

bwHPC: Concept, Infrastructure and State-wide User Support

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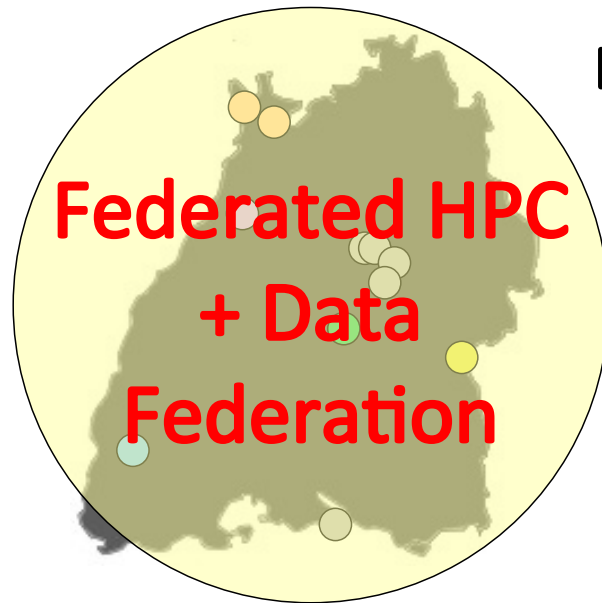
KIT
Karlsruher Institut für Technologie



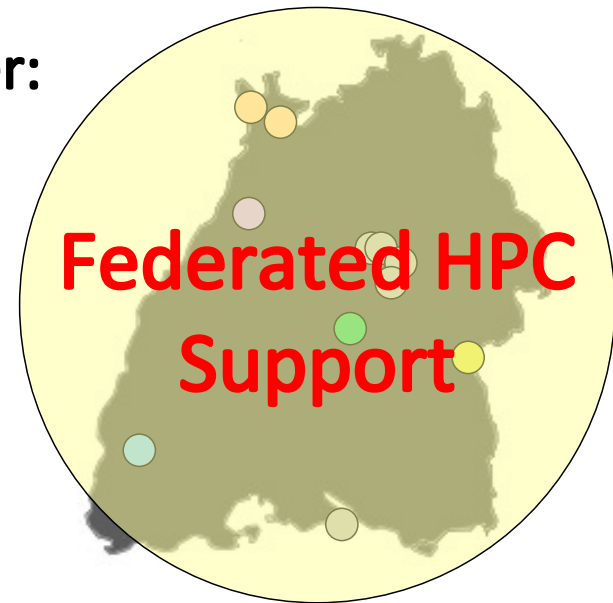
ulm university universität
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What is **bwHPC**?
What is **bwHPC-S5**?
Where do I get / What kind of **Support**?

