HIFIS HELMHOLTZ FEDERATED IT SERVICES

HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

From License Consultation to Software Spotlights

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RDA DE 2022
Session: Reproduzierbare Wissenschaft – Forschungsdaten und Research Software im Zusammenspiel

24. Februar 2022
DOI:10.5281/zenodo.6248895

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

HIFIS - Helmholtz digital Services for Science

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

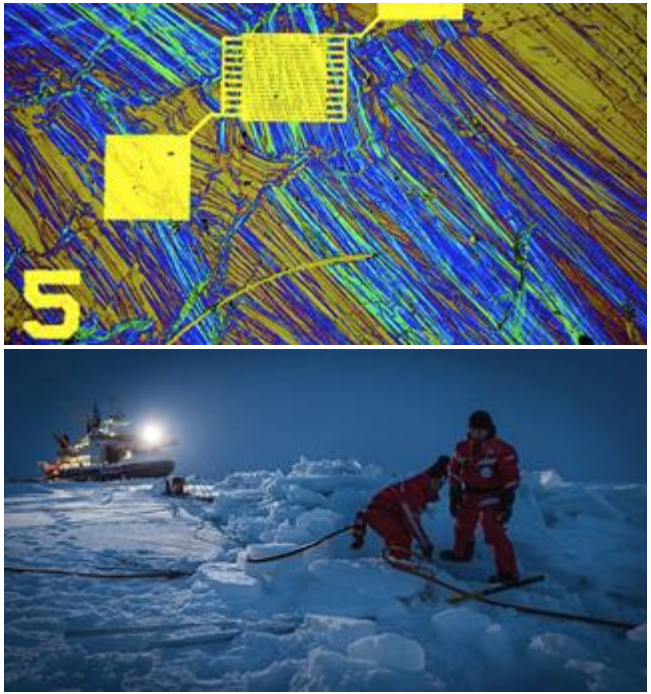
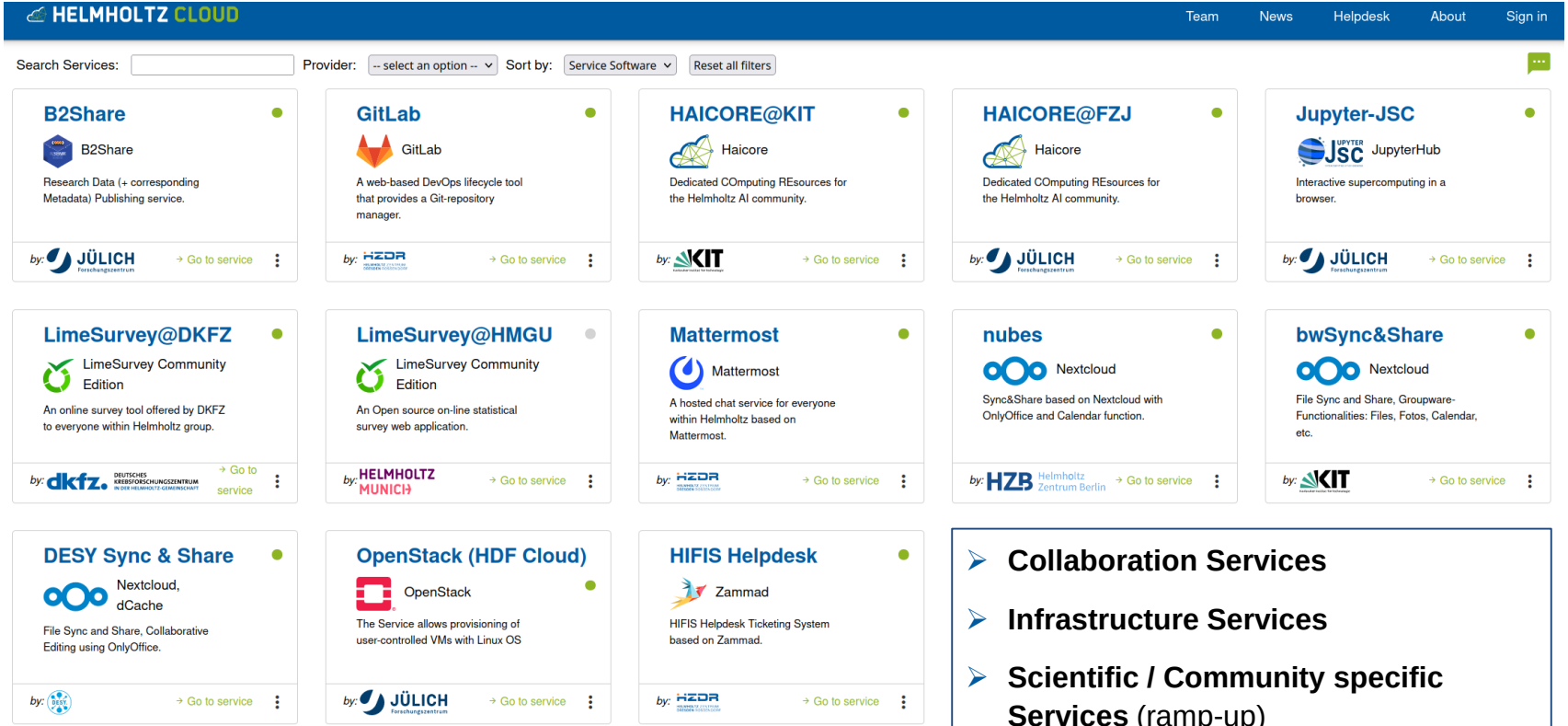


