pyrolite: Python for geochemistry

@metasomite

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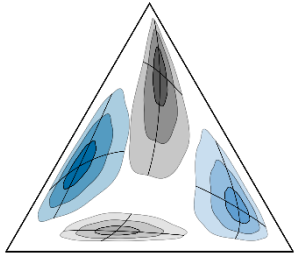
Workshop - Intro

Facilitators:

- Morgan Williams (CSIRO)
- Hayden Dalton (U. Melb)
- Louise Schoneveld (CSIRO)

1. What is pyrolite? Why does it exist?
2. Core functions:
   - Handling geochemical data
   - Visualisation
   - Putting geochem data to work
3. Installation, Ecosystem & Tools
4. Get Involved
5. **Demonstration**
   - *Starting with some basics*

What is pyrolite?



- A set of tools for working with geochemical data
- An open source Python package (a bundle of reusable code)
- A project under active development, aiming to eventually be community-driven
- Part of a broader ecosystem of interoperable tools within the scientific Python ecosystem

The Journal of Open Source Software

pyrolite: Python for geochemistry

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Software

- Review
- Repository
- Archive

`pyrolite` is a Python package for working with multivariate geochemical data, with a particular focus on rock and mineral chemistry. The project aims to contribute to more robust, efficient and reproducible data-driven geochemical research.

What's the bigger idea?

Encouraging a programmatic approach to geochemical data analysis:

- Defining explicit workflows
- Reproducibility and reuse of research code
- Interoperability and automation
- Scalability and flexibility

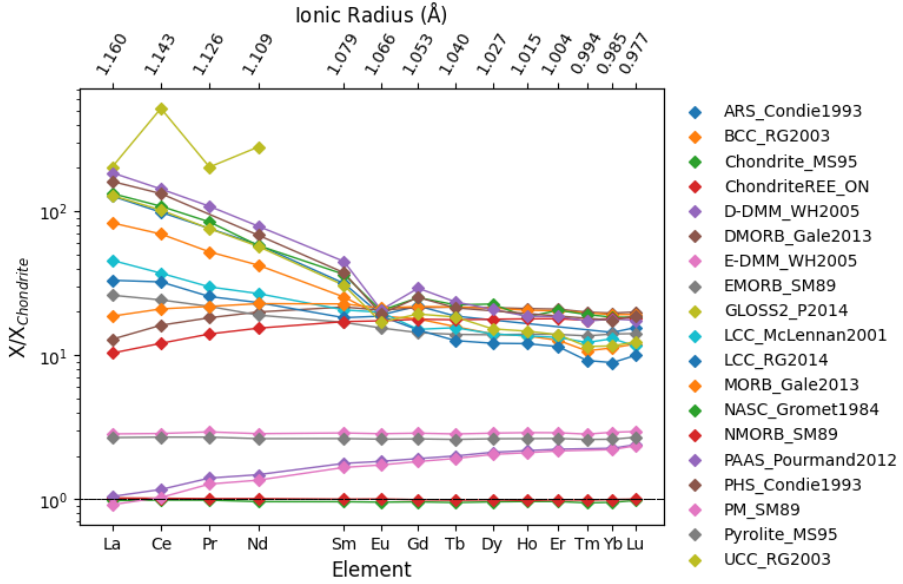
To support this:

