HELMHOLTZ

RESEARCH FOR
GRAND CHALLENGES


# Research Software Development @ Helmholtz

Dr. Uwe Konrad, Helmholtz-Zentrum Dresden-Rossendorf
and the HIFIS Team

# What was our vision in 2018?

Provide services to users in Helmholtz & Partners

## I. Helmholtz Cloud & Backbone Services

- Provide high performance **collaboration and community services**
- **Connect all centres** and their world-wide collaboration partners!

## II. Establish **best-practices** for **Research Software Engineering**:

- High level of knowledge, quality, visibility and sustainability
- State-of the-art SW development infrastructures

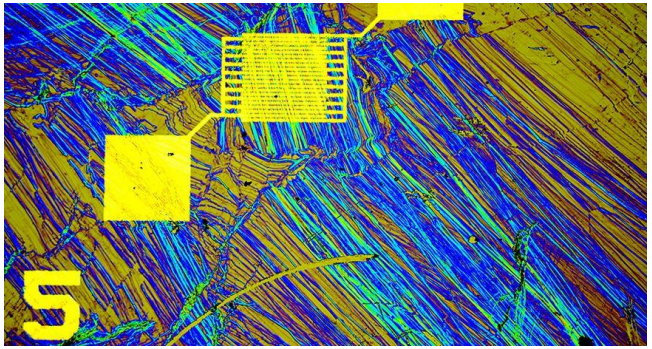
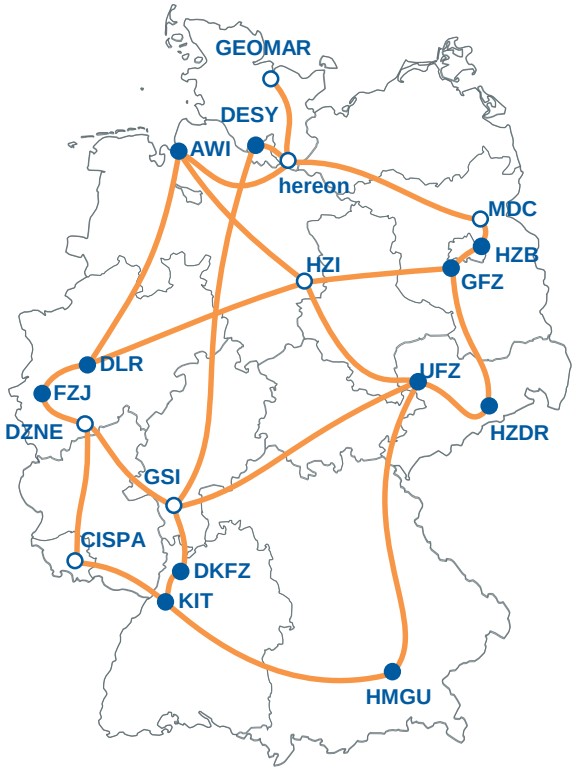


Bild 1: Strukturen aus organischen Halbleiter-Polymeren/ Himani Arora/HZDR
Bild 2: Mosaic Expedition/Stefan Hendricks/AWI

# Who is HIFIS?

- **Team: 11 (out of 18) Helmholtz centres**
- Main Coordination: DESY
- Three Clusters:
  - **Backbone Cluster** (head: DESY)
    Core Services for Authentication, Authorisation, Large Data Transfer, etc.
  - **Cloud Cluster** (head: HZB)
    Helmholtz Cloud Platform
  - **Software Cluster** (head: HZDR)
    Platform, Training, Support for high quality, sustainable Research Software Engineering




- https://hifis.net/team

# Helmholtz Digital Services for Science - Collaboration made easy

**HIFIS has become major provider for science-oriented digital services**

- **All Helmholtz Centres**, all research fields and external **Partners use the Services**.
- Research **Communities offer own Services** on the HIFIS platform.
- **Blueprint** e.g. for **NFDI**. Several Consortia already use HIFIS services.

