

bwHPC: Concept, Infrastructure and State-wide User Support

Robert Barthel, SCC, KIT



UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386

Hochschule Esslingen
University of Applied Sciences

Universität
Konstanz



UNIVERSITÄT
MANNHEIM



Universität Stuttgart

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



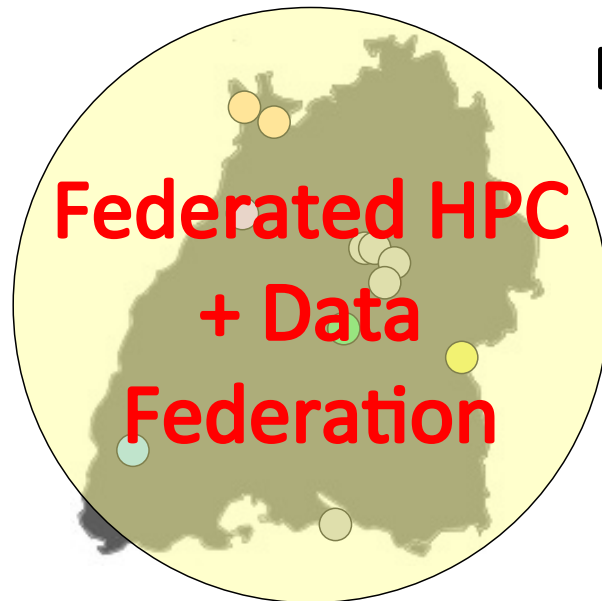
KIT
Karlsruher Institut für Technologie



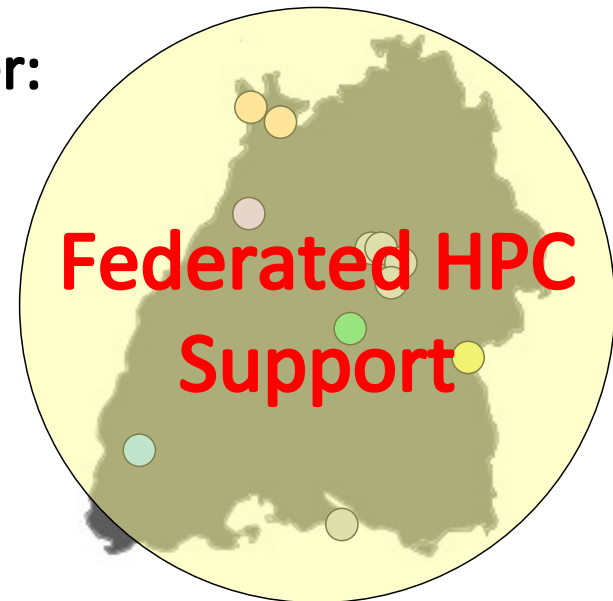
ulm university universität
uulm



What is **bwHPC**?
What is **bwHPC-S5**?
Where do I get / What kind of **Support**?

