

The aims of the Workshop were to:

- Try to push the research frontier in the most urgent questions in soil science such as connecting biotic and abiotic processes, soil organic matter dynamics, and utilizing X-ray and neutron sources to answer these questions;
- Provide basic knowledge about different X-ray and neutron imaging techniques, comparing pros and cons of the different approaches;
- Give scientific inspiration in form of various application examples of the techniques in the field;
- Establish a network between international soil scientists and beamline scientists, which could
- Lead to new collaborations.

In the workshop, we had an introductory lecture (Stephen Hall) which introduced briefly the basics of X-ray and neutron imaging techniques and the ways they can be used complementarily to obtain comprehensive information about structure, chemistry and dynamic processes of otherwise obscure sample systems. Stephen also gave an overview of the synchrotron (www.lightsources.org) and neutron (www.neutronsources.org) sources worldwide, and a particular look on the possibilities offered (or to be offered) by MAX IV and ESS.

In the first keynote speaker session, Jeffrey Warren (Oak Ridge National Lab), Sascha Oswald (Potsdam University) and Daniel Uteau Puschmann (University of Kassel) gave talks about applications of X-ray and neutron tomographic imaging and their applications for observing rhizosphere water dynamics in situ, monitoring soil moisture, locating organic matter in the 3D CT images of soil, etc.

In the second keynote speaker session, Juergen Thieme (Brookhaven National Laboratory), Kristin Boye (SLAC National Accelerator Laboratory) and Derek Peak (University of Saskatchewan) introduced X-ray spectroscopy and nano- to micro-spectroscopic imaging techniques, their pros and cons, particularly related to up-scaling, sample preparation, radiation damage and suitable beamline access, as well as their applications for characterization of nutrients (such as nitrogen or phosphorus) and tracking of contaminants in soil, or looking a single microbial cells.

One of the key points mentioned by all the speakers was the importance of complementary use of various techniques –based on X-ray and neutron sources and table-top - for obtaining comprehensive information about the samples.

The presentation material of the workshop can be found here, by pressing a *Download material* button in the top-left corner of the window: <https://indico.linxs.lu.se/event/123/>.

The main points discussed in the four discussion groups (newbies' group, nano- to micro-spectroscopic imaging, bulk spectroscopy and X-ray/neutron tomographic imaging groups) and the subsequent panel discussion:

- Appropriate beamlines around the world can be found via www.lightsources.org
- Before writing a proposal for any beamline, **talking to the beamline scientists** about the feasibility of the study, sample preparation, requirements for the application, beamtime needed, the size of the team necessary to take the most use of it, etc. is of utmost importance;

- **Acquiring as much knowledge as possible about your sample** using more conventional techniques prior applying for experiments at large scale facilities is necessary;
- **Sample preparation:** sample thickness and geometry, state, compatibility with beamline hardware (e.g. sample holders, vacuum, transferability of sample to different beamlines or more conventional techniques after having visited a facility, etc.), possible radiation damage to the sample has to be considered before the experiments; labelling can be considered for organic matter in soils for better contrast;
- **Data analysis** and image reconstruction can be quite complicated and produce artefacts, which a user should be aware of, particularly for CT data. To catch biological variety, many images/measurements and statistical treatment of those are needed, treated with understandable, user-friendly codes. In spectroscopy, having spectra of reference materials is important, and the need for databases has been discussed. However, with beamlines constantly improving, and them being different in different facilities, it is a difficult aim to achieve. Appropriate data treatment routines should be discussed with beamline scientists;
- The need to use **complementary techniques** for sample analysis was stressed throughout the workshop (multimodality by combining different beamlines, both within X-ray and neutron facilities, but also table-top techniques such as MRI, LIBS, nano-SIMS, infrared and Raman microspectroscopy, etc.). For example, bulk spectroscopy measurements performed prior imaging can be helpful in getting a good idea of a sample in a broad sense, and different techniques may be needed to combine to zoom in and out over different scales;
- Choosing the right scale for measurements to answer a particular question can be really important. **Up-scaling** the information obtained at nano- to micro-scale to larger scales is not a trivial, but essential task, particularly in soil sciences. It could be tackled by combining different techniques that work at different scales on the same sample or sampling site, or embedding cartridges/sample holders in larger sample, which could be scanned at larger scale (including the cartridges). Then the cartridges could be retrieved for analysis in higher detail;
- An important goal of beamline scientists is to **improve their beamline labs** to the point, that even users with little experience can use it with high efficiency. This can be achieved through automatization of equipment and creation of standardized protocols both for the measurements and the data treatment. However, it is important that the user community is active in learning both the measurement and data analysis techniques for best results.
- A wide variety of **research questions** were addressed during the group discussions, and large potential to advance scientifically with help of X-ray and neutron techniques were identified in the field of physical stabilization of soil carbon, microplastics in soil, and microsite conditions for biogeochemical processes including the fate of toxins.