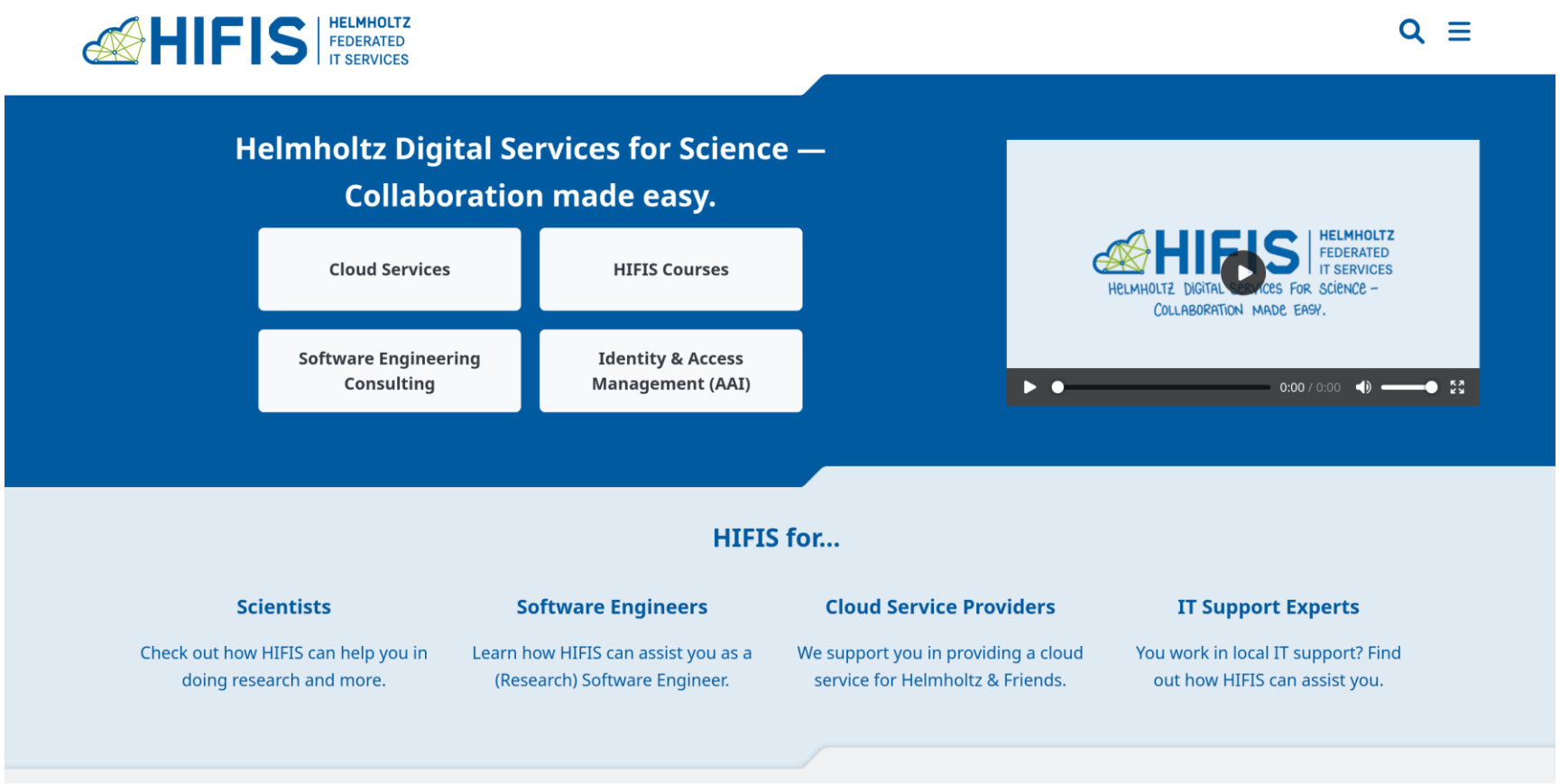
**Helmholtz AAI and Helmholtz Cloud Services**

- AAI enables **group management** and access to **common cloud services** through credentials of the **home institution**. Compatible with int'l standards.
- >20 **collaborative**, **infrastructure** and **scientific cloud services** onboarded and in use by thousands of Helmholtz plus external users.

**Training, Consulting and Community Building for Software Engineers,**

- Widely used throughout Helmholtz: >1.000 requests for **Training**
- Central contact point for **RSE Consulting** with lots of consultations performed in 2021.

