User-provided reproducible publication

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Presenter: Thomas Vincent

ESRF

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Study of ultramarine blue pigment

SCIENCE ADVANCES | RESEARCH ARTICLE

CHEMISTRY

Sulfur K-edge micro- and full-field XANES identify marker for preparation method of ultramarine pigment from lapis lazuli in historical paints

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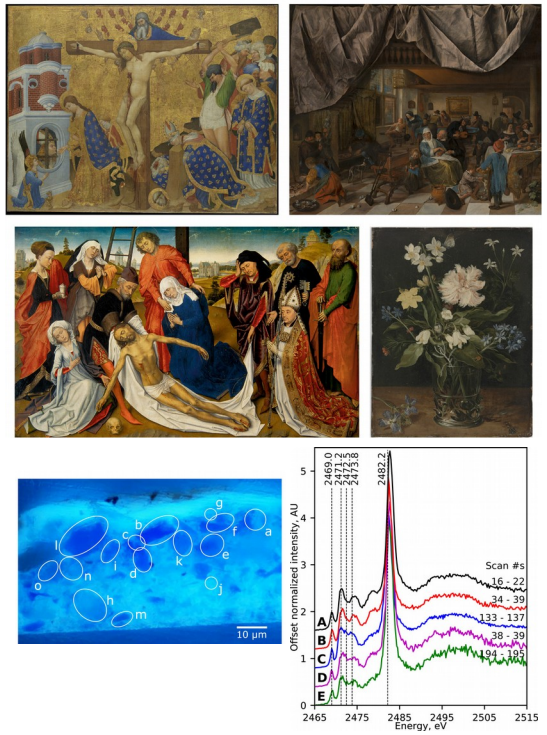
Ultramarine blue pigment, one of the most valued natural artist's pigments, historically was prepared from lapis lazuli rock following various treatments; however, little is understood about why or how to distinguish such a posteriori on paintings. X-ray absorption near-edge structure spectroscopy at the sulfur K-edge in microbeam and full-field modes (analyzed with nonnegative matrix factorization) is used to monitor the changes in the sulfur species within lazurite following one such historically relevant treatment: heating of lapis lazuli before extracting lazurite. Sulfur signatures in lazurite show dependence on the heat treatment of lapis lazuli from which it is derived. Peaks attributed to contributions from the trisulfur radical—responsible for the blue color of lazurite—increase in relative intensity with heat treatment paralleled by an intensified blue hue. Matching spectra were identified on lazurite particles from five historical paint samples, providing a marker for artists' pigments that had been extracted from heat-treated lapis lazuli.

https://advances.sciencemag.org/content/6/18/eaay8782



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Use case

Reprocessing the experiment

- Experiment with a true effort from the authors to provide:
  - Open-data: https://data.datacite.org/10.15151/ESRF-DC-186933507
  - Open-source data analysis material: https://github.com/alessaan/rhapsody-in-blue

- => How to bridge the gap between reproducible and reproduced results?

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Data and data analysis

- Data: 23 datasets, 48GB including:
  - Raw data: 28.7GB
  - Pre-processed data: 9.7GB
  - Intermediary results: 9.3GB
- Analysis: 19 steps
  - Jupyter Python Notebooks: 14 steps
  - Graphical User Interface (PyMca, GIMP): 5 steps
  - Data analysis: 13 steps, producing figures: 6 steps

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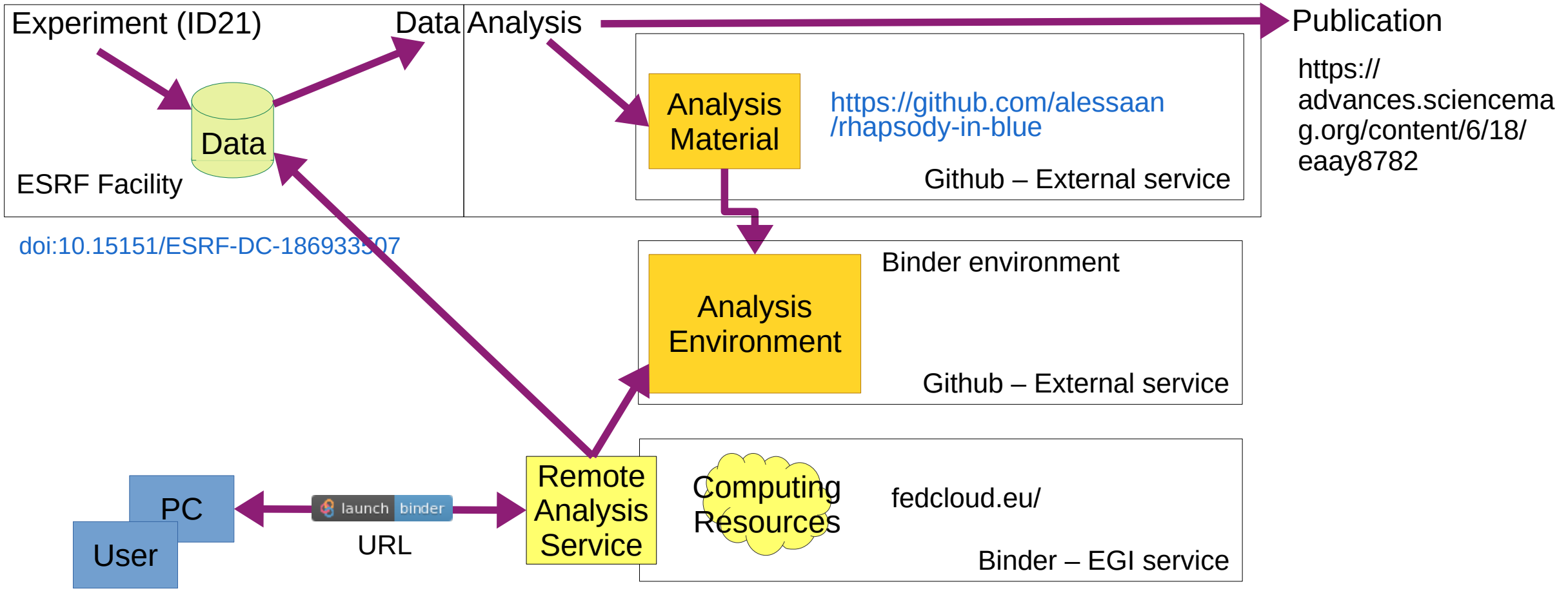
Resources