- Accessibility
- Community
- Education

pyrolite’s Core Features

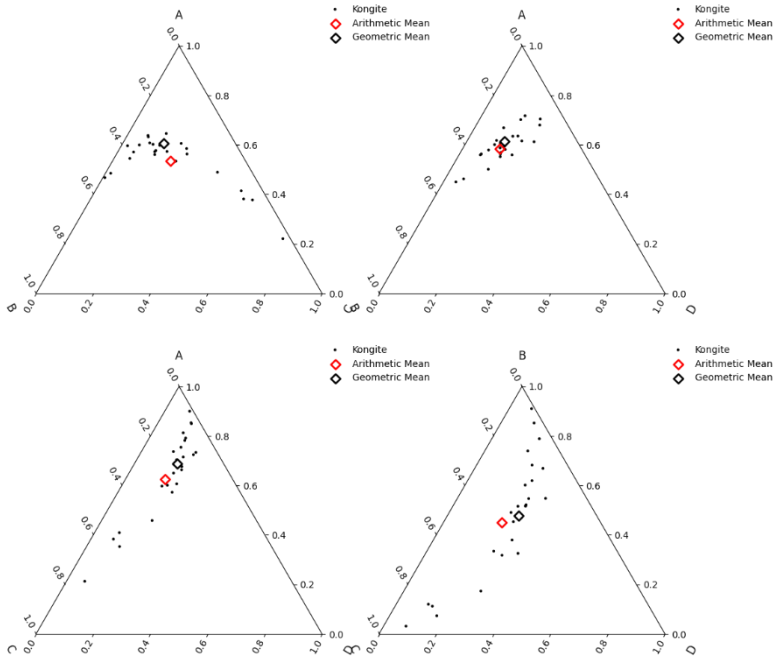
Handling Geochemical Data

- Transformation (elements, oxides, minerals, normalization)
- Reference compositions and mineral composition databases



Handling Geochemical Data

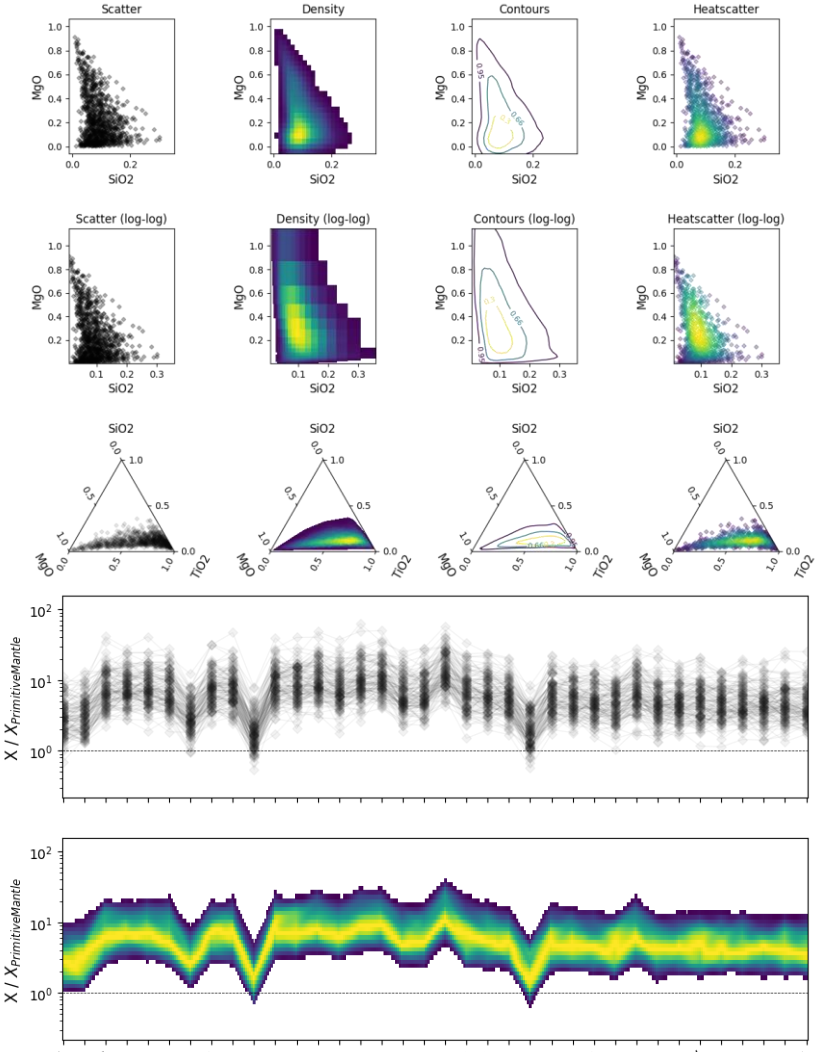
- Transformation (elements, oxides, minerals, normalization)
- Reference compositions and mineral composition databases
- Compositional data – logratio transforms!
- Provide some specialized functionality to complement general tools
- Linking all of this directly to your dataset (data-centric, via Pandas)