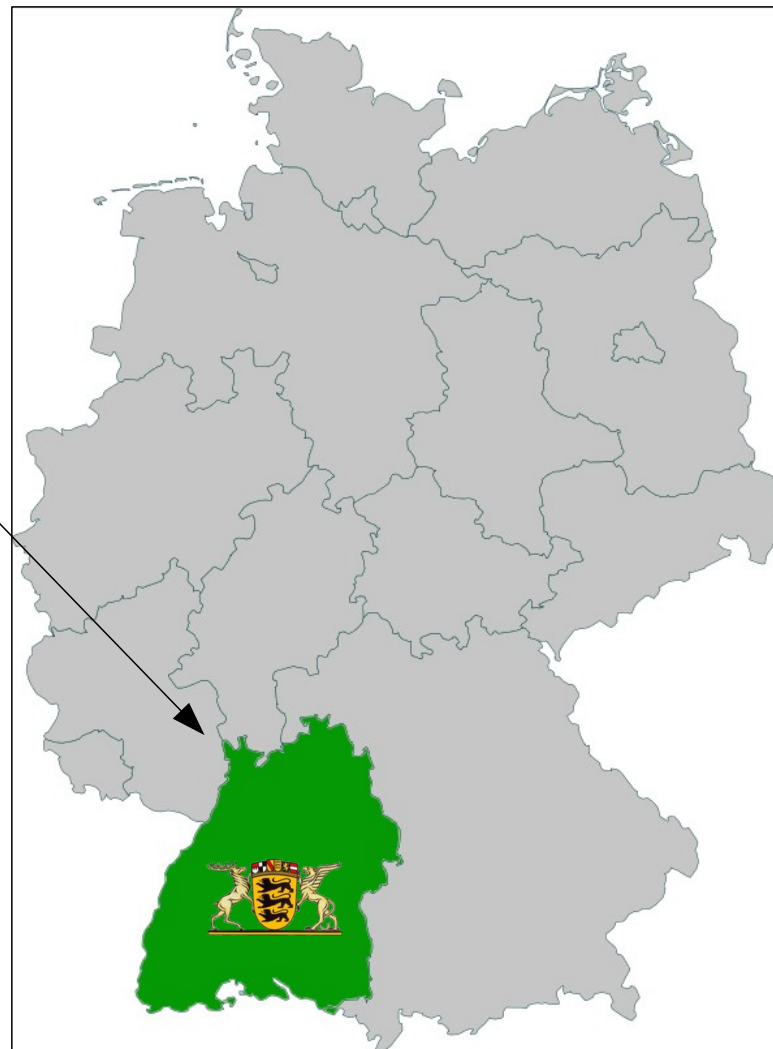


Brief answer:



1. bwHPC

What is bwHPC/bwHPC-S5?



bw = Baden-Württemberg

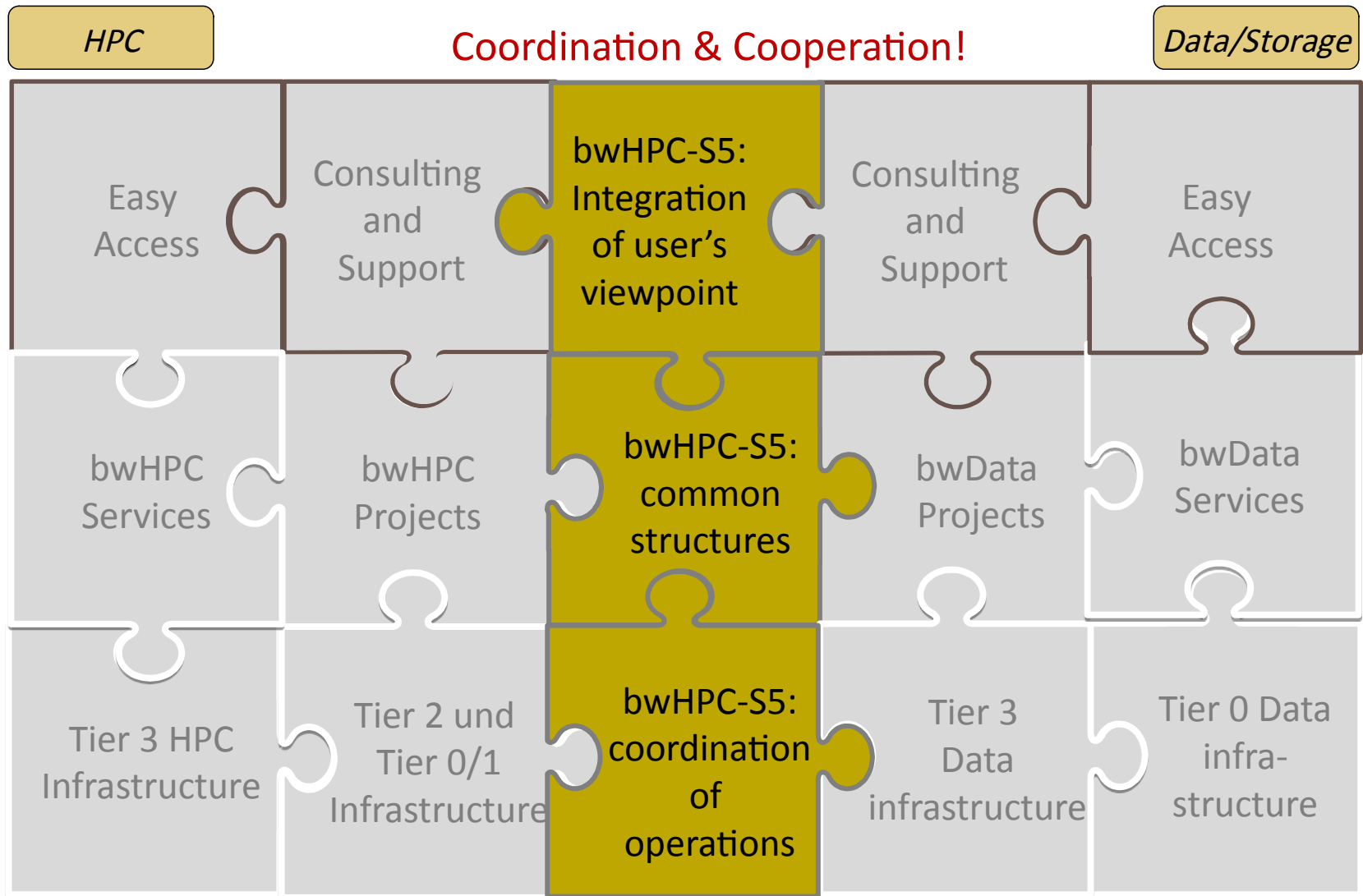
bwHPC = Initiative for implementing high performance computing cluster and data federation and corresponding support infrastructure

