Scientific Software Center

IWR Interdisciplinary Center for Scientific Computing

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

Scientific Software Center

2025 Annual Report

Scientific Software Center: Mission Statement

Development & Sustainability

Teaching & Consultation

Outreach & Communication

The Scientific Software Center strives to improve research software development practices at Heidelberg University and beyond, to promote reproducible science and research software sustainability.

Current state of the SSC

Current status
The Scientific Software Center (SSC) has been successfully established within the university and is fully operational. Rapid growth in funded projects led to new hires and increased administrative effort. As Research Software Engineering gains recognition among funding agencies, Heidelberg aims to strengthen institutional best practices. This will be reflected in the planned transition of the SSC to become a core facility.

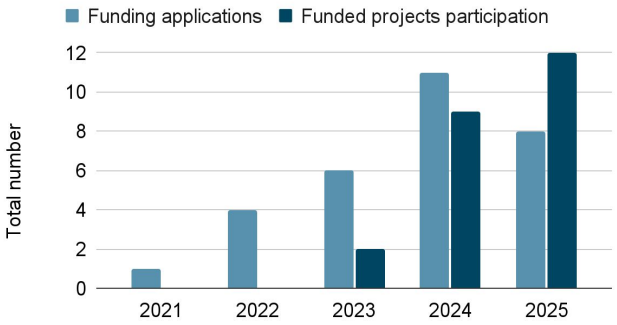
Who we are
Originally founded in 2020 with three Research Software Engineers (RSEs), we are a team of eleven RSEs in December 2025.

Success story
The SSC functions like a core facility of the university. The Open Call allows researchers to gain access to research software development capacities at no cost to the researchers. In 2025, the Open Call was oversubscribed by a factor of two.

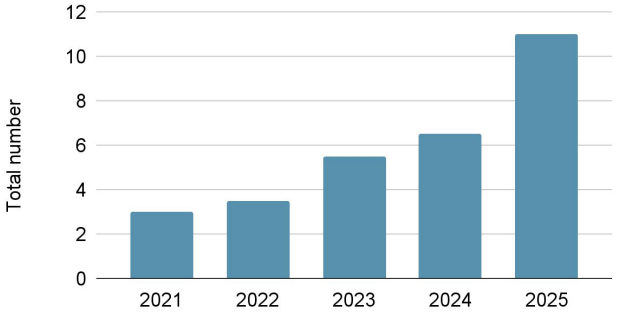
Additionally, the SSC is part of several third-party funding applications, with a large increase in ongoing third-party funded projects and a slight decrease of grant proposal participation.

In 2025, we submitted eight proposals and participated in twelve third-party funded projects. The decrease in submitted grant proposals is a natural consequence of reaching a capacity limit due to the ongoing projects.

Third-party funded projects

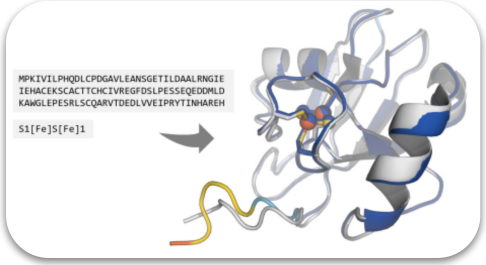


Number of FTE RSEs



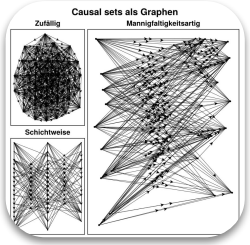
New SSC sub-units

Bio-Structure Hub
The Bio-Structure Hub offers a wide range of services and resources in the field of computational structural biology for scientists at research institutes in Heidelberg. Researchers are supported in setting up and using structure prediction models as well as in interpreting the predictions. The Bio-Structure Hub is made possible through funding from the Klaus Tschira Foundation.



bwRSE4HPC
The bwRSE4HPC unit implements projects across the state of Baden-Württemberg in collaboration with the KIT RSE team, with a focus on the use of the region's high-performance computing (HPC) infrastructure. Efficiently utilizing the diverse HPC landscape in Baden-Württemberg can be challenging for many university research groups. To address this, support is provided for improving existing code in terms of performance, efficiency, and maintainability, as well as for developing new software for use on HPC infrastructure. This program is funded by the Ministry of Science, Research and the Arts of Baden-Württemberg.

