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https://github.com/JYU-IBA/jabs

DOI 10.5281/zenodo.6362701

JaBS: Open source RBS, EBS, NRA simulation and fitting code

INTRODUCTION

A code to simulate RBS, EBS, NRA and ERD spectra has been developed. The GPL licensed open source software is computationally similar to other popular codes e.g. SIMNRA.

Although some features are still missing, the code is able to simulate e.g. typical RBS spectra by taking into account screened Rutherford cross sections, stopping, straggling etc. The code can simulate and fit arbitrary number of detector spectra in arbitrary geometries simultaneously, but is currently limited to modeling a single experiment (same incident beam, fluence).

The program is intended to be used by human readable (and writable) scripts, providing a degree of flexibility for various use cases and providing means to perform semi-automated analysis. The scripts can be edited and run using a graphical user interface or using a command line interface.

The code is hosted at GitHub, see the page for latest list of features and bug reports.

TECHNICAL STUFF

The code is written in C (command line version) and C++ (Qt6 based GUI). In case of popular demand the simulation backend can be turned into a library, to be used by other programs. The code runs on Windows, macOS and Linux. Fitting uses nonlinear least-squares Levenberg-Marquardt algorithm from GNU Scientific Library (GSL) with some modifications for parallel processing.

JIBAL

Stopping forces, electronic straggling and isotopic data are provided by Jyväskylä Ion Beam Analysis Library (JIBAL), also used by Potku. The library allows user to provide files for e.g. stopping for a particular Z_1, Z_2 combination. Files containing SRIM2013 and DPASS electronic stopping and Chu and Yang straggling data are available and bundled with the binary versions of JaBS.

WHERE CAN I GET IT? IS IT CHEAP?

Source code is available from GitHub *(https://github.com/JYU-IBA/jabs/)*, ready-to-use binaries for macOS and Windows are also available, see *releases* in GitHub. There is some built-in help available, but the documentation is quite poor. *Getting started* guide is available from the author. Examples are included in the distribution. IDF/XNRA files can be converted into JaBS scripts.

JaBS is free software, you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, version 2. There is no warranty.

GRAPHICAL USER INTERFACE

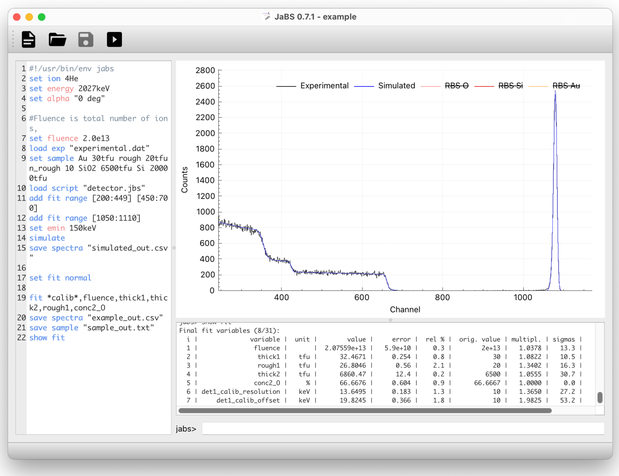


Fig. 2: Qt 6 based GUI offers syntax highlighting and plotting features.

COMMAND LINE INTERFACE

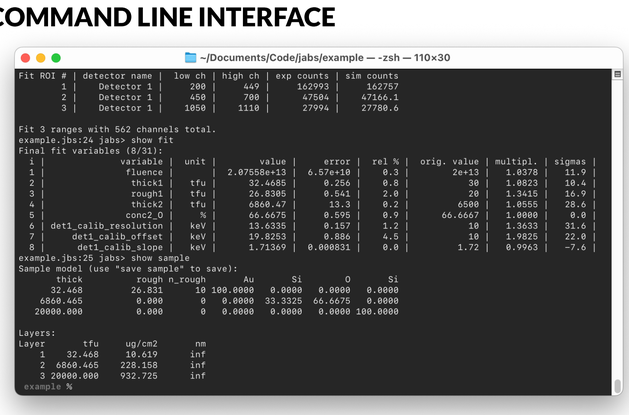


Fig. 3: Running scripts on the command line is an easy way to process large batches of measurements. Interactive use is also possible.

