

High-Performance Computing and Coordinated Compute Cluster Competence Centers in Baden-Württemberg

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Baden-Württemberg's initiative on high-performance computing (**bwHPC**) has been establishing a permeable HPC ecosystem throughout all performance levels (i.e., tiers) including a federated and purpose customized, multi-cluster entry level as well as state-wide coordinated HPC support and competence centers. Clusters, implementation activities and support services are co-funded by Baden-Württemberg's Ministry of Science, Research and the Arts and largely coordinated by the corresponding project **bwHPC-C5**. Driven by a successful and positively reviewed transition phase (i.e., from 2013 until 2015) the project bwHPC-C5 Phase 2 aims between 2016 and 2018 for continuation and expansion of Baden-Württemberg's HPC tier-3 services.

1 Introduction

High-performance computing in the state of Baden-Württemberg has a long tradition. The current implementation concept for Baden-Württemberg's high-performance computing from 2013 until 2018, officially labelled **bwHPC** [1], has been aiming for the implementation of HPC clusters covering all HPC performance and scalability levels, i.e., HPC tiers, (Fig. 1) for permeability throughout all HPC tiers, differentiation/customization of tier-3 services to the requirements of scientific areas, and providing federated HPC support via competence centers. The initiative bwHPC recommended by the German Research Foundation (DFG) for funding is considered a model concept for Germany advancing the impact of HPC.

The accompanying state-wide project of bwHPC – officially labelled “bwHPC-C5” which is short for bwHPC: Coordinated Compute Cluster Competence Centers [2] – coordinates all associated provisions and activities to establish HPC competence centers and cooperative HPC operations, unify user environment, pool HPC expertise, as well as identify and implement HPC innovations. Moreover, bwHPC-C5 raises awareness of Baden-Württemberg's HPC, helps to embed the scientific communities into the HPC world and creates synergies for the development of state-wide user support. The project bwHPC-C5 is co-funded by Baden-Württemberg's Ministry of Science, Research and the Arts (MWK).

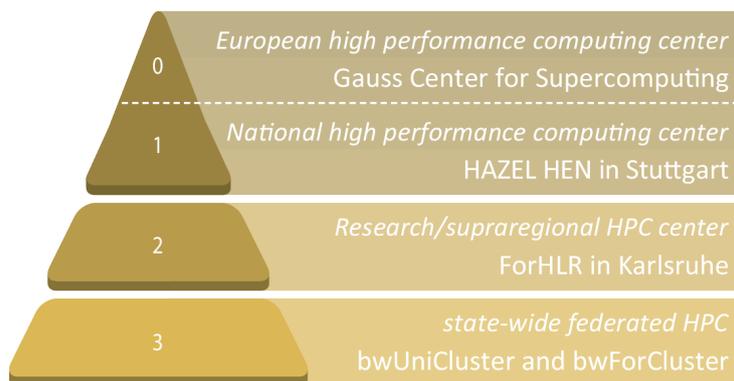


Figure 1: HPC performance pyramid in the state of Baden-Württemberg, Germany: from top (tier 0) to bottom (tier 3) with decreasing scalability and performance level.

2 Federated HPC tier-3

Since late 2016 all clusters of Baden-Württemberg’s HPC tier-3 are operational. The HPC entrance level consists of the bwUniCluster (bw = Baden-Württemberg, Uni = Universal/University) and 4 bwForClusters (For = Forschung, German for Research). The latter ones are tailored to the needs of particular scientific communities and their specific applications while the former one provides the resources of Baden-Württemberg’s universities for general purpose computing covering teaching and all science communities without a dedicated bwForCluster (Tab. 1).

Cluster	Location	Start date	Purpose
bwUniCluster	Karlsruhe	Jan 2014	General purpose, teaching
bwForCluster JUSTUS	Ulm	Dec 2014	Computational chemistry; high I/O, large MEM jobs
bwForCluster MLS&WISO	Heidelberg / Mannheim	Dec 2015	Molecular life science, economics and social science; method development
bwForCluster NEMO	Freiburg	Sep 2016	Neuro science, elementary particle physics, micro systems engineering; VM image deployment
bwForCluster BinAC	Tübingen	Nov 2016	Astrophysics, bioinformatics; 60 dual GPU nodes

Table 1: bwHPC tier-3 clusters: location, operational start date and their main purpose.

3 Services and achievements of bwHPC-C5

bwHPC-C5 offers a comprehensive and demand-oriented service for users in Baden-Württemberg for the existing HPC systems. The bwHPC-C5 project assembles a team of more than 30 people from 11 Baden-Württemberg universities¹.

¹Universities of Freiburg, Tübingen, Ulm, Heidelberg, Hohenheim, Konstanz, Mannheim, Stuttgart, the KIT and the universities of applied sciences in Stuttgart and Esslingen.