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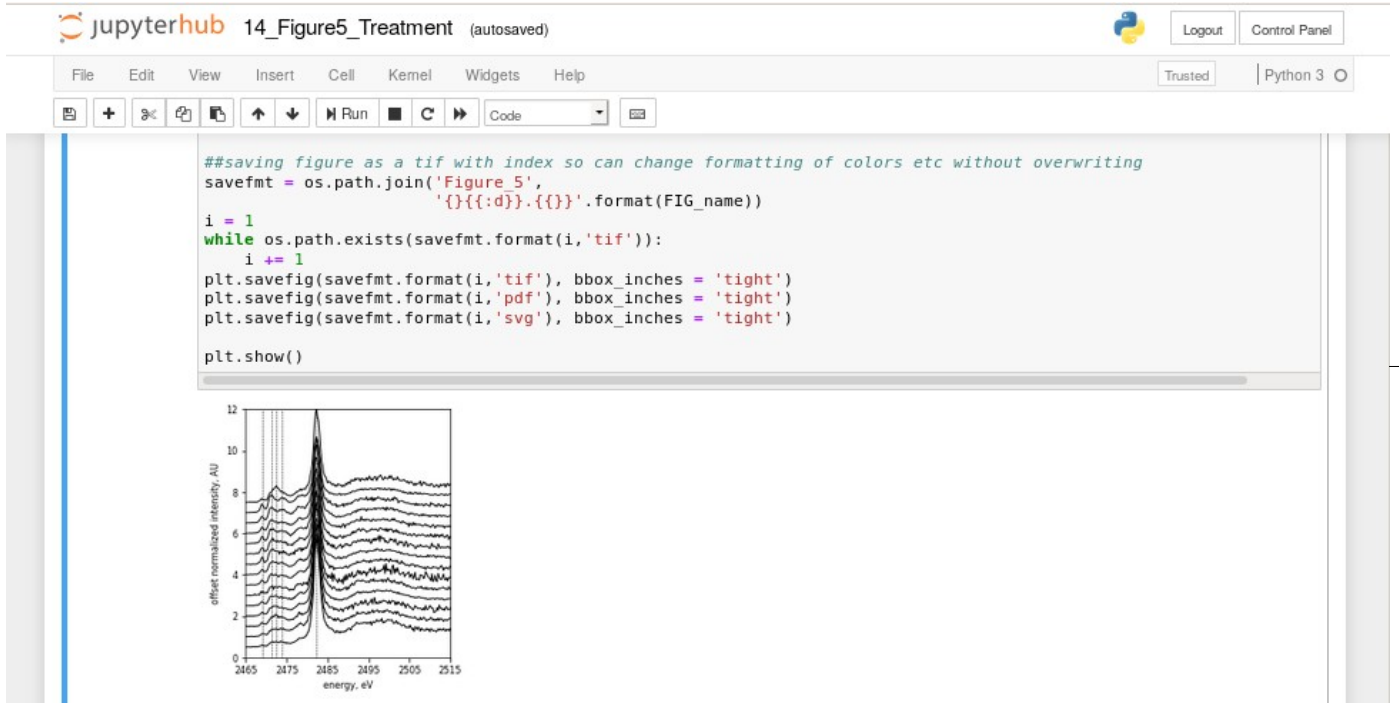
Demo

https://binder-panosc.fedcloud-tf.fedcloud.eu/v2/gh/t20100/rhapsody-in-blue/binder?filepath=introduction.ipynb



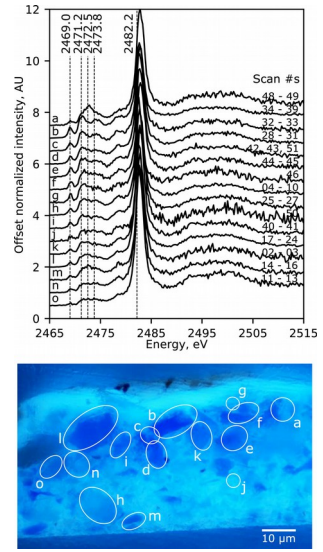


Fig 5.

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Concluding remarks

- This data analysis requires both remote desktop AND notebooks.
- There is a bit of work to bridge the gap between reproducible and reproduced results.
- Using freely available computing resources is fine for demonstration purpose but not for large amount of data and/or compute intensive data analysis.
- => PaNOSC enables providing tools to ease and promote producing reproducible results.

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Thank you

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