IWR
Interdisciplinary Center
for Scientific Computing

UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386

Scientific Software Center

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2025.04.30

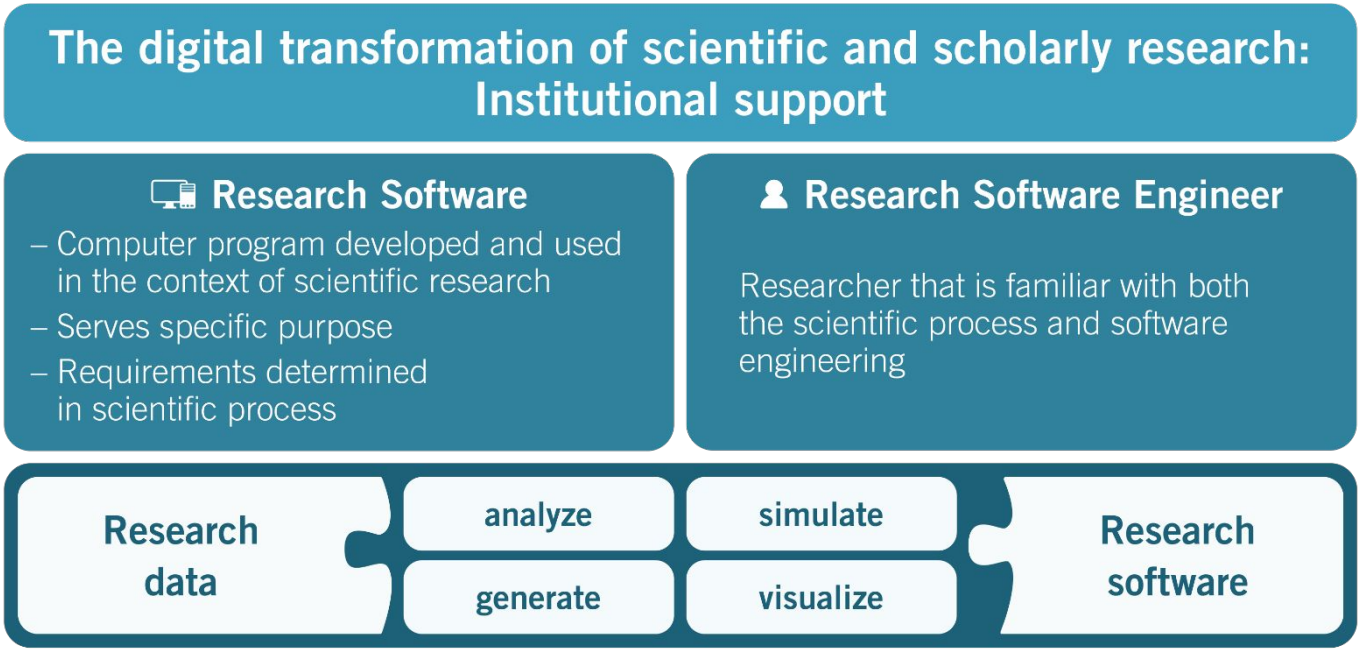
ssc.uni-heidelberg.de

What we do

Mission Statement

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

Research software, research software engineers, and research data



Types of support needed for research data and software

Scientific Software Center

SSC

- Research software development
- Software engineering best practices
- Training in software engineering and software project management
- Software sharing and publication
- Machine-learning based research software
- ...

RDU/ library

- Research data management
- Planning and implementing data analysis
- Storage and archiving
- Data publication
- Establishing standard practices
- ...

New: BioStructure Hub@SSC

- Research software service: Biostructure Hub
  - Structure prediction of biomolecules
  - Support with running the research software/ interpreting the results
  - ...

New: Data Science Unit@SSC

- Data Science support
  - Data quality/accuracy
  - Data pipelines
  - Data modelling/model training
  - ...

Currently funded by FoF2

URZ

- Software operations
- Deployment
- Operating and supporting software applications
- Installing, configuring, testing, releasing, monitoring and maintaining software products in operational environments
- ...

