BETTER SOFTWARE BETTER RESEARCH

```python
import heat as ht                    # HeAT for distribu
import opencarp as oc                # Hypothetical Oper

# Initialize tissue domain (e.g., 1000 cardiac cells)
num_cells = 1000
domain = ht.zeros(num_cells, split=0)  # distributed over

# Set up initial membrane potential (e.g., -85 mV)
Vm = ht.full((num_cells,), -85.0, split=0)

# Load a simplified OpenCARP cell model (e.g., ten Tussch
model = oc.models.TenTusscher()

# Time stepping loop (simplified)
dt = 0.01  # ms
for t in range(1000):  # simulate 10 ms
    I_ion = ht.array([model.compute_ionic_current(v) for
    Vm += dt * (-I_ion)  # Update Vm based on ionic curre

# Output final Vm
if ht.comm.rank == 0:
    print("Final Vm snapshot:", Vm[:10])
```

2nd Workshop on Research Software Engineering (RSE) @ KIT

René Caspart

LP9.1.4 Research Software: Work Package 1: Identification of Services and Offers for Research Software at KIT

In diesem AP sollen die für die Entwicklung, Veröffentlichung und Pflege von Forschungssoftware wichtigen und nötigen Dienste und Unterstützungsangebote identifiziert werden.

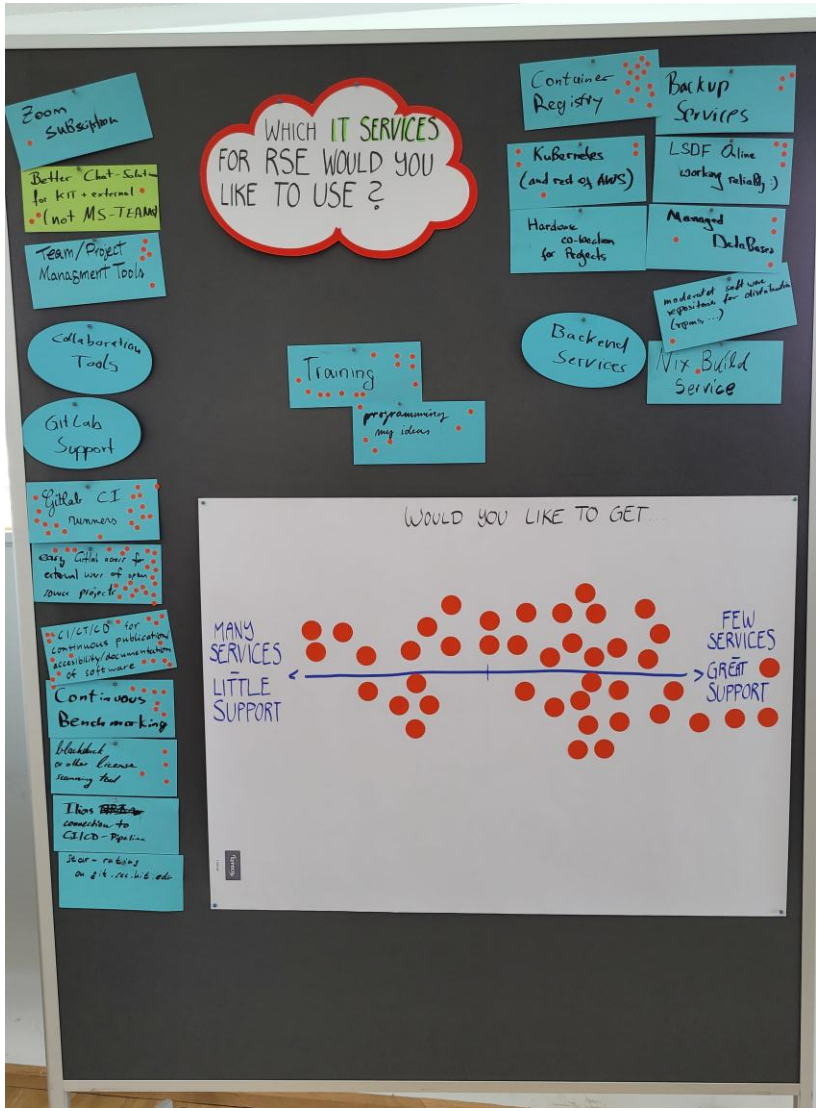
The aim of this WP is to identify services and support offerings that are important and necessary for the development, publication and maintenance of high quality research software.

