

# BETTER SOFTWARE BETTER RESEARCH

```
import heat as ht
                                      # HeAT for distrib
                                      # Hypothetical Oper
import opencarp as oc
# Initialize tissue domain
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])
```

## Research Software Engineering (RSE) @ KIT Requirements and Communication

## Work Package 2: Requirements and Communication

Building a RSE community @ KIT
Bringing various activities on RSE @ KIT closer together
Helping newcomers
Supporting the communication in our RSE community



## First Workshop on Research Software Engineering @ KIT



#### Methodology at workshop

- Gathering of wishes and requirements (yellow cards)
- Ranking of ideas (green buttons)

## Digitalization and grouping of results

Addressing of high-ranked wishes



https://indico.kit.edu/event/3461/overview (May 2023)



## **New Chat Channel**



New Matrix chat channel for RSE@KIT

Join here: https://matrix.to/#/#derse-rse@kit:kit.edu

General information on Matrix: <a href="https://www.scc.kit.edu/en/services/matrix.php">https://www.scc.kit.edu/en/services/matrix.php</a>

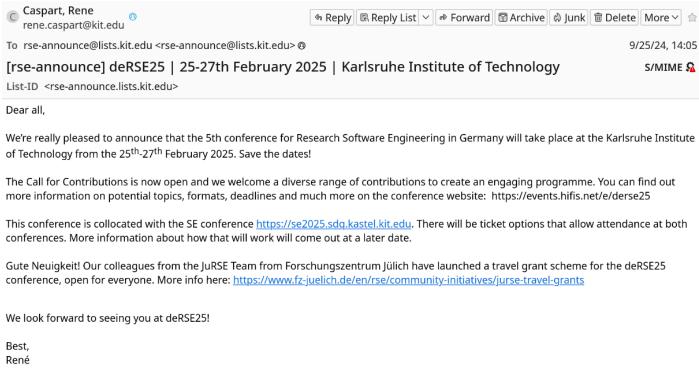


## **New Mailing List**

#### rse-announce@lists.kit.edu

Subscribe here: https://www.lists.kit.edu/sympa/subscribe/rse-announce



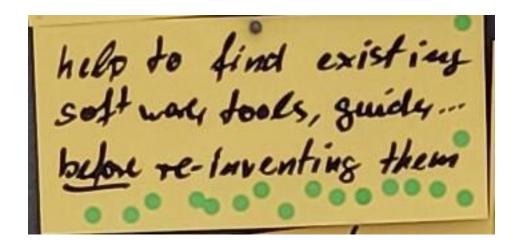




## **New Web Page**

### https://www.rse-community.kit.edu/

- About RSE
- Further information and links
- Events
- Services for RSE





Research Software Engineering (RSE) at KIT

## RSE@KIT

Welcome to the community page for Research Software Engineering (RSE) at KIT. This page aims to serve as the starting point, if you are looking for information, events, services and knowledge exchange in the context of research software engipeering.



#### What is Research Software?

- For hundreds of years the basis for science are theory and experiments; since a about 50 years simulations allow to investigate questions where experiments are too expensive, too complex, too long-lasting or can not be done. Since about 10 years the extraction of knowledge from data is seen as the 4<sup>th</sup> paradigm IZ in science.
- Hence, software in research is a key component of scientific work and scientists have today the same rigorous requirements towards research software as they have towards data, devices, and technologies that they are using. Research software have become valuable assets in many research disciplines and can be seen as research infrastructure itself, which need to be financed and further developed in a long-lasting way like other research infrastructures, e.g. research vessels and stations, particle accelerators, laboratories and the like.
- The importance of research software has e.g. been addressed in a strategy paper by the Netherlands eScience Center in 2019 entitled "Raising the Profile of Research Software: Recommendations for Funding Agencies and Research Institutions \( \mathref{Z}^n\), which stats "If open science is to truly lead towards better, more transparent, and reproducible research, then research software needs to be treated in equal footing to research data and publications at the policy level and in practice"
- The Software Sustainability Institute 