Visualisation

- Ternary diagrams
- Spider diagrams
- Addressing overplotting with data density-based visualisation methods

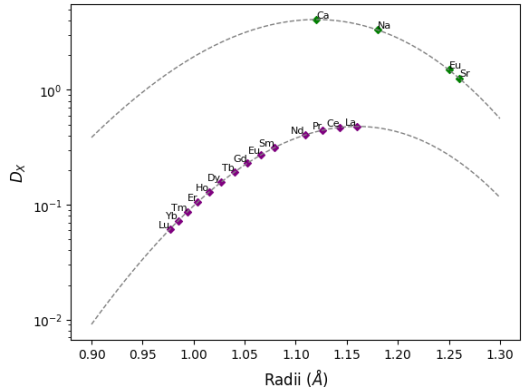
- Interface reflects the tools it's built on top of (e.g. matplotlib) in order to be interoperable
- Highly customisable

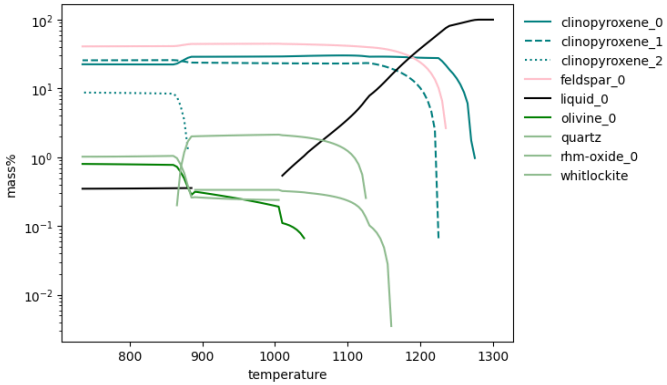


Linking Geochem Data to Modelling and ML

- To get the most out of our geochemical data, we'll need to be able to link it to a variety of different tools
  - Modelling (e.g. lattice strain, alphaMELTS)
  - Machine learning

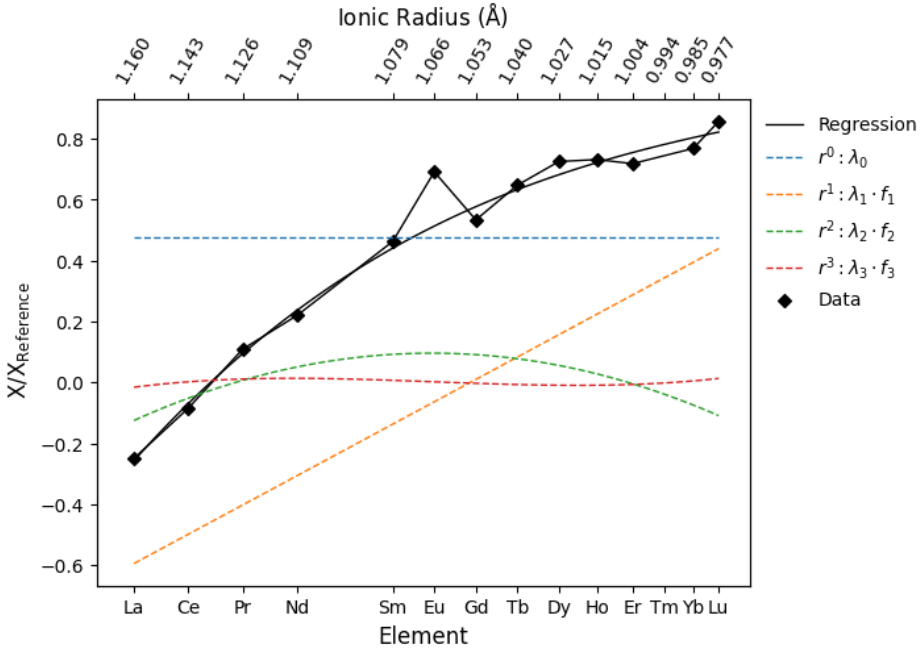
- The scientific Python ecosystem comes with 'batteries included'