Access services: bwHPC-C5 is committed to install new levels of federated service management which in particular provides enhancement for users. For logging into bwHPC clusters via home organisation credentials bwHPC-C5 has integrated Baden-Württemberg’s federated identity management (bwIDM) in the cluster infrastructure. To transparently apply the usage policies of bwHPC, hence process compute project applications for all bwForClusters, the bwHPC-C5 team has developed and is using the central application site (ZAS) [3] as well as assembled the cluster assignment team.

Software services: bwHPC-C5 has managed to set up the same environment and behaviour throughout all tier-3 HPC clusters. Moreover, comprehensive HPC software stacks – in case of bwUniCluster and bwForCluster JUSTUS over 200 and 100 software modules, respectively – together with extensive help built-ins and installation description have been installed which have been expanding upon demands and user requests.

Support services: Competence centers for bwHPC, which have been established by the project bwHPC-C5, play a central role in the science specific HPC support as these centers unite technical experts and field specialists and coordinate the high-level support projects (aka tiger team projects). bwHPC competence centers match the scientific fields of the bwForClusters, but also cover areas of expertise without dedicated cluster resources (Fig. 2). Tiger team projects are

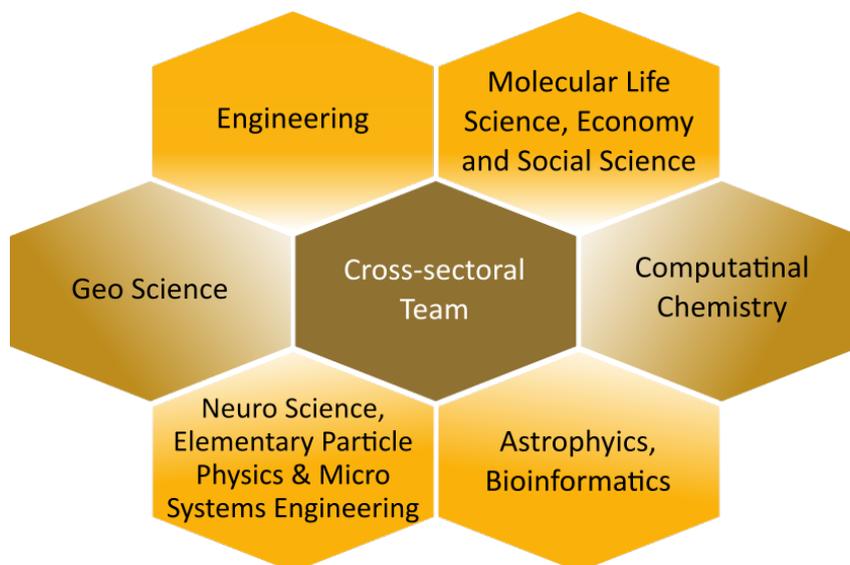


Figure 2: bwHPC competence centers covering the dedicated scientific areas of the bwForClusters, but also three areas of expertise without cluster resources.

the project’s most elaborated support activities resulting in 30 collaborations with the scientific communities since 2013 [4]. Other support activities of the bwHPC competence centers are: providing online best practice and user guides [5], aiding in parallelization of application codes and in accessing HPC or traversing to higher HPC tiers, provisioning development tools and scientific software on the HPC systems, and providing tools to manage scientific data. Together with other members of the bwHPC-C5 team HPC courses (incl. materials) [6] have been organized and held at the Baden-Württemberg universities with 36 HPC introductory, 7 programming, 21 HPC tools, 25 parallel programming, 3 visualization, and 7 compiler and debugging courses

since 2014. Furthermore, the current support infrastructure of bwHPC-C5 has more than 20 state-wide HPC support units dealing with all kind of HPC related second level support issues.

Dissemination: bwHPC-C5 has been publishing all results of bwHPC (e.g. user's publications [7]), reporting and answering to the (user) steering committees as well as promoting the bwHPC infrastructure to raise awareness of HPC (and bwHPC in particular) to all science communities. To enhance the impact of the scientific communities on bwHPC, the bwHPC-C5 team provides the platform for an annual meeting between users and support/operations teams, namely the bwHPC symposium.

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References

- [1] Hartenstein, H., T. Walter, and P. Castellaz. "Aktuelle Umsetzungskonzepte der Universitäten des Landes Baden-Württemberg für Hochleistungsrechnen und datenintensive Dienste." *Praxis der Informationsverarbeitung und Kommunikation*, Band 36, Heft 2 (2013): 99-108. <http://dx.doi.org/10.1515/pik-2013-0007>
- [2] Barthel, R., T. König. "Landesprojekt "bwHPC-C5" gestartet: Föderative Fachkompetenzzentren unterstützen Landesnutzer beim Einstieg ins Hochleistungsrechnen". *SCC-News*, 02-2013, pp 6-9.
- [3] <http://www.bwhpc-c5.de/en/ZAS>
- [4] http://www.bwhpc.de/en/tiger_team_projects.php
- [5] <http://www.bwhpc.de/wiki>
- [6] <http://training.bwhpc.de>
- [7] http://www.bwhpc.de/en/user_publications.php