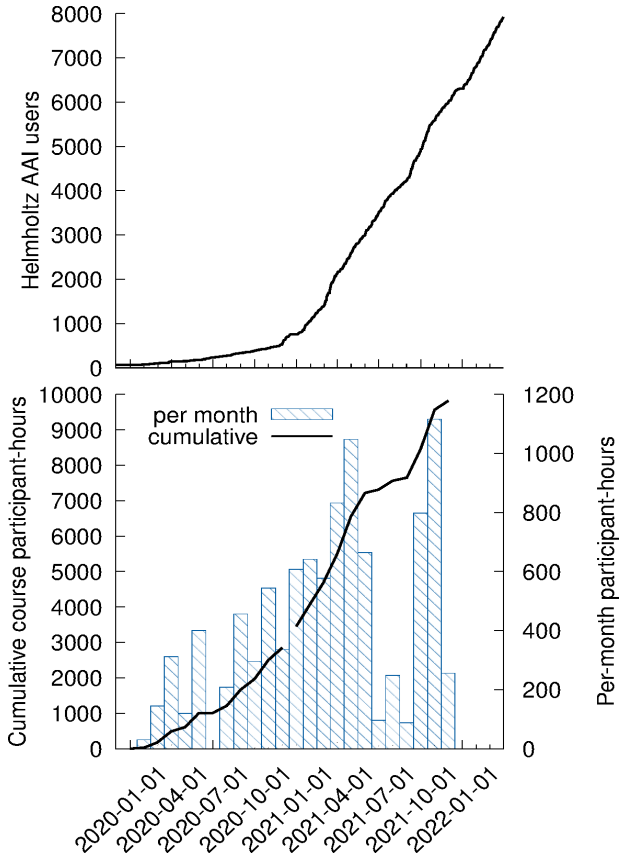
# HIFIS Services in a nutshell



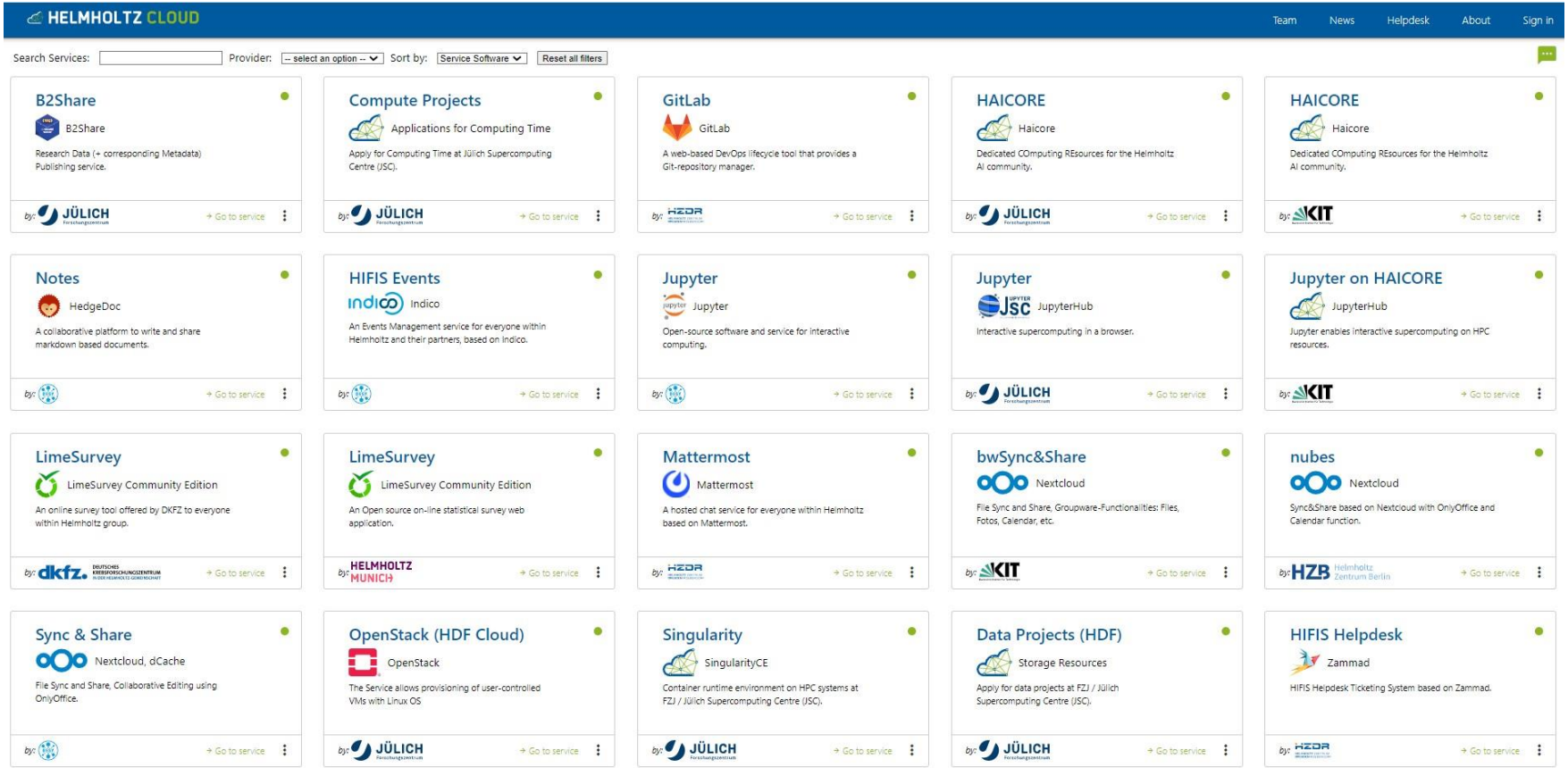

- https://hifis.net

# HIFIS — Fact Check

- More than **7.500 Helmholtz AAI / Cloud (pilot) users**, increase by factor ~8 (to 2020), including ~1.500 externals.
- **22 Helmholtz Cloud Services** of 7 Helmholtz Providers, offered via the new ➢helmholtz.cloud Portal.
- **38 Training Courses** and **Events** organised, ~800 attendees (demand: ~1.100). Increase by factor ~2.5.
- **HIFIS Support** processed **~500 tickets**; **35 Consulting requests** completed, 86% with “excellent” ratings.
- **Research Software Spotlights**: nucleus to upcoming Research Software Catalogue with >100 Lighthouses.
- **All-Helmholtz Survey** conducted on IT services usage.
- All centres and research fields represented



# Cloud Services & Portal




- https://helmholtz.cloud/services

# Software Services - Overview

## Best-practices for sustainable Research Software Engineering on multiple levels:

### 1. Consulting

- **Contact points** for researchers for questions and problems in the context of RSE.

### 2. Technology

- Provide a sustainable, well integrated and easy to use **technology infrastructure** for research software development.

### 3. Education & Training

- **Courses, material** and **workshops** for getting you started or boosting your software engineering practice.