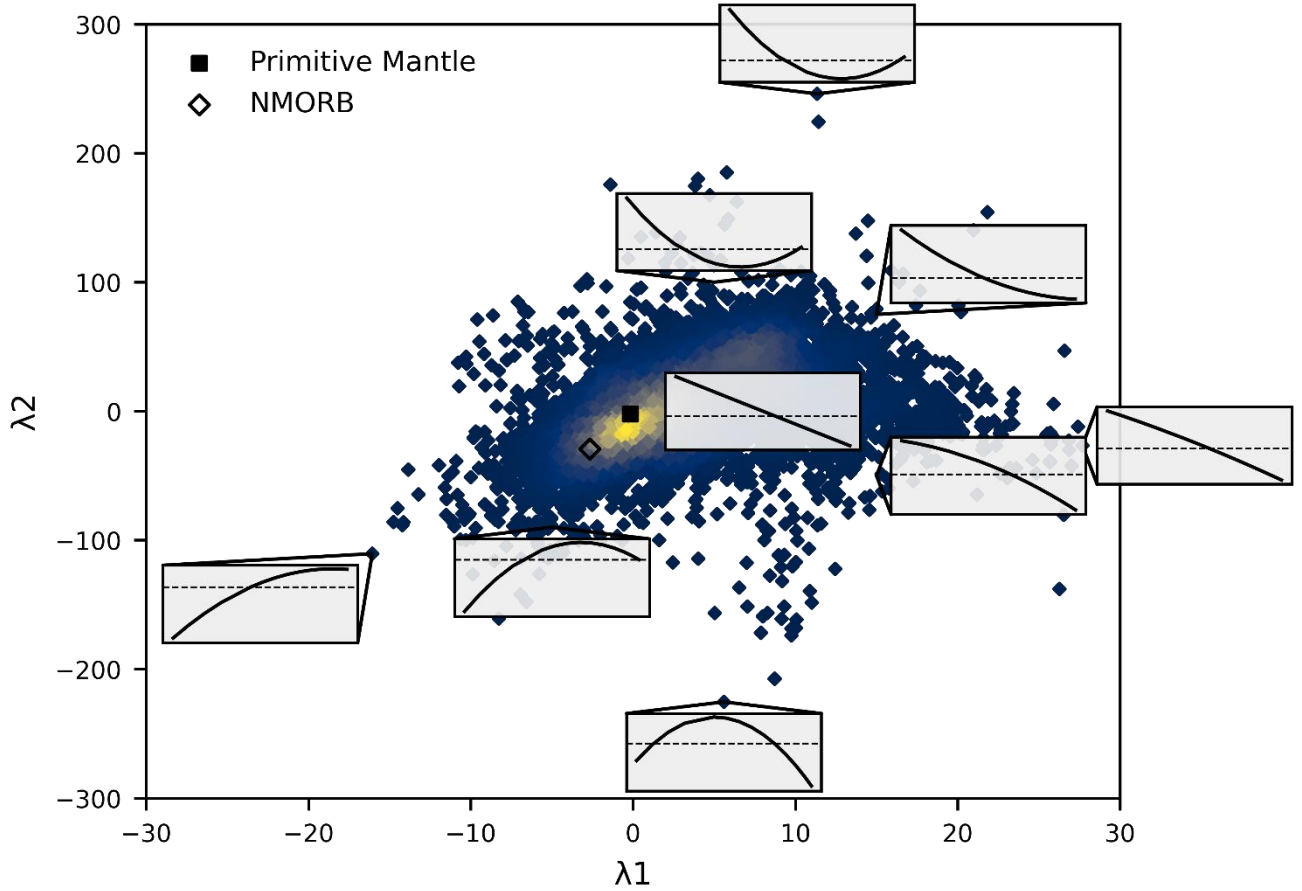




Lambdas: Parameterising REE Profiles

- Quantitative description of REE profiles closely linked to geological processes
- Customisable implementation of orthogonal polynomial regression, after O'Neill (2016)
- Tetrads, anomalies, fit measures and parameter uncertainties released in v0.3.0




