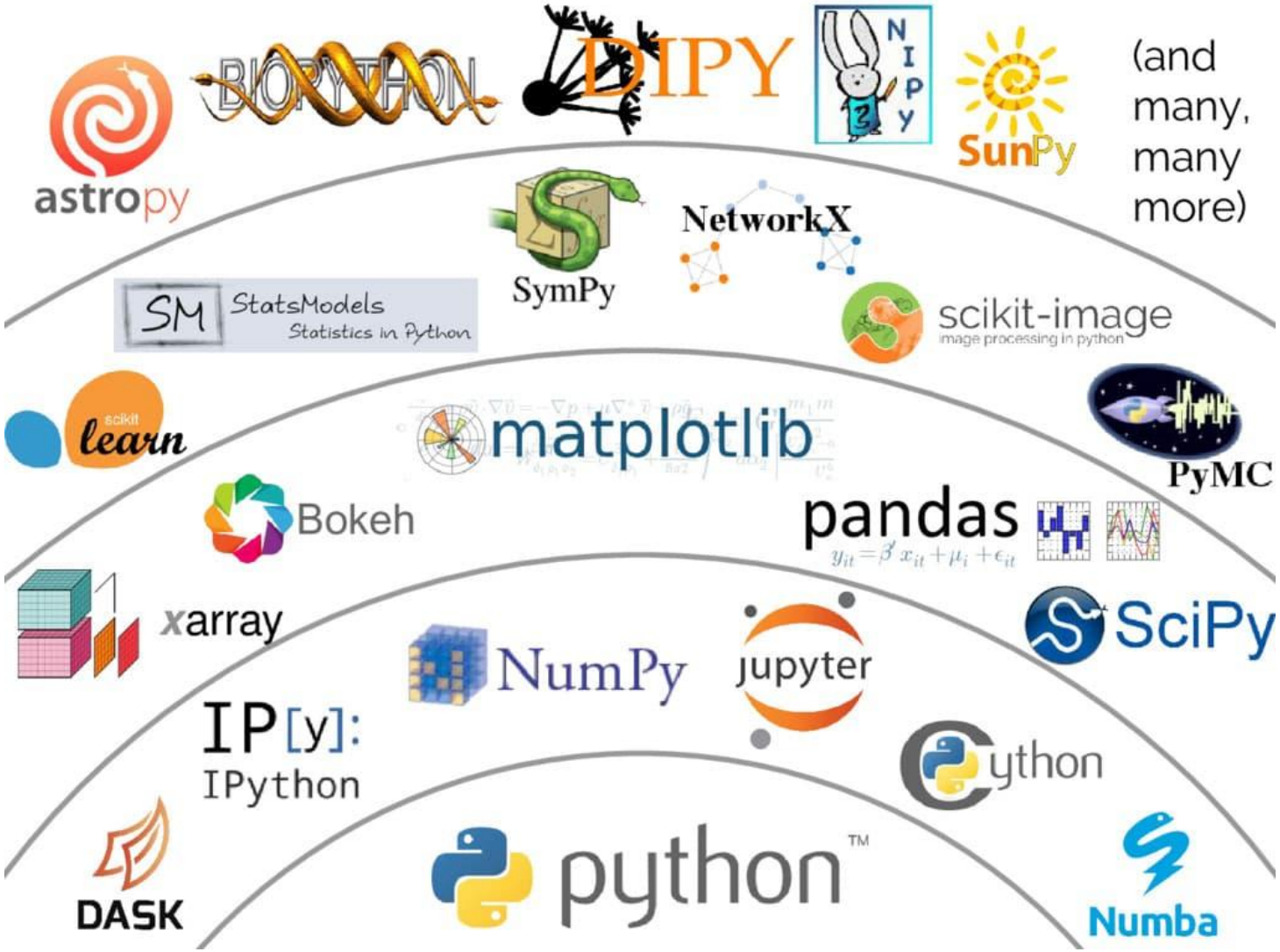
Roots For Resilience Program

November 24, 2025

Environmental Sciences Colloquium

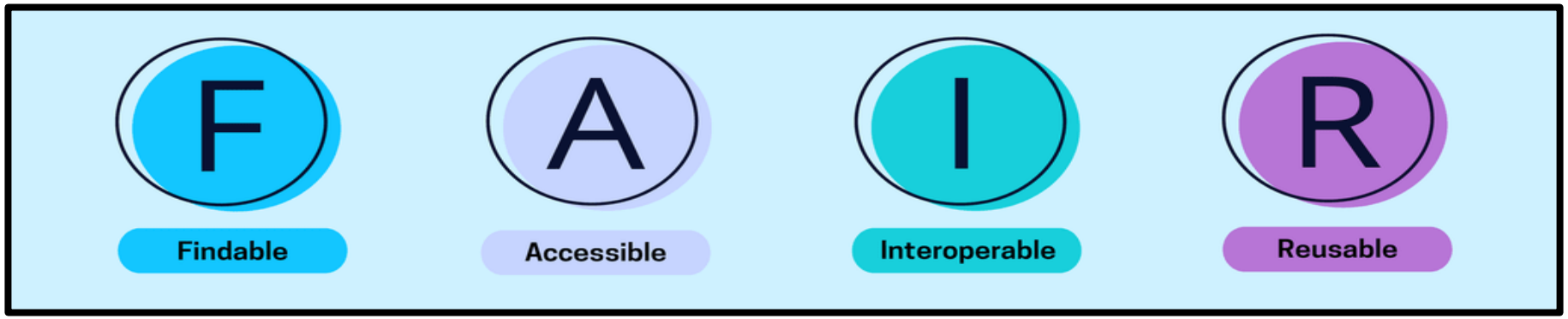
Outline

- Roots for Resilience Program
- Jupyter notebooks for our workflows
- LARCH, a python-based tool for XAS analyses
- Github repos for sharing workflows