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

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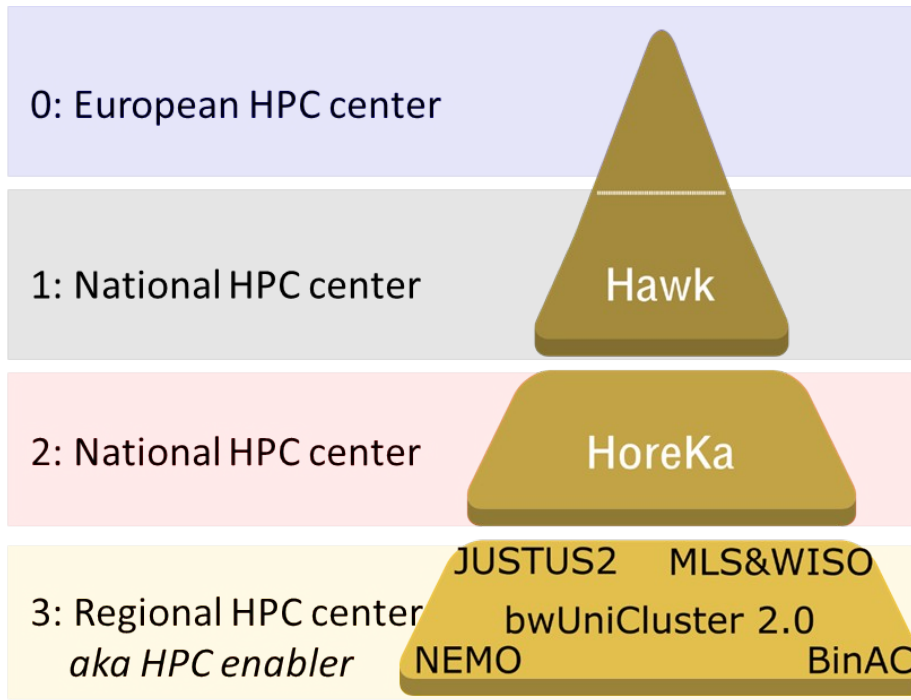
Cooperated activities

What is bwHPC-S5?