  Thas put it simply in short: "Better Software, Better Research"

#### What is Research Software Engineering?

- Many answers exist to this question, so let's look at what is written on Wikipedia 27. "Research software engineering is the use of software engineering practices in research applications. The term was proposed in a research paper in 2010 in response to an empirical survey on tools used for software development in research projects, projects. It started to be used in United Kingdom in 2012, when it was needed to define the type of software development needed in research. This focuses on reproducibility reusability, and accuracy of data analysis and applications created for research.
- This encompasses a sustainable/long-lasting paradigm shift in developing software for research through using Continuous Integration/ Testing/Delivery (CI/CT/CD), through educating, training and promoting (young) Research Software Engineers, through adapting common key performance metrics and indicators to reflect the importance of research software, as well as through a co-design approach with an early integration of computers scientists, mathematicians and – possible also hardware operators in the development of community software in science.
- At KIT the importance of research software and research software engineering is reflected in "Dachstrategie KIT 2025", which states in chapter 9 about "Digitalisierung" under aim 9.1.5 (page 33, in German only): "KIT understands Research Software Engineering (RSE) and the development of research software as an essential task in the digitized research process and strives for new research projects, which are increasingly data and computation intensive.
- To address this aim a KIT-internal small project without funding, called "Leitprojekt 9.1.4", was initiated. More information about this RSE-related project as well as the other projects in the domain of "Digitalisierung" is here, again only in German.



## Web Page: KIT links

#### **KIT**

- Handbook Free/Libre Open Source Software (in German)
- LP 9.1.4 Research Software (in German)
- SSPE team at the Scientific Computing Center (SCC)
- Working Groups/Arbeitskreis Open-Source-Software
- RSE announce mailing list <u>subscribe</u>
- RSE@KIT Community Matrix Channel join here



## Web Page: National links

#### **National**

- Helmholtz Open Science Policy
- Helmholtz Working Group Open Science Task Group Research Software
- Helmholtz Working Group Open Science Task Group Helmholtz Quality Indicators for Data and Software Products
- Research Software Directory
- HIFIS Software Services
- Helmholtz Platform for Research Software Engineering Preparatory Study (HiRSE\_PS)
- HiRSE Seminar Series
- de-RSE e.V. Society for Research Software
- NFDI Sektion Common Infrastructure, Working Group Research Software Engineering
- Access to and Reuse of Research Software Position paper of the Helmholtz Association Open Science Working Group
- Helmholtz Information & Data Science
- <u>Digitalization Strategy of the Helmholtz Association</u>
- JuRSE, the Community of Practice for Research Software Engineering at Forschungszentrum Jülich



## Web Page: International links

#### International

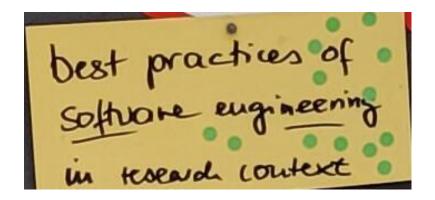
- US Research Software Engineer Association (US-RSE)
- Society of Research Software Engineering (UK)
- Research Software Alliance ReSA
- FAIR for Research Software (FAIR4RS) WG of the Research Data Alliance
- Linux Foundation: Open Source Licensing Basics for Software Developers (LFC 191)



## **HiRSE Seminar Series**

#### https://www.helmholtz-hirse.de/series.html

- Seminar on RSE topics
- Started in April 2022
- 44<sup>th</sup> edition tomorrow!
- You missed it so far? → youtube channel



#### **Events**

• July 08, 2025 (virtual)

#### 44th HiRSE Seminar

On Tuesday 8th July at 11am CEST, Judith Hartstein from the German Centre for Higher Education Research and Science Studies (DZHW) will join us at the HiRSE Seminar Series to talk about 'Research practices in a digitalized world: Research software, mundane software and programming languages in research.'