### 4. Community

- Build and foster communities to support the necessary **cultural change** when dealing with research software.

# Software Services @ Helmholtz

HIFIS Services for the **Research Software Lifecycle**:

**1. Consulting**

Research Software Directory

Zammad

GitLab

INVENIO


**4. Community Services**

**2. Development Infrastructure**

ANSIBLE

Mattermost

CI – CD Pipelines

indico

THE CARPENTRIES

**3. Education & Training**

# Software Services - Consulting

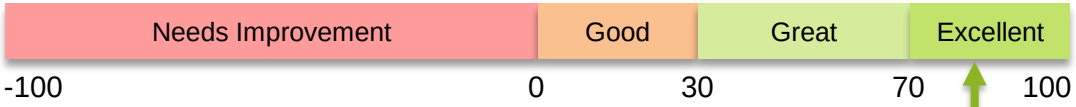
- Free-of-charge **software consulting** for research groups within the Helmholtz umbrella
- Possible topics include, but are not limited to **Licensing and Open Source**, setting up new projects, code migrations etc.

- **References** (Examples):
  - Making a project **HPC** ready
  - Setting up and introducing **Continuous Integration**
  - Frequent requests about **Licensing and Open Source**
  - **DevOps Development** using Ansible

Katerina Limpitsouni via undraw.co

# Software Services - Consulting

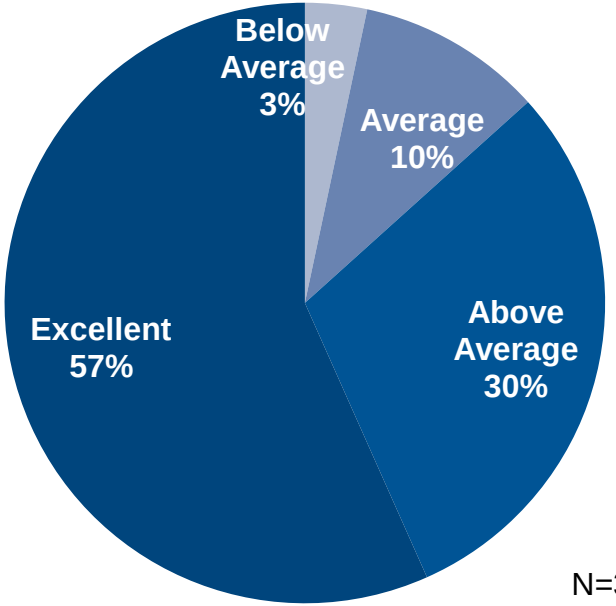
Net Promoter Score




80

*This was a great experience. Having worked at a Helmholtz institution for many years, it is a bit difficult for senior staff to understand that this is really a free and open service meant to support research groups in different fields. This is quite uncommon in "old Helmholtz" and it may take a while before HIFIS becomes widely known and accepted…*

Impact of the consultation on your project or work




N=30

# Software Services - Technology

*Provide a sustainable, well integrated and easy to use technology infrastructure for research software development.*

Transparency | Accessibility | Reliability | Reusability

- Everything we implement is shared as Open Source software
  - https://gitlab.com/hifis/ansible
- Infrastructure as code, Remove manual components, Transparently visible for Helmholtz employees
  - https://gitlab.hzdr.de/hifis-software-deployment/

# Software Services - Education & Training

**Basic**

- First Steps in Python-Programming
- Project Management with GitLab
- Version Control using Git

**Intermediate**

- GitLab for Software Development in Teams
- Let us Make Your Script Ready for Publication
- OOP Programming with Python (available in 2022)
- Continuous Integration (CI) using GitLab CI (available in 2022)

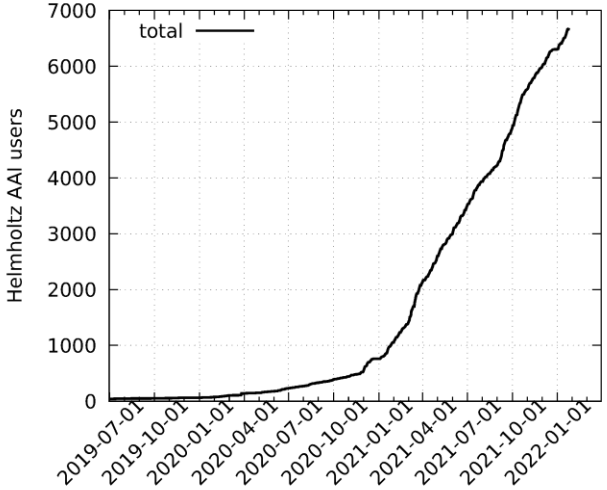
**Advanced**

- Using Containers in Science
- Test Automation with Python

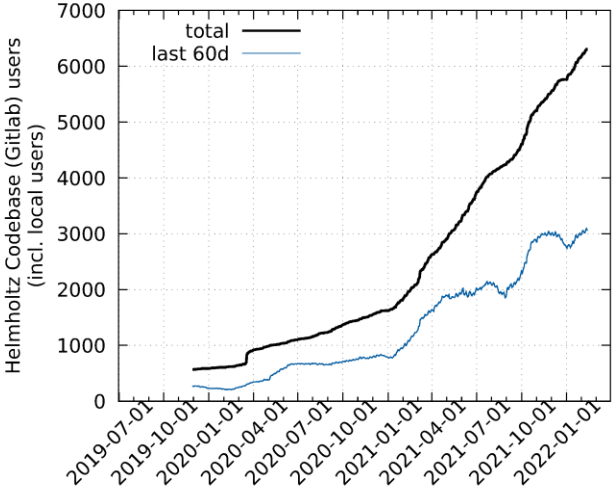
➢ https://hifis.net/events

# Usage of the Services

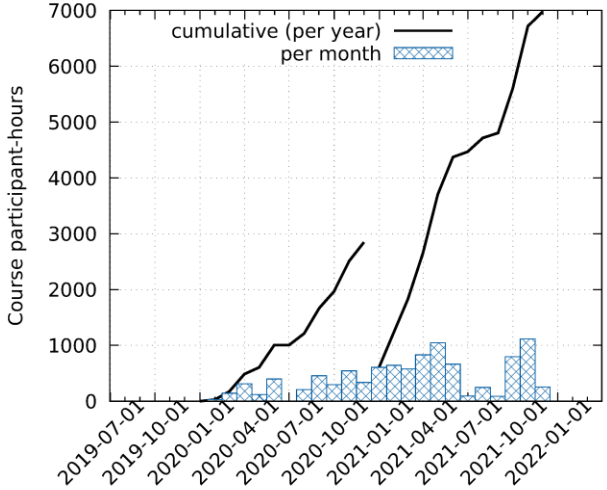
## Development of selected KPI (07.2019 – 01.2022)




AAI & Cloud Services

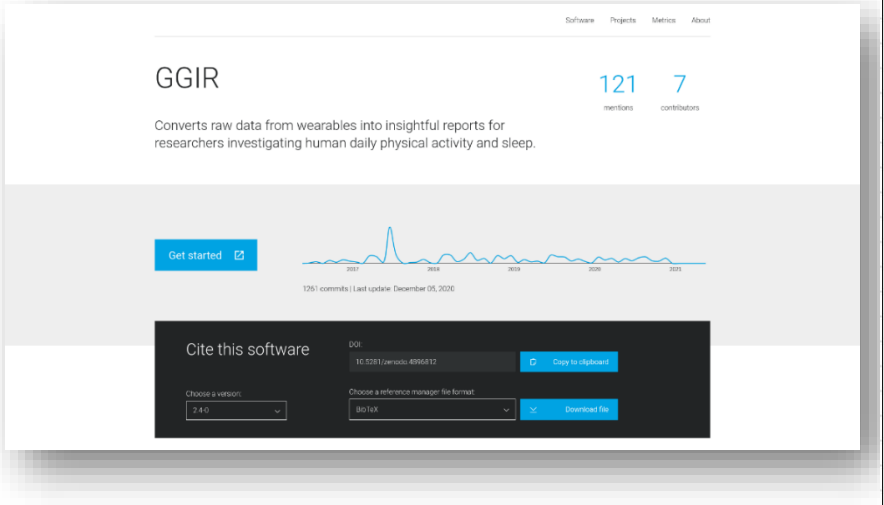


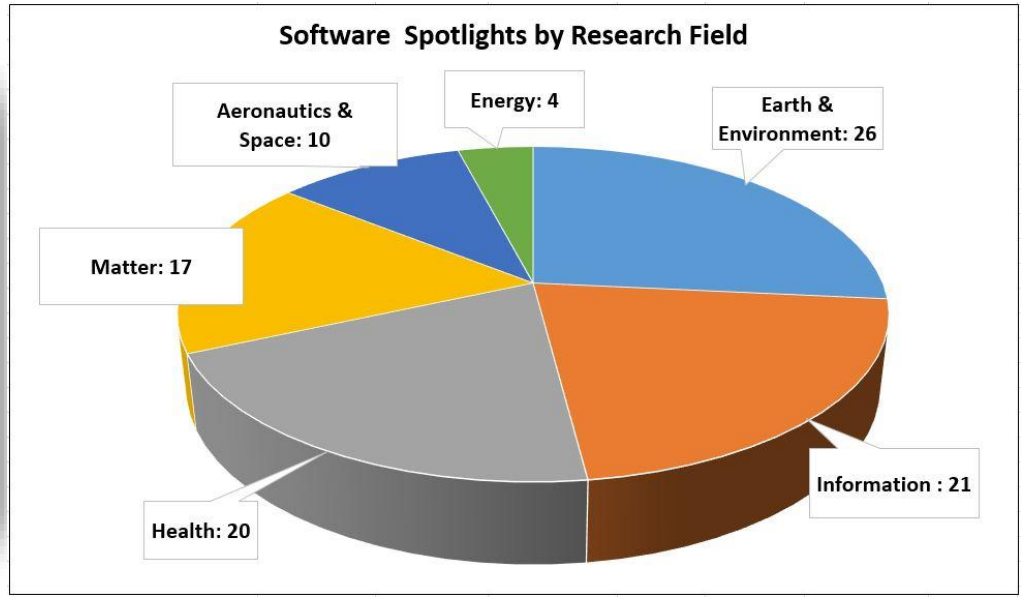

Gitlab @HZDR




Course participant hours

# Software Services - Community




- Development of a **Research Software Directory** for Helmholtz
- Built on top of and in cooperation with the Netherlands eScience center solution

- Present & Promote top success stories of Research Software Engineering in Helmholtz
- > **100 Proposals** so far, being presented in: hifis.net/spotlights

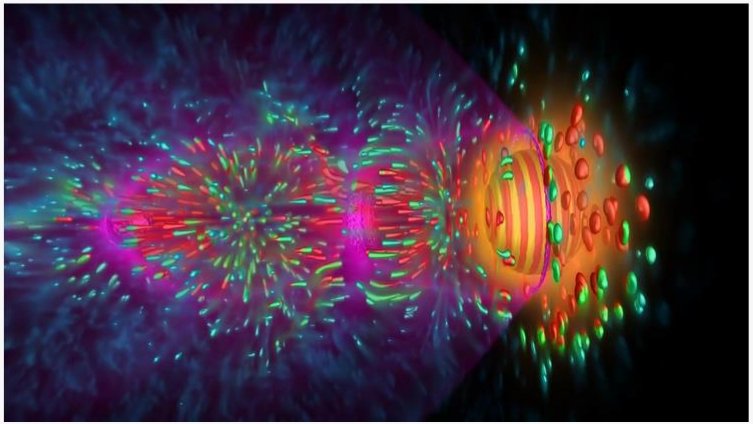
# Software Services - Community

◀◀ Back to Software Spotlights Overview ◀◀

## 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.



**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**

- https://hifis.net/spotlights/picongpu

- **Promote** Success Stories and Best Practices using Spotlights
- **Find** Stories, Metadata, Videos, Libraries used, Licenses and …
- **Connect** Communities and Experts
- **Get Visibility** of the Top Management

- https://hifis.net/spotlights/picongpu

# HIFIS Services – Use Cases


The HIFIS Transfer Service (HTS) has been implemented and is in use. Colleagues from HZDR and DESY were among the first to use HTS for the transfer and sharing of Datasets in the context of HelmholtzAI.


The Helmholtz AAI supports PUNCH4NFDI by providing AAI components. This offers a working solution on a strongly connected AAI, which follows already the recommendations and guidelines for participating in the EOSC.


The Earth and Environment DataHub was one of the first project groups to use nubes as a sync+share service of the Helmholtz Cloud. Since then, the number of user groups has been growing steadily.


The German Center for Infection Research (DZIF) builds a platform collecting methodologies and results of coronavirus antibody studies. In cooperation with HIFIS and led by scientists at the Helmholtz Centre for Infection Research (HZI), the project

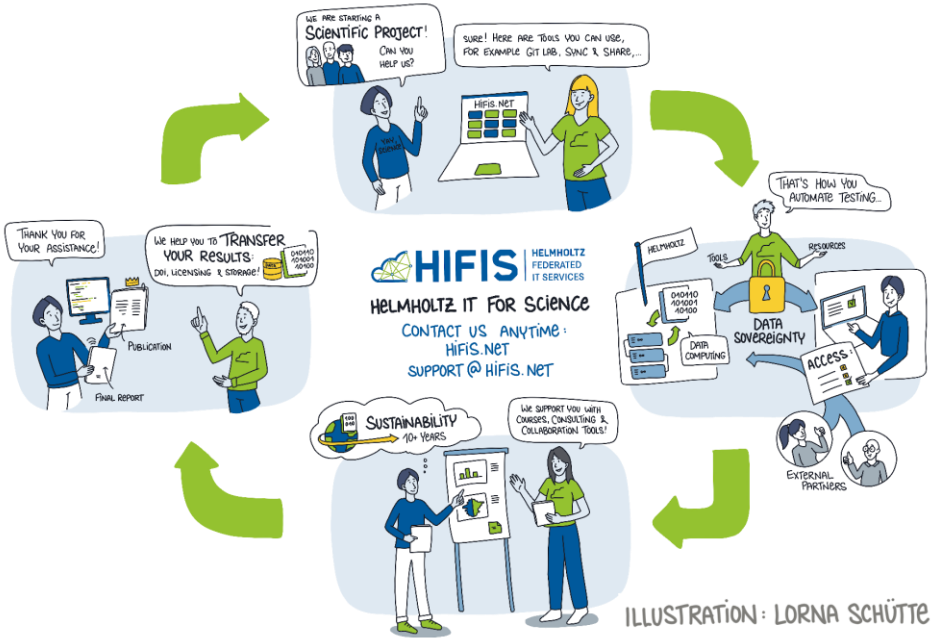

The Helmholtz platform HIFIS, the HZDR and the Center for Advanced Systems Understanding (CASUS) support the world-wide project Folding@Home in developing an antibody based therapy to prevent a respiratory infection by the virus.

- https://www.hifis.net/usecases

## Consult us:

- https://hifis.net
- support@hifis.net
- Resonator Podcast

# THANK YOU!
# QUESTIONS?




Podcast

Poster