

# From License Consultation to Software Spotlights

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Research Software im Zusammenspiel

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- 1) Helmholtz-Zentrum Dresden-Rossendorf (HZDR)
- 2) Deutsches GeoForschungsZentrum Potsdam (GFZ)
- 3) Deutsches Elektronen-Synchrotron (DESY)

## Helmholtz Cloud + Backbone Services

- Provide high performance collaboration and community services based on an unified AAI
- Connect all centres and their world-wide collaboration Partners
- Secure, simple access and easy-to-use

## Services for Research Software Engineering

- Achieve high level of knowledge, quality, sustainability and visibility of research software through training and consultation services
- Provide state-of-the-art SW development infrastructures

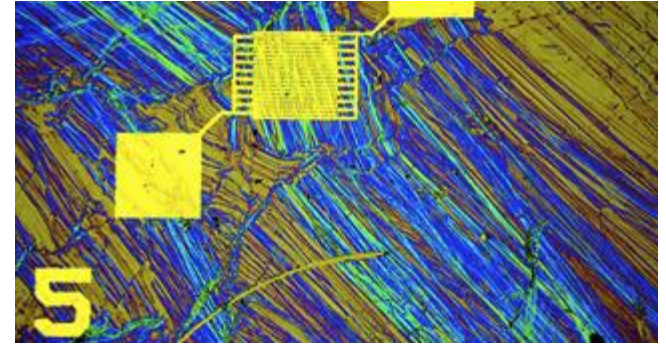




























Bild 1: Organische Halbleiter-Polymere/ Himani Arora / HZDR  
Bild 2: Mosaic Expedition / Stefan Hendricks / AWI

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<b>DESY Sync &amp; Share</b> <span style="float: right;">●</span>  Nextcloud, dCache File Sync and Share. Collaborative Editing using OnlyOffice. by:  <a href="#">Go to service</a> <span style="float: right;">⋮</span>	<b>OpenStack (HDF Cloud)</b> <span style="float: right;">●</span>  OpenStack The Service allows provisioning of user-controlled VMs with Linux OS by:  <a href="#">Go to service</a> <span style="float: right;">⋮</span>	<b>HIFIS Helpdesk</b> <span style="float: right;">●</span>  Zammad HIFIS Helpdesk Ticketing System based on Zammad. by:  <a href="#">Go to service</a> <span style="float: right;">⋮</span>	<div style="border: 1px solid black; padding: 10px;"><ul style="list-style-type: none"><li>➤ <b>Collaboration Services</b></li><li>➤ <b>Infrastructure Services</b></li><li>➤ <b>Scientific / Community specific Services (ramp-up)</b></li></ul></div>	

# Services for the Research Software Lifecycle

Consulting

Research Software Directory 

Community Services

INVENIO 

  
Mattermost



Education & Training

 Zammad

Development Infrastructure

 GitLab

 THE CARPENTRIES

- Research software is a fundamental part of reproducibility
- Software is often times cited badly or not at all
- Software developed by scientists is rarely published
- FAIR principles implemented?