Primitive Mantle
NMORB
300
200
100
0
−100
−200
−300
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−20
−10
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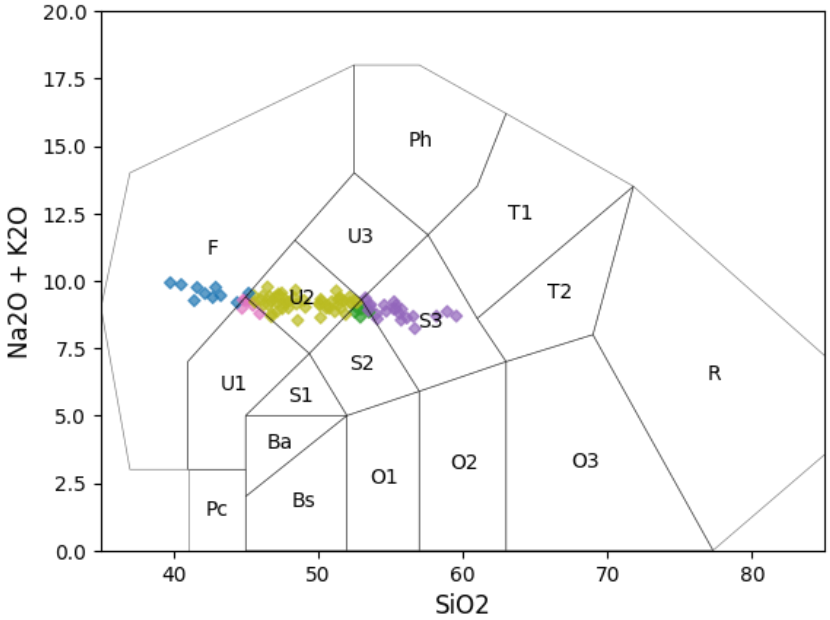
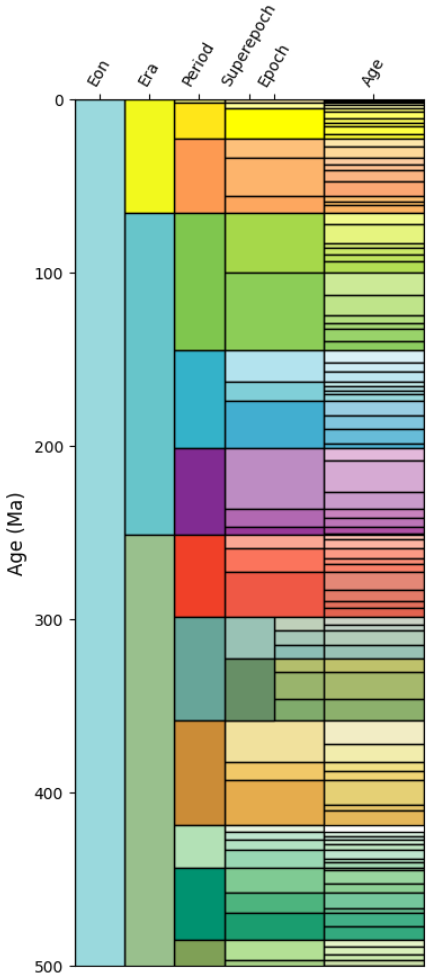
30
λ1
λ2

And a range of other utilities…





Extensions

pyrolite-meltsutil

- Working with alphaMELTS and its outputs
- Automating batch calculations over a grid of parameters and compositions.

pyrolite-datasouce (not yet released)

- Directly accessing data from GEOROC and EarthChem

Installation, Ecosystem & Tools

```
> pip install pyrolite
```

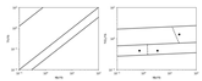
Pyrolite is hosted on the Python Package Index (PyPI), and each new release (≈ every few months) will be uploaded there and on GitHub. In the future it will also likely be released via conda-forge.

Docs

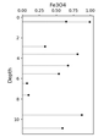
pyrolite.rtfd.io

Plotting Examples

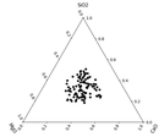
pyrolite provides some functionality for basic plotting of geochemical data in the form of spidergrams (pyrolite.plot.spider), ternary diagrams (pyrolite.plot.tern) and density diagrams (i.e. 2D histograms, pyrolite.plot.density).