SOME IMPLEMENTED FEATURES

- Multidetector support
- IDF import and export (partially)
- Arbitrary cross sections and reactions from R33 files. Both EBS (Q-value is zero) as well as p-p NRA are implemented.
- Point-by-point and layered sample models. Automatic normalization of concentrations to 100%.
- Roughness (gamma or user defined distribution of thicknesses)
- Arbitrary geometries, calculation of geometric broadening even for detectors outside IBM or Cornell geometry
- Non-linear detector calibration (polynomial) and constant detector energy resolution or timing resolution (for ToF)
- Z-specific calibrations, foil in front of detector
- Fitting to experimental spectrum (L-M)
- Tunable speed /accuracy
- Dual scattering (large angle)
- Layer specific stopping, straggling and yield corrections can be supplied by the user
- Two-phase fitting, where faster physics model is used in the beginning and more accurate model is turned on after the first phase is starting to converge.
- Multiprocessing using OpenMP

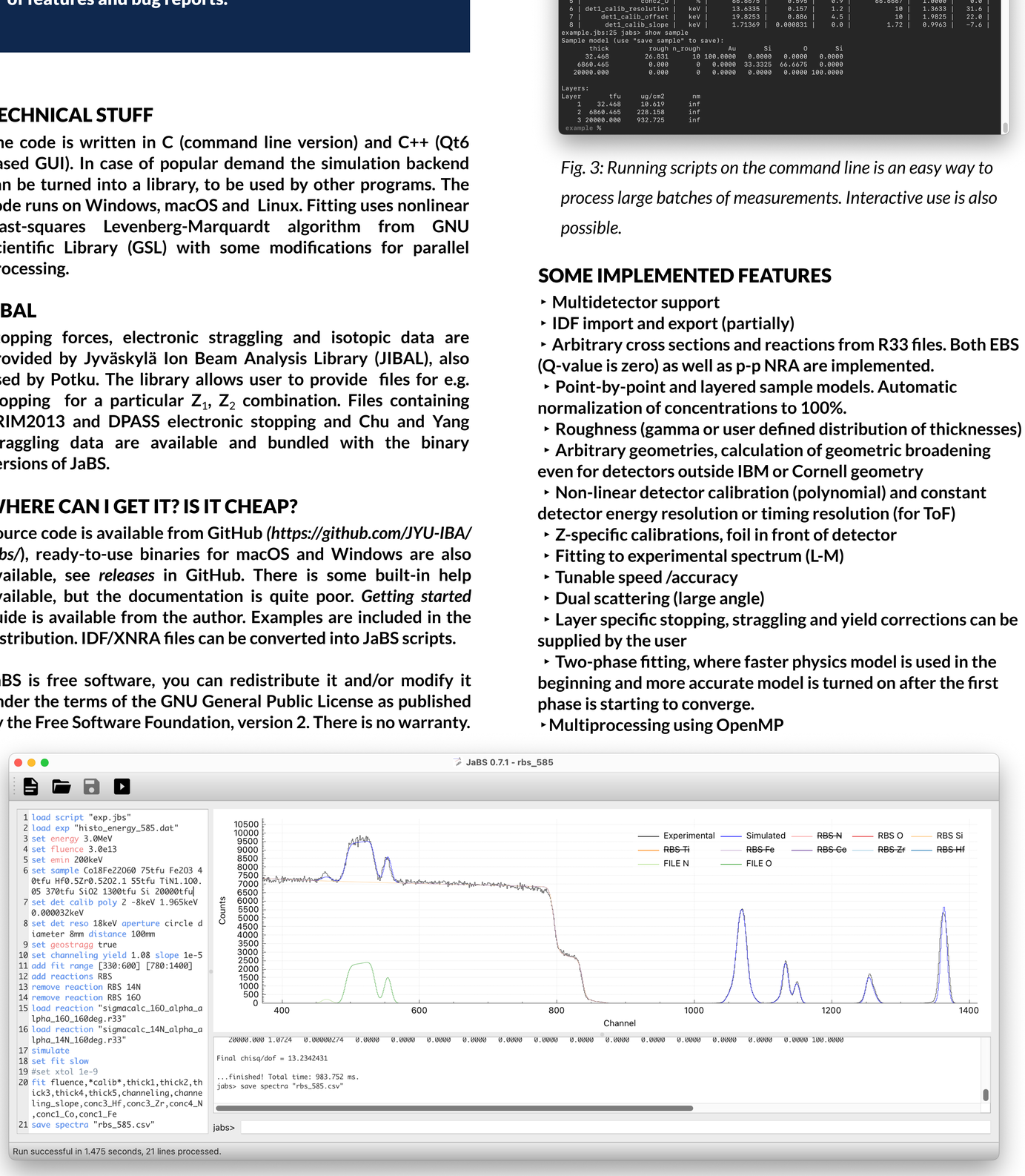


Fig. 1: RBS spectrum of a multilayer sample being fitted with JaBS. The fit is far from perfect, but the system is quite complex and channeling plays a role.