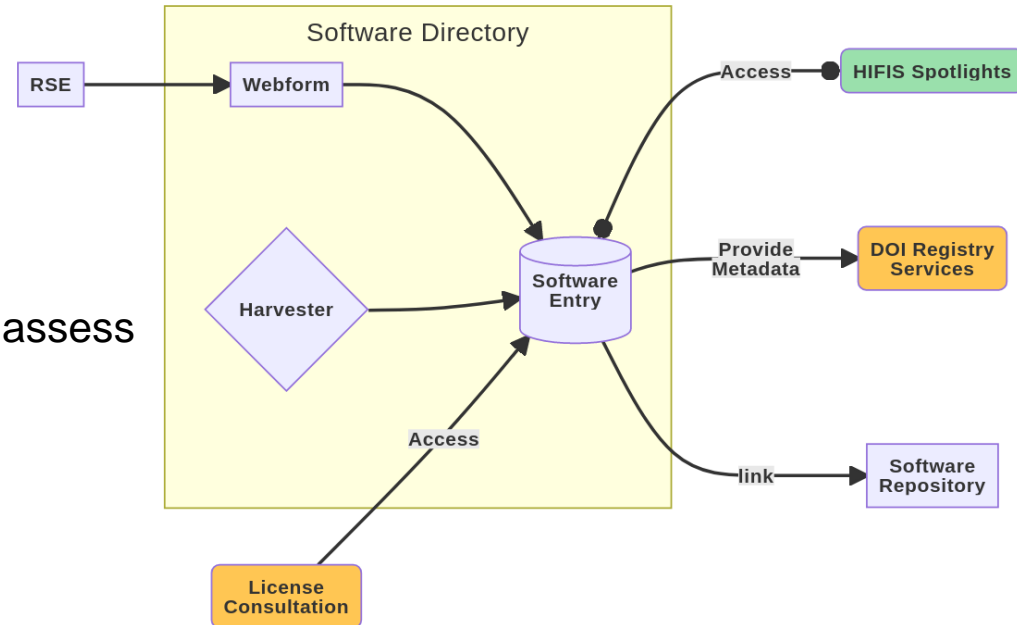


## Goal

- Provide support to scientists and developers so they can publish and (re)use Software within the meaning of FAIR principles

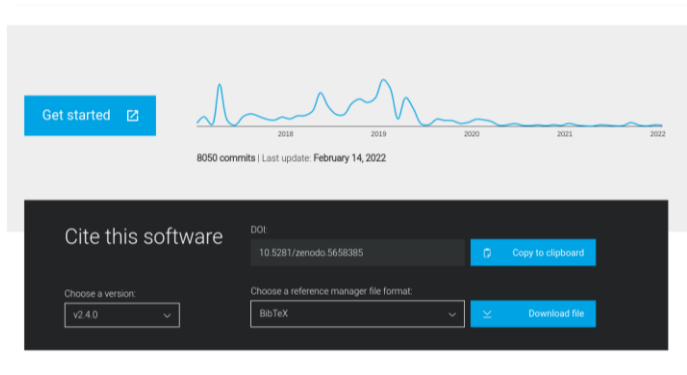
# Increasing the visibility of research software

- Create a process around a software directory
- Goal: every software developed at a research center will be added to the directory
- Allow access for other services, e.g.
  - License consultation
  - DOI registry services
- Automatically collected metrics help to assess software impact



# Research Software Directory

- Build on top of open-source project **Research Software Directory**
- Developed at Netherlands eScience Center
- Features
  - Harvesting information
  - Visual representation of development activity
  - Citation support
- Currently setting up collaboration



netherlands **Science center**

Software Projects Metrics [Fork me on GitHub](#)

This website is powered by the [Research Software Directory](#) – the content management system for research software.

Start typing here to search for software



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Tags -

- Big data (37)
- GPU (6)
- High performance computing (30)
- Image processing (6)
- Inter-operability & linked data (16)
- Machine learning (18)
- Multi-scale & multi model simulations (8)
- Optimized data handling (26)
- Real time data analysis (6)
- Text analysis & natural language processing (19)
- Visualization (30)

ESMValTool

ES

The Earth System Model eValuation Tool is a community diagnostics and performance metrics tool for the evaluation of Earth System Models that allows for routine comparison of models and observations.

8 days ago

★ Featured

DIANNA

DI

Deep Insight And Neural Network Analysis, DIANNA is the only Explainable AI, XAI library for scientists supporting Open Neural Network Exchange, ONNX - the de facto standard models format.

9 days ago

★ Featured

GGIR

GG

Converts raw data from wearables into insightful reports for researchers investigating human daily physical activity and sleep.

Noodles

No

Task-based parallel programming model in Python that offers the same intuitive interface when running complex workflows on your laptop or on large computer clusters.

# Adding software to the RSD using a web form

GFZ  
Helmholtz-Zentrum  
POTSDAM

IT-Services and Operation GFZ-Webpräsenz Other

Forms portal / Other / Software distribution

### About the Software

Name of the software \*

Version \*

Is it new or existing? \*    Is it simple or complex? \*    Can it be commercialised?    Scope of usage \*

-- Select property --    -- Select property --    -- Select property --    -- Select property --

Case group

-- Select a case group --

Please refer here: [http://intranet.gfz-potsdam.de/fileadmin/intranet/doc/Arbeitskreise/AM\\_Software/Guidelines\\_Software\\_ENG\\_Layout\\_20190319.pdf](http://intranet.gfz-potsdam.de/fileadmin/intranet/doc/Arbeitskreise/AM_Software/Guidelines_Software_ENG_Layout_20190319.pdf)