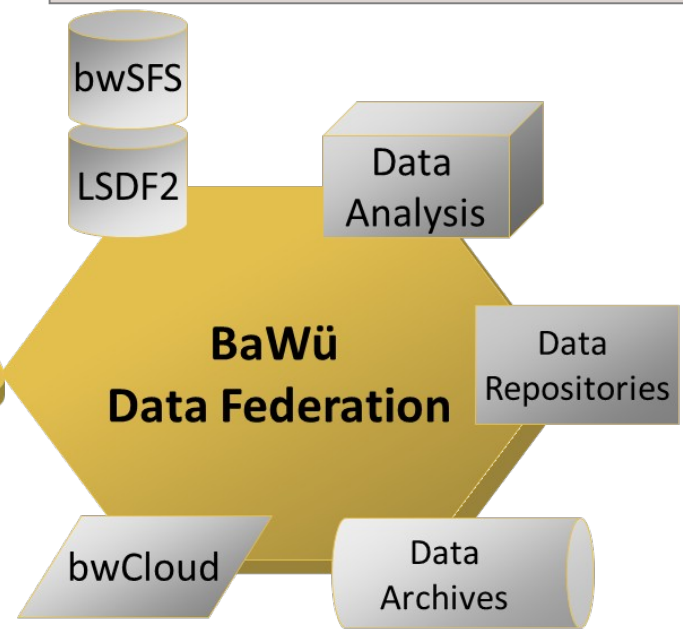


bwHPC 2.0 (2018 - 2025)

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 MLS&WISO (10/2015):

Structural and Systems Biology, Medical Science, Comp. Humanities & Soft Matter
Successor: **Helix**, approved by DFG

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):

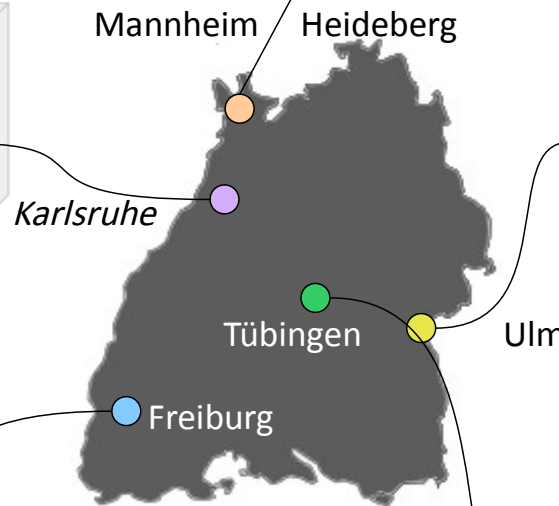
NeuroSc, Micro Systems Eng., Elementary Particle Phys.,
Successor: **NEMO 2**, approved by DFG

bwSFS (FR/TU)

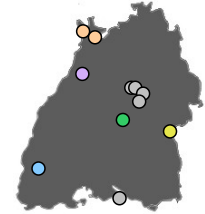
Bioinformatics, Elementary Particle Physics, Micro Systems Eng., NeuroSc., Systems Biology

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)

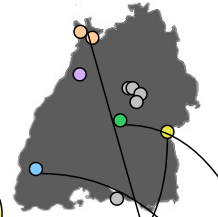
■ Access:

- 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 MLS& WISO

(10/2015):

Economics & Social Science, Molecular Life Science, ...

bwForCluster BinAC

(11/2016):

Bioinformatis, Astrophysics, ...

bwForCluster NEMO

(09/2016):

Neurosciences, Micro Systems Engineering, Elementary Particle Physics, ...