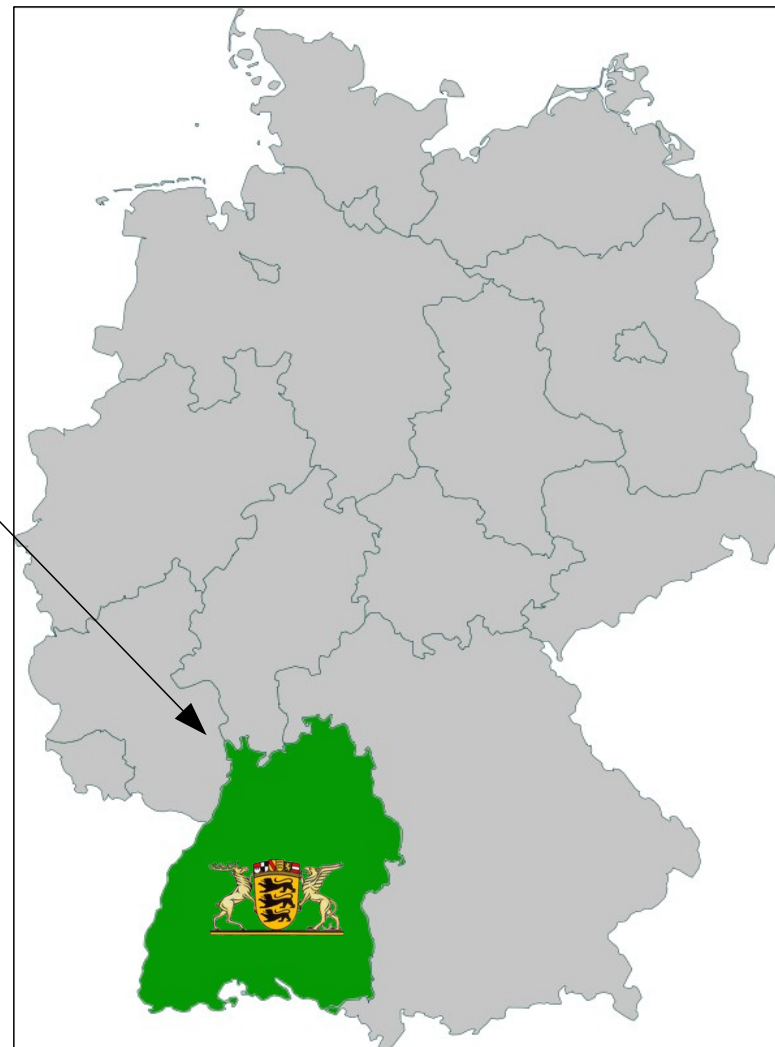


Brief answer:



1. bwHPC

What is bwHPC/bwHPC-S5?



bw = Baden-Württemberg

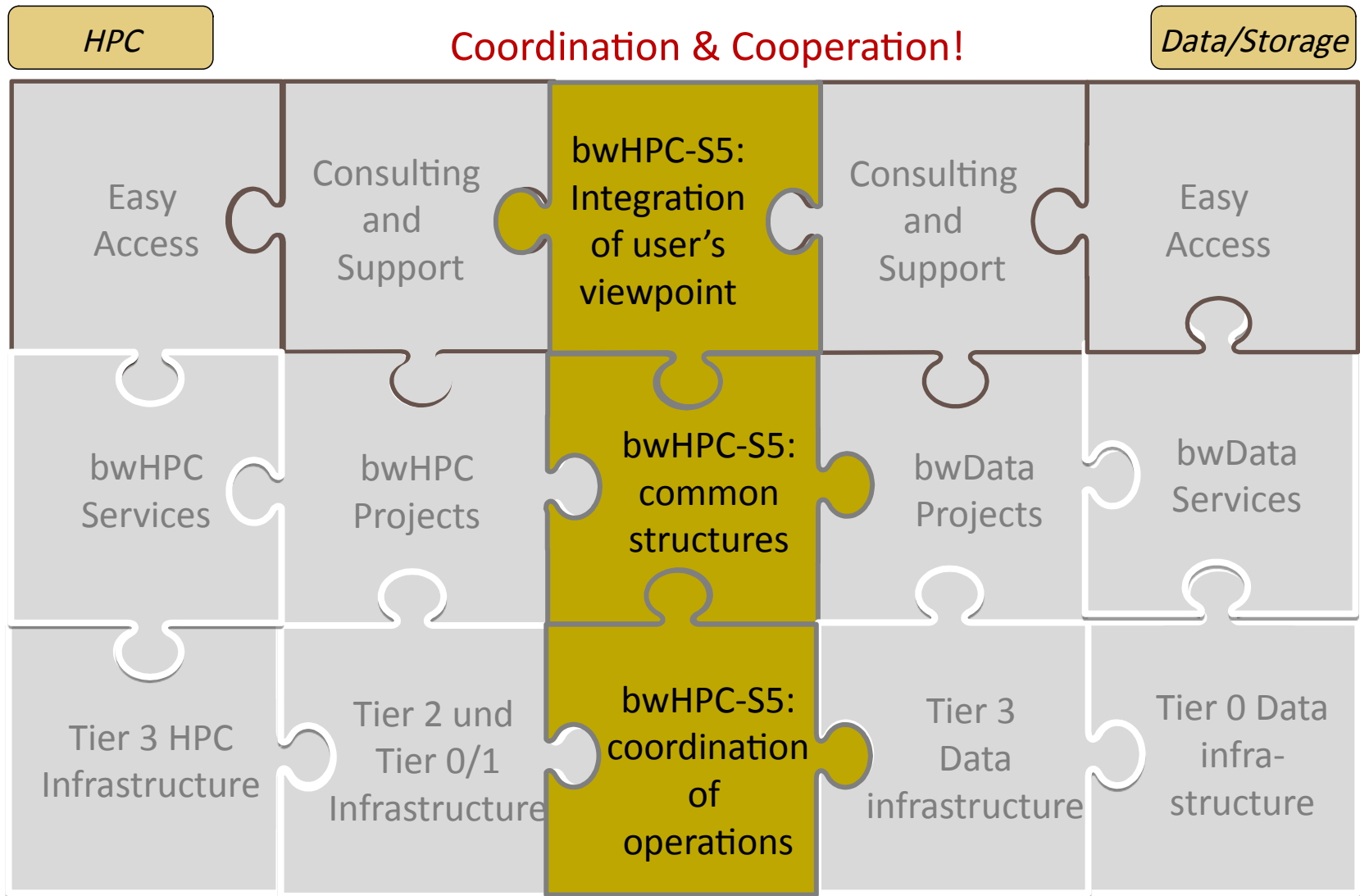
bwHPC = Initiative for implementing high performance computing cluster and data federation and corresponding support infrastructure