REAL WORLD EXAMPLES

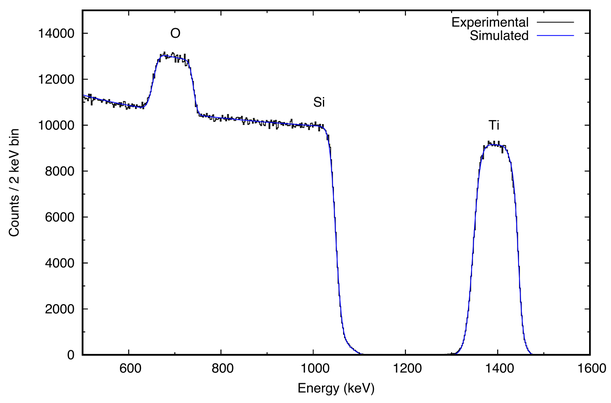


Fig. 4: RBS spectrum of 100 nm thick ALD-TiO_2 sample measured with 2 MeV ^{4}He beam. JaBS was used to fit layer thickness (areal density), roughness etc. Insert: HIM image.

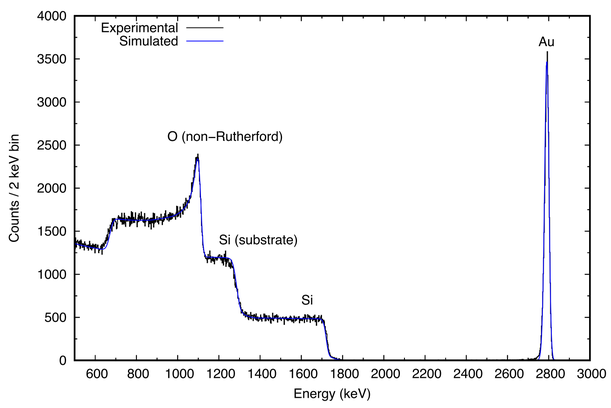


Fig. 5: RBS spectrum of a thin gold film on 1 µm thick SiO_2 layer measured with 3.035(3) MeV ^{4}He beam. Cross section R33 file for $^{16}O(a,a)^{16}O$ reaction was obtained from SigmaCalc.

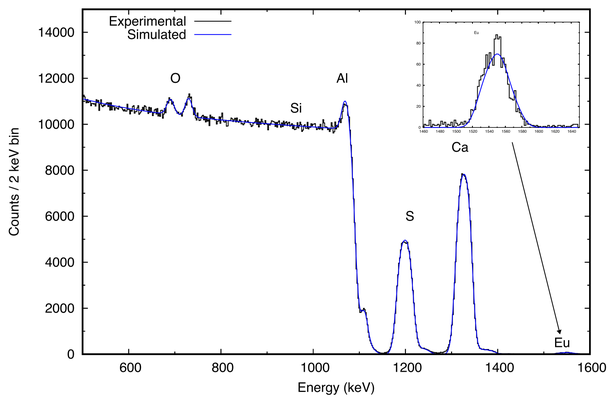
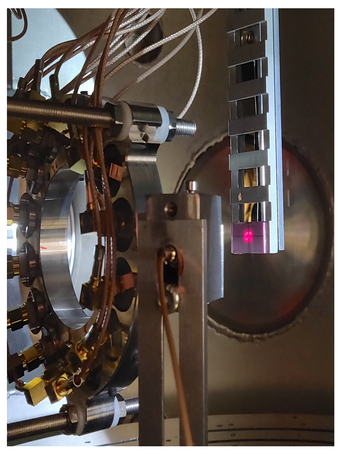


Fig. 6: RBS spectrum of a CaS:Eu film with Al_2O_3 cap layers.

EXPERIMENTAL



The multidetector RBS setup in Jyväskylä used for the experimental spectra above features:

- 14 detectors (Canberra PIPS PD50) in a ring, **θ**=160°
- 1 movable detector, **θ** from 10° to 145°
- rotating vane beam chopper
- 2 preamplifiers (CAEN A1422), 8 channels each
- 2 digitizers (CAEN N6725)
- sample manipulator, 2 axises (to be replaced soon)
- accelerator (NEC Pelletron 5SDH-2) (to be replaced)

Fig. 7: RBS setup in Jyväskylä

ACKNOWLEDGEMENTS

Thanks to S. Kinnunen, J. Rosa and M. Napari for the samples, K. Kinnunen and FYSS5455 autumn semester 2021 project group 3 for the HIM image, M. Laitinen for setting up the multidetector RBS together with the author and T. Sajavaara and the COVID-19 pandemic for making this work possible.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 824096.