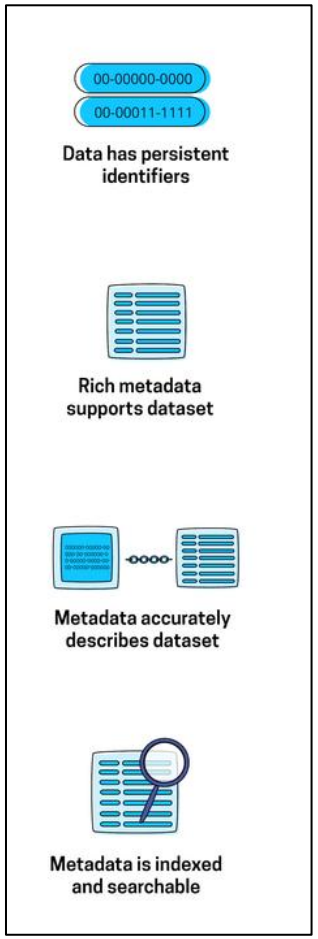


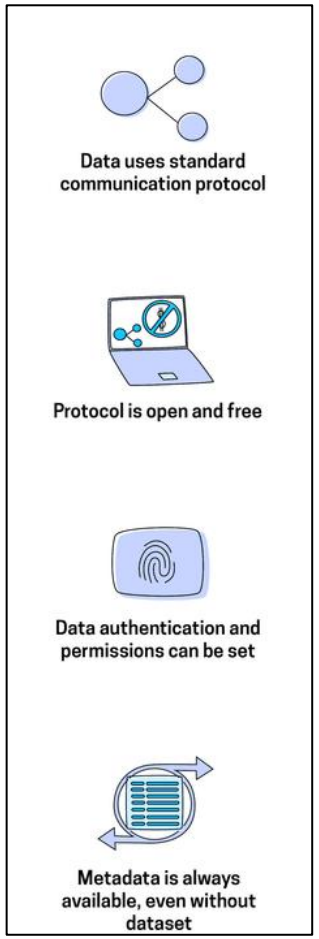
Roots for Resilience Program

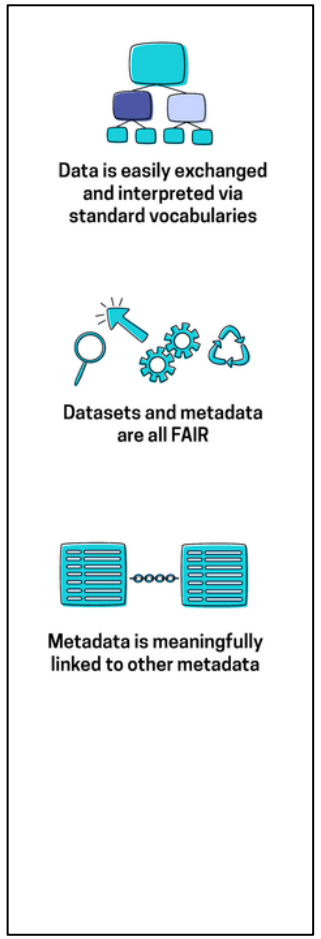
- Training to grad students (Meetings twice a week)
- Discuss: Open, reproducible science, computational infrastructure and AI tools
- Objective: Enhance research focused on environmental and societal resilience.
- Administered by: the Data Science Institute (DSI), CyVerse, & Arizona Institute for Resilience (AIR)

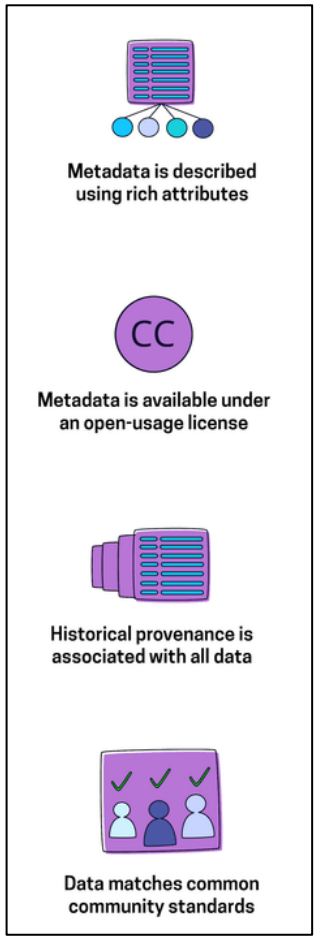


They teach us to create FAIR data!