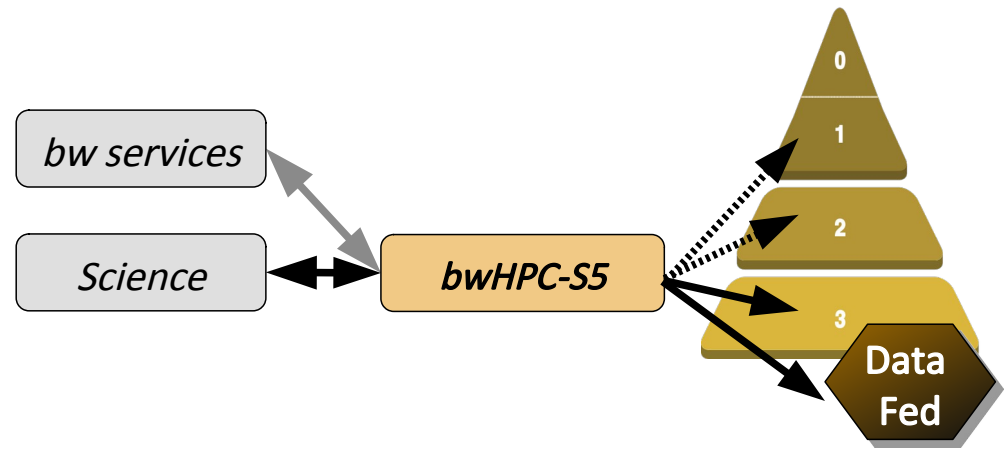
2. bwHPC-S5

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

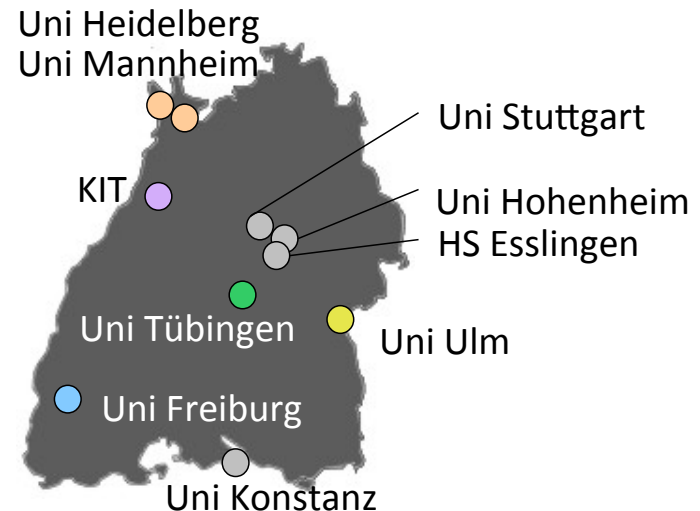


■ Where are these Competence Centers?

→ Organised by 8 Universities

■ Who ?

→ Experts from 10 Universities



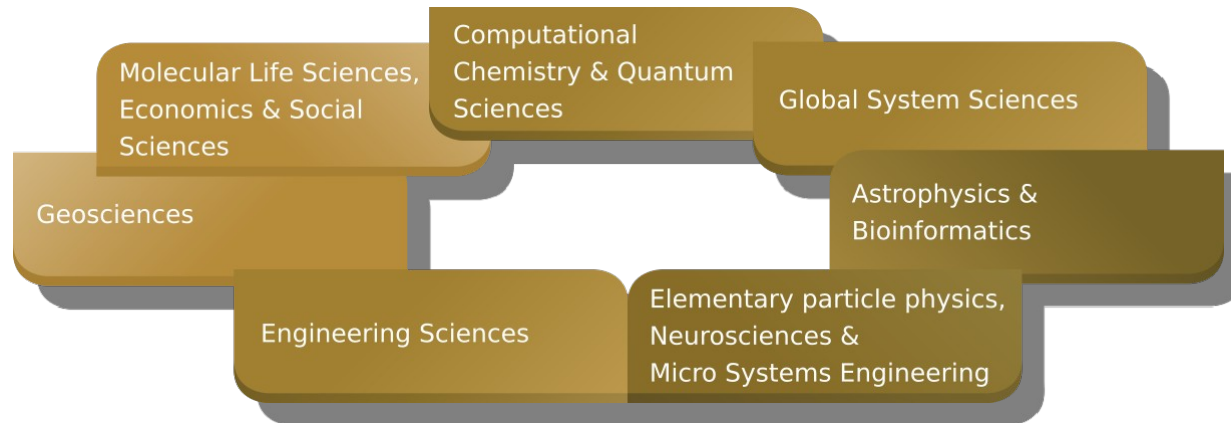
bwHPC-S5: What kind of support?

