



import heat as ht
import opencarp as oc

HeAT for distribu
 # Hypothetical Open

Initialize tissue domain (e.g., 200 corduac cell

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 current * (-I ion) # Update Vm based on ionic current * (-I ion) * (-I

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

<u>1st Workshop on RSE at KIT</u>

- 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



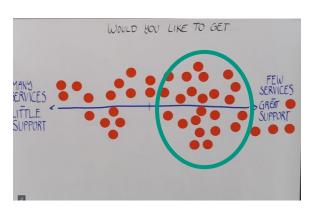


GitLab at KIT

- <u>GitLab</u> 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

GitLab

- Integration in full operational mode (e.g., including deprovisioning)
- Scalable/redundant backend architecture
- Information on the service and link to documentation <u>https://www.scc.kit.edu/en/services/16888.php</u>
- 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

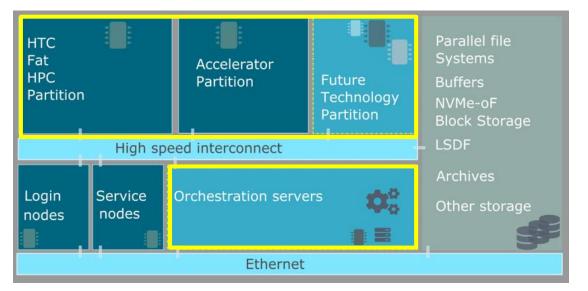
Name/tag		Concurrency	Cores	Memory	Disk
kgr2-inst	ance-hugedisk	1 (low)	1 - 2	8	128

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









Guidelines to support and help with certain aspects

Two different approaches:

Support and Guidelines

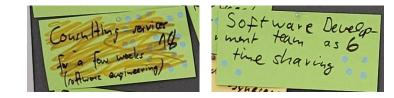
- E.g. guideline for choosing a suited open source license (more see later)
- Incorporating (open) research software in KIT guidelines for open science
- Offering hands-on support and consulting for researchers in RSE aspects
 - Similar to "RSE for hire" but with a limited scope
 - As of now two offers at KIT (SCC)
 - Software Sustainability and Performance Engineering Team
 - The <u>bwRSE4HPC</u> project



The Software Sustainability and Performance Engineering (SSPE) team supports scientific software developers in selecting the right tools to make scientific codes fit for the future, to make optimal use of the available computing resources and advises on porting, testing and benchmarking on new architectures, for example the Future Technologies Partition systems.