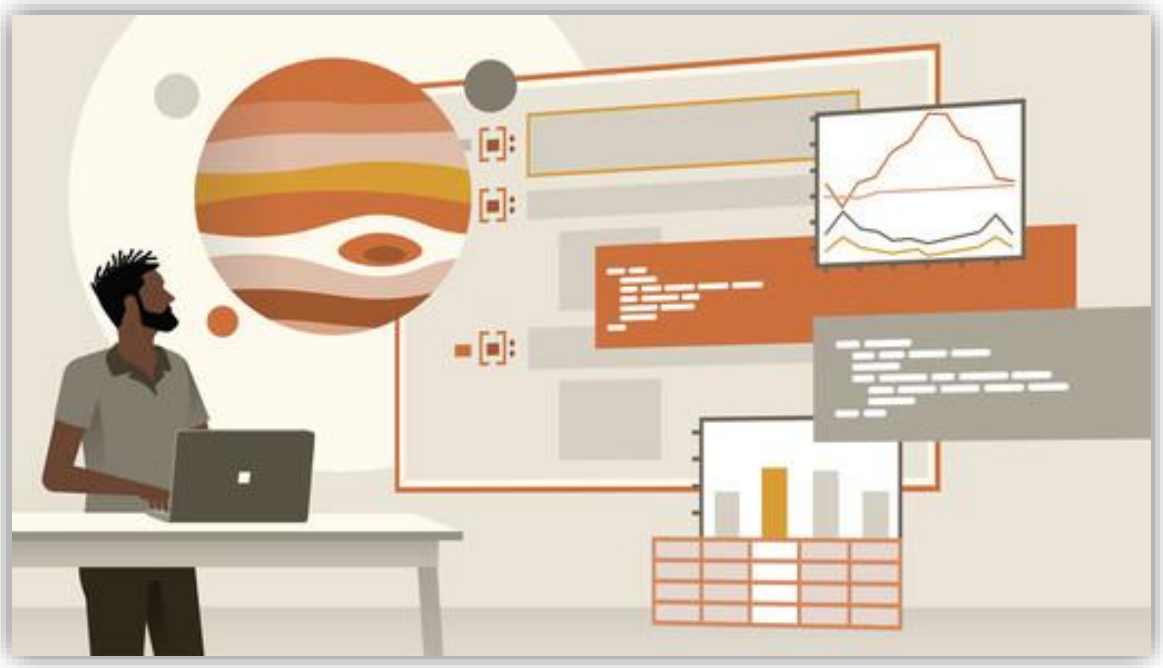




Doubleday, K. (2024, August 29). *Making data FAIR*. Fluree. https://flur.ee/fluree-blog/making-data-fair/

Jupyter Notebooks

- Integrates text with code
- Add your analysis right after your plots
- Show results in a self-explanatory way
- Share your workflow