Bild 1: Organische Halbleiter-Polymere/ Himani Arora / HZDR
Bild 2: Mosaic Expedition / Stefan Hendricks / AWI

HIFIS Cloud Services + Portal



- **Collaboration Services**
- **Infrastructure Services**
- **Scientific / Community specific Services** (ramp-up)

https://cloud.helmholtz.de

Services for the Research Software Lifecycle

HIFIS

Consulting

Research Software Directory

Zammad

Community Services

Development Infrastructure

INVENIO

GitLab

Mattermost

THE CARPENTRIES

Education & Training

Research reproducibility and research software

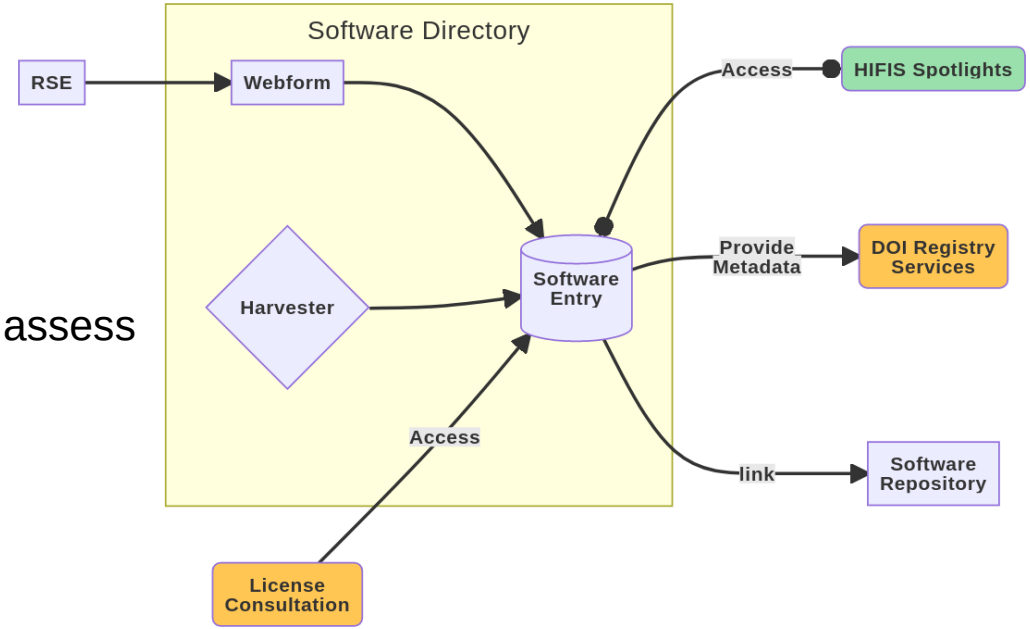
- Research software is a fundamental part of reproducibility
- Software is often times cited badly or not at all
- Software developed by scientists is rarely published
- FAIR principles implemented?