Previous users

Please list users or groups that used the software

Description \*

Please write a description and use of the software (max 1000 characters)

Reference

Where can the software be accessed, e.g. a repository or a website link

Previous step **Next step**

GFZ  
Helmholtz-Zentrum  
POTSDAM

IT-Services and Operation GFZ-Webpräsenz Other

Forms portal / Other / Software distribution

### Contributors and funding

First contributor *	Second contributor	Third contributor	Fourth contributor
Full name: Role	Full name: Role	Full name: Role	Full name: Role

Are there more than four contributors? \*

-- Select confirmation --

Funding \*

If multiple funding exist, list them comma separated

Previous step **Next step**

GFZ  
Helmholtz-Zentrum  
POTSDAM

IT-Services and Operation GFZ-Webpräsenz Other

Forms portal / Other / Software distribution

### Dependencies

Used programming language(s) \*

C  
 C++  
 Fortran  
 Java  
 JavaScript  
 Python  
 R  
 Other

Is the software part of a larger software package? \*

-- Select a confirmation --

This may be the case, if this software is a submodule designed for another software.

Provide a list of dependencies and their licenses

library\_name: SPDX-identifier

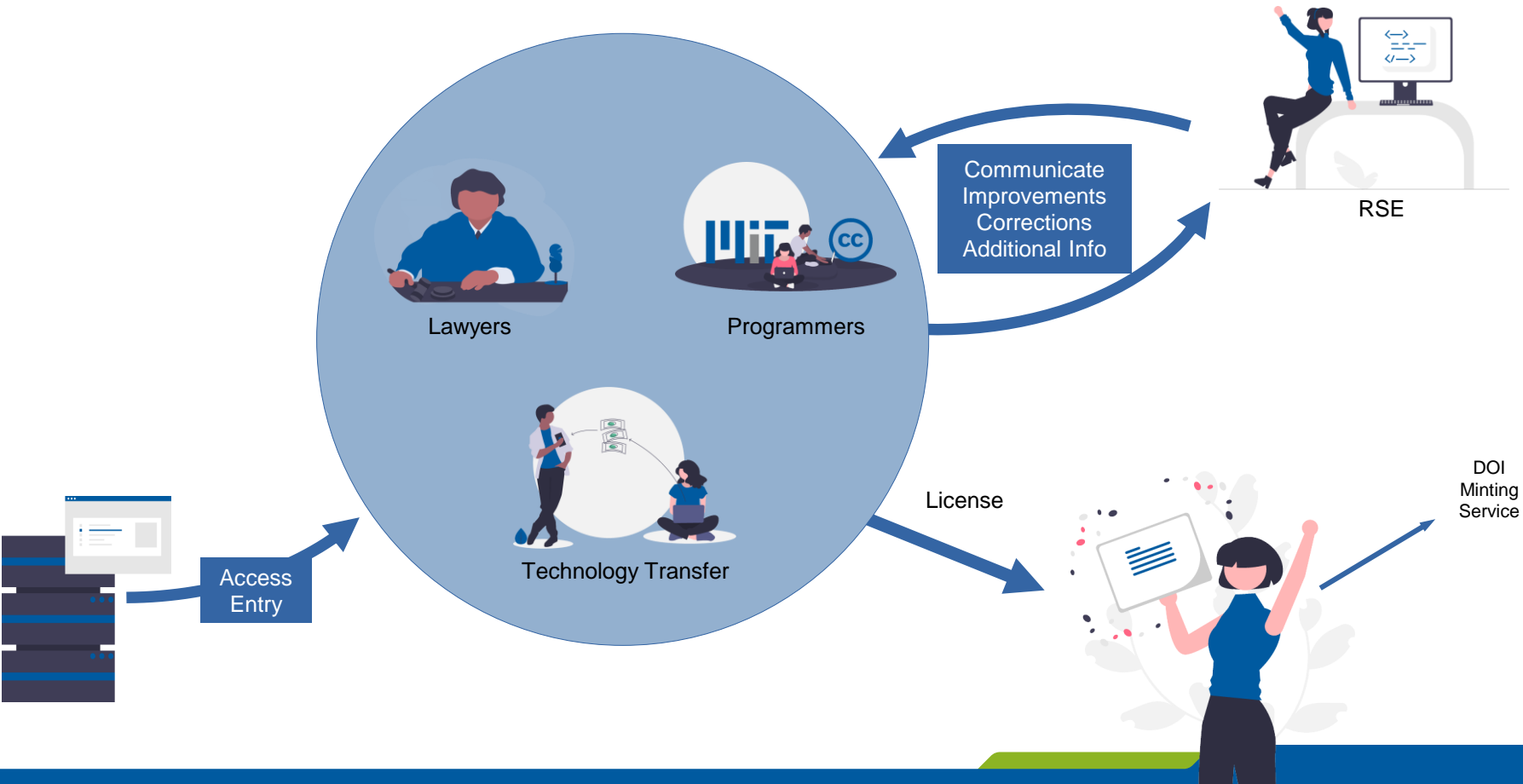
### Filling out the dependency list

- Use one line per dependency
- The license of the dependency should be listed on the corresponding website or repository
- For a full list of SPDX-identifiers please refer to <https://spdx.org/licenses/>
- Fill out only primary dependencies of your software (not the dependencies of your dependencies)
- We provide a framework that helps you to generate a list of dependencies: <https://git.gfz-potsdam.de/id2/software/services/fair/software-quality-assurance>
- If you do not know the license of a library, please write "unknown"