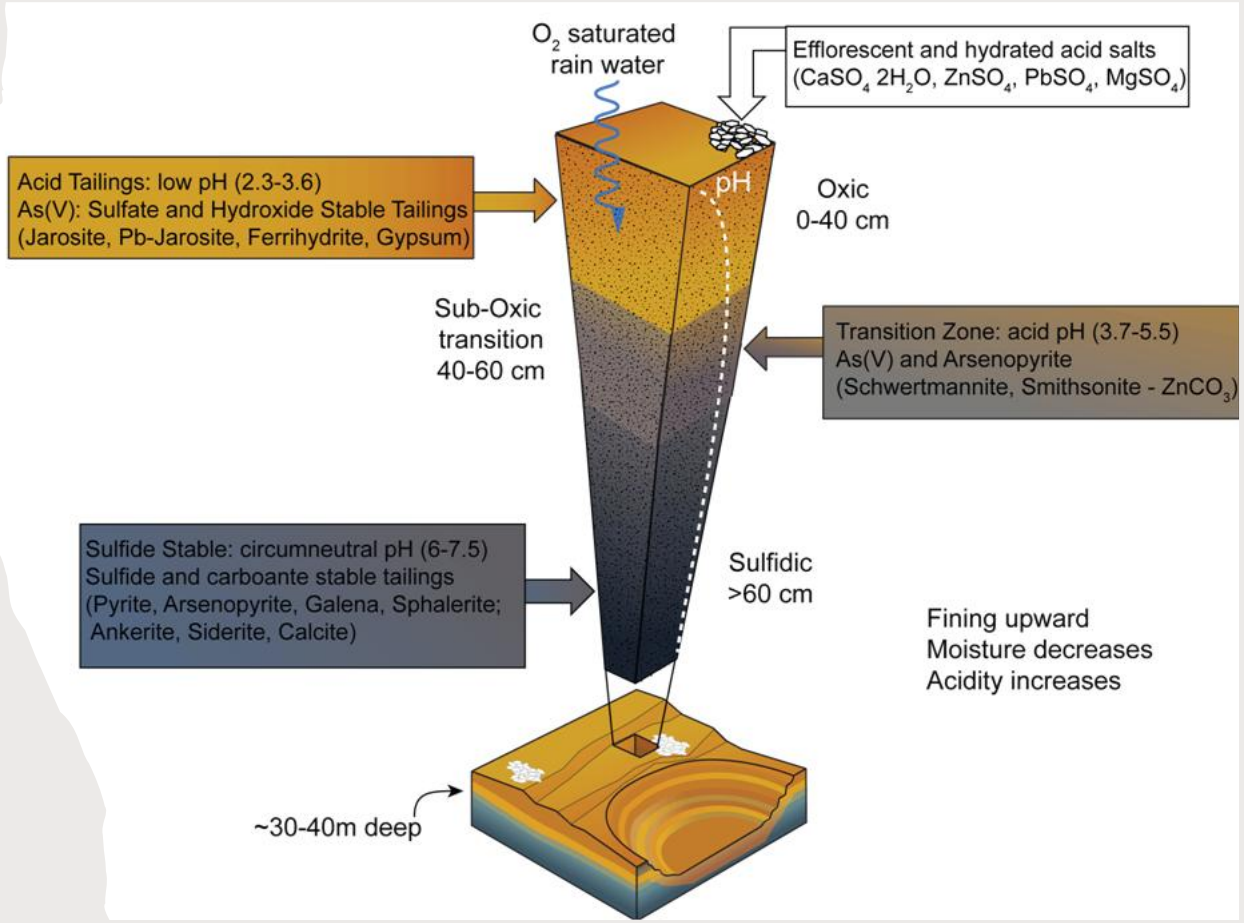


Let's apply it to mine tailings research!

Sulfur XANES Spectroscopy

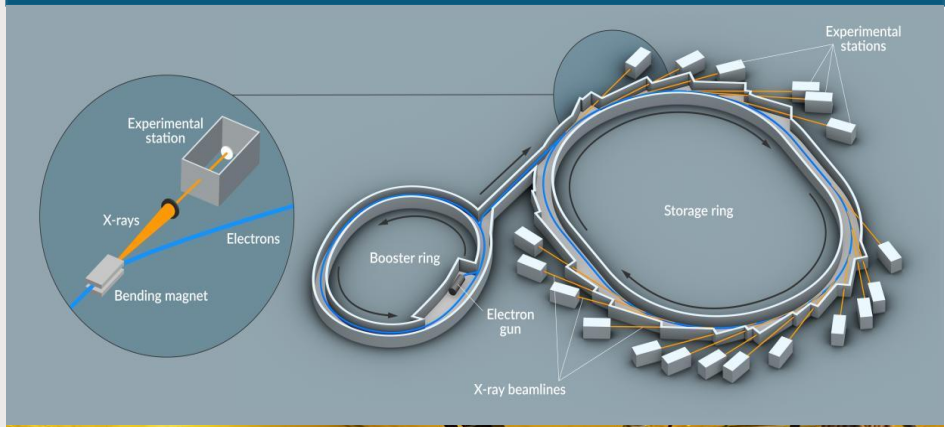
(XANES = X-ray absorption near edge structure)

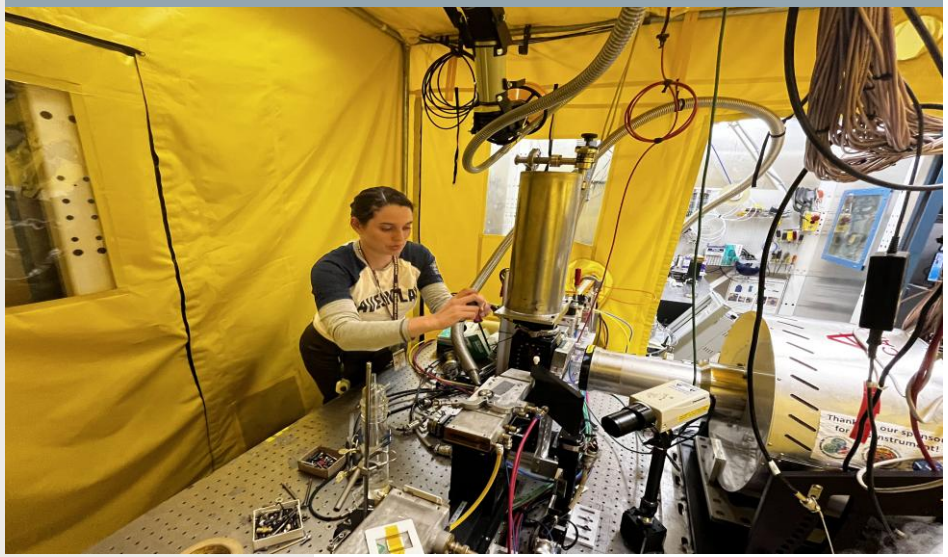
For oxidation state analyses of mine tailings



Data obtained in Synchrotron facilities

Synchrotron facility: high-intensity x-rays





LARCH (python tool) for Sulfur XANES

This Jupyter Notebook:

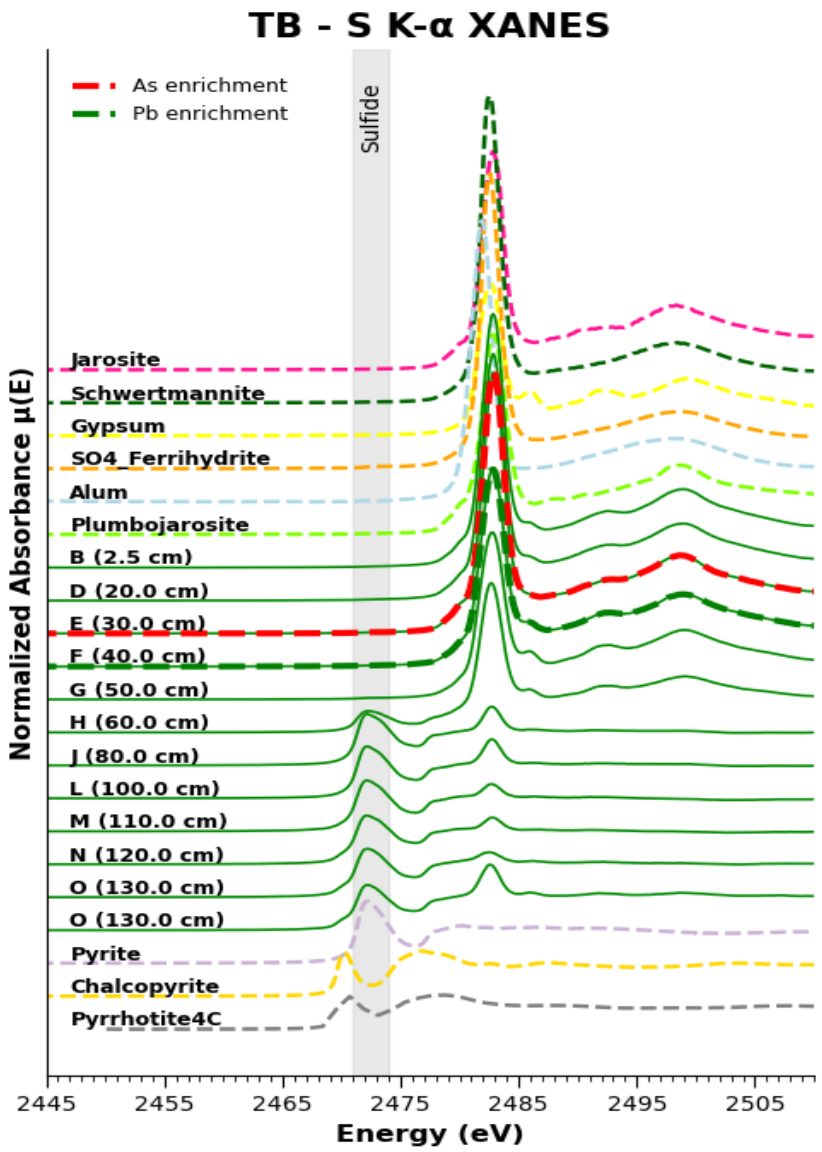
- 📁 Loads CSV files,
- ➗ Averages replicates,
- ✨ Normalizes XANES (with E_0 detection),
- 🔬 Analize the S-XANES pre-edge features,
- ✨ Creates a Principal Component Analysis (PCA) for the XANES data,
- 🔬 Linear Combination Fitting with XANES references,
- 🖼️ Plots everything.

```
references_xanes_results = {}
for reference, df in averaged_references.items():
    energy = df['energy'].values
    mu = df['mu_avg'].values

    # Create a Larch Group and store data
    g = Group()
    g.energy = energy
    g.mu = mu

    # ✅ Lookup custom post-edge bounds, or use defaults if not specified
    pre1, pre2 = pre_edge_bounds.get(reference, (-50, -20))  # default fallback
    norm1, norm2 = post_edge_bounds.get(reference, (40, 600))  # default fallback

    # Apply pre-edge normalization (this modifies 'g' in place)
    pre_edge(g.energy, g.mu, group=g, # energy, intensity, and the group to treat
                    pre1 = pre1, # the lower bond of the function to fit the pre-edge       # 🎯 customized per reference
                    pre2 = pre2, # the upper bond of the function to fit the pre-edge
                    norm1 = norm1, # the lower bond of the function to fit the post-edge    # 🎯 customized per reference
                    norm2= norm2, # the upper bond of the function to fit the post-edge
                    nnorm= 2, # degree for the polynomials
                    nvict= 4 # energy exponent to use for pre-edge fit.
                    )

    # Store results in DataFrame
    df2_result = pd.DataFrame({
        'energy': g.energy,
        'mu': g.mu,
        'pre_edge': g.pre_edge,
        'post_edge': g.post_edge,
        'norm_mu': g.norm,
        'flat': g.flat,
    })

    # Plot XANES normalization
    plt.figure(figsize=(8, 5))
    plt.plot(g.energy, g.pre_edge, label='Pre-Edge', color='gold', linestyle='--')
    plt.plot(g.energy, g.post_edge, label='Post-Edge', color='cornflowerblue', linestyle='--')
    plt.plot(g.energy, g.mu, label='Raw mu(E)', color='black')
    plt.plot(g.energy, g.norm, label='Normalized', color='green')
    plt.axvline(g.e0, color='r', linestyle='--', label=f'E0: {g.e0:.1f} eV')
    plt.title(f'Sulfur XANES Norm. - {reference}', fontsize=14, fontweight='bold')
    plt.xlabel('Energy (eV)', fontsize=14, fontweight='bold')
    plt.ylabel('mu(E)', fontsize=14, fontweight='bold')
    plt.xlim(2425, 3000)
    plt.legend()
    plt.show()
```