Data Science Unit
The Data Science Unit provides specialized support in the fields of machine learning and data science. Its services cover the full spectrum of research support—from developing machine learning solutions from the ground up, through refining existing models and pipelines, to targeted consultations addressing specific challenges. These services are offered in close collaboration with the other sub-units as well as the SSC core team, and are made possible through funding from Field of Focus 2 and IWR.



Development & Sustainability

Aim

- Support researchers with high-quality, sustainable research software that generates reproducible data
- Provide access to well-trained RSEs
- Provide career option and community to RSEs
- Adapt the latest software engineering standards in research software development

type of support	small-scale project	open call project	third-party funded project
time scale	1 week	1 – 12 months	> 1 month
cost	free of charge	free of charge	determined though consultation
availability	throughout the year	proposal submission (till mid-June)	throughout the year (on availability)

“Development” pillar in numbers

2 Open Call projects completed

12 Small scale projects completed

9 Ongoing/completed third-party funded projects

2 Small open source contributions

2 Data science projects

9 Bio-Structure Hub projects completed

3 bwRSE4HPC projects

Open Call and small scale projects
The SSC provided development support for researchers through two open call projects:

MONDEY: We developed an online platform mondey.de which parents and professionals can use to document and evaluate the developmental progress of children.

“PIRATES”: We developed a reusable web component that displays objects from the Heidelberg media database HeidICON. It is used in a Neo4J graph database dashboard application about maritime predation in the mediterranean developed by Heidelberg historians. Additionally, we enhanced this dashboard with map visualizations.

Third-party funded projects
Research projects supported as service or as co-PI on funding applications, including:

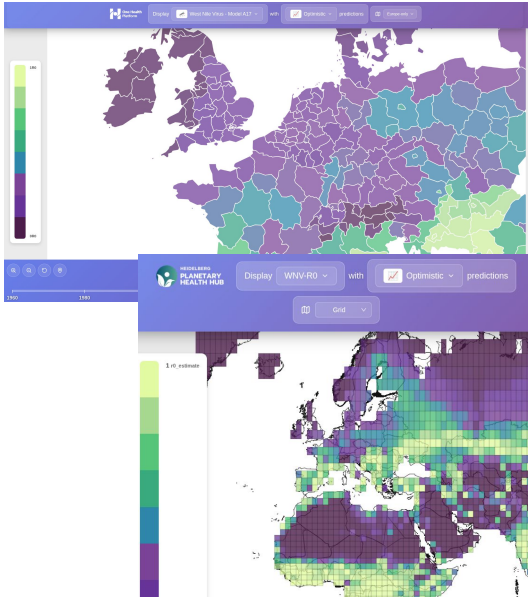
BioCypher: Analysing biochemical and medical information in a knowledge graph provides many insights, but harmonizing different data sources represents a challenge. We are working on an adapter registry and metadata standards to streamline workflows and make them accessible to researchers in bioinformatics.

predicTCR: Researchers worldwide can use the predictcr.com web service to predict tumor-reactive T cells and TCRs from their scRNA-seq data using a DKFZ machine learning model.

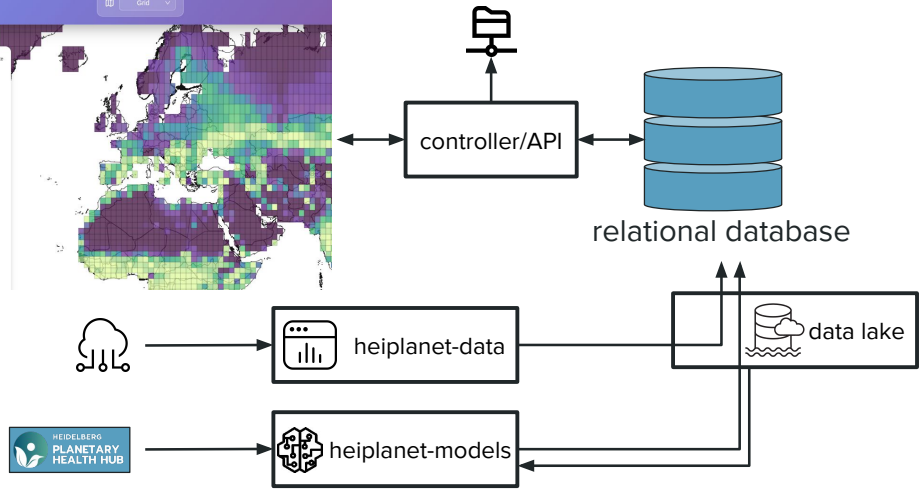
“Development” highlight: Hei-Planet platform

