

bwRSE4HPC

*A blueprint for better research
software in Baden-Württemberg*

Jasmin Hörter, Dominic Kempf, Marcel Koch

Motivation



Research software is an integral component in modern research, but

- it is usually developed by domain researchers with little formal education on best practices
- the publishable outcome is prioritized over sustainability of software

Bad software poses a risk to research

- can lead to non-reproducible results
- waste of researcher's time, waste of energy, ...

Identifying needs



HPC in BW: 5 Tier-3 Cluster (bwHPC), 1 Tier-2 Cluster (HoreKa, NHR), 1 Tier-1 Cluster (Hunter, GCS)

bwHPC-S5: federated support

- domain specific competence centers and HPC cluster operators
- centralized bwSupportPortal and complementary courses and workshops
- Focus on cluster management, rapid response/short term support

NHR@KIT: Call-for-Collaboration

- domain specific research projects with added support component
- mainly PhD students and early career researchers
- Not enough RSE expertise, primary focus is individual research

- Need for dedicated RSEs that work together with user groups (>2 weeks)

bwRSE4HPC

- 5 fully funded RSEs at KIT and Uni Heidelberg
- Funding period: 01.2025-12.2027

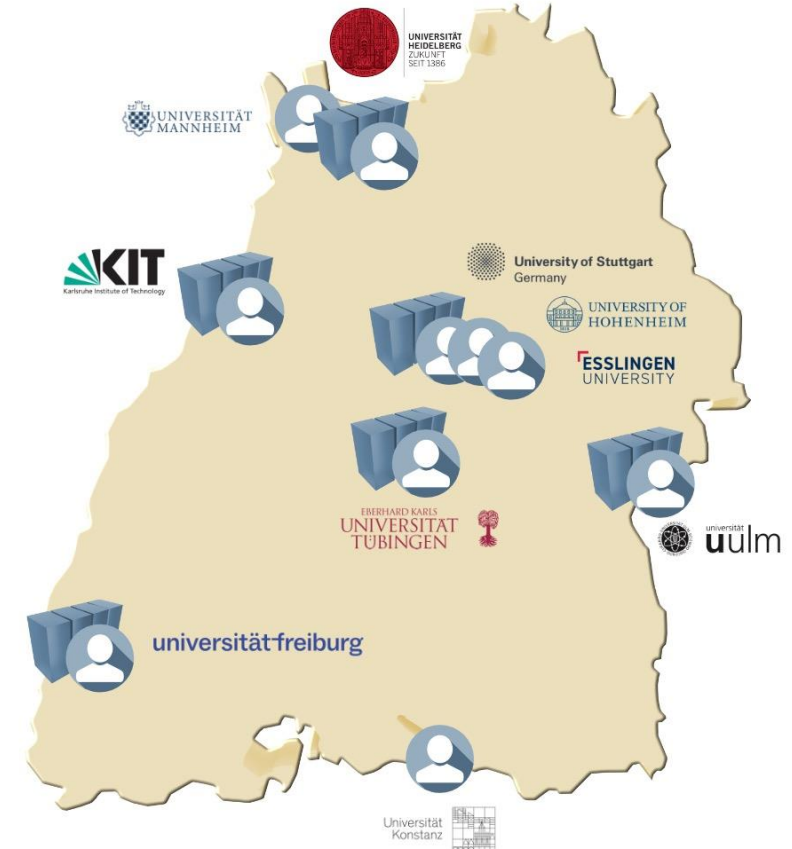


Baden-Württemberg
Ministerium für Wissenschaft,
Forschung und Kunst



Goals

- Provide software development services for (prospective) HPC users and strengthen RSE practices
- Complement the existing support services
- Cover all application fields and universities
- Demonstrate the scientific value of research software development → cooperation on equal terms, co-authorship



Software Development Areas



Performance

- Algorithmic development
- Interfacing with optimized libraries
- Generic optimizations

Usability

- Language bindings

Sustainability

- Modernizing the build system
- Refactoring to remove code debt

Emerging HPC

- Adding parallelism, shared and/or distributed memory

From Laptop to HPC

Workflow Software Projects



First contact via mail or bwSupportportal

Issues: Performance, Useability, Sustainability,
From Laptop to HPC, Emerging HPC

Team of 2 RSEs; check if request is in scope (BW? HPC? Too extensive? ...)



Introductory consultation

Discuss status quo and preferred outcome; get access to code, data, cluster, ...

Work plan (suggested solution, milestones, expected contributions from users) → cooperation on equal terms



Approval and working phase

1.5 RSEs work on the project for up to 6 months, regular progress updates and meetings with users

Internal reporting and quarterly meeting of the bwRSE4HPC team



Final report

Ensure sustainability of solution, publish results, collect feedback from the users

Publish project report; follow-up after 6 months

Long-Term Projects



- Some projects need more time and attention than we can cover in 6 months
 - Long-term research projects with a significant software component
 - Long-term maintenance
 - We cover the RSE aspects in exchange for additional funding
 - Joint third-party funding proposal
 - RSE as a Service
- Diversify funding and growing our team



Integration into HPC landscape in BW

- Regular exchange with other support initiatives (bwHPC-S5, Helmholtz AI, NHR@KIT, NFDI, ...)
- BW HPC user committee as sounding board for ideas and user needs

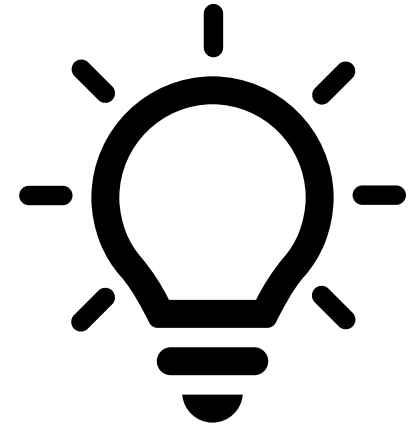
Example: Training

- Complement the existing bwHPC training landscape with specialized courses
- Address most common questions/issues from user projects
- New workshop „Sustainability in research software for HPC“

Difficulties and Lessons learned



- Advertisement, advertisement, advertisement, ...
- There is a lot of demand, but it is difficult to reach users
 - targeting inefficient jobs via cluster monitoring
- Working with and complementing existing initiatives/ infrastructure saves time and resources
 - bwSupportportal, cluster mailing lists for advertisement
- Improving software requires time from both the RSE and the user group



Contact



<https://www.bwrse4hpc.de>

support@bwrse4hpc.de

