Gwaihir: Jupyter Notebook Graphical User Interface for Bragg Coherent Diffraction Imaging

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Analysis workflow

**Introduction**

- **Open-source tool** to process and analyse Bragg Coherent X-ray Diffraction data.
- **Integrates bcdi** [Carnis et al. 2021] for phase retrieval and bcdi [Carnis et al. 2021] for data pre- and post-processing.
- **Creates workflow** promoting data reproducibility.
- **Python 3.9**, GNU General Public License v3.0.

**Data visualisation**

Large scale facilities seek to:
- provide remote-access to high powered computing services,
- combine solutions in an interactive and accessible environment.

JupyterHub, a cloud computing service:
- heavy computations without relying on specific hardware,
- Jupyter Notebook, versatile and user-friendly IDE supporting many programming languages (Kluyver et al. 2016),
- browser-based data analysis interfaces,
- command-line scripts for advanced users,
- pre-configured data analysis environment managed efficiently by system administrators.

Chosen by:
- Google (Google Colab),
- European Synchrotron (Simple Linux Utility for Resource Management – SLURM),
- SOLEIL (GRADES).


**References**

1. Favre-Nicolin, Vincent et al. (2011). “Fast computation of scattering maps of nanostructures using graphical processing units”. In: Journal of Applied Crystallography

**Conclusion**

- Local or remote use with JupyterHub,
- User-friendly web-interface,
- Data visualisation in two or three dimensions,
- Compatible with cluster resources,
- Enables on-site fast data analysis,
- Data sharing in the CXI format
- Unique workflow.

In a world where data is steadily made more available, Gwaihir is a tool that overcomes multiple issues by bridging remote access, cluster computing and, a user-friendly interface, consequentially improving the link between synchrotrons and their users.

**Acknowledgements**

This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 818823).

**GitHub.com/DSimonne/Gwaihir**

**References**

1. Favre-Nicolin, Vincent et al. (2011). “Fast computation of scattering maps of nanostructures using graphical processing units”. In: Journal of Applied Crystallography