Who we are

- Research Software Engineers
- Founded 4 years ago with 3 RSEs
- Growth through third party funding
- Current team of 11 RSEs

Development

- Consultation
  - Researchers can come to us for a free consultation on any software development issue
- Small scale projects
  - One week of developer time, often as follow-up work to a consultation
- Open call projects
  - Annual competitive call offering several months of developer time for projects without cost
- Funded projects
  - SSC as service partner or co-PI on grant applications for software development work

Example: Small-scale project

Hammingdist

Topological data analysis of the genomic structure of variants of the SARS-CoV2-virus (Physical Mathematics)

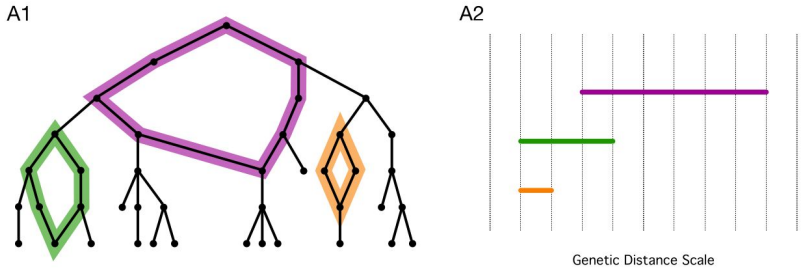
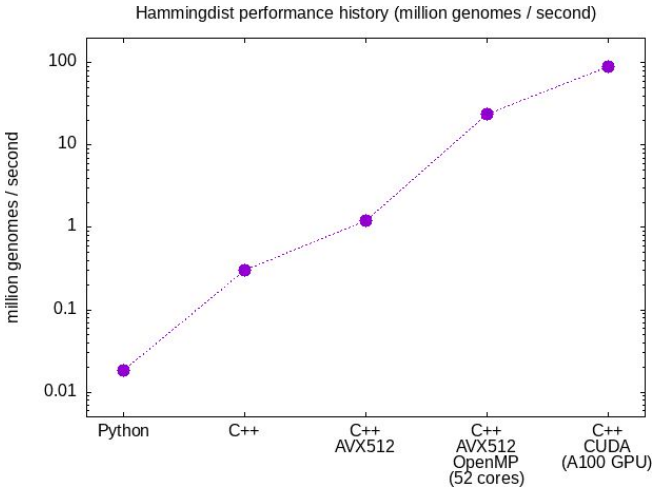


Figure 2. Topological data analysis quantifies convergent evolution.

Compute genetic distance scale of reticulate events in viral evolution.
https://arxiv.org/pdf/2106.07292.pdf



Improved implementation currently handles 10 GB of genome data (≈350k genomes each of length ≈30k).
https://github.com/ssciwr/hammingdist

Example: Open call project

ammico

AI Media and Misinformation Content Analysis Tool (Social/Political Sciences)

https://github.com/ssciwr/AMMICO
https://osf.io/preprints/socarxiv/v8txj
https://doi.org/10.57967/hf/0603

TextDetector

Analyse text

Select models for text_summary, text_sentiment, text_NER or leave blank for default:

Select model revision number for text_summary, text_sentiment, text_NER or leave blank for default:

Run Detector

filename	../../data/Image_some_text/109237S_spa.png
text	29 de septiembre CONFÍAN EN LA REUNIÓN DE HOY 0:10/0:14
text_language	es
text_english	September 29th THEY TRUST IN TODAY'S MEETING 0:10/0:14
text_clean	September 29th THEY TRUST IN TODAY 'S MEETING
text_summary	September 29th THEY TRUST IN TODAY'S MEETING 0:10/
sentiment	POSITIVE
sentiment_score	0.99
entity	
entity_type	

Scientific Software Center

Selected SSC projects

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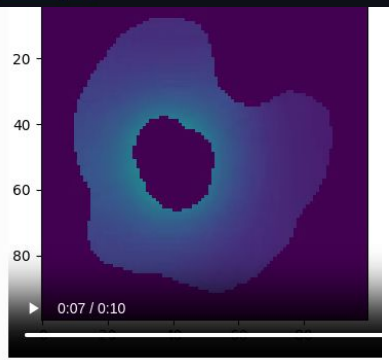
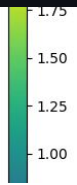
Spatial Model Editor

release v1.5.0 | pypi v1.5.0 | Open in Colab | docs passing | GUI/CLI Release Builds passing | codecov 88%

quality gate passed | DOI 10.5281/zenodo.10246531

A GUI editor to create and edit spatial SBML models of bio-chemical reactions and simulate them using the dune-copasi solver for reaction-diffusion systems.