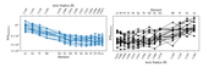
Plot Templates



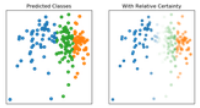
Stem Plots



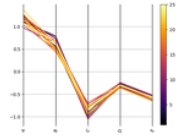
Ternary Plots



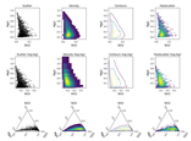
REE Radii Plots



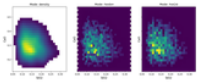
Using Manifolds for Visualisation



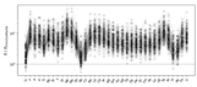
Parallel Coordinate Plots



Heatscatter Plots



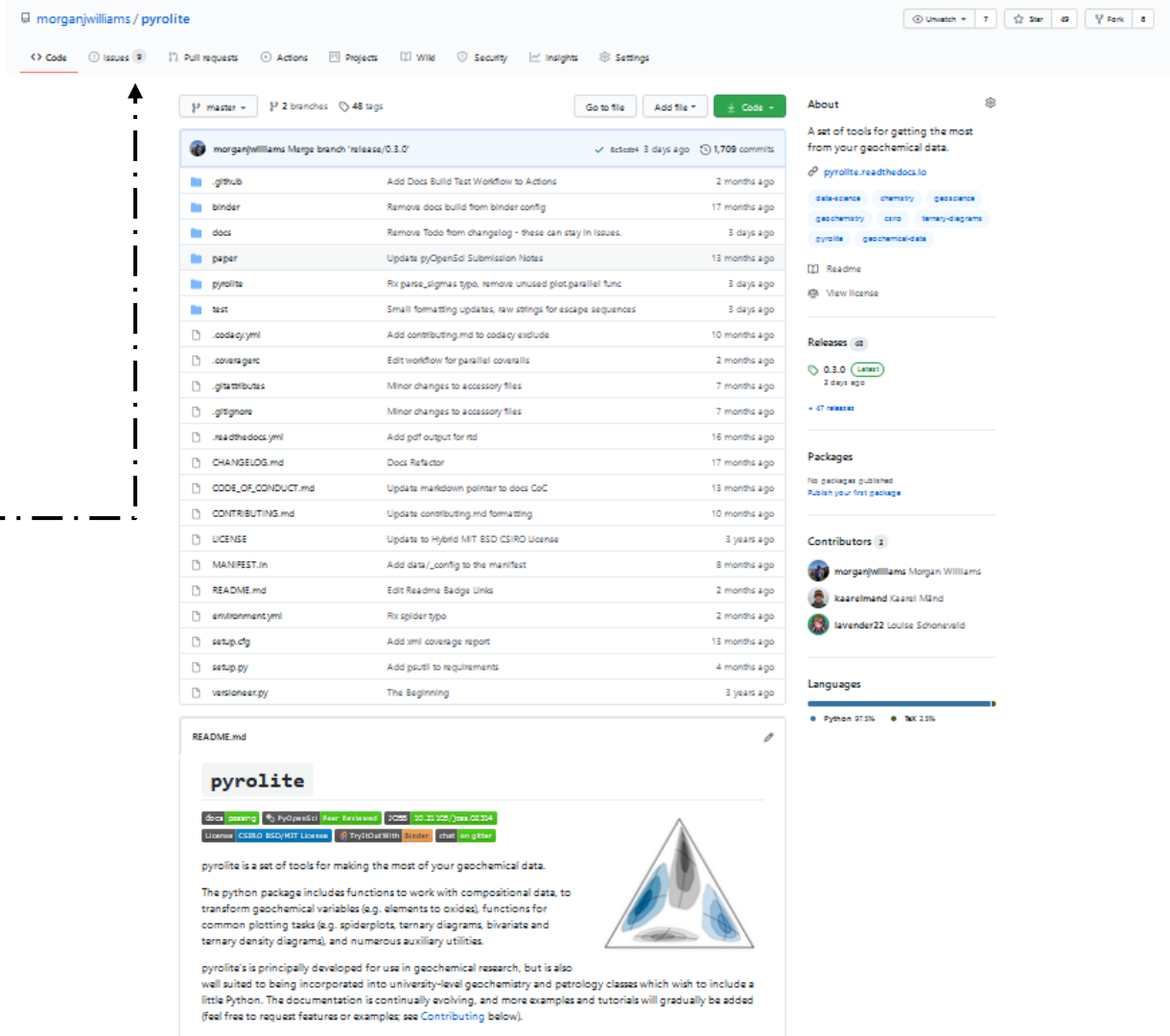
Density and Contour Plots



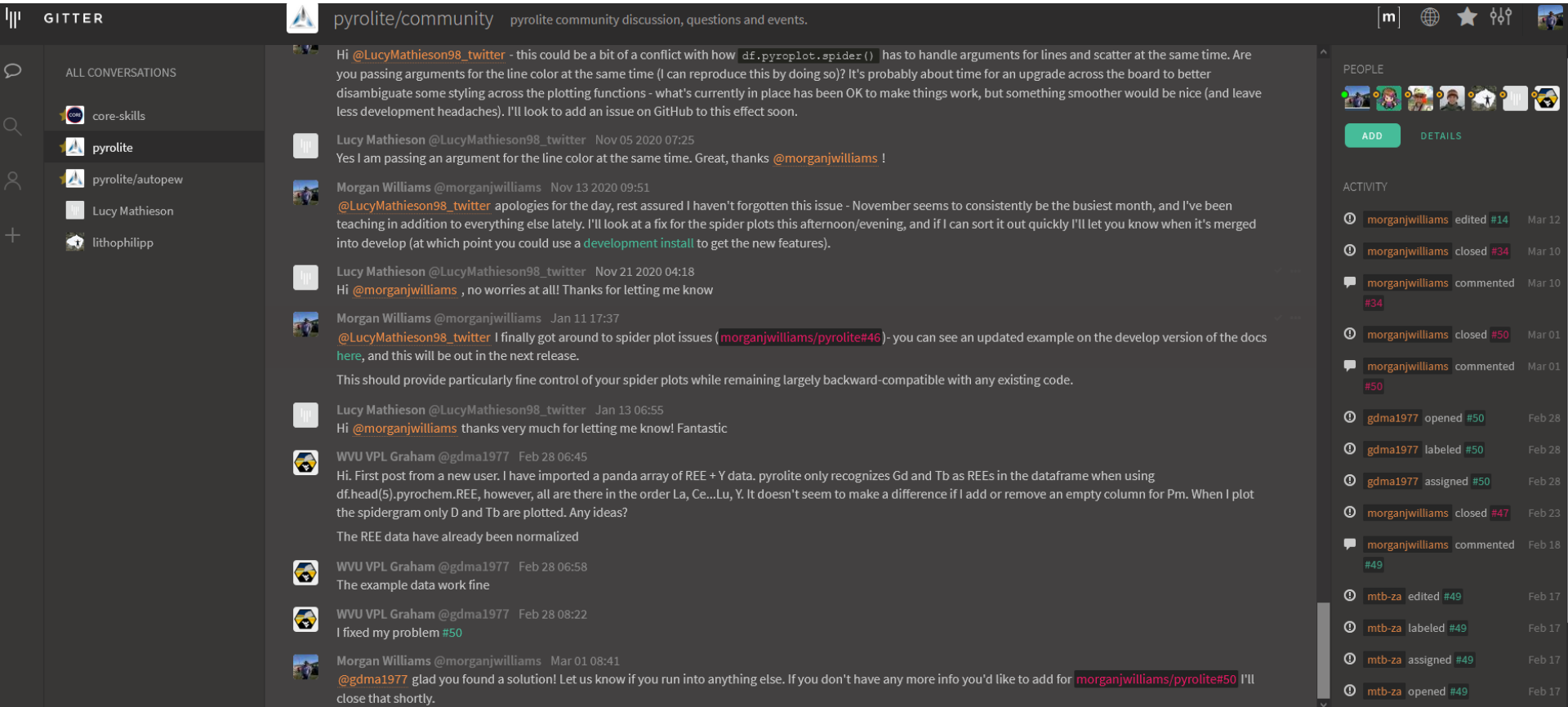
Spiderplots & Density Spiderplots

GitHub

- **Code repository**
- **Issue Tracker**
- **Version archive (also on Zenodo)**



Gitter – a simple forum linked to GitHub



Get Involved