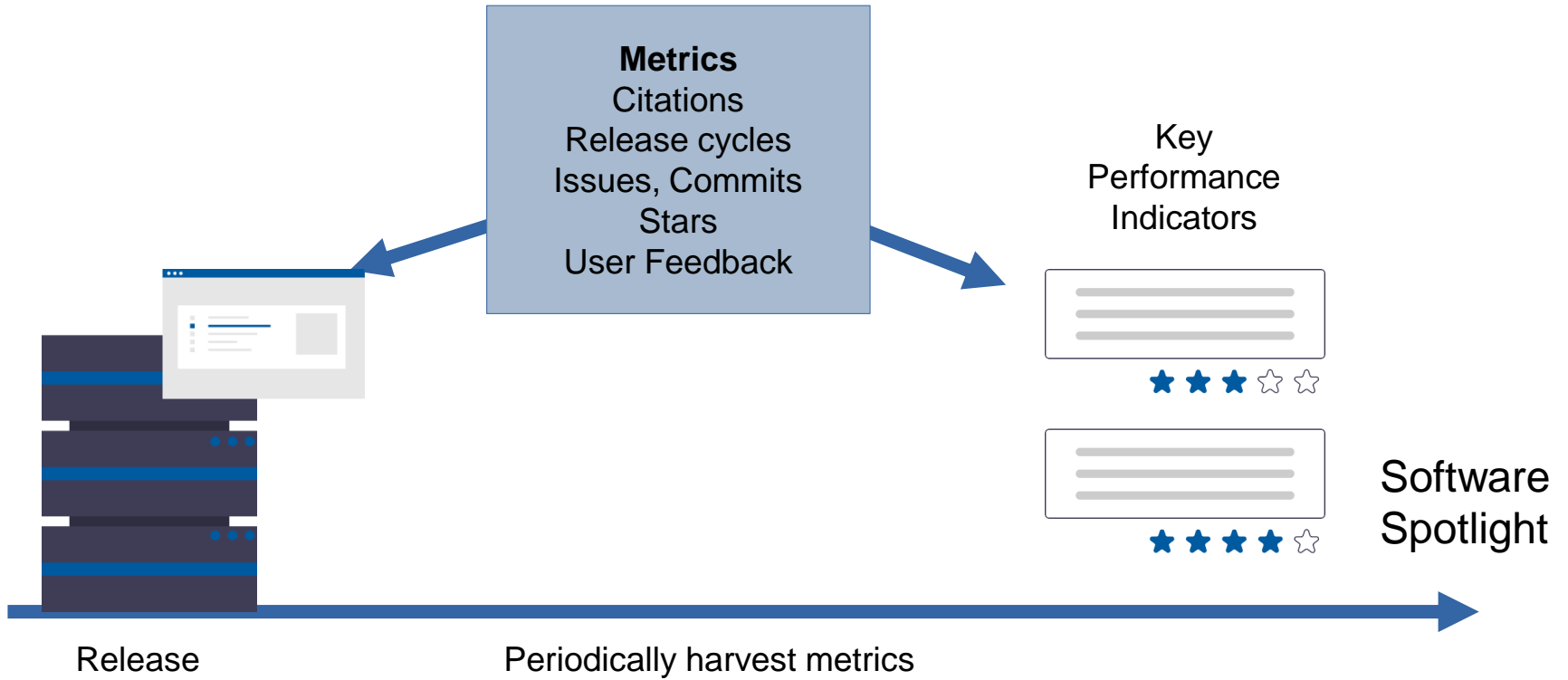
Previous step **Next step**



# License consultation process



# Becoming a Software Spotlight

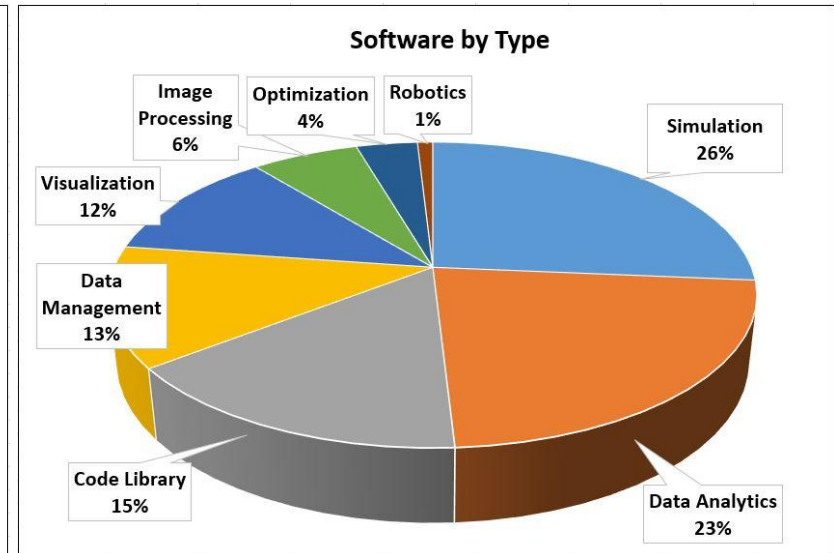