- Seminars and workshops
 - coordinated by 10 BaWü universities
- Documentation + **best practices repository** → Wiki
- HPC and Data Competence Center:
 - Coordination of **Tiger Teams**
 - Help concerning:
Code/workflow adaptation, porting and parallelisation
 - 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 tabs for 'Main page', 'Discussion', 'Read', 'View source', and a search box. The main content area features a large graphic of the state of Baden-Württemberg, Germany, with several icons of people representing different HPC centers. Below the graphic, the text reads 'bwHPC Wiki of Baden-Württemberg's HPC, DIC and LS2DM'. A sidebar on the left contains a list of links and resources, including 'Home', 'Best Practices', 'Wiki help', 'Best Practice Guides', 'Overview', 'Batch Jobs', 'Software Modules', 'Compiler', 'Numerical Libraries', 'Parallel Programming', 'bwHPC tier 3', 'bwUniCluster_2.0', 'bwForCluster JUSTUS_2', 'bwForCluster MLS&WISO', 'bwForCluster NEMO', 'bwForCluster BinAC', 'bwHPC tier 1+2', 'Hawk', 'HoreKa', 'bwHPC Support Services', 'bwHPC courses', 'Support/Ticket System', and 'Software Search'.

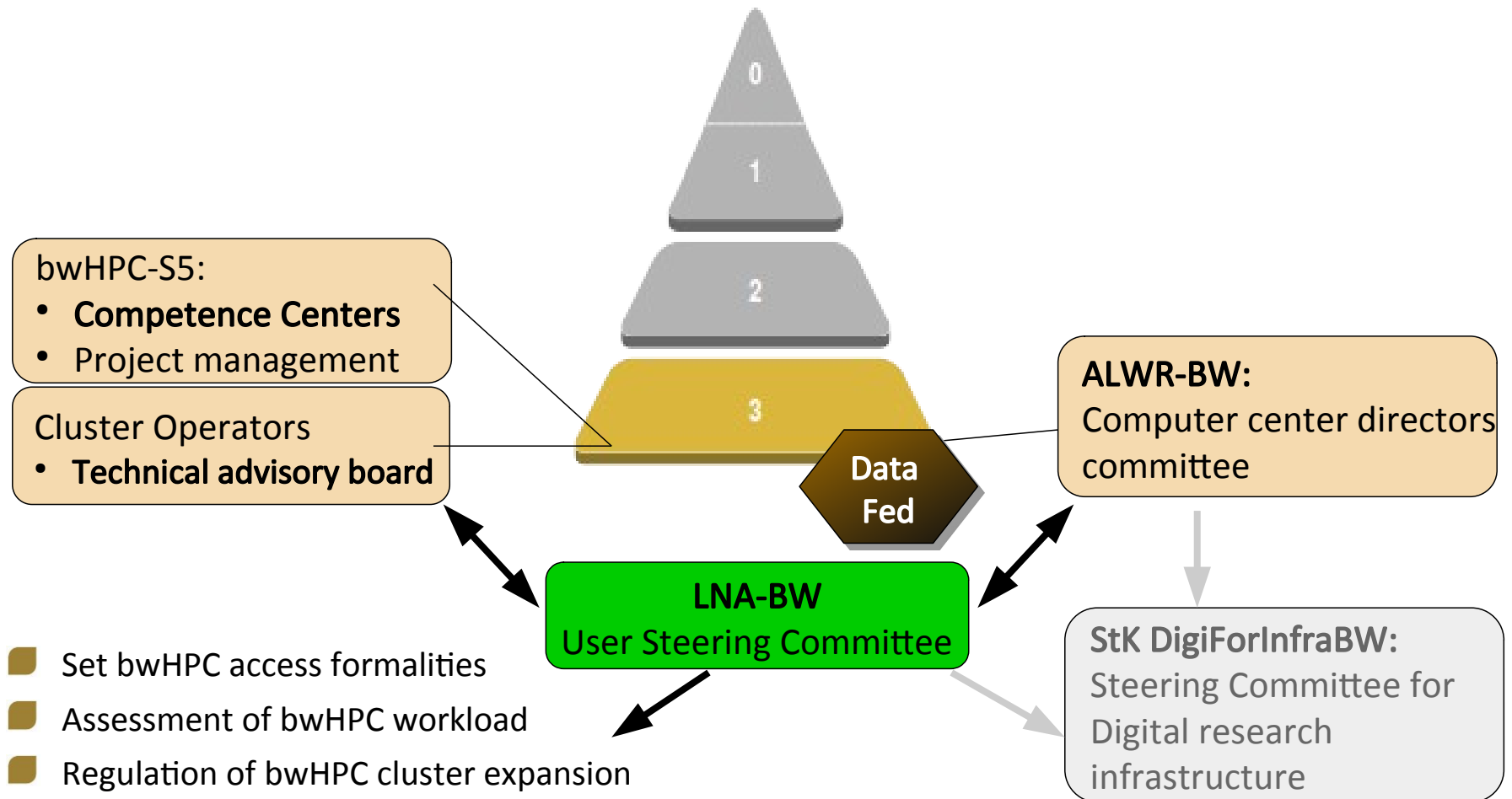
How to get support?



