Scientific Software Center

IWR Interdisciplinary Center for Scientific Computing

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

Scientific Software Center

2024 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.

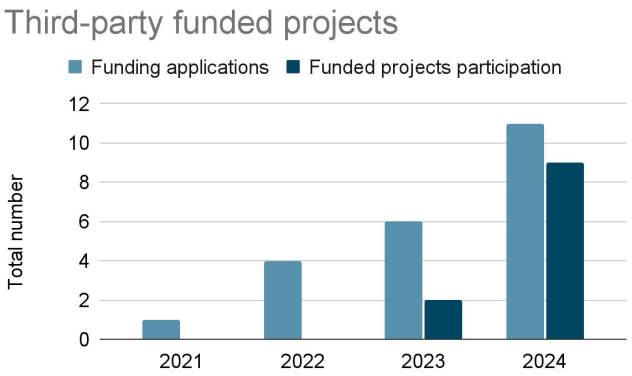
Current state of the SSC

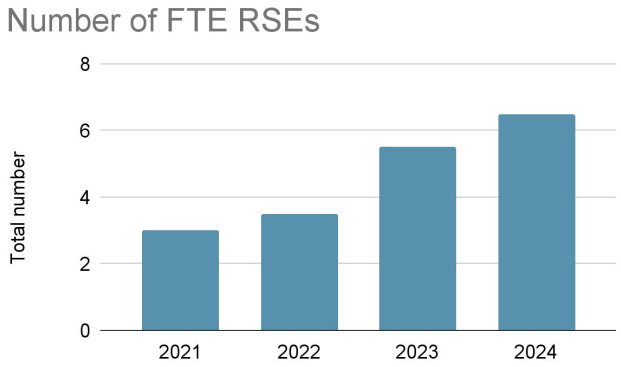
Establishment
The Scientific Software Center (SSC) has been successfully established within the university and is fully operational. It is in regular dialogue with other internal service providers that have thematic overlaps with research software. Through active advertisement and networking with other faculties, the SSC is becoming increasingly well known among researchers at Heidelberg University.

Who we are
Originally founded in 2020 with three Research Software Engineers (RSEs), we are a team of six RSEs in December 2024, growing to eleven in early 2025.

Success story
The SSC's Open Call allows researchers to gain access to research software development capacities at no cost to the researchers, after a successful application. The Open Call is regularly oversubscribed, highlighting the need of support from all faculties.

Additionally, the SSC is part of several third-party funding applications, with a large increase in grant proposals as well as involvement in ongoing third-party funded projects. In 2024, we had eleven applications and were involved in nine running projects. This also indicates the need and demand for research software development within the university.





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

5 Open Call projects completed

4 Small scale projects completed

9 Ongoing/completed third-party funded projects

11 Small open source contributions

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

- Quantifying organelle geometry and morphology based on volume electron microscopy data (biology)
- Identification of cultural heritage objects with computer vision methods (cultural heritage)
- Modernisation of the Potsdam Wolf-Rayet Stellar Atmospheres Code (astrophysics)
- Performance improvements for the toolkit for Simulation and Image Processing for Photonics and Acoustics (biophysics)
- Virtual telescope GPU computing in astronomy (astrophysics)

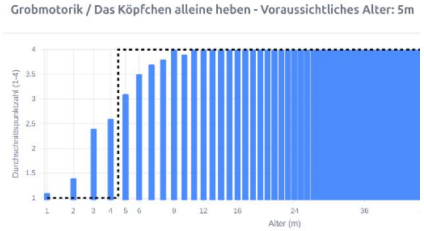
Ongoing and completed third-party funded projects
Through various funding agencies, the SSC received the means to support additional research projects as service or as co-PI on funding applications. Most funding is provided through the DFG, in particular for the two projects that were successful in the call “Research software: Quality assured and re-usable”. Many smaller projects make use of ExploreTech funding (Health + Life Science Alliance Heidelberg Mannheim), which is a smaller grant to support joint projects of research groups with core units.

“Development” highlight: MONDEY

Background
The “Mondey (Milestones of Normal Development in Early Years)” project provides a standardised instrument for documenting early childhood development for the age range 0-6 years. MONDEY contains descriptions of more than 200 milestones, which are assigned to eight different areas of development (gross and fine motor skills, perception and thinking, language, social relationships, self-regulation, emotions), which in turn are intended to reflect general development in early childhood. Previously, the researchers used a platform developed by an external company, but over time no longer met the state of the art modern security requirements.

SSC contribution
Thanks to the development by the SSC as part of the Open Call, it is possible to further develop the project. The SSC supports the project by developing an online platform, which parents and professionals can use to document the developmental progress of children in that age group. The perceptions of parents and carers are included into the documentation, allowing targeted support and early identification of the needs of the children.

Some enhancements by the SSC include expanding the applicable range from 0-3 to 0-6 years, improving the accuracy of the prediction algorithm, a more intuitive user experience as well as meeting security requirements. MONDEY will be integrated into larger health and education software programmes in the future, with prospect of nationwide use in Baden-Württemberg by kindergartens and parents to support the development of young children.