bwHPC-S5 = User and IT support for bwHPC and data federation

||

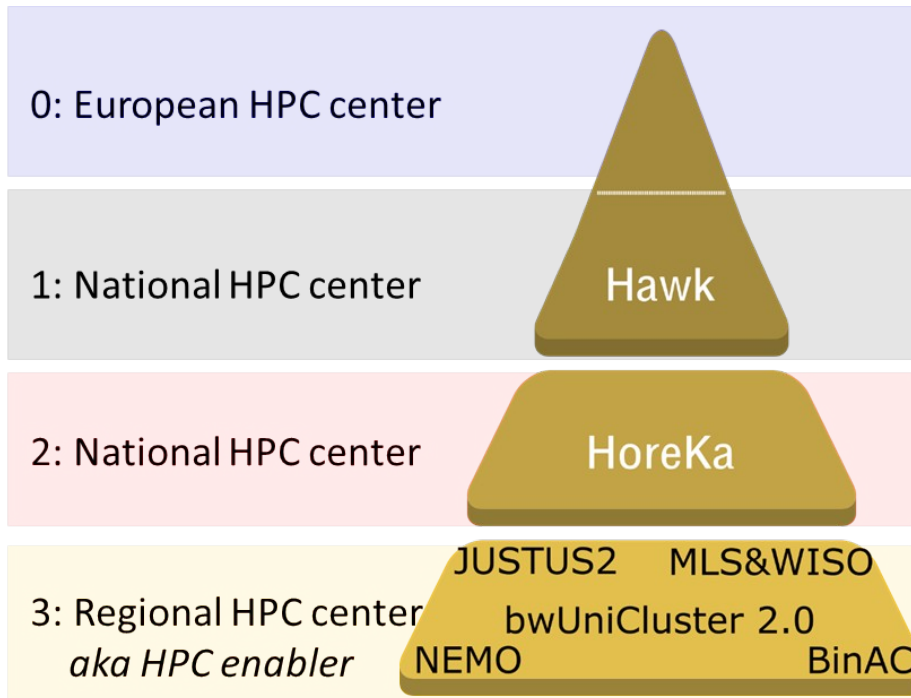
Cooperated activities

What is bwHPC-S5?