• June 23, 2025 (virtual)

#### 43rd HiRSE Seminar

On Monday 23rd June at 2pm CEST, Sabine Grießbach from Jülich Supercomputing Centre (FZI) will join us at the HiRSE Seminar Series to talk about 'Leveraging Earth System Science to Exascale' and the German National Earth System Modelling Support Team.

May 15, 2025 (virtual)

#### **42nd HiRSE Seminar**

On Thursday 15th May at 11am CEST, we will celebrate the 'Young RSE Award' winners from 2023, 2024 and 2025 with a presentation from each of them on the research topic that won them the award. If your RSE career has just started you can get involved in the Young RSE competition which occurs annually organised by the deRSE Association and takes place at the deRSE Conference. We welcome the 2023 Award Winner - Yudong Sun, the 2024 Award Winner - Florian Sihler, the 2025 Award Winner - Anna Lena Schaible.

April 02, 2025 (virtual)

#### 41st HiRSE Seminar

On April 2nd, 2025, 2pm CEST, Mascha Schmidt, Victor Haguet and Fritz Niesel from the Applied Machine Learning Group based at the Jülich Supercomputing Centre will join us at the HiRSE Seminar Series with their talk about Bridging the Gap Between Private Data and AI: A Beginner's Guide to Retrieval Augmented Generation (RAG).

March 07, 2025 (virtual)

#### 40th HiRSE Seminar

On March 7, 2025, 11am CET, Samantha Wittke from CSC - IT Center for Science will continue the HiRSE Seminar with her talk about CodeRefinery: A Community for Teaching, Learning, and Growing Together

• February 21, 2025 (virtual)

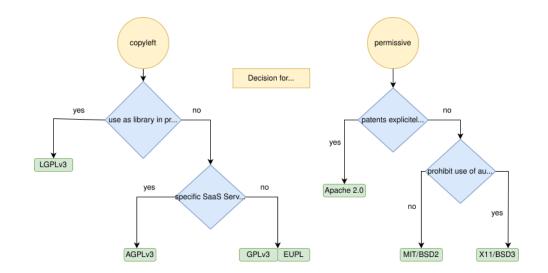
#### 39th HiRSE Seminar

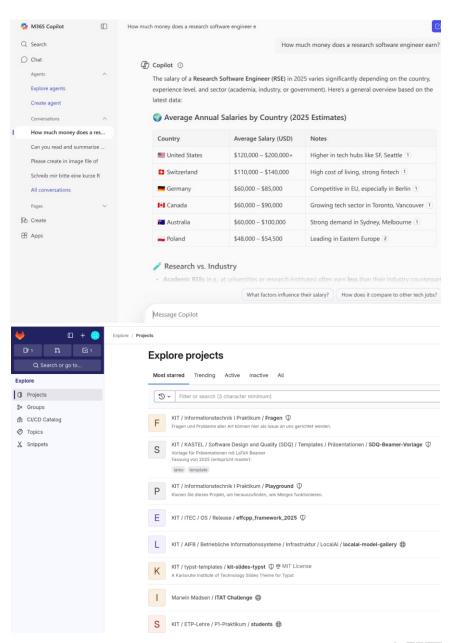
On February 21, 2025, 11am CET, Guido Juckeland from Helmholtz-Zentrum Dresden-Rossendorf will continue the HiRSE Seminar with his talk about Introduction of a quality indicator for research software publications



## Web Page: Services for RSE

- Gitlab at KIT
- Continuous Integration/Testing/Delivery/Benchmarking (CI/CT/CD/CB) on the HPC clusters at KIT
- Service Catalogue on the Helmholtz Cloud Portal
- Assistance in finding a suitable open source license
- Microsoft Copilot







## **Community – That's you!**

#### A community thrives on participation

- Make use of the offered RSE tools and communication channels
  - Exchange of experiences, best practices, ...
- Already many RSE activities at KIT
  - We hope LP9.1.4 helped in supporting and linking research software engineers







12