- Want help getting started?
- Find something which looks like a bug?
- Want to be able to do something, but not sure how/if its possible?
- Want to get involved with the project, or have ideas where it should go?
- Keen to make the project more sustainable?

- Want a sticker?
  Catch me when we get back to in-person conferences..

Discussion:

gitter.im/pyrolite/community

Bugs and Features:

github.com/morganjwilliams/pyrolite

Some Perspectives on Getting Started

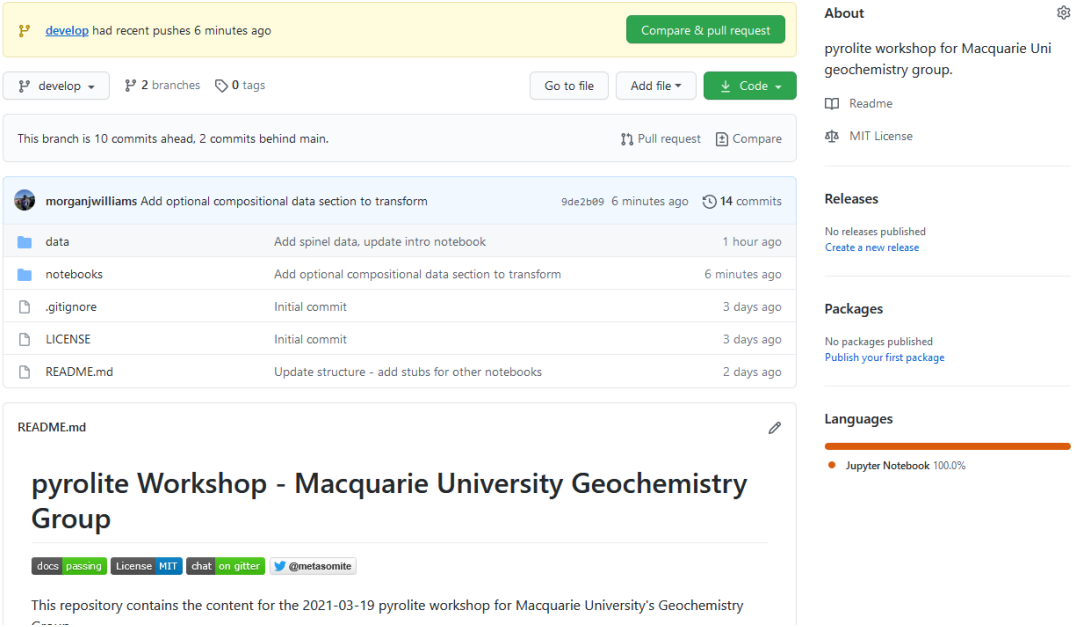
- Start where you are. For new coders, it'll take a while to get used to. Don't expect to learn everything overnight.

- Play around with the examples, then try working with your own data. Having a project or objective in mind helps with the learning process!

- I still have to look up & copy-paste lots of things, even for my own code. This probably won't change!

Quick Demo

- Python Basics
- Pulling in and transforming some data
- Visualisation
- Working with mineral data
- lambdas



Repo: github.com/morganjwilliams/202103-MQ-pyrolite-workshop

Play along:

tinyurl.com/202103-MQ-pyrolite

Thank you

@metasomite

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pyrolite Contributors:

- Hayden Dalton
- Louise Schoneveld
- Adam Bath
- Yajing Mao
- Justin Gosses
- Kaarel Mand
- Laura Miller
- Steve Barnes
- Lucy Mathieson

This is the first official pyrolite workshop we've run! How'd we go?

Q&A, Feedback