Tutorial "Tips, tricks, and tools for reproducible materials science"

Wednesday, 15 September 2021 14:00 (1 hour)

The ability to replicate results is a key characteristic of quality science, and is growing ever more important in light of the replication crisis [1, 2].

A study can rarely be repeated using only the minimalistic descriptions provided in the "Materials and methods" section in a paper.

It is therefore important to properly document the entire knowledge generation pipeline in such a way that it could be repeated by anyone with minimal effort.

In this tutorial we will look at the tools and techniques by which we can improve the reproducibility of an experimental study through a single comprehensive example from electron microscopy.

The session will cover:

- eLabFTW, an electronic lab notebook application with a python API, which can be used to document samples and experiments.
- Various strategies of working with experimental metadata, including the HDF5 file format and JSON.
- Strategies and best practices for reproducible data analysis pipelines in jupyter notebooks, using git, conda-forge, mybinder and docker.

<div id="ioannidis">[1] Ioannidis JPA (2005) Why most published research findings are false. PLoS Med 2(8): e124.</div>

<dif id="schooler">[2] Schooler, J. Metascience could rescue the ,'replication crisis'. Nature 515, 9 (2014).</div>

Primary author:CAUTAERTS, Niels (Max-Planck-Institut für Eisenforschung GmbH)Presenter:CAUTAERTS, Niels (Max-Planck-Institut für Eisenforschung GmbH)

Session Classification: Learning from Complex Data