Outstanding Research Software requires access to excellent services and support.

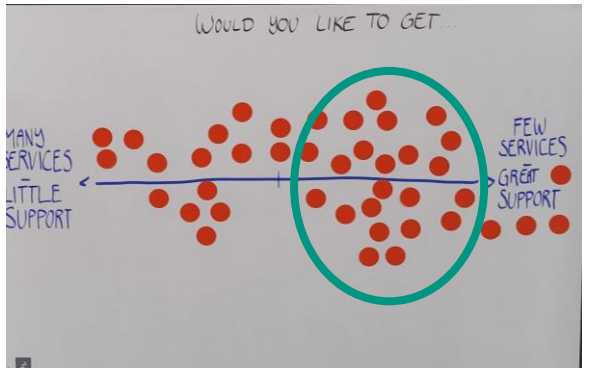
Looking back at the 1st Workshop on RSE at KIT

- 1st Workshop on RSE at KIT
  - Key part: World-Café style boards to identify baseline and direction forward

- For services and offers two key findings
  - Already some services offered for KIT researchers (not just from KIT)
  - Visibility can be improved
  - And especially training and support can be improved
  - In general: few, selected lighthouse services with outstanding support



GitLab at KIT



- GitLab is a full central service at KIT
  - Operated by SCC
  - Over 12.000 users, 26.000 projects and 5000 groups
- Features
  - Login via Federated Login Service (FeLS) incl. access for externals
  - Integration in full operational mode (e.g., including deprovisioning)
  - Scalable/redundant backend architecture
  - Information on the service and link to documentation https://www.scc.kit.edu/en/services/16888.php
- In preparation: bwGit – GitLab as a state level service

- GitLab Runner
  - In the KIT GitLab
    In 2025 up to 500 active Runners, 318.144 Piplelines run (till mid of May)
  - For HPC users (next slide)

Available runners overview

KGR1 runners

- **Platform:** Kubernetes
- **Timeout:** 1 hour

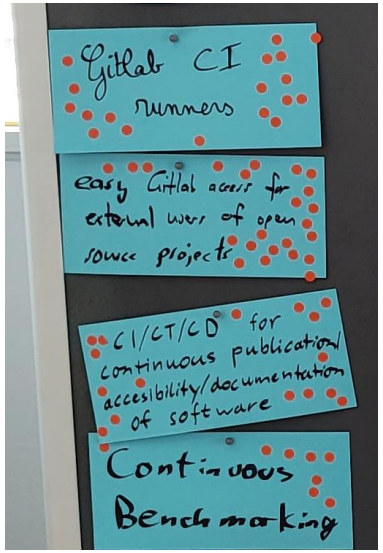
Name/tag	Concurrency	Cores	Memory	Disk
`kgr1-instance-mini`	20 (high)	0.5 - 0.5	1.6 - 2	4 - 13
`kgr1-instance-standard`	16 (high)	1 - 1	2.8 - 3.7	10 - 26
`kgr1-instance-experimental`	(medium)			
`kgr1-instance-extraordinary`	1 (low)	4 - 6	44 - 45	44 - 92