Goal

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

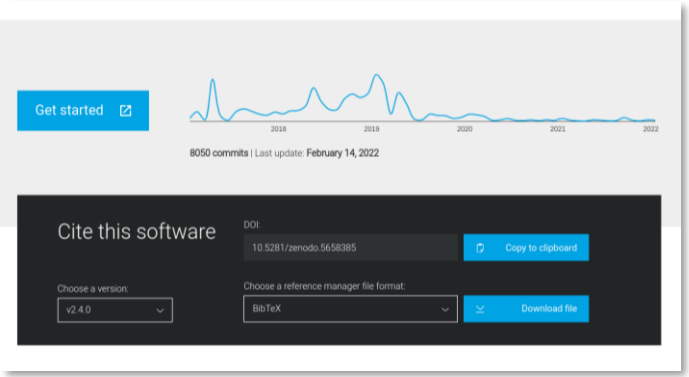
Increasing the visibility of research software

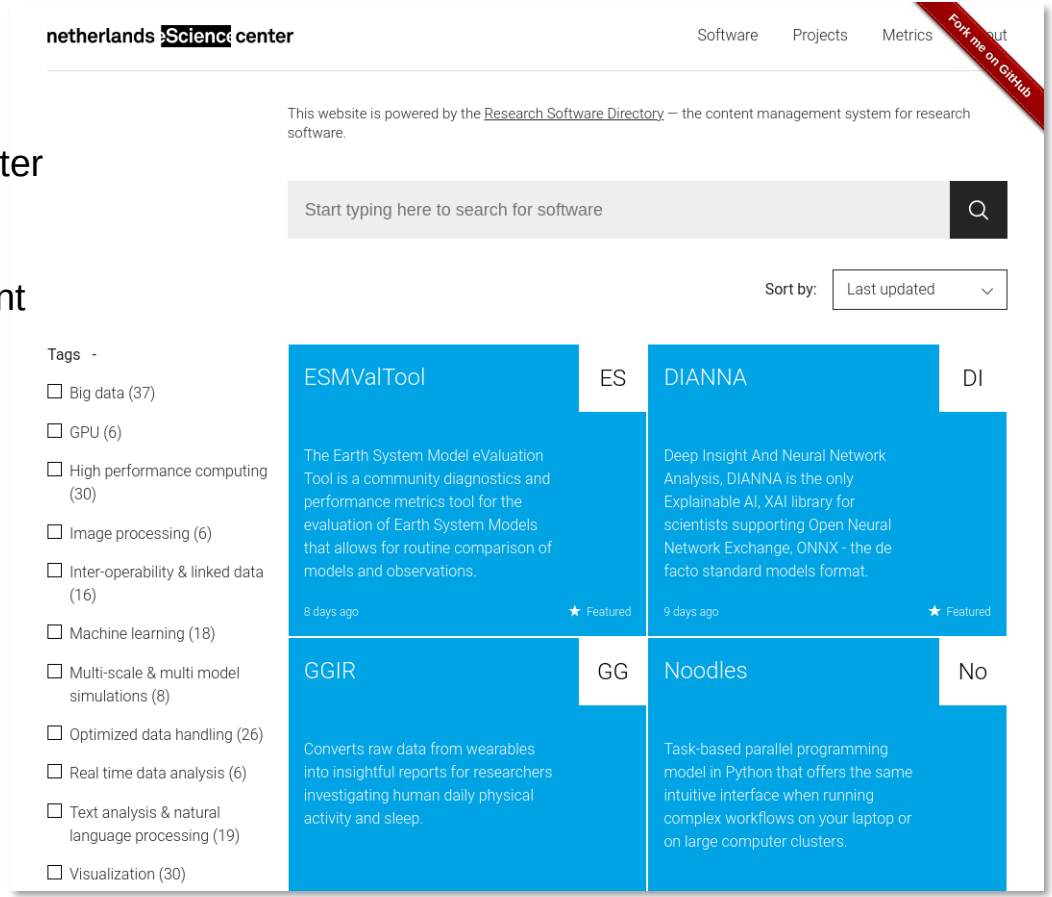
- Create a process around a software directory
- Goal: every software developed at a research center will be added to the directory
- Allow access for other services, e.g.
  - License consultation
  - DOI registry services
- Automatically collected metrics help to assess software impact