Background
The Heidelberg Planetary Health Hub (Hei-Planet) is working with the SSC to build an interactive climate-health platform. This platform will support decisions, strategies and measures in the climate-health nexus, with the goal of providing a surveillance and early warning system. Ideally, it should further enable policy- and decision-makers with predictive power about the outcome of interventions and measures.

The Hei-Planet group has previously developed models to predict suitability and risk factor spread, such as certain types of mosquitoes, for vector-borne diseases. These models are made available to the public through the platform.



SSC contribution
The SSC supports the Hei-Planet group by developing sustainable and reproducible data pipelines, robust model implementations, a lean architecture of the database backend and interactive easy-to-use frontend.
http://platform.hei-planet.com/



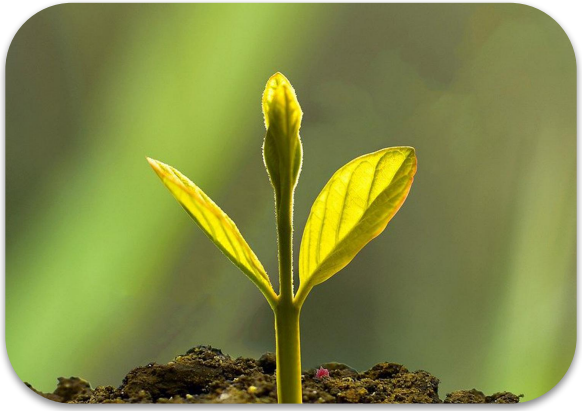
Teaching & Consultation

Aim

- Provide access to training in software engineering best practices
- Spread the use of best practices in the community
- Provide an easy, low-barrier entrance point for researchers, directly provide feedback on software quality or software-related questions

Block courses	On-demand courses	Mentoring program	Consultations
Template repositories	Guidelines	Compact courses	Seminars

“Teaching” pillar in numbers



13 Compact courses on Software Engineering Best Practices

1 Block course on Scientific Software Development

2 Workshop contributions

4 Bio-Structure Hub workshops

Courses
The SSC offers courses open to all students and researchers at the university, aiming to improve knowledge and skills of participants. The courses are very hands-on, motivating participants to try out their newly obtained insights and becoming confident in handling new tools and frameworks.
Furthermore, the SSC hosts a seminar series called Lunch-time Python, where participants can learn about new libraries in an informal setting.

- AI in research software: Best practices for developing and using ML models
- Building software with CMake
- Containers in Science: Using Docker and Singularity
- Continuous Integration with Github Actions
- Data Exploration with Python and Jupyter
- Effective Software Testing
- Expert Topics in Version Control with Git
- Intermediate Topics in Version Control with Git
- Python Packaging
- Scientific Software Development
- The Unix Shell + Version Control with Git
- ...

“Teaching” highlight: SSC Fellows program

The program
SSC Fellows receive individual training in state-of-the-art software engineering and tools for improving their research software development skills. Each Fellow is assigned an RSE mentor from the SSC with whom they meet on a monthly basis, to track and support their research software engineering project. Fellows further engage in community events and educational efforts organized by the SSC. In addition, Fellows receive a travel stipend to participate in a national RSE conference, with the opportunity to engage in the research software engineering community, and present their contribution.

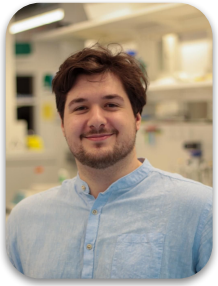
The Fellows
The Fellows are current PhD students and Postdocs at Heidelberg University, and spend a substantial amount of their time on creating research software, to carry out their research. The connection to the SSC will extend the Fellow’s academic identity profile with the attribute of a Research Software Engineer.

