Quasi Elastic Neutron Scattering (QENS) model library

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Outline

- Motivations
- Description
  - Repository, build system, tests
  - User experience
- Conclusion & future developments
QENS library - Motivations

Workflow of data treatment

Experiment → Reduction → $S(q, \omega)$ → Analysis/Fitting → Results

Existing software, libraries

*Software:* mantid, Lamp (strfit), Dave (pan), Modes, Frida, Qclimax (SNS)...

*Fitting tools:* ufit, bumps, lmfit...

*Python library:* qef...
QENS library - Motivations

Workflow of data treatment

Coverage of data treatment

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<th>Software / libraries</th>
<th>Reduction</th>
<th>Fitting</th>
<th>Results</th>
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<tr>
<td>mantid</td>
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** https://github.com/jmborr/qef
QENS library - Motivations

Workflow of data treatment

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QENS library - Description

- Requirement of work-package 10

- Aim
  
  "develop an exhaustive library of dynamical models, to allow rapid and easier prototyping"

- Similar approach in Small Angle Scattering
QENS library - Description

Repository on GitHub: https://github.com/QENSlibrary/QENSmodels

License
- GPL
- Free as in Freedom

Code quality
- flake8

Tests
- Doc tests
- Unit tests
- Reference data

Continuous integration
- Travis CI

Models
- Python scripts
- 100% of models from strfit

Documentation
- Read the Docs
- SPHINX
- README files

Examples
- Jupyter notebooks
- “Fitting engines”: Lmfit, Bumps, scipy

Users’ contribution
- CONTRIBUTING file

How to start?
- https://qensmodels.readthedocs.io/
Help for users

- Documentation
  
  ![Read the Docs](readthedocs.org) → nothing to build neither install

- Examples
  ![Jupyter notebooks](jupyter.org)

  - Name
    
    **bumps_BrownianDiff_fit.ipynb**
    
    Fitting engine QENS model
  
  - Installation of minimizer if not already installed
  
  - Widgets → display options for minimizers, plot different settings
  
  - Output
    - values of refined parameters
    - Plots
  
  - Trying without installing → ![binder](binder.org)
Demo

Example from QENS library ➔ jupyter notebook
Models

- Issue with Mantid (transition Python2 ↔ Python3)
- Choice of default units? default values?
- Add derivative in models (required by some minimizers)
- Method to combine models (one example, not straightforward)
- 🐚 / 🐍 python™

Software development

- Need agreement on good implementation of δ function
- How to deal with ☕ Jupyter notebooks in Git?
- ☞ Binder is slow. Any other option?

⇒ Need of users’ feedback
Conclusion / Future developments

**Future developments**

Documentation: physical description of models

Implement first users’ feedback

Please test the library [https://github.com/QENSlibrary/QENSmodels](https://github.com/QENSlibrary/QENSmodels)