The 8th International Workshop on Magnetic Resonance Sounding, Strasbourg, France

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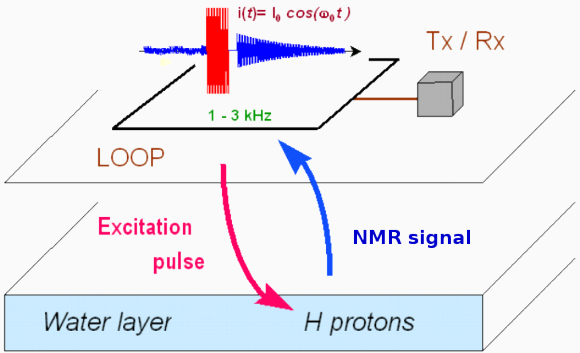
Trevor Irons[1]

27 November 2021

[1]Montana Technical University

surface NMR



- earth's field B_0
- hydrogen spins align with B_0
- precessing at Larmor frequency ($\in$ 1-3 kHz)
- rf pulses tip magnetization out of equilibrium
- inductive voltage response
- hydrologic properties (ϕ, κ)

Adapted from *iris-instruments.com*

Akvo features

- **FLOSS** Akvo is freely released under a copyleft license (GPL V. 3) and is available via anonymous download with no proprietary dependencies.
- **User friendly** Akvo is trivial to install for most users and requires no programming or scripting.
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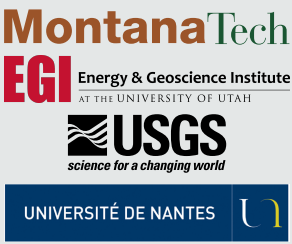
- **Reproducible** Akvo records all processing steps and parameters in human-readable yaml files facilitating the release of reproducible results.

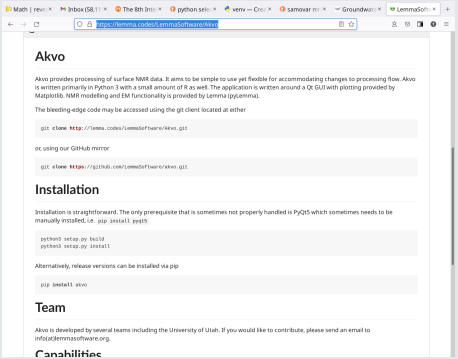
Organisations



FLOSS

Download

- `lemma.codes/`



- `github.com/LemmaSoftware/akvo`
- `pypi.org/project/Akvo/`

Python Dependencies

- numpy, scipy
- pandas, seaborn, matplotlib, cmocean
- ruamel.yaml
- pyQt5

All available on PyPi

C++ Dependencies

- Qt - Graphical user interface
- Lemma - Lemma is an Electromagnetics modelling API
- Merlin - Surface NMR forward modelling

Wheels available for CPython 3.7 & 3.8

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User friendly

For users on 64 bit Linux, macOS, or Windows 10 under CPython 3.7 or 3.8

use pip

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pip install akvo
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git pull https://lemma.codes/akvo.git && cd akvo
python setup.py build
(sudo) python setup.py develop
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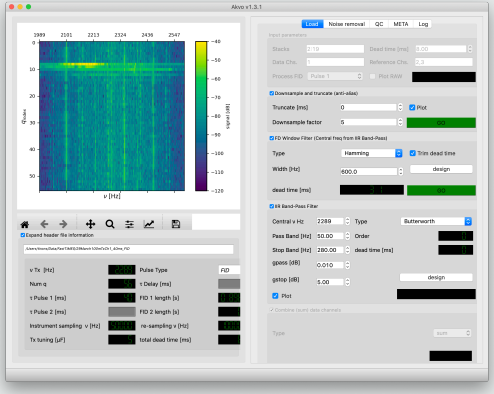
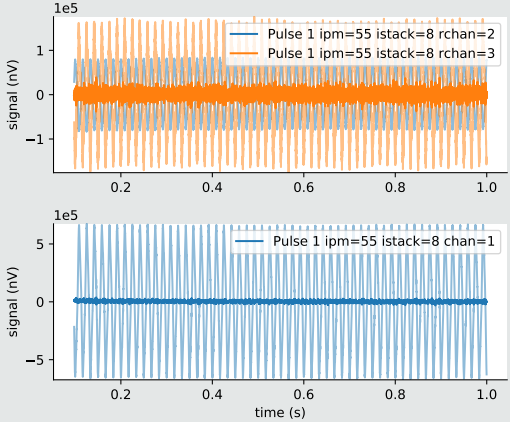
User friendly