Niklas Baumgarten
Postdoc (maths)

Anamaria Elek
Postdoc (biology)

Stanley Scott
PhD student (physics)

Maximilian Friedrich
Researcher (medicine)



Luca Monari
PhD student (biology)

Outreach & Communication

Aim

- Improve recognition of research software as scientific output, support and shape RSE career paths
- Develop and mantain official guidelines and policies for research software development
- Actively participate in national and international software engineering initiatives and communities
- Contribute to open-source software and open science

de-RSE	GI	URZ	HIFIS/Helmholtz
NHR/bwHPC	Carpentries	University library	Research Data Unit

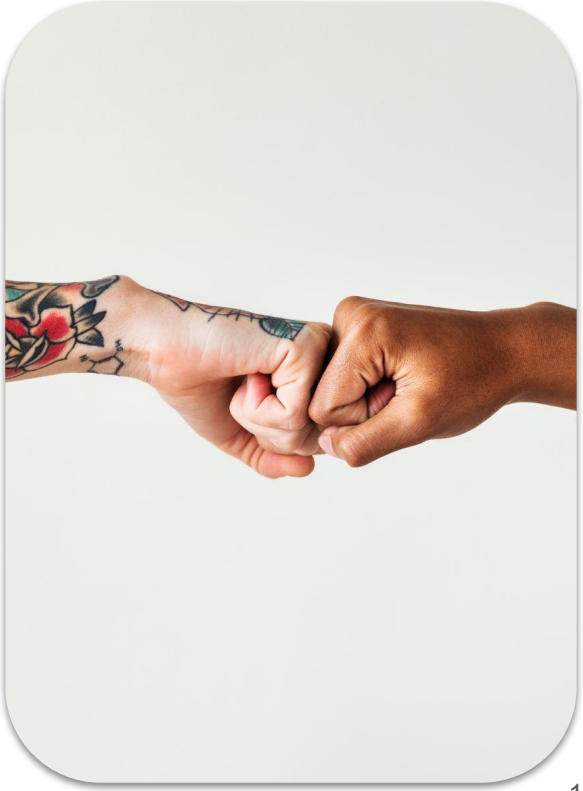
“Outreach” pillar: Contributions

Networking
Through the ongoing third-party funded projects, the SSC is becoming more connected within RSE-embedded research communities such as bioinformatics, for example in initiatives like BioCroissant, metadata standards and findability, and information fusion.

Sustainability
The SSC supports the Sustainable Development Goals #3 ("Good Health and Well-Being") and #13 (Climate action) through dedicated projects. Further, by building sustainable and robust research software, the SSC also supports goals #9 (Resilient infrastructure) and #12 (Responsible consumption).

Recognition of Research Software Engineering as fundamental pillar of modern and excellent research
Through the participation in several working groups of the de-RSE e.V. and the RSE work group of the GI e.V., the SSC supports RSE Advocacy, Research Software Management Plans, and AI4RSE initiatives.

deRSE Conference Organization
SSC members participated in the program and sponsor committee of the deRSE25 conference in Karlsruhe, and also in the program committee of the upcoming deRSE26 conference in Stuttgart. The RSE community is not supported by a network of academic permanent staff, due to the lack of RSE career pathways in the academic landscape, and therefore relies on RSEs giving back to the community.



“Outreach” highlight: Large SSC delegation attends deRSE25

Image taken by Erik Burger (KIT), CC-BY 4.0

From February 25 to 27, the annual conference on Research Software Engineering took place at KIT in Karlsruhe. The Scientific Software Center attended the conference with a large delegation and presented a total of five talks and co-organized one birds-of-a-feather session.

The RSE developers were also joined by two SSC fellows: Stefan Maurer presented his poster on *"Designing Intuitive and Flexible Software for a Novel Image-Based Cell Sorting Method"* and Anna-Lena Schaible gave a talk on her work on *"Fast GPU-powered and auto-differentiable forward modeling for cosmological hydrodynamical simulations"*.

Anna-Lena's talk was not only well-received by the audience, but also by the reviewers of the jury for the young RSE prize. At the end of the poster session, she was awarded this years prize together with a prize money of 512 Euros. Congratulations, Anna-Lena!

Edwin Carreno: Effective workflows for community engagement of users and developers in open-source software development
Liam Keegan: What researchers need vs what they ask for
Dominic Kempf: Better research software through better research software competencies - a symposium report
Harald Mack: The SSC fellowship program - Personalized support and RSE education for young researchers
Inga Ulusoy: A research software engineering department at a German university: Four years and counting