KGR2 runners

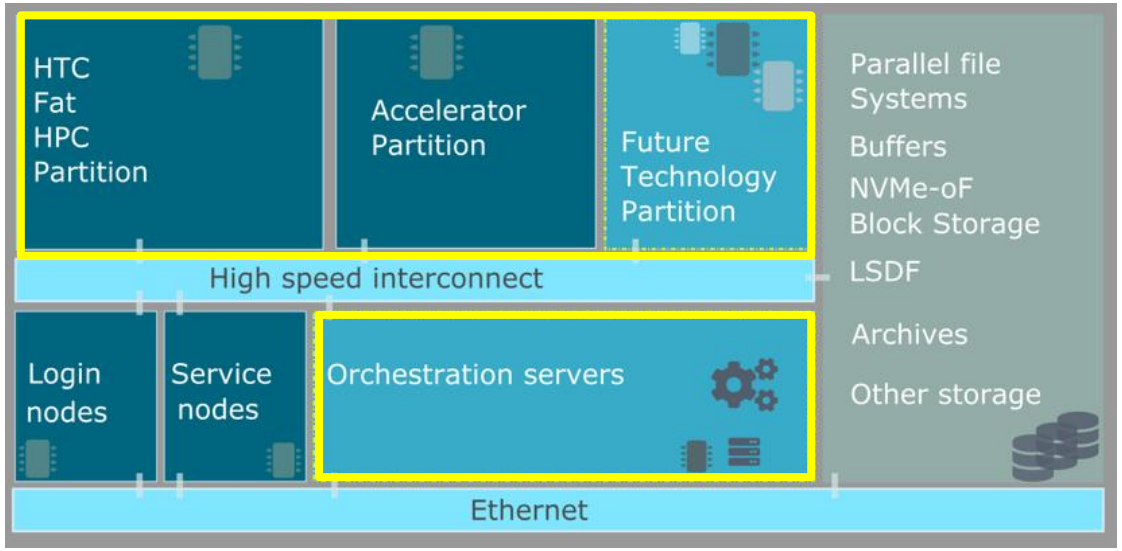
- **Platform:** Docker
- **Timeout:** 1 hour

Name/tag	Concurrency	Cores	Memory	Disk
`kgr2-instance-hugedisk`	1 (low)	1 - 2	8	128

Continuous X Services on HPC at KIT

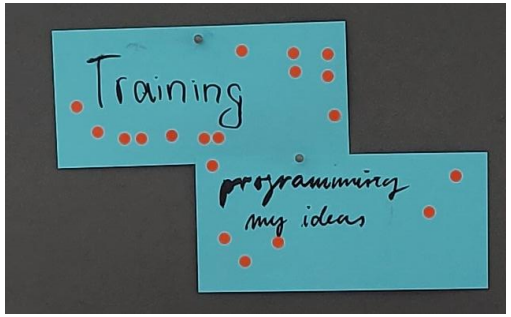


- Enabling Continuous Integration, Testing, Deployment and Benchmarking for software development on HPC
  - Available on bwUniCluster 3.0, HoreKa and Future Technology Partition:
    - For all users of these clusters
    - Wide range of computing platforms, including disruptive ones
  - Covering different usage models:
    - Limited resources with fast response time (e.g. CT)
    - up to large jobs with medium response time (e.g. CB)
- Easily integratable in any GitLab project (on KIT GitLab, Codebase, gitlab.com, …)
  - Steadily growing userbase
  - Support can be provided by the SSPE team



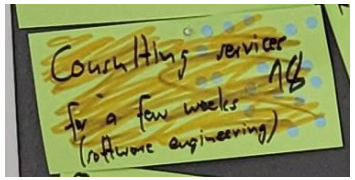
Details see https://www.nhr.kit.edu/userdocs/ci/