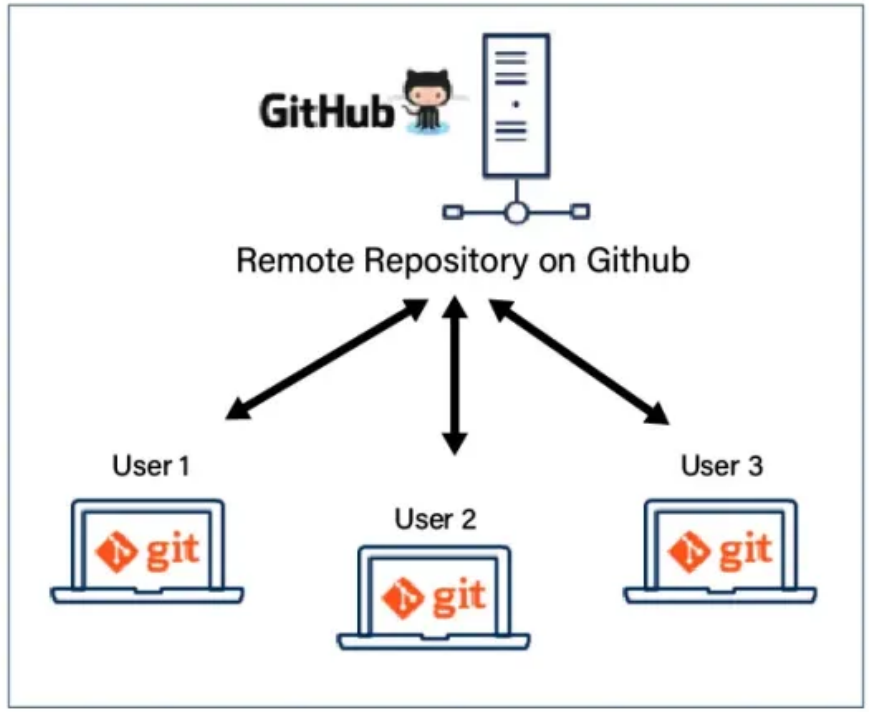
Newville, M. (2013). LARCH: an analysis package for XAFS and related spectroscopies. Journal of Physics Conference Series, 430, 012007. https://doi.org/10.1088/1742-6596/430/1/012007

Sulfur XANES results: Mine Tailings Oxidation state

We can determine the oxidation state of mine tailings at different depths and compare mineral shapes in our material to assess their presence.



GitHub repos



Chaurasia, N. (2024, December 17). How to use Git- a beginner Step-by-Step guide. Sprintzeal.com. https://www.sprintzeal.com/blog/how-to-use-github

Table of contents

Tailings Atlas

AUTHORS

Xenia De Gracia Medina

Rob Root

Ma'In Alghzawi

Boyoung Song

Jon Chorover

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Sunday, November 9, 2025 18:01:52

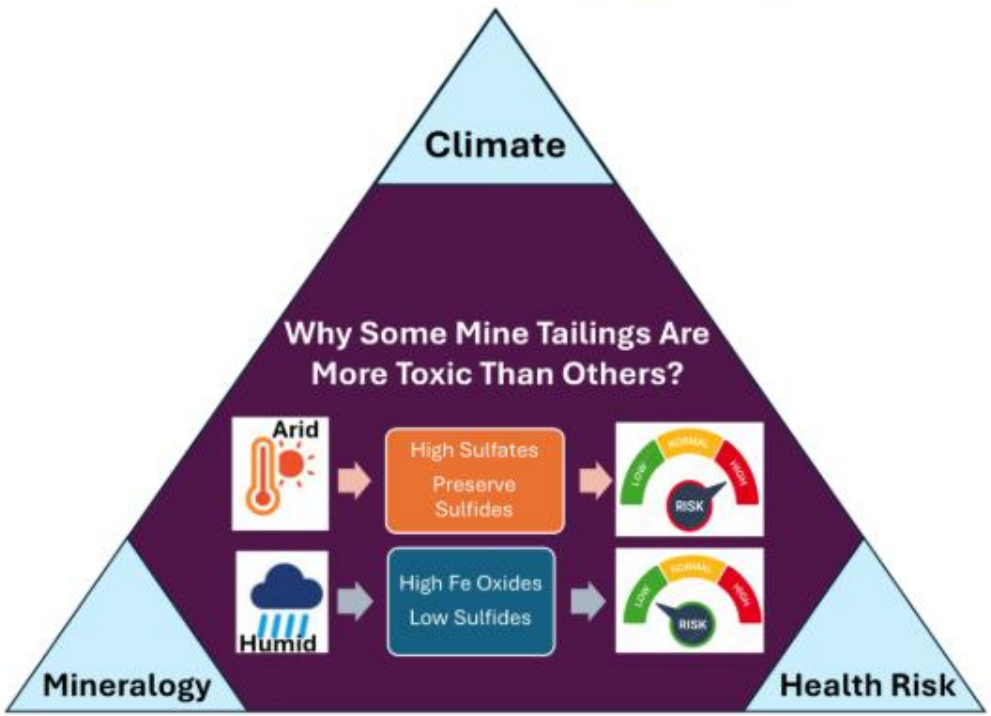
THE UNIVERSITY OF ARIZONA College of Agriculture, Life & Environmental Sciences