Research Software Directory

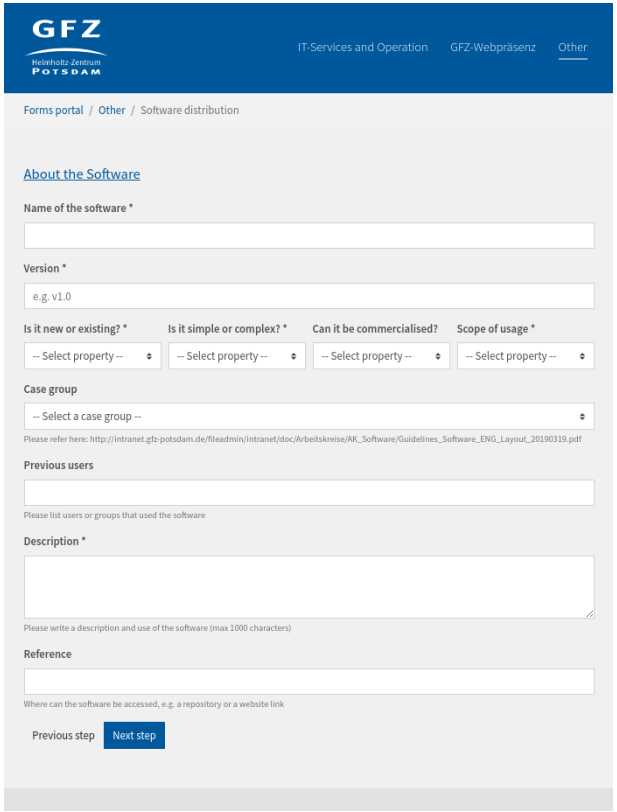
- Build on top of open-source project **Research Software Directory**
- Developed at Netherlands eScience Center
- Features
  - Harvesting information
  - Visual representation of development activity
  - Citation support
- Currently setting up collaboration

