MS41-1-2 Data treatment at Synchrotron SOLEIL: automation, IA, on-demand computing, packaging
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Abstract
We shall present the reduction and analysis initiatives undertaken at Synchrotron SOLEIL. In terms of data treatment automation, we have implemented automatic data reduction pipe-lines for surface diffraction (using libHKL and Binoculars), auto-processing for MX beamlines, and a set of Jupyter Notebooks for absorption spectroscopy data.
We are also developing new AI algorithms targeted to automatic data reduction. Examples include de-noising of microscopy images as well as inelastic ARPES data sets, classifying SAXS datasets into scatterer model groups for further fit (based on SASmodels and McXtrace [1]). Further studies include an element identification and oxidation state estimator for absorption spectroscopy (XANES), as well as a Bravais lattice/space group estimator for powder diffraction.
Last, we provide computing resources in the form of a JupyterHub portal, and the DARTS service [2] with virtual machine on-demand for data treatment computing. Our strategy is to keep in touch with beam-lines to inquire for their software needs, feed these services with this software that we push as X/neutron Debian packages [3], and always favour simplest solutions.

References
[1] McXtrace <http://mcxtrace.org/>
[2] DARTS/qemu-web-desktop <https://gitlab.com/soleil-data-treatment/soleil-software-projects/remote-desktop>
[3] Photons-and-Neutrons Debian packaging <https://salsa.debian.org/pan-team/soleil-packaging-overview>

McXtrace beam-line modelling

DARTS on-demand computing