Tailings Atlas

Xenia De Gracia Medina

Department of Environmental Sciences
University of Arizona

For Lab Procedures used, check out my SOP repo on GitHub

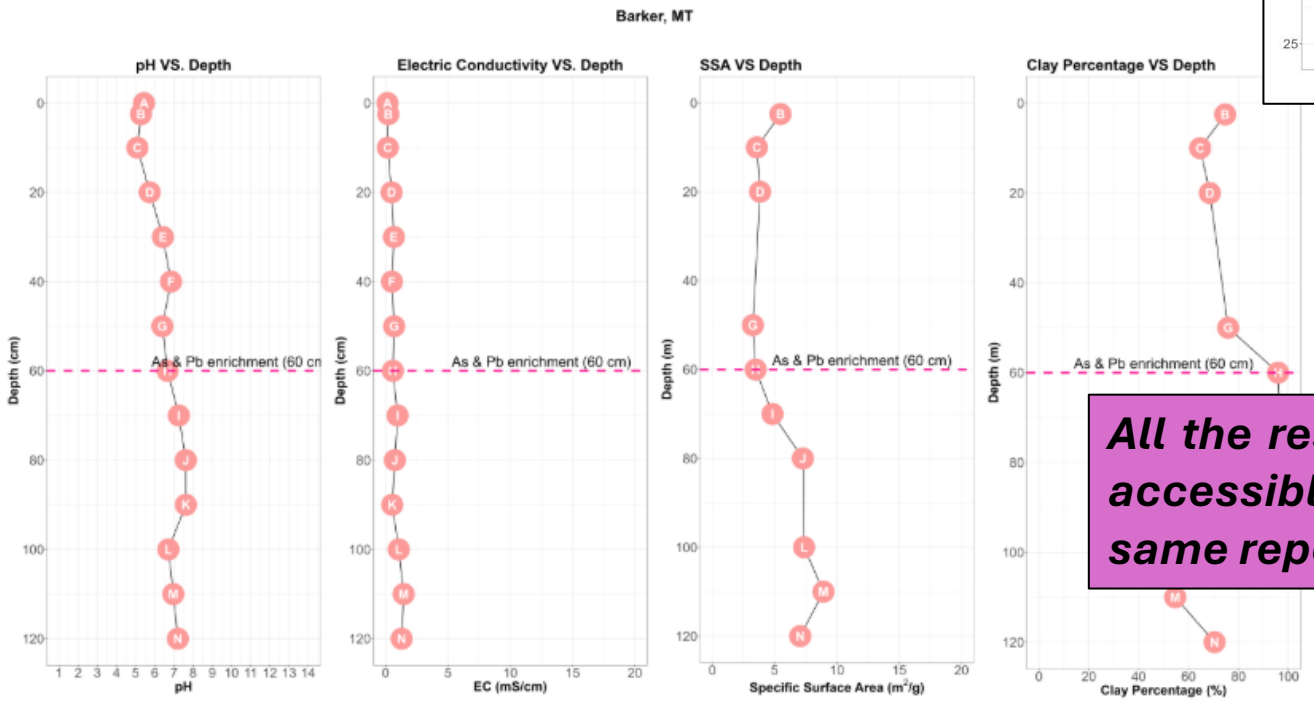


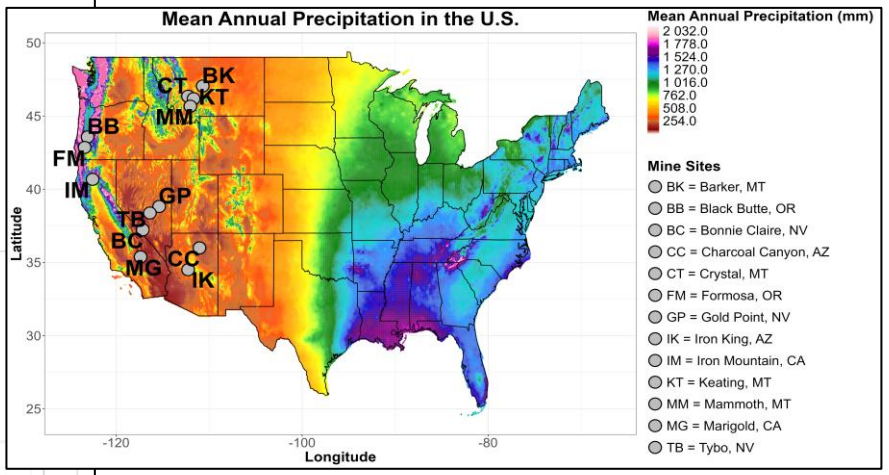
Repo I created to share our mine tailings results with research collaborators from different departments (Toxicology, Environmental, Mining).