Signal processing

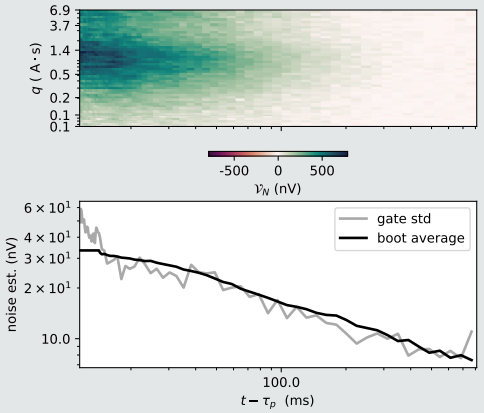


Noise removal



User friendly

Signal processing



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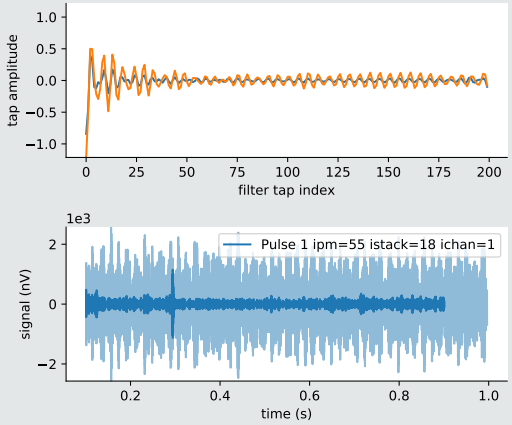
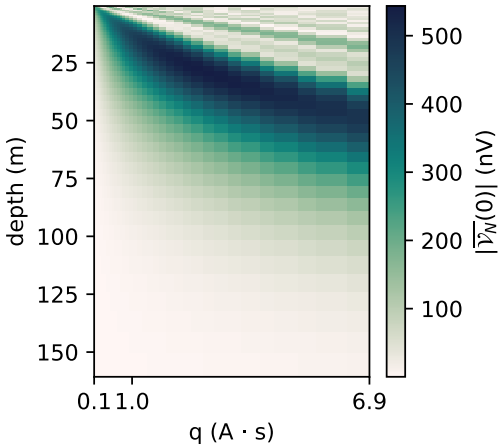
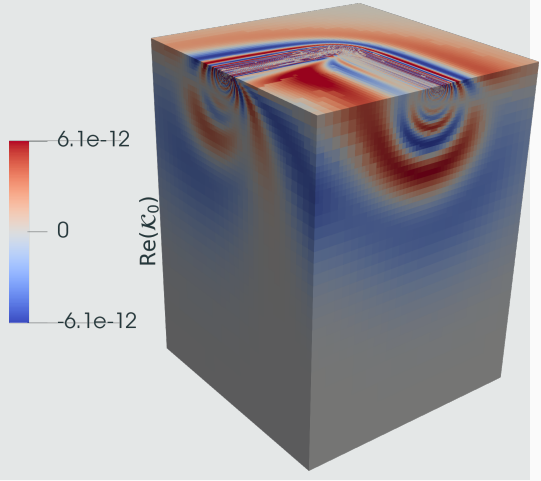