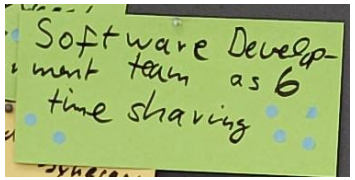
Support and Guidelines



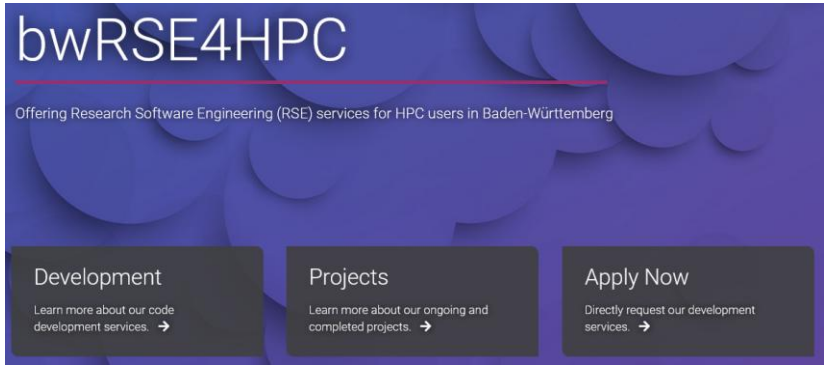
Two different approaches:

- Guidelines to support and help with certain aspects
  - E.g. guideline for choosing a suited open source license (more see later)
- Incorporating (open) research software in KIT guidelines for open science

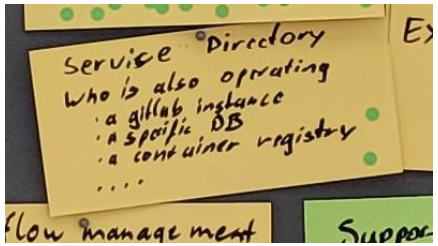




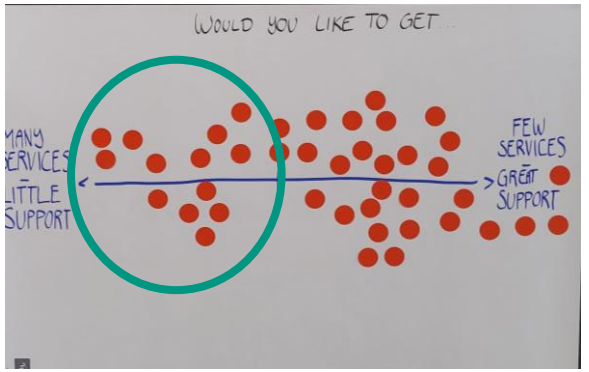
- Offering hands-on support and consulting for researchers in RSE aspects
  - Similar to “RSE for hire” but with a limited scope
  - As of now two offers at KIT (SCC)
    - Software Sustainability and Performance Engineering Team
    - The bwRSE4HPC project