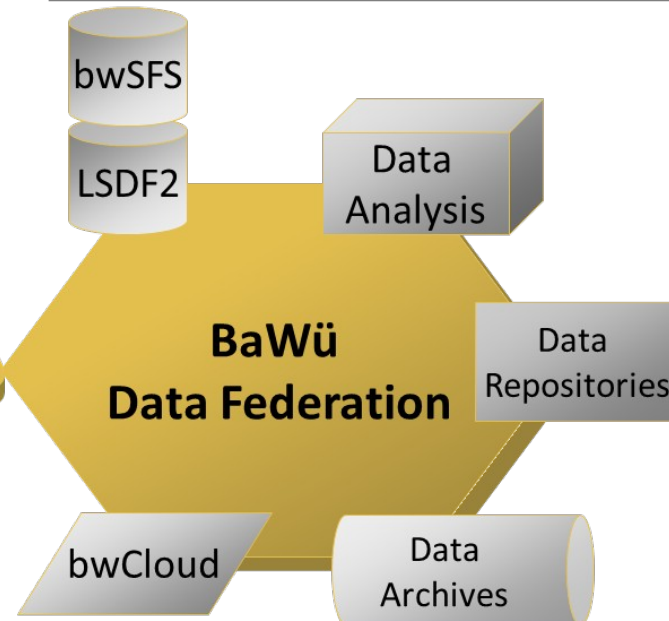


bwHPC 2.0 (2018 - 2025)

Baden-Württemberg's implementation strategy for **HPC**, **Data Intensive Computing** & **Large Scale Scientific Data Management**



- *Advancement of federated HPC@tier3*
- *Establishing the BaWü data federation*
- *Advancement of support project focusing on integration of HPC & Data*
- *Competence centers for HPC & Data*



HPC and Data Facilities: Purpose

LSDF 2 (SDS@hd/ LSDFOS)

Hot Data: Life Sciences, Medical Science, Hydro-mechanics, Humanities, Astrophysics, Scientific Computing / GP

bwForCluster Helix (08/2022):

Structural and Systems Biology, Medical Science, Comp. Humanities & Soft Matter
Successor of: **MLS&WISO**

bwUniCluster 2.0 (03/2020):

General purpose, Teaching & Education

bwForCluster JUSTUS 2 (07/2020):

Computational Chemistry, Quantum Sciences

bwDataArchive (KA)

Cold Data: General purpose

Future Data Facilities

bwForCluster NEMO (09/2016):

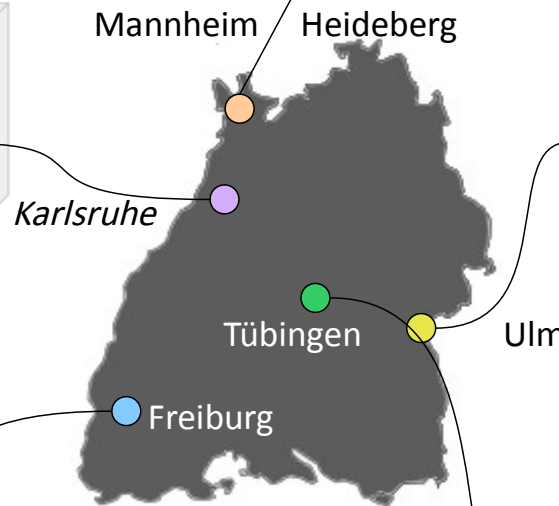
NeuroSc, Micro Systems Eng., Elementary Particle Phys.,
Successor: **NEMO 2**, approved by DFG

bwSFS (FR/TU)

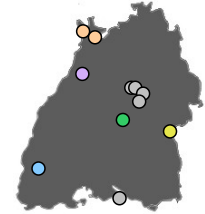
Bioinformatics, Elementary Particle Physics, Micro Systems Eng., NeuroSc., Systems Biology

bwForCluster BinAC (11/2016):

Bioinformatics, Astrophysics, Geosciences
Successor: **BinAC 2**, approved by DFG



bwUniCluster 2.0



■ Shareholders:

- Freiburg, Tübingen, KIT, Heidelberg, Ulm, Hohenheim, Konstanz, Mannheim, Stuttgart, and HAW BW e.V. (an association of university of applied sciences in Baden-Württemberg)
- Baden-Württemberg's ministry of science, research and arts (MWK)

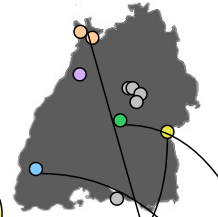
■ Access:

- For all members of **shareholder**'s university in BW
 - For all members of the universities of applied sciences in BW
- How?** → Entitlement → Registration → Questionnaire → Login
(Details: 2. Talk today)

■ Usage:

- Free of charge
- For general purpose, teaching & education
- For technical computing (sequential & weak parallel) & parallel computing

4x bwForClusters



- Shareholders
 - German Research Society (DFG)
 - Baden-Württemberg's ministry of science, research and arts
- Access (*Details: 2. Talk today*):
 - All university members in Baden-Württemberg
 - How? → Entitlement +
Compute Project Proposal →
Registration → Login
- Usage:
 - Free of charge
 - **Approved** Compute Project Proposal **to only 1 bwForCluster matching cluster's subject fields**

bwForCluster JUSTUS 2

(07/2020):
Theoretical Chemistry, Condensed matter physics, Quantum physics

bwForCluster Helix

(08/2022):
Structural and Systems Biology, Medical Science, ...

bwForCluster BinAC

(11/2016):
Bioinformatics, Astrophysics, ...

bwForCluster NEMO

(09/2016):
Neurosciences, Micro Systems Engineering, Elementary Particle Physics, ...

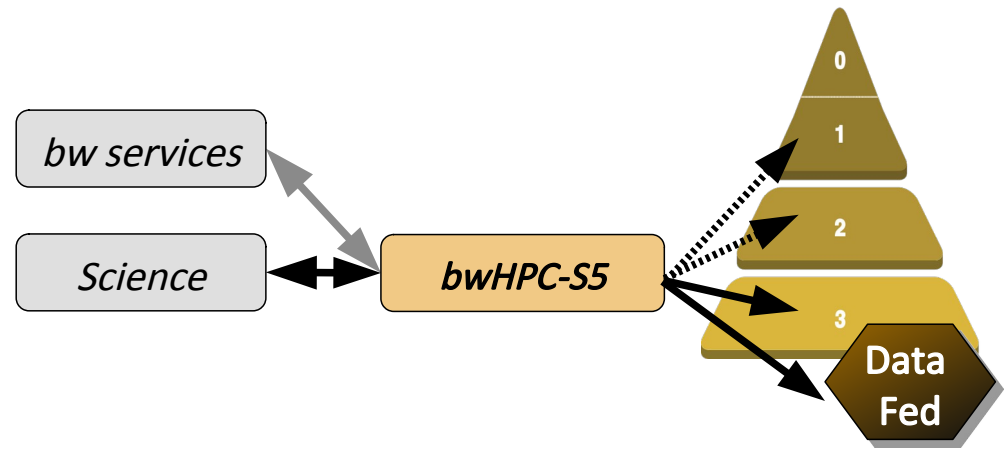
2. bwHPC-S5

Scientific Simulation and Storage Support Services (bwHPC-S5)

HPC & Data Fed. @ BaWü

■ Goal?

- Bridging science & HPC
- Bridging HPC tiers and Large Scale Scientific Data Facilities (LS²DM)
- Embedding services