- 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



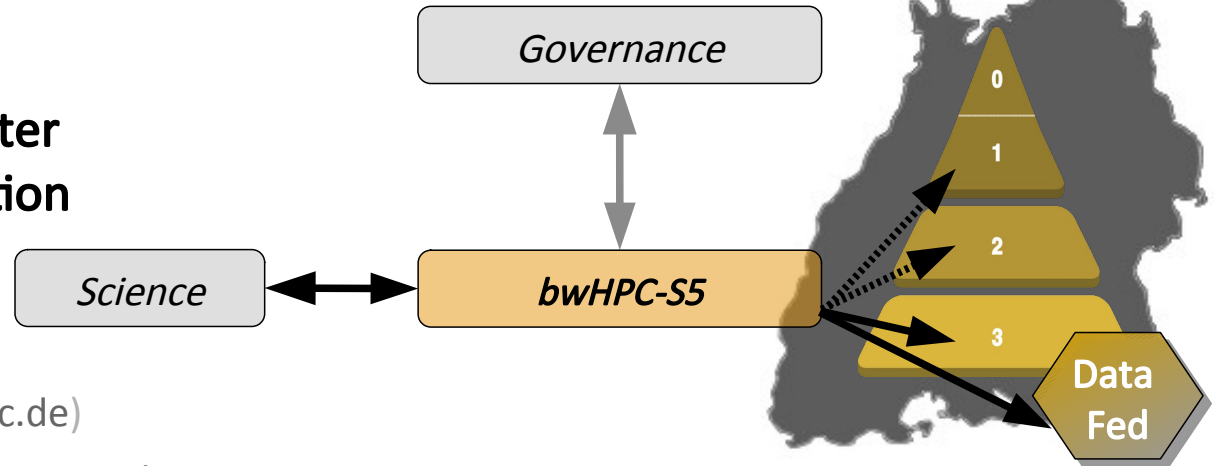
- Set bwHPC access formalities
- Assessment of bwHPC workload
- Regulation of bwHPC cluster expansion
- Assignment