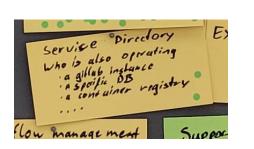








Helmholtz Cloud



Cloud

Q Text Search serv

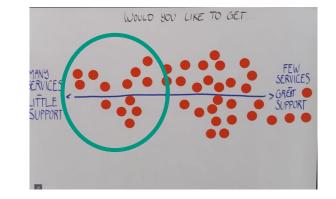
AWI DESY

Helmholtz Al cor

- 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)
 - ---

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



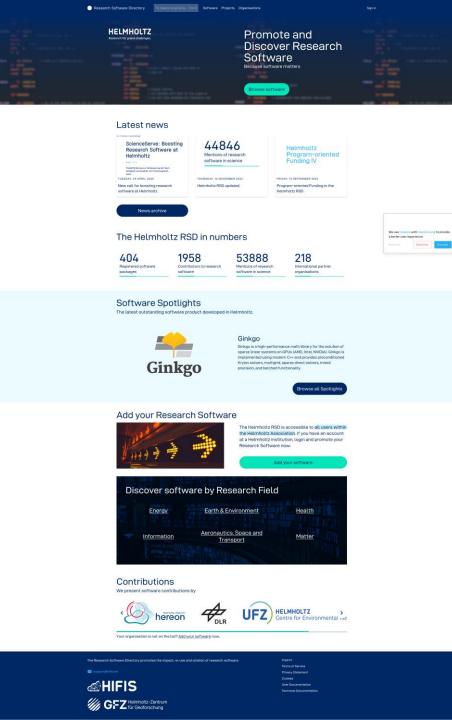


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			Sort by Popularity
	₩	*	INDIO
	GitLab Helmholtz Codebase	Heimholtz Knowledge Graph Heimholtz KG & unHIDE	Indico HIFIS Events
e	A web-based DevOps Iffecycle tool that provides a Git-repository manager.	Explore Heimholtz KG & Limmbe Explore Heimholtz data, digital assets, resources and infrastructure in one place!	An Events Management service for everyone within Helmohat and their partners, based on indico.
sh	٢	đ	000
z	Mattermost	Overleaf Collabtex	Nextcloud Sync & Share
UFZ	A hosted chat service for everyone within Heimholtz based on Mattermost.	Collaborative document writing with LaTeX	File Sync and Share, Collaborative Editing using Collabora.
	ď	• RSD	⊜ Jsc
	LimeSurvey CE LimeSurvey	Research Software Directory Helmholtz RSD	JupyterHub
	An online survey tool offered by DKFZ to everyone within Helmholtz Association.	Promote and discover research software developed in the Helmholtz Association.	Interactive supercomputing in a browser.
	File Sender	000	•
	FileSender	Nextcloud	HedgeDoc Notes
	FileSender by DKFZ for Heimholtz.Cloud is a secure way to share large files with enyone!	Sync&Share based on Nextcloud with Office for Web and Calendar function.	A collaborative platform to write and share markdown based documents.
	-	1	
	Timeseries Timeseries Management	Sensor Management System	Sensor Management System
	Visualise, monitor, combine, analyse and share time series data from multiple sources	Manage metadata for devices, platforms, measurement configurations and sites.	Manage metadata for devices, platforms & measurement configurations.
		2	
	OpenStack OpenStack (JSC Cloud)	dCache dCache InfiniteSpace	Jupyter GPU compute Service
	The Service allows provisioning of user- controlled VMs with Linux OS	Store large-scale scientific data and access it through different protocols.	Jupyter Notebooks on GPU Nodes containing Nvidia A100 GPUs
	(C) Solitow	@ (A)	٢
	SciFlow	Apptainer Container Runtime on HAICORE	B2SHARE, based on Invenio B2Share
	SciFlow is a collaborative text editor for academia.	Container runtime environment on KIT HAICORE HPC systems.	Research Data (+ corresponding Metadata) Publishing service.
	20	н	н
	BLABLADOR The Large Language Model Inference server of the Helmhoitz Association, with privacy bulk-in	Earthquake Explorer Integrate existing 0EOFON earthquake Information products with other services e.g. shake maps.	GIPP Experiment Database Access information on all geophysical experiments supported by the GIPP.
	€GraviS eset⊠	6 HACORE	HA-CORE
	Gravity Information Service (GravIS)	HAICORE	HAICORE
	GravIS provides user-friendly products to	Dedicated COmputing REsources for the	Dedicated COmputing REsources for the

Helmholtz Research Software

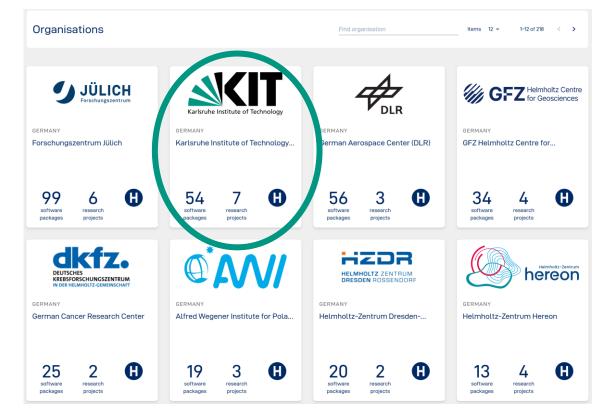
help to find existing software tools, guide ... before re-inventing them

- 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

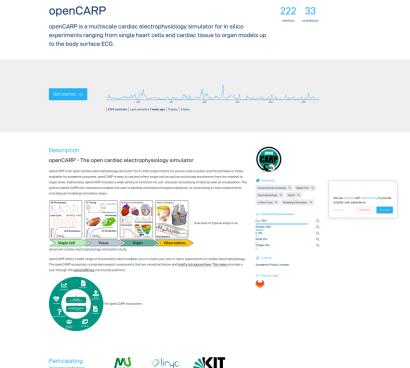
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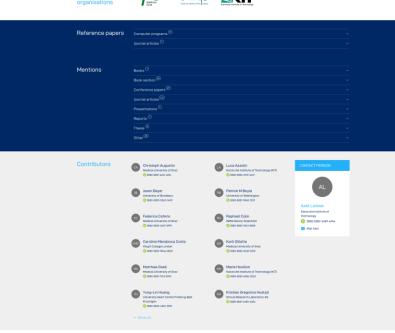




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Trainings

- 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