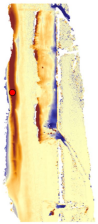


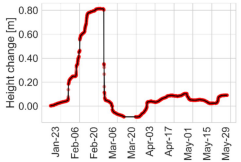
SampleFlow

Multiplexed nanopore DNA sequencing.

About | My samples | Login

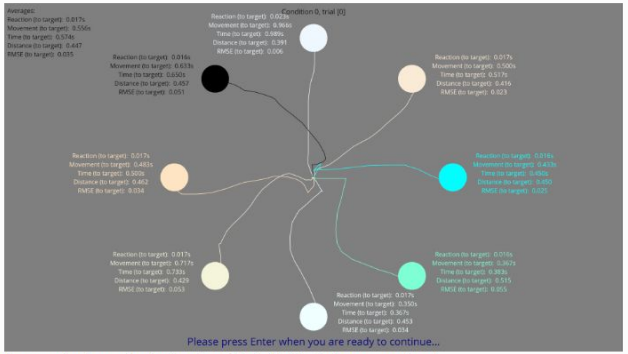
py4dgeo





4D objects-by-change extraction

Visuomotor Serial Targeting Task (VSTT)



An example of a results display after a block of trials during an experiment.

E-mails - Dynamics of standardization

MailCom

ESCRIBIR DESPUÉS DE LA CULTURA LETRADA
A ESCRITA DEPOIS DA CULTURA DAS LETRAS
ÉCRIRE APRÈS LA CULTURE ÉPISTOLAIRE

Building a knowledge graph community

biocypher

a unifying framework for biomedical knowledge graphs

Data Science Unit@SSC

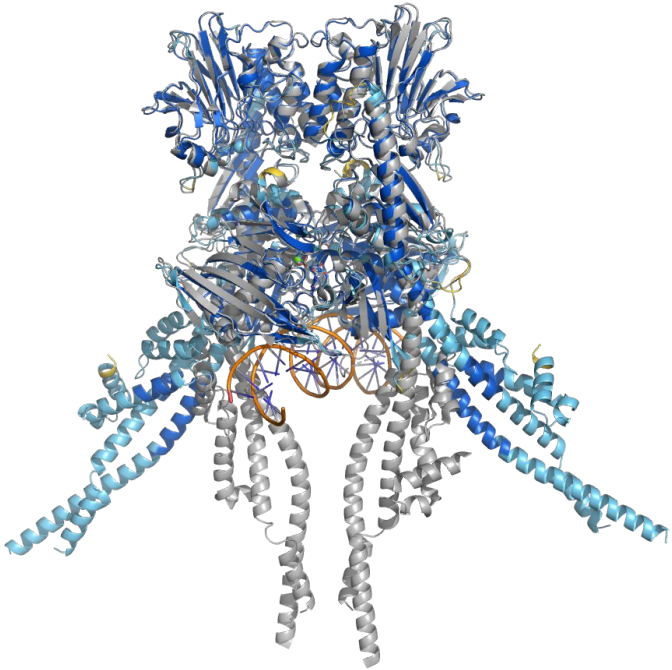
- Apply data science to specific scientific questions
  - Build a new data science system based on research project
  - Augment or enhance existing systems to tackle new questions
- Integrate data science into the scientific process
  - Make machine learning systems more interpretable
  - Data science for knowledge extraction or hypothesis generation