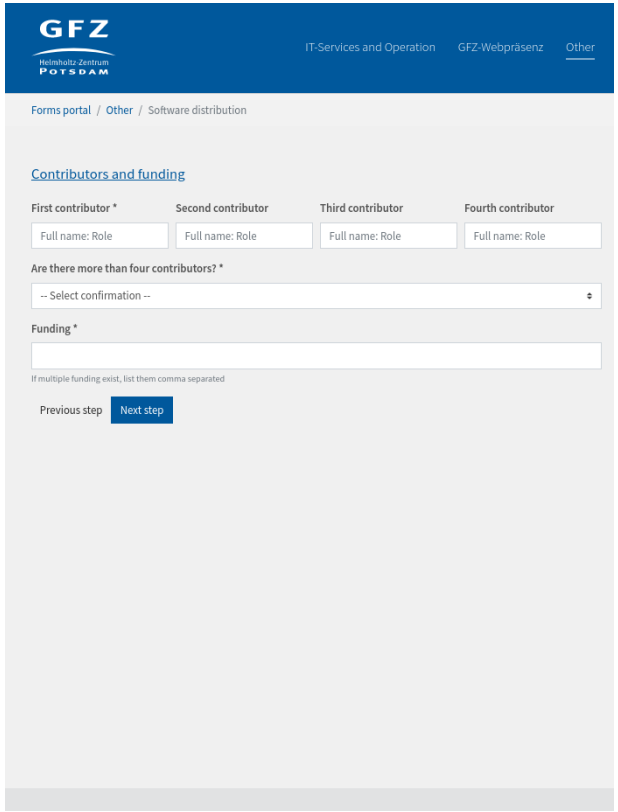


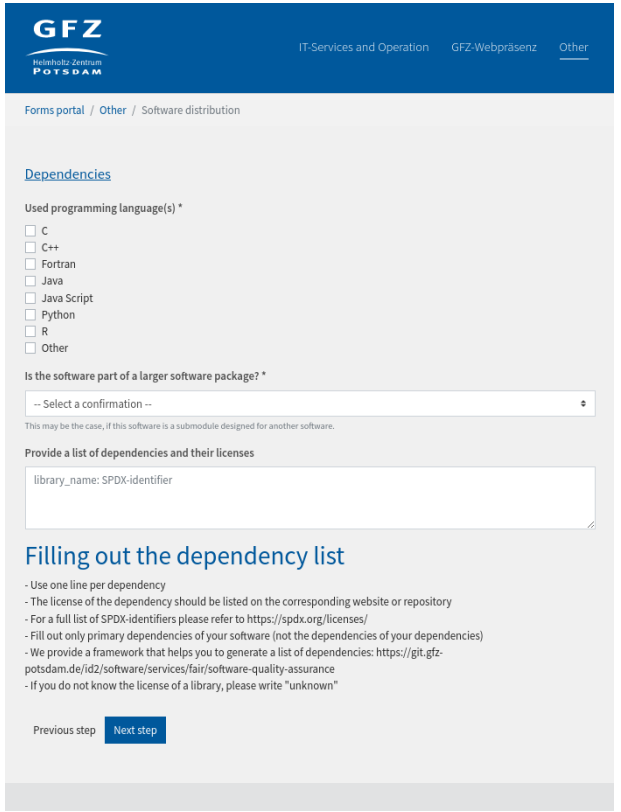


research-software.nl