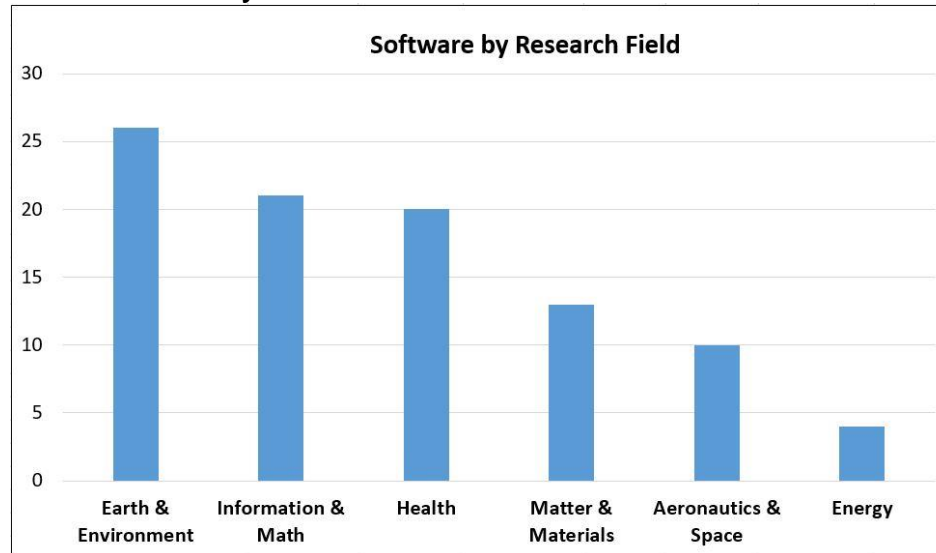


## Initiative of the Helmholtz Software Forum:

- platform to exchange knowledge, present ideas & results and define policies and incentives.