BioStructure Hub@SSC

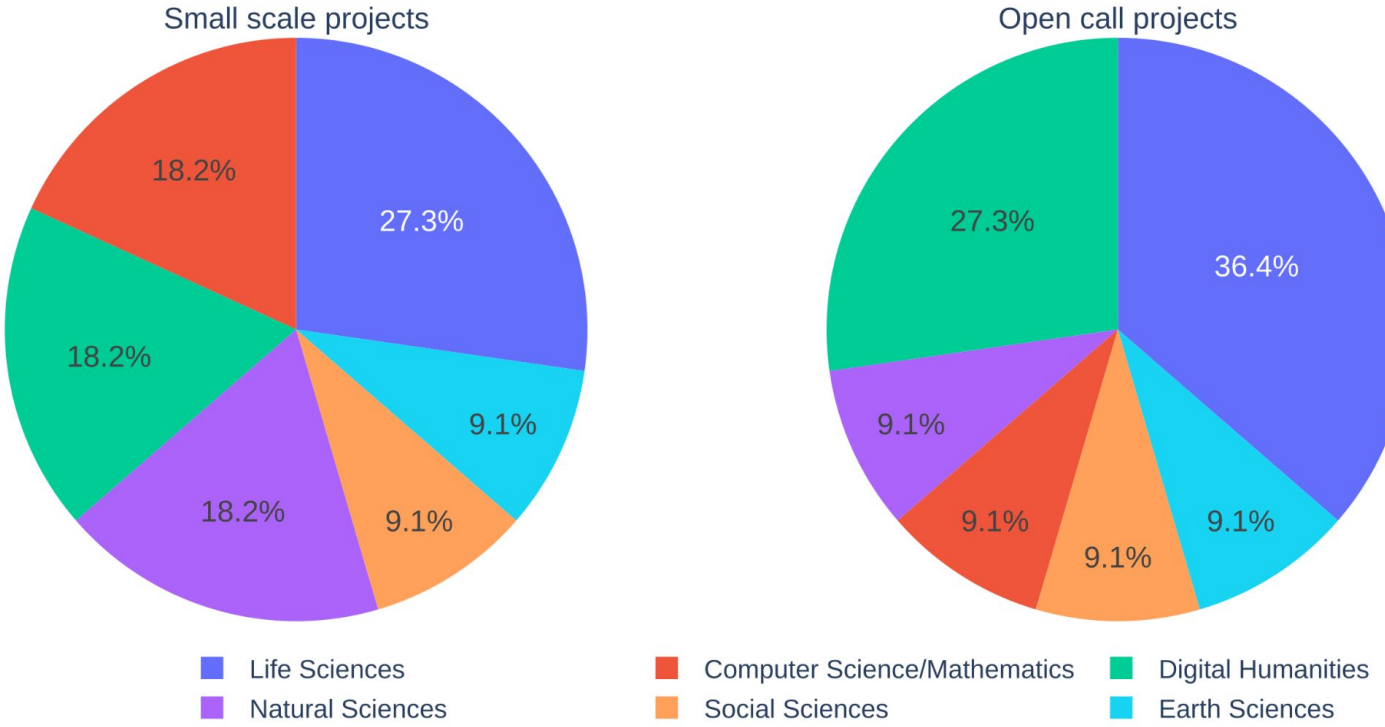
Structure prediction of biomolecules

Protein structures, DNA / RNA,
small molecules

From small scale projects to long term
collaboration



Distribution of small-scale and open call projects 2021-2023



Training

- Consultation
  - Researchers can come to us for a free consultation on any software development issue
- Compact courses
  - We offer regular courses on a variety of software development topics
- Fellows
  - Annual fellowship offering one-to-one mentoring to early career researchers
- HiWis
  - Our HiWis contribute to our projects and learn best practices

Example: Courses

Compact Courses: Software Engineering Best Practices

- The Unix Shell
- Version Control with git
- Open Source Licensing
- Automated Testing with GitHub Actions
- A short tour of sustainable software development
- Containers in Science: Using Docker and Singularity
- Advanced Topics in Version Control with git
- Effective Software Testing
- AI in research software
- Generative AI for writing (research) software

Compact Courses: Language-specific

- Python Best Practice
- Introduction to Python Testing
- Data Exploration with Python and Jupyter
- Python Packaging

Compact Courses: High-performance computing

- Performance Benchmarking C++ Applications
- High Performance C++

Seminar Series

- Lunch-time Python

Block Courses

- Scientific Software Development

Outreach

- Contributing to “*A guidelines and policy template for the development of research software at German research institutions*” (GI e.V., de-RSE e.V.)
  - https://doi.org/10.18420/2025-gi_de-rse
- SSC Whitepaper
  - https://doi.org/10.5281/zenodo.10867902
- Position papers
  - Co-authors of several de-RSE / GI position papers
- Attending and organising conferences
  - deRSE25, Code for Science symposium
- National organisations
  - We’re active in the national organisations such as de-RSE

Getting in touch

- Our website: ssc.uni-heidelberg.de
- Our email: ssc@uni-heidelberg.de
- Our offices: 4/410, 4/408, 1/222, Mathematikon, Im Neuenheimer Feld 205

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