Helmholtz Cloud

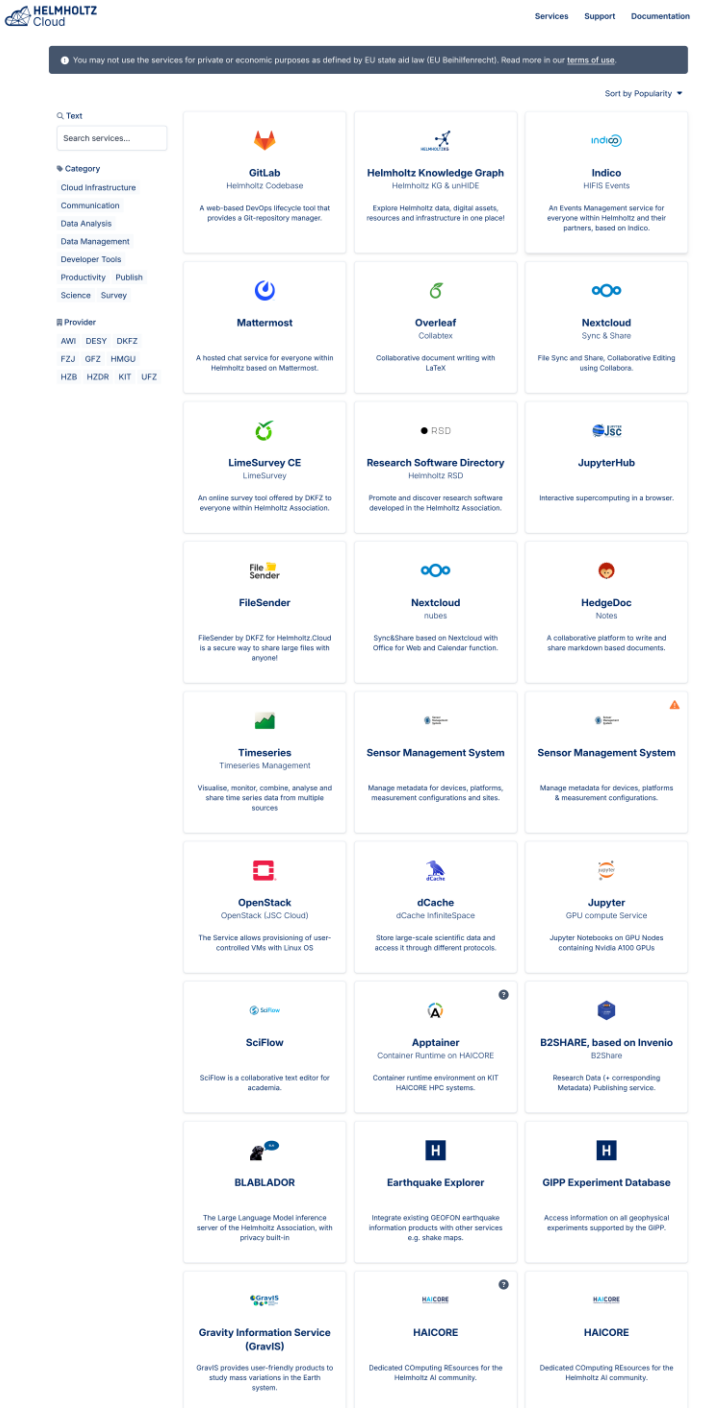


- Part of HIFIS (Helmholtz Federated IT Services)
  - Plethora of services offered by Helmholtz Centers for Helmholtz Members
  - Focusing not just RSE but also other
    - Admin
    - Compute
    - Fileshare (e.g. bwSync&Share)
    - …

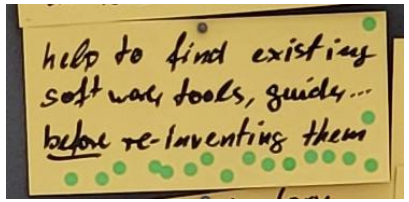


- Some example for services for RSE
  - Helmholtz Codebase (GitLab Instance)
  - Research Software Directory
  - Timeseries Databases
  - …