## Helmholtz Lighthouse Projects:

- First Call: **94 great software projects** representing top success stories, about 50% for Simulation and Data Analytics



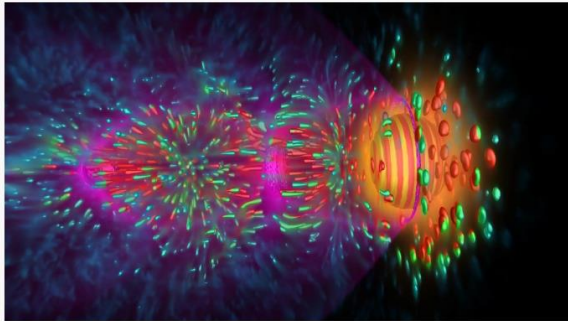
# HIFIS Software Spotlights



## PICONGPU

PICongPU is an extremely scalable and platform portable application for particle-in-cell simulations. While we mainly use it for studying laser-plasma interactions, it has also been used for astrophysics studies of the Kelvin-Helmholtz-instability.

PICongPU has been a finalist for the prestigious Gordon-Bell-Award in 2013 and has been one of the flagship applications for a number of leading edge high performance computing (HPC) systems since then (Titan, JUWELS Booster, Frontier1, Frontier2, Frontier3). Through this work, PICongGPU has established strong ties with a lot of national and international partners, especially the underlying hardware agnostic libraries like Alpaka and Llama are now adopted in the CERN LHC software stack as well. Another collaborative effort also driven by PICongGPU is a standardization in data formats for plasma physics via openPMD, which is becoming one of the leading data standards in the community.



A snapshot from a simulation of an ultrashort, high-intensity laser pulse (orange-striped sphere) driving a plasma wave in ionized helium gas on the Oak Ridge Leadership Computing Facility's (OLCF) Summit supercomputer. Purple areas highlight the electron density. Streams depict the stronger (red) and weaker (green and blue) electric fields. See also [this video](#) on this [Link to Youtube](#). This image was generated using ISAAC, a tool for visualizing simulations in real time on the Frontier supercomputer being built at OLCF. Image Courtesy of Felix Meyer/Helmholtz-Zentrum Dresden-Rossendorf.

### CENTRES

HZDR

### CONTRIBUTING ORGANISATIONS

Center for Advanced Systems  
Understanding, University of  
Delaware, Oak Ridge National Laboratory

### KEYWORDS

GPU CPU Particle-in-Cell  
Simulation

### RESEARCH FIELD

Matter

### SCIENTIFIC COMMUNITY

Matter / Photon Science

### FUNDING

HZDR, CASUS, ORNL CAAR project

### PROGRAMMING LANGUAGES

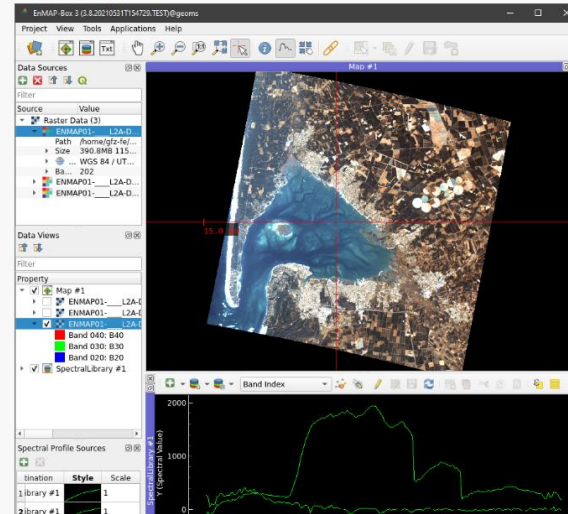
C++

### LICENSE

GPL-3.0-onlv

## ENPT - ENMAP PROCESSING TOOL

The Environmental Mapping and Analysis Program (EnMAP) is a German hyperspectral satellite mission that aims at monitoring and characterising the Earth's environment on a global scale. The EnPT Python package is an automated pre-processing pipeline for the new EnMAP hyperspectral satellite data. It provides free and open-source features to transform EnMAP Level-1B data to Level-2A. The package has been developed at the German Research Centre for Geosciences Potsdam (GFZ) as an alternative to the processing chain of the EnMAP Ground Segment.