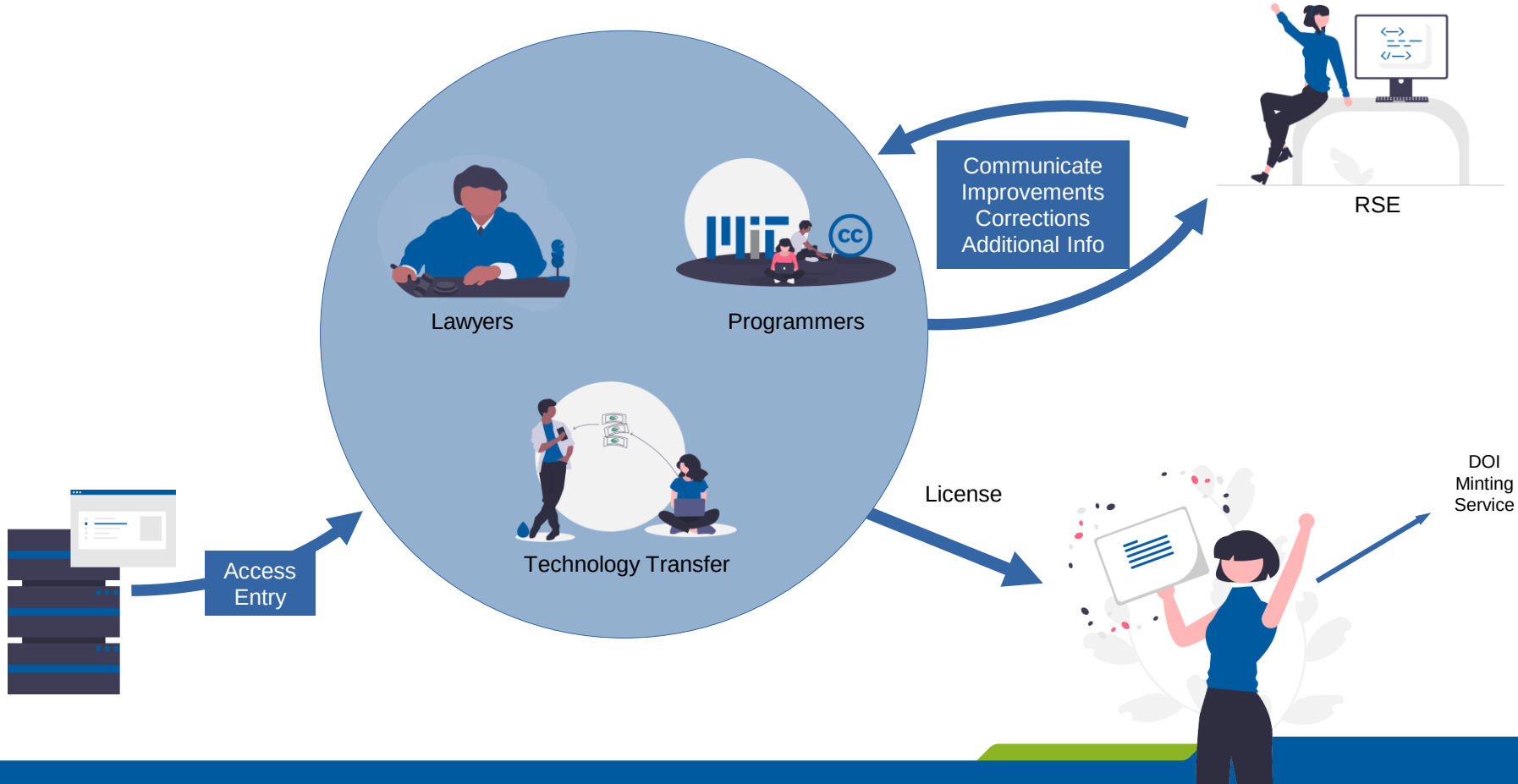
Adding software to the RSD using a web form