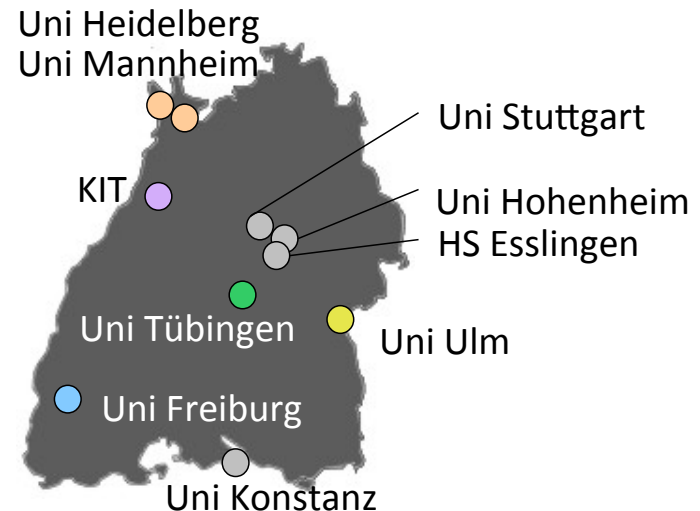


■ Where are these competence centers?

→ Organised by 8 universities

■ Who ?

→ Experts from 10 universities



bwHPC-S5: What kind of support?

- Seminars and workshops
 - coordinated by 10 BaWü universities
- Documentation + best practices → wiki
- HPC and Data Competence Center:
 - Coordination of tiger teams
 - Help concerning: Code/workflow adaptation, porting and parallelization
 - Identify of user key topics
 - Help to access tier 2 (HoreKa) and 1 (Hawk)
 - Establish state-wide experts pool
- Providing/maintaining:
 - Community specific & HPC generic software and tools,
 - Data management tools for using e.g. [bwDataArchive](#) or [SDS@hd](#)



The screenshot shows the main page of the bwHPC Wiki. At the top, there is a navigation bar with links for 'Main page', 'Discussion', 'Read', and 'View source', along with a search box labeled 'Search bwHPC Wiki'. The main heading is 'Main Page'. Below this, a welcome message reads: 'Welcome to the bwHPC Wiki. bwHPC represents services and resources in the State of Baden-Württemberg, Germany, for High Performance Computing (HPC), Data Intensive Computing (DIC) and Large Scale Scientific Data Management (LS2DM). The main bwHPC web page is at <https://www.bwhpc.de/>. Many topics depend on the cluster system you use. First choose the cluster you use, then select the correct topic.'

There are three main sections highlighted with colored backgrounds:

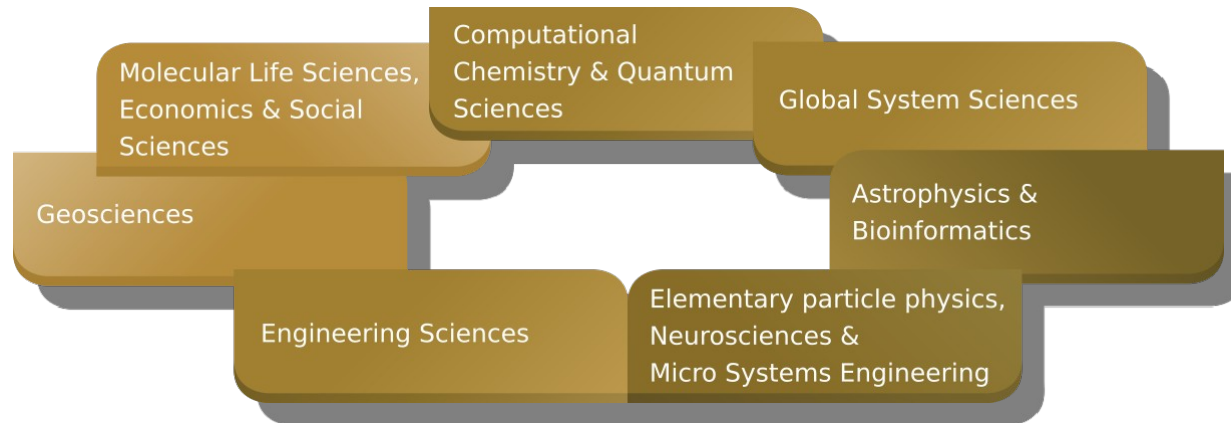
- Courses / eLearning** (purple background):
 - [eLearning and Online Courses](#)
 - [Introduction to Linux in HPC \(external resource\)](#)
- Need Access to a Cluster?** (green background):
 - [Registration](#)
- HPC System Specific Documentation** (light green background):

bwHPC Clusters are dedicated to [specific research domains](#). Documentation differs between compute clusters, please see cluster specific overview pages:

bwUniCluster 2.0	General Purpose, Teaching
bwForCluster JUSTUS 2	Theoretical Chemistry, Condensed Matter Physics, and Quantum Sciences
bwForCluster	Computational Humanities, Structural and Systems Biology, Medical Science, and Soft

