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ParSeq –a Tool for Creation of Comparative Data Analysis Pipelines

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Package ParSeq is a python software library for _Parallel execution of _Sequential data analysis. It implements a general analysis framework that consists of transformation nodes –intermediate stops along the analysis propagation to visualize data, display status and provide user input –and transformations that connect the nodes. It provides an adjustable data model (a collection of data objects that supports grouping, renaming, moving and drag-and-drop actions), tunable data format definitions, plotters for 1D, 2D and 3D data, cross-data analysis routines and flexible widget work space suitable for single- and multi-screen computers. It also defines a structure of Python modules to implement particular analysis pipelines as relatively lightweight Python packages.

ParSeq is intended for synchrotron based techniques, first of all spectroscopy.

In this contribution, I present the basic ideas about the analysis framework, go through the list of centralized facilities (data import/export, plotting, project saving/restoring, undo, dynamically built html help pages etc) and show examples of a few ready pipelines for XAS, XES and XRD.

The main ParSeq package and a few analysis ParSeq pipelines are available on GitHub [github.com/kklmn/ParSeq]. Its online documentation can be viewed on parseq.readthedocs.io .

Fig 1. A screenshot of ParSeq-XAS (an EXAFS analysis pipeline, github.com/kklmn/ParSeq-XAS) as an application example that builds on top of ParSeq framework. The XAS pipeline itself is a relatively lightweight package of less than 2500 lines; it includes all standard EXAFS analysis steps up to EXAFS FT/BFT with atomic shell fitting.

I plan to submit also conference proceedings

Yes

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