4 DATA BY TECHNIQUE

Physico-chemical properties | Particle size distribution | Flow-through reactive mini-column experiment results | XRD Mineralogy | Arsenic XAS | Iron XAS | Sulfur XAS | ATR-FTIR | pH, EC, SSA combined

Enrichment data extracted from Alghzawi, 2025.





All the results from different techniques are accessible to collaborators, anytime, in the same repository.

I created another repo to host our methods and explain the use of lab equipment to future users.

GitHub repos for Lab Standard Procedures

Link to the repo:
https://xeniadegraciam.github.io/sop_chorover_lab/SOP.html

Table of contents

1 ADMINISTRATIVE PROCEDURES

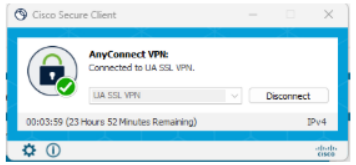
BuyWays: Buy Lab Supplies | Chemical & Biohazard Waste Pickup Request | Printing Posters | RLSS | Chemical Inventory | Cryogenics & Compressed Gas Facility | Remote Access to 518 computer | ENVS Business Office

Note

- This procedure is valid if you are **on campus**, but if you are not, you can connect to the university VPN, through the following app: Cisco Secure Client.

Connect to VPN (just if you are off campus)

- Download Cisco Secure Client here
- Set it up as follows:



VPN AnyConnect

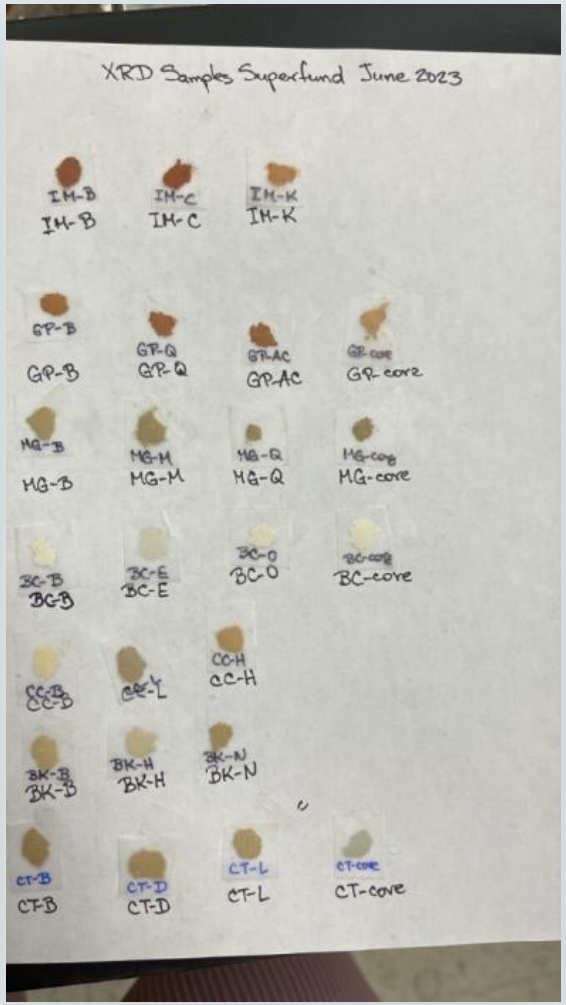
- Sign in with your university NetID

BuyWays

- Uacces
- Financial
- NetID
- More Items
- Orders
- Shop catalogs
- In the search tool, write what you're looking for (Catalog number, Product number or SKU number)
- Add to cart
- View my cart
- ***You can only do one supplier at a time***
- Proceed to Uaccess Financials
- Document overview (Description, Explanation
- Delivery -> Search -> Building Code = 38 -> Return value -> Room # = 518 ->
- Items -> Setup distribution -> Account number. *Check that the name of your project is under the account

In there, I explain the procedures and sample-preparation formats required for the different lab facilities we use.

Sample prep formats required by facility



XRD at Brookhaven National Lab

XAS at Stanford Synchrotron Research Lab

REFERENCES

- **Roots for Resilience Program (R4R). Data Science Institute.** **https://datascience.arizona.edu/r4r**
- Team, C. S. Home - CYVERse Foundational Open Science Skills 2025. https://foss.cyverse.org/
- Newville, M. (2013). LARCH: an analysis package for XAFS and related spectroscopies. Journal of Physics Conference Series, 430, 012007. https://doi.org/10.1088/1742-6596/430/1/012007
- Gräfe, M., Donner, E., Collins, R. N., & Lombi, E. (2014). Speciation of metal(loid)s in environmental samples by X-ray absorption spectroscopy: A critical review. Analytica Chimica Acta, 822, 1–22. https://doi.org/10.1016/j.aca.2014.02.044
- **De Gracia Medina, X. Lab Procedures & notes.** **https://xeniadegraciam.github.io/sop_chorover_lab/SOP.html**

Thanks!

Tybo mine, Nevada. 2021.
The highest lead-contaminated site out of the 13 legacy mine sites we are currently studying.