A sidebar on the left contains various navigation links: Home, bwHPC Systems, bwUniCluster 2.0 JUSTUS_2, Helix, NEMO, BinAC, Documentation, Batch Jobs, Software Modules, Software Search, Support, eLearning, Ticketing System, Feedback, Data Storage, SDS@hd, bwDataArchive, Tools, What links here, Related changes, Special pages, Printable version, Permanent link, and Page information.

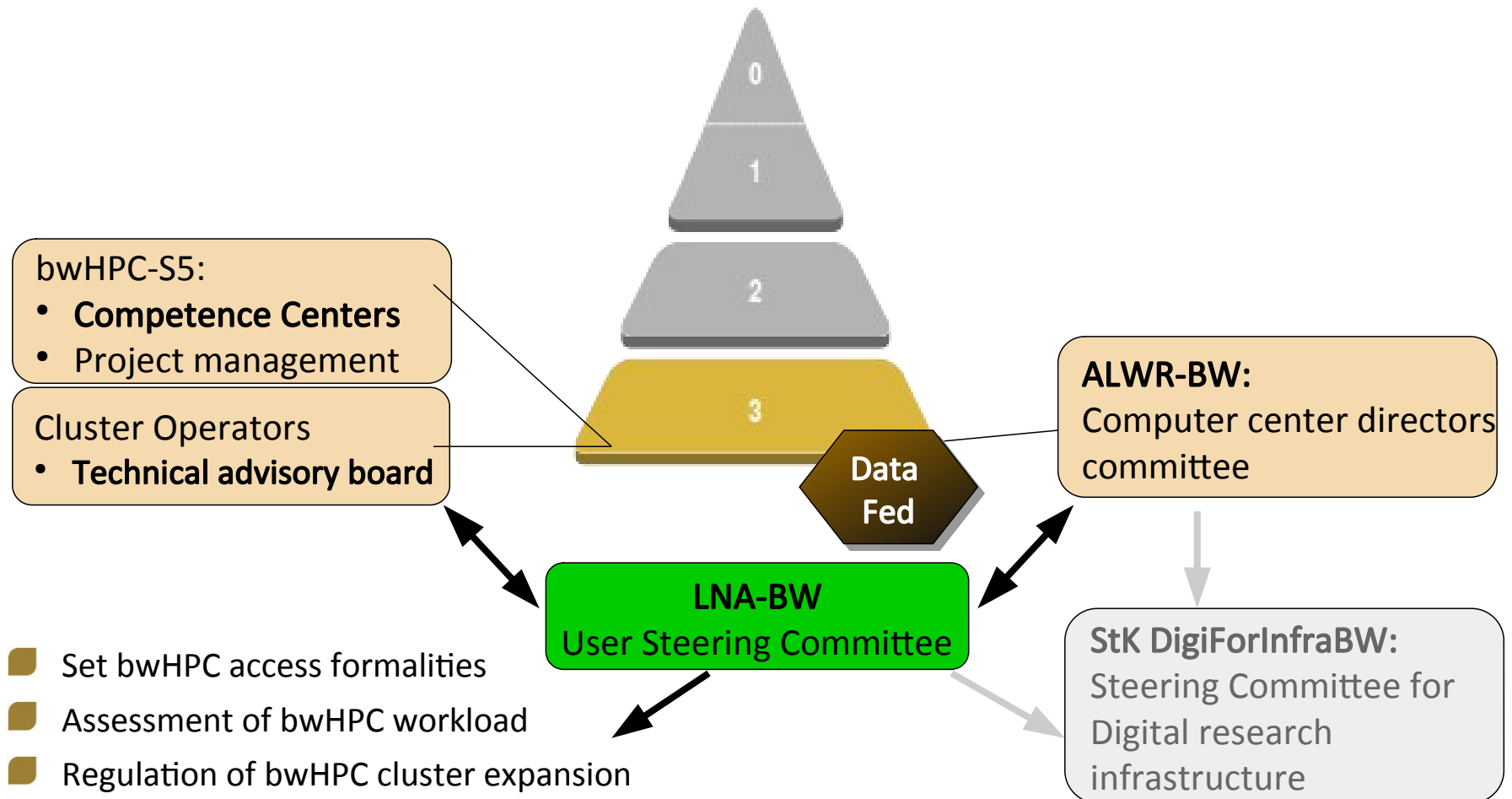
How to get support?