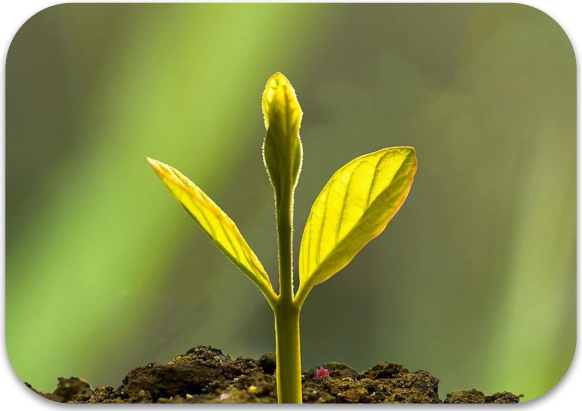
Teaching & Consultation

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



10 Compact courses on Software Engineering Best Practices

4 Language specific compact courses

1 Block course on Scientific Software Development

1 Seminar series: Lunch-time Python

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.

- The Unix Shell + Version Control with Git
- Intermediate Topics in Version Control with Git
- Expert Topics in Version Control with Git
- Effective Software Testing
- Open-source licensing
- Generative AI for writing (research) software
- AI in research software: Best practices for developing and using ML models
- Data Exploration with Python and Jupyter
- Python Packaging
- Python Best Practices
- Introduction to Python Testing
- ...
- Block course “Scientific Software Development”

“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.

Anna Lena Schaible, PhD student (astrophysics)

Stefan Maurer, PhD student (biophysics)

Solène Gerwann, PhD student (sport psychology)

Chris Byrohl, Postdoc (astrophysics)

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

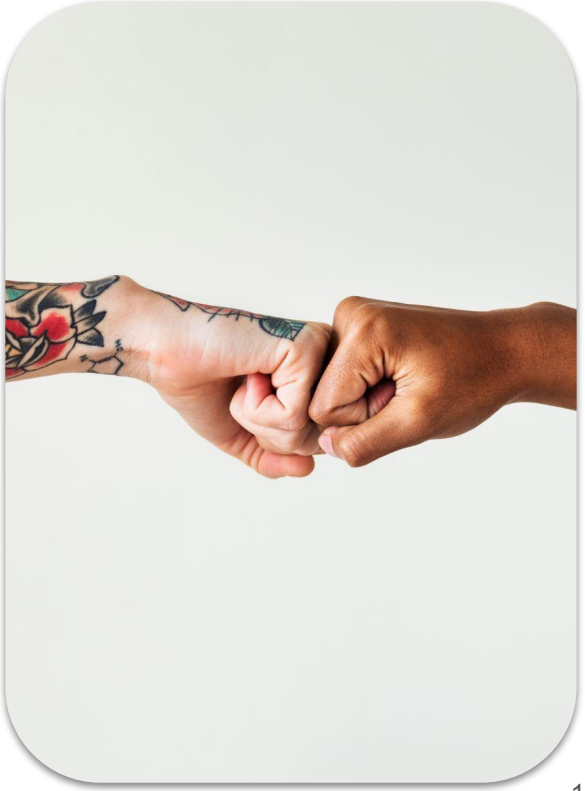
“Outreach” pillar: Contributions

Networking
The SSC is excellently connected within Heidelberg University, at national and international level, e.g. Heidelberg Forum Digital Humanities, RWTH Aachen University and the NHR (National High Performance Computing) Association, as well as Queen’s University Belfast (UK), the eScience Center (NL) and the Research Software Alliance ReSA (international).

The SSC’s involvement and contribution in transregional and national projects has increased significantly over the past year. Among other projects, a collaboration with the KIT “bwRSE4HPC” will start in 2025, in which state funds will be used to provide Baden-Württemberg-wide, long-term support for researchers in the development of research software.

Recognition of Research Software
The SSC supports the visibility of research software through the “Research Software Directory”. Software packages developed by researchers at Heidelberg University are listed in this database. The Research Software Directory serves the purpose of networking and supports the recognition of research software as a scientific achievement.

Guidelines
The SSC’s intensive collaboration on the “GI and de-RSE Guidelines Template for the Efficient Development of Research Software” has demonstrated the SSC’s pioneering role as one of the first German dedicated RSE departments at a university, leading to support requests from other universities of how to establish this type of infrastructure.



“Outreach” highlight: Symposium Code for Science

Under the title “**Code for Science or: Better research through better research software skills**”, around 30 representatives of the German research software engineering community met for a 3-day workshop on improving research software skills. The workshop was part the of the Volkswagen Foundations themed week on “Digital competencies in Science”, which took place in December 2024 in Hannover. The central aim of this event was to develop multiple recommendations on how to empower different actors and their institutions to deal more effectively with research software and the corresponding acquisition of expertise.

The results of this workshop have been presented at deRSE25, and can also be found here. In total, 40 recommendations for different target groups have been developed, providing insights on preparing learning opportunities, promoting the RSE community and creating incentives and frameworks for quality assurance.