### CENTRES

GFZ, AWI, DLR

### KEYWORDS

Remote sensing Hyperspectral  
Satellite data EnMAP

### RESEARCH FIELD

Earth and Environment

### SCIENTIFIC COMMUNITY

Remote sensing

### FUNDING

German Federal Ministry of Economic  
Affairs and Energy (50 EE 0850)

### PROGRAMMING LANGUAGES

Python

### LICENSE

GPL-3.0-or-later

### CITE

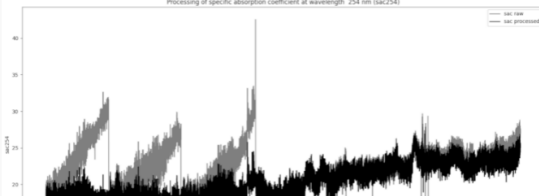
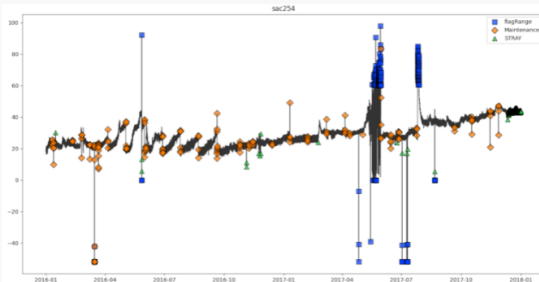
10.5281/zenodo.3742344

### CONTACT

## SAQC IN A NUTSHELL

Anomalies and errors are the rule, not the exception when working with time series data. This is especially true if such data originates from *in situ* measurements of environmental properties. Almost all applications, however, implicitly rely on data that complies with some definition of 'correct'.

In order to infer reliable data products and tools, there is no alternative to quality control. SaQC provides all the building blocks to comfortably bridge the gap between 'usually faulty' and 'expected to be corrected' in an accessible, consistent, objective and reproducible way.



### CENTRES

UFZ Leipzig

### KEYWORDS

- Time series
- Quality control
- Data analysis

### RESEARCH FIELD

Earth and Environment

### FUNDING

UFZ

### PROGRAMMING LANGUAGES

Python

### LICENSE

GPL v3

### COSTS

free

### CONTACT

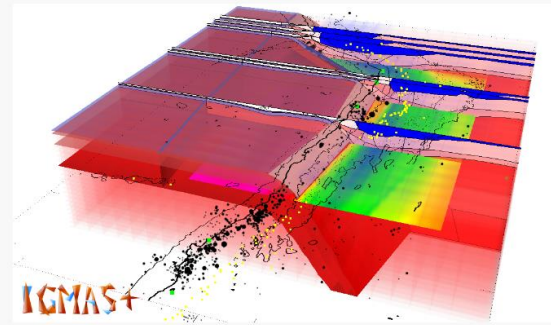
david.schaefer@ufz.de

### RESOURCES



## IGMAS+ IN A NUTSHELL

Modern geophysical interpretation requires an interdisciplinary approach and software capable of handling multiple inhomogeneous data like seismic, FTG gravity, magnetic and magnetotelluric in complex geological environments.



3D flat model of the central Western South American margin, modelled gravity, and modelling constraints.

IGMAS+ (Interactive Gravity and Magnetic Application System) is a geo-modelling software for three-dimensional joint inversion of potential fields and its derivatives under the condition of constraining data and independent information.

Three-dimensional gravity and magnetic modelling appreciably improves the results of distinct depth imaging projects. This regards especially to areas of strong lateral seismic velocity and density contrasts and corresponding imaging problems. Typical areas where grav/mag modelling has been successfully used are sub-salt and sub-basalt settings.

What makes IGMAS+ highly efficient and user-friendly is that it allows adjusting the geometries and

### CENTRES

GFZ Potsdam

### KEYWORDS

- Gravity
- Magnetic
- Modelling

### RESEARCH FIELD

Earth and Environment

### SCIENTIFIC COMMUNITY

Structural Modelling

### FUNDING

GFZ

### PROGRAMMING LANGUAGES

Java

### LICENSE

Proprietary

### COSTS

Free

### CITE

10.1190/1.1442546

- The **Helmholtz Platform HIFIS** supports the entire software life-cycle in order to increase quality, sustainability and visibility. Consulting, in particular licensing consulting, is an integrated service.
- The **Helmholtz Software Forum** is a platform to exchange knowledge, present ideas & results and define policies, key indicators and incentives.
- With its partners Helmholtz is building up a **Research Software Directory** and selects best practice software projects representing success stories; top projects are highlighted and prominently featured via spotlights