Modelling

1D Kernel

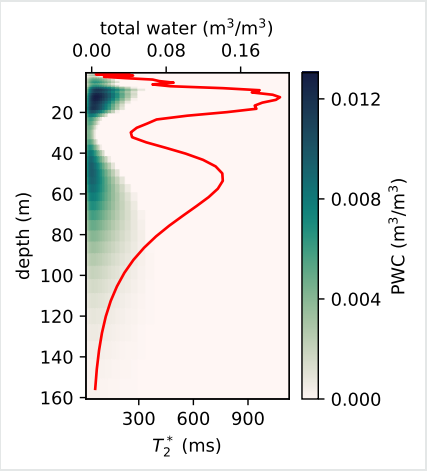


3D Kernel

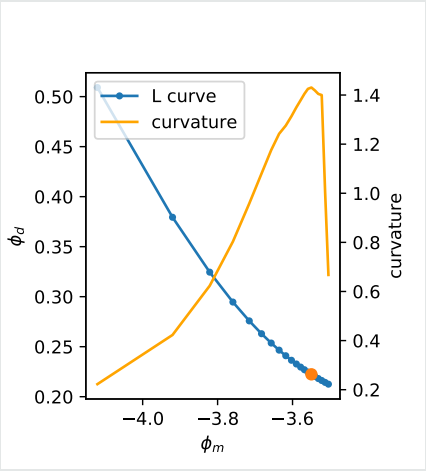


Inversion

1D Qt



Optimal λ^*



Inversion

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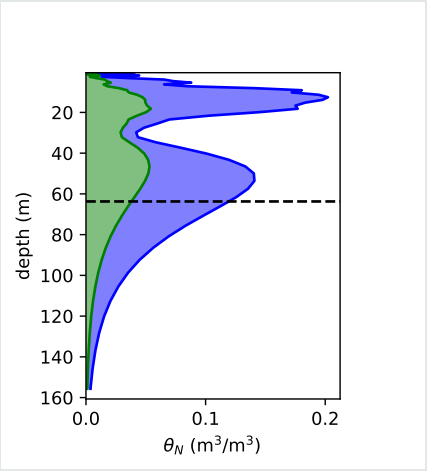
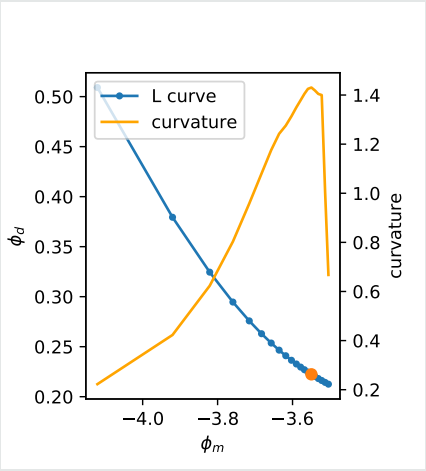


Optimal λ^*



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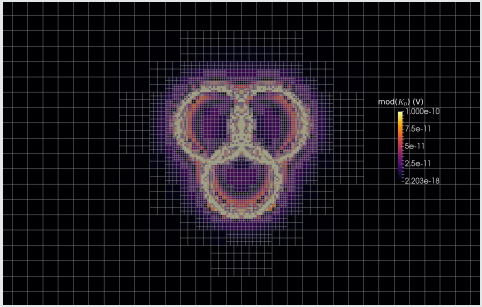
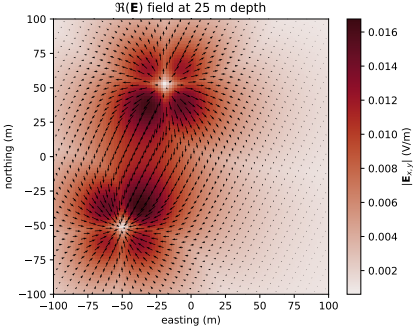
Flexible

Arbitrary transmitters



Grounded sources



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Reproducible

```
!<AkvoData>
Akvo_VERSION: 1.4.3
TuneCapacitance: 5.0
headerstr: /home/tirons/Data/Ne/58b/FastTimes/29March100mTxCh1_40ms_FID
nPulseMoments: 56
processed: Akvo v1.4.3, on 29/10/2019
pulseLength: [0.04]
pulseType: FID
transFreq: 2289.0
Import:
  GMR Header: /home/tirons/Data/Ne/58b/FastTimes/29March100mTxCh1_40ms_FID
  opened: '2019-10-28T22:25:36.182739'
  pulse Type: FID
  stacks: [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]
  data channels: [1]
  reference channels: [2, 3]
  pulse records: Pulse 1
  instrument dead time: 0.008
META:
  Location: Lexington, NE, Site 58A
  Coordinates: {UTM: Local, LatBand: Local, ellipsoid: Local}
  DateTime: 2010-03-29T12:00
  Temp: 20.0
  B_0: {inc: 68.0, dec: 0.0, intensity: 53761.0}
  Field Notes: 'Reference loop locations are approximate. '
  Loops: {Ch.1: Ch.1.yml, Ch.2: Ch.2.yml, Ch.3: Ch.3.yml}
Processing:
- {STEP 0: Resample, downsample factor: '5', truncate length: '0'}
- {STEP 1: Window filter, centre: '2289.0', trim: 'True', type: Hamming, width: '600.0'}
- {PCA: No, STEP 2: TD noise cancellation, lambda: 0.99, mu: 0.01, n_Taps: 200, truncate: 800.0}
Stacking:
  Calc Q: true
  TD stack: {cutoff: '1.48', outlier: MAD}
```