- Scientific specific support?
 - Choose your competence center → contact via [email](#), [trouble ticket](#)
 - Wiki: [best practice guides](#)
- Extensive support needed?
 - [Tiger team support](#)
- Cluster specific support?
 - Choose your cluster → [email list of cluster](#), [trouble ticket](#), [telephone](#)
- Complaints / policy issues?
 - [email](#) or [trouble ticket](#) @ project management
 - Contact your university member of the [LNA-BW \(User Steering Committee\)](#)

Governance

bwHPC: Governance



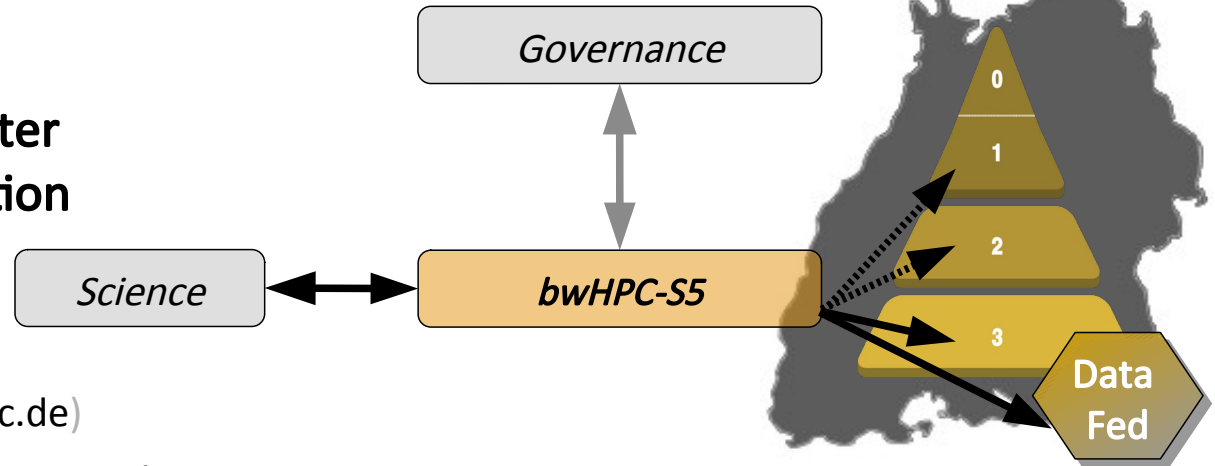
- Set bwHPC access formalities
- Assessment of bwHPC workload
- Regulation of bwHPC cluster expansion
- Assignment of science communities to science clusters and data facilities
- Representation of HPC users interests concerning:
resource demands, HPC technologies and software licences, adjustment of resource quota

Summary

Summary

■ bwHPC:

→ bwUni- & bwForCluster
+ BaWü Data Federation



→ **bwHPC-S5** (www.bwhpc.de)

= Support & Service integration, User Support

- Training courses
- User and Best Practice Guides (wiki.bwhpc.de)
- HPC and Data software maintenance & Code migration / optimisation aid
- HPC and Data innovation evaluation

→ **Governance**

- LNA-BW (user steering committee)
- Competence Centers

Thank you for your attention!

Questions?