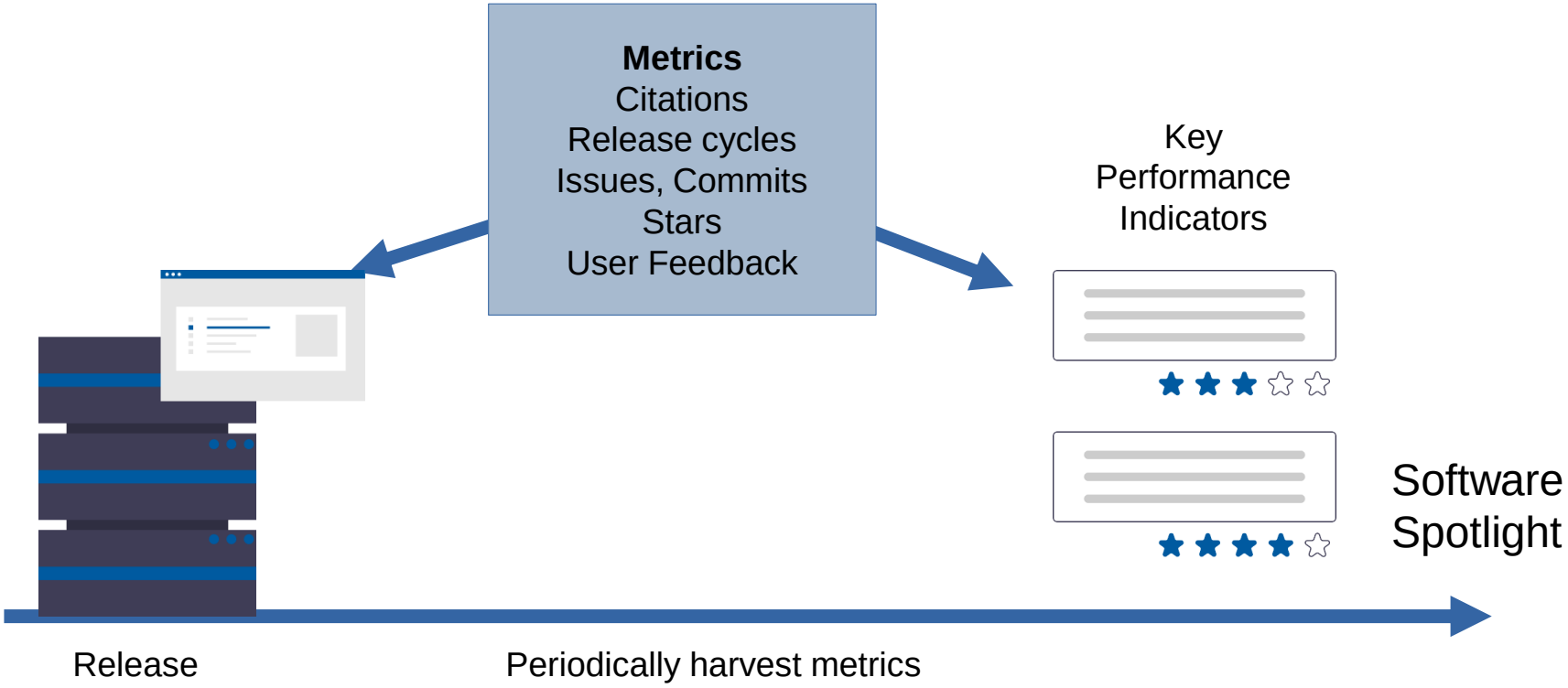




License consultation process



Becoming a Software Spotlight



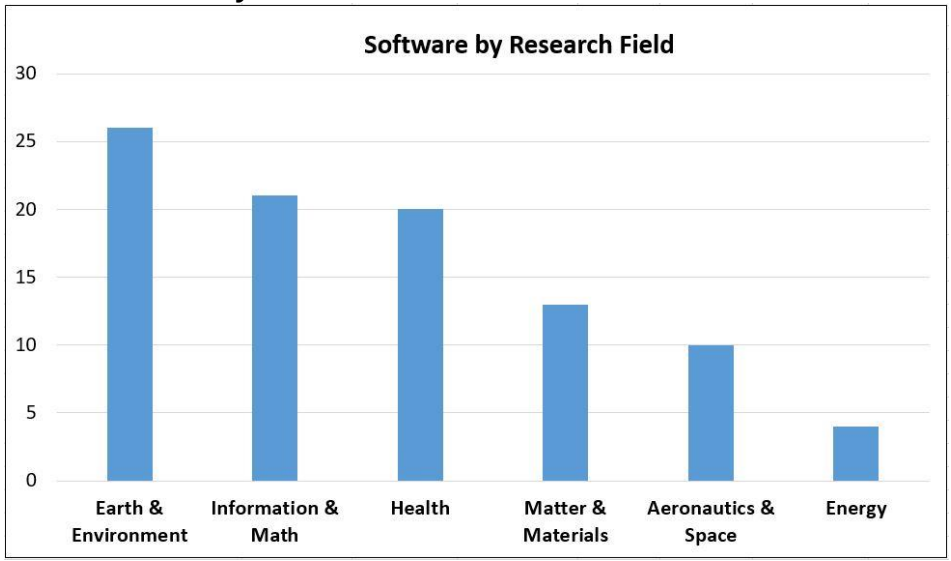
HIFIS Software Spotlights 2021

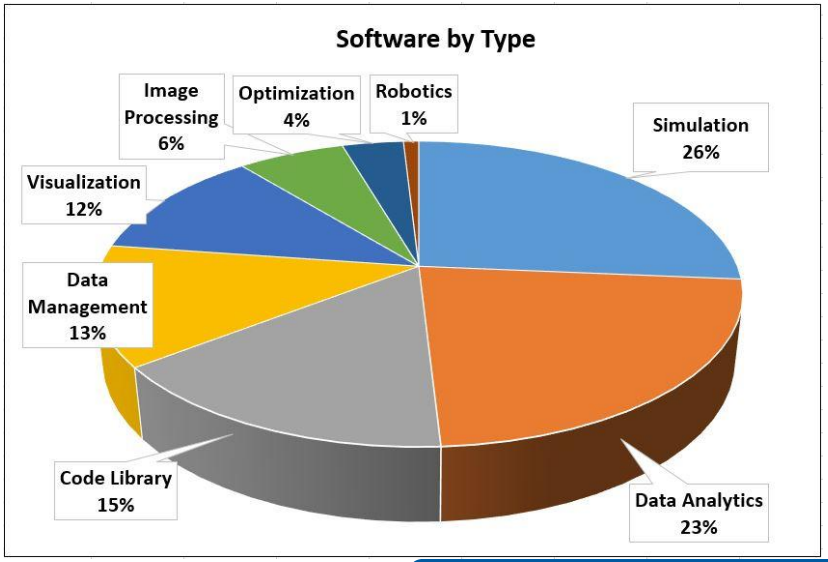
Initiative of the Helmholtz Software Forum:

- 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



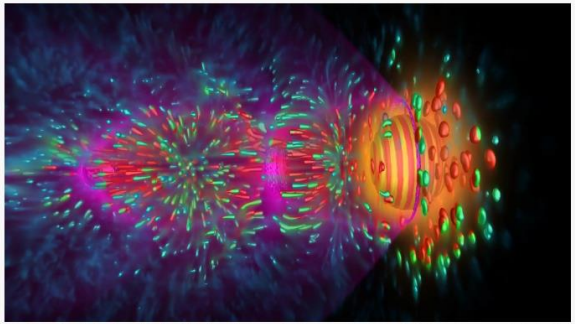


HIFIS Software Spotlights

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, PIConGPU 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 PIConGPU 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 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

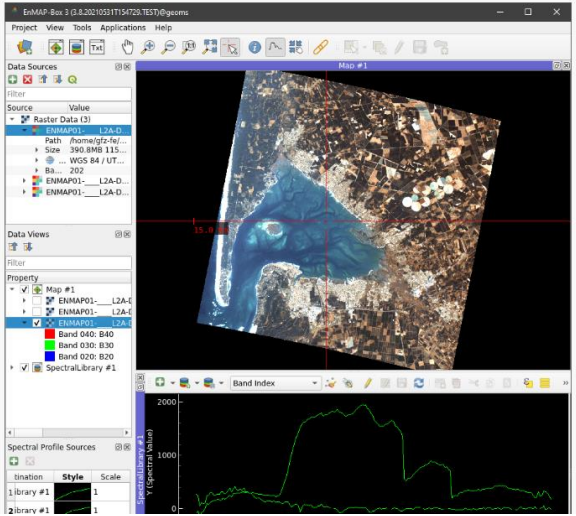
C++

LICENSE

GPL-3.0-only

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

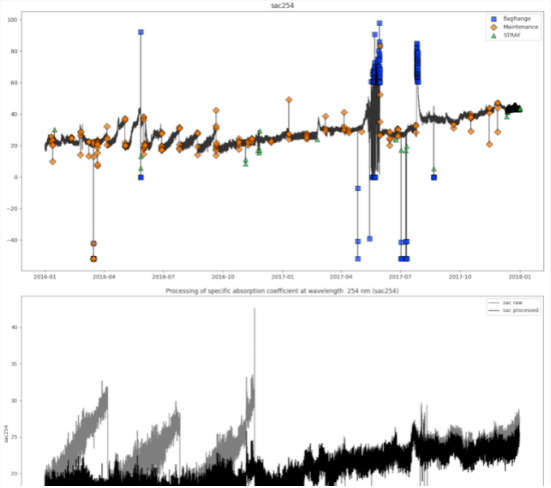
hifis.net/spotlights

HIFIS Software Spotlights

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
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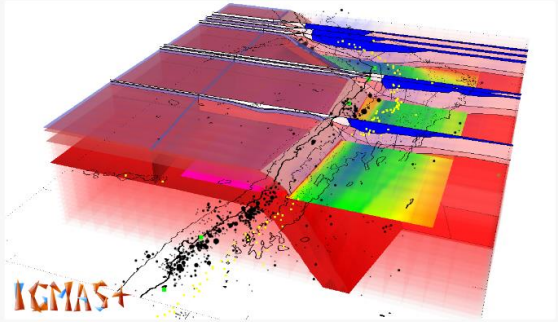
RESOURCES

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 constraings.

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

Take home messages

- 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