More information

- https://akvo.lemmasoftware.org
- https://pypi.org
- FastTIMES article in current issue, eegs.org
- Trevor.Irons@lemmasoftware.org

Akvo: a Surface NMR Workbench

Trevor Irons
Department of Geophysics
Montana Technical University
Butte MT, USA
irons@mtech.edu
Bio»
Benjamin R. Bloss
United States Geological Survey, Geology, Geophysics, and Geochemistry Science Center, Denver CO, USA
bbloss@usgs.gov
Bio»
Thomas Kremer
University of Nantes, Univ Angers, CNRS, LPG, UMR 6112, F-44000 Nantes, France
Thomas.Kremer@univ-nantes.fr
Bio»
M. Andy Kass
Hydrogeophysics Group, Dept. of Geoscience, Aarhus University, Denmark
andykass@geo.au.dk
Bio»

Abstract

Akvo is a software project for processing, modelling, and inversion of surface nuclear magnetic resonance (sNMR) data which is being released as a resource for the community. The signal processing, inversion, front-end, and Qt5-based graphical user interface code are written in Python 3 and released under the GNU v3.0 public license. Akvo seamlessly interfaces with Merlin, an open source (Mozilla Public License) sNMR modelling API written in C++-14 for high-performance back-end functionality. Precompiled binaries and Python wrappers for Merlin are provided through pip as part of the Akvo package, allowing for simplified installation on Linux, macOS, and Windows 10 platforms. The installer also provides a standalone executable entry point, meaning that users can bypass direct interaction with the Python interpreter, which can be helpful for newcomers to Python. Akvo is entirely open source. There are no external dependencies on proprietary runtime environments. The code is managed in a public git repository (https://akvo.lemmasoftware.org). Anyone can anonymously access, read, edit, and use the code. Akvo is flexible—Akvo processing, modelling, and inversion supports multiple channel data and arbitrary transmitter configuration. All processing steps are configurable so that they can be adapted to varying survey conditions. Akvo processing is reproducible and transparent. The processing workflow is documented along with the data in self-describing human readable YAML files. This encourages reproducible publications and reports. Akvo seeks community engagement. We are looking for new users and collaborators. This runs the gamut from code development, to testing and reporting of tickets for enhancements or bugs reports, and documentation.

Keywords: hydrogeophysics, Python, open source, surface NMR
2010 MSC: 00-01, 99-00

Introduction

Free/libre and open source software (FLOSS) projects serve a vital role in the geoscience community where they facilitate the exchange of ideas and allow for greater scrutiny when validating research findings. However, in many sub-fields non-free and proprietary software remain the only viable options for processing and inversion of data. This is fundamentally damaging as findings cannot be freely replicated and reproduced without the expenditure of great effort. Building the software infrastructure to facilitate the dissemination of research findings in a verifiable and reproducible manner is therefore of paramount concern. The Python programming language continues to be widely adopted by the scientific community, and usage statistics suggest that it is the language of choice for a large portion of open source projects (Borges et al., 2016). Additionally, software must be easy to use for a variety of users, not just experts, in order to gain a sufficiently large userbase.

Surface nuclear magnetic resonance (sNMR), also called magnetic resonance sounding (MRS), is a non-invasive geophysical method that is directly sensitive to liquid-phase water in the top~100 m of the subsurface (e.g. Behroozmand et al., 2015). Processing and inversion of these data are typically performed using proprietary binary codes provided by instrument manufacturers and a few dominant research institutions which tend to not widely disseminate source codes. As such, newcomers to the field face a large barrier to entry. For a fledgling technique such as sNMR this limits the widespread adoption of the method and may even drive off interested parties. There are also no established standards for releasing sNMR data associated with publications which further fractionates the community.

We are aware of only three other software packages providing sNMR capabilities with freely available source code.

- **MRSmatlab**[1] is self-described as being an 'open platform' package which provides much of the same functionality as Akvo including signal processing as well as 1D modelling and inversion (Müller-Petke et al., 2016). While a useful tool, MRSmatlab has several limitations: 1) the licensing is

Corresponding author
Email address: irons@mtech.edu (Trevor Irons)
[1] available at https://github.com/mrepetke/MRSmatlab

T. Irons, B. R. Bloss, T. Kremer, and M. A. Kass (2019). "Akvo: a Surface NMR Workbench". In: FastTIMES 24.4, pp. 101–115.