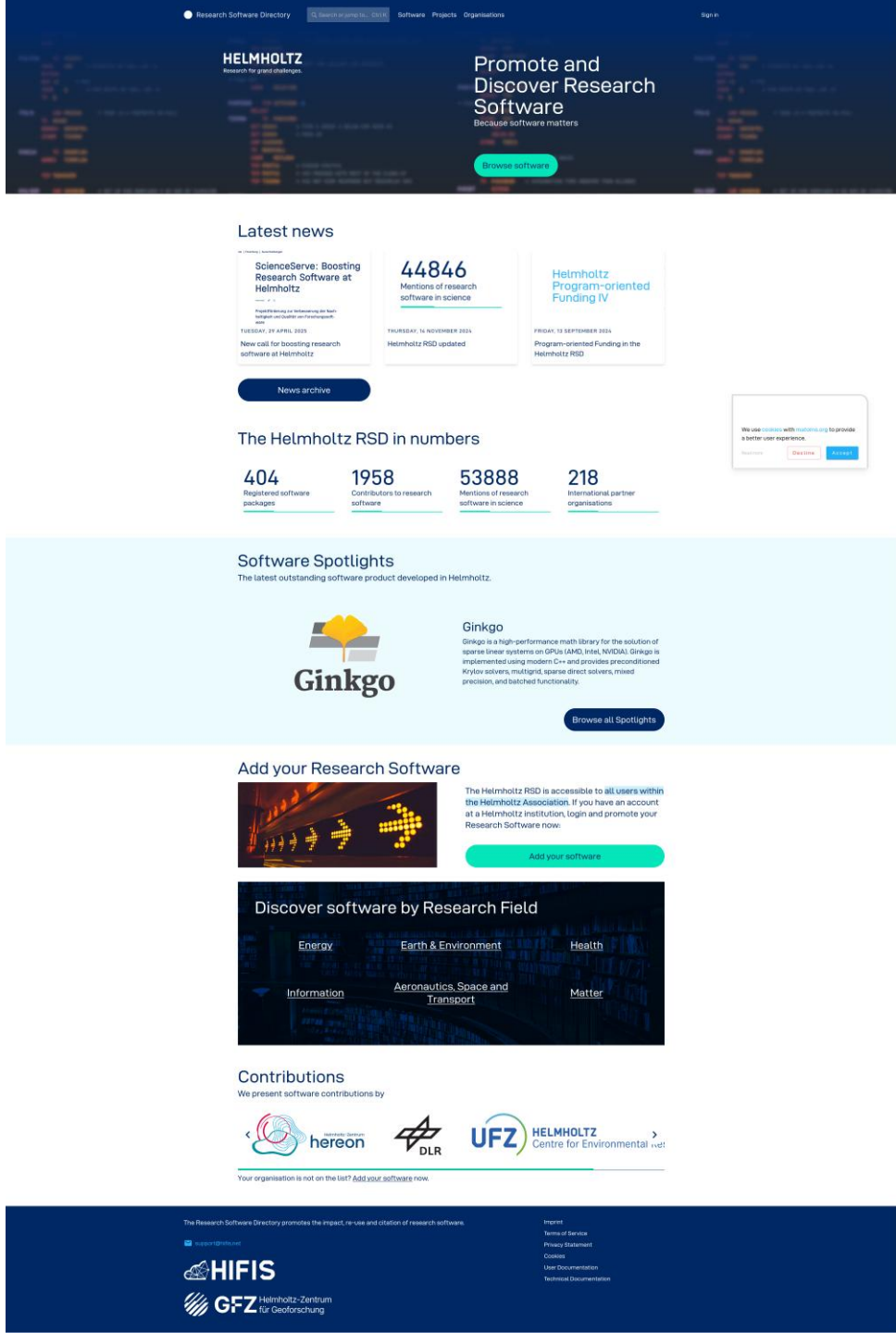
HIFIS
HELMHOLTZ DIGITAL SERVICES FOR SCIENCE – COLLABORATION MADE EASY.



Helmholtz Research Software Directory

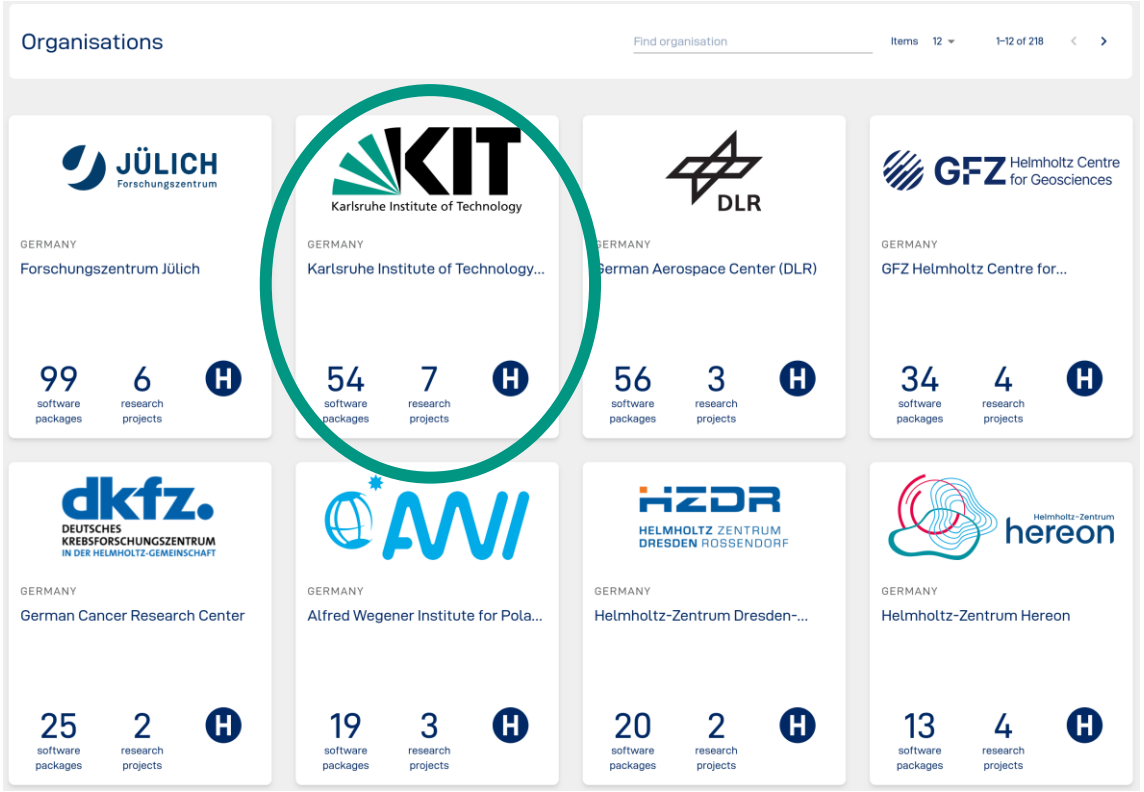


- Making your Software Visible
  - Central (Meta-)repository for research software in Helmholtz
  - Collects information like releases, citations, …
  - Forked from a project by the Netherlands eScience Center
  - Operated and further developed by a team at GFZ Potsdam
  - Over 400 software packages entered
- Entries are basis for e.g. the Helmholtz Software Award
- KIT has the third most software projects registered on the RSD
  - Anyone from KIT can add their software



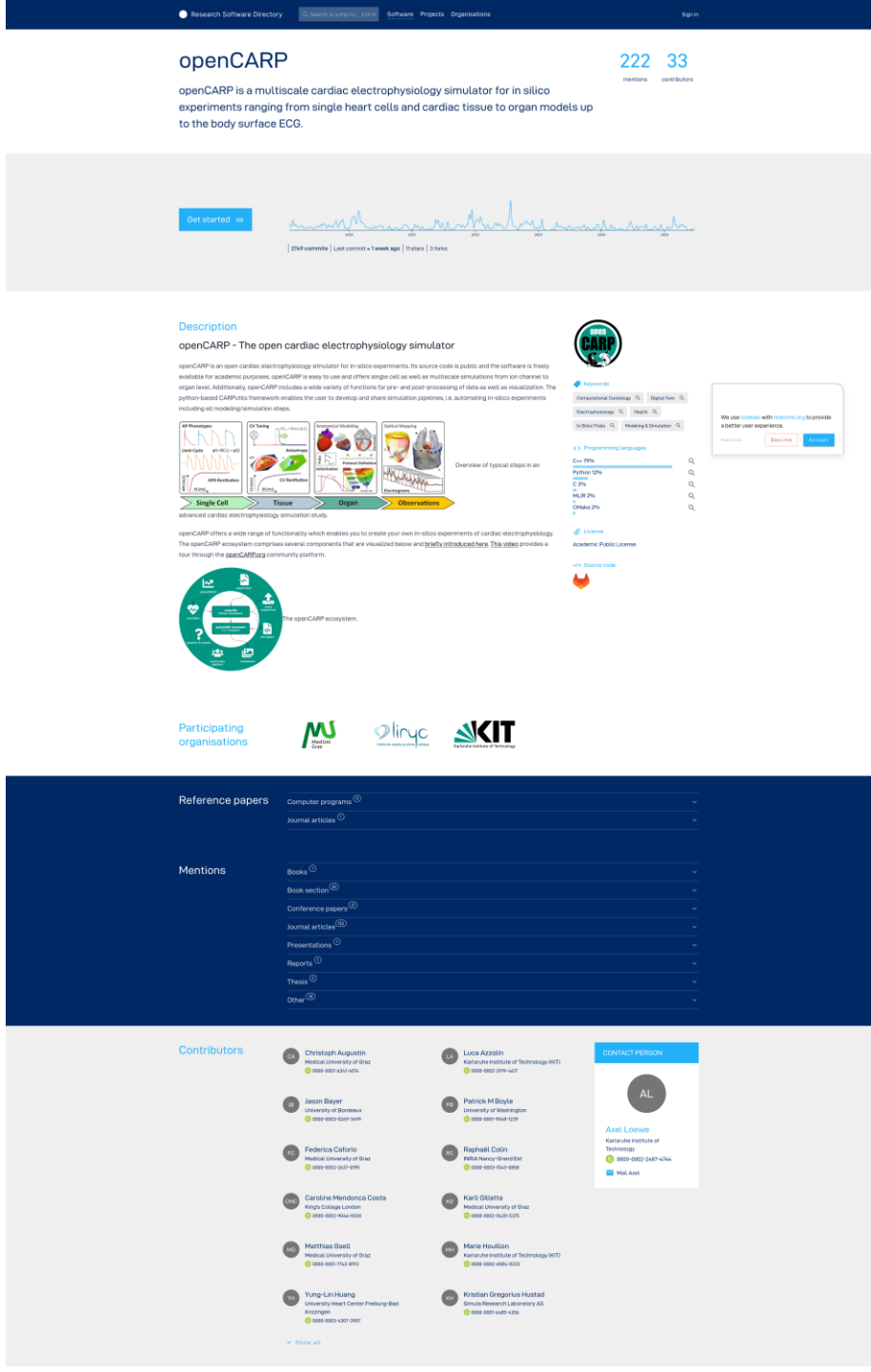
Helmholtz Research Software Directory

- Making your Software Visible
  - Central (Meta-)repository for research software in Helmholtz
  - Collects information like releases, citations, …
  - Forked from a project by the Netherlands eScience Center
  - Operated and further developed by a team at GFZ Potsdam
  - Over 400 software packages entered
- Entries are basis for e.g. the Helmholtz Software Award
- KIT has the third most software projects registered on the RSD
  - Anyone from KIT can add their software



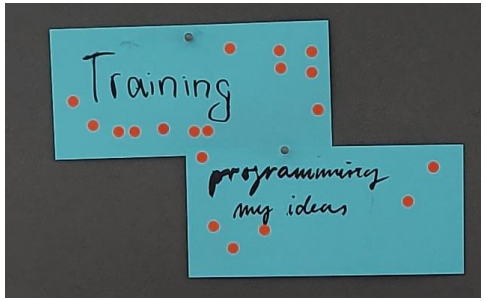
Helmholtz Research Software Directory

- Making your Software Visible
  - Central (Meta-)repository for research software in Helmholtz
  - Collects information like releases, citations, …
  - Forked from a project by the Netherlands eScience Center
  - Operated and further developed by a team at GFZ Potsdam
  - Over 400 software packages entered
- Entries are basis for e.g. the Helmholtz Software Award
- KIT has the third most software projects registered on the RSD
  - Anyone from KIT can add their software



Trainings

- Many different trainings around RSE already available for RSEs at KIT
  - Trainings at KIT, e.g. Software Carpentries jointly organized by SCC and IBT
  - Courses in the scope of HIFIS
  - And many more in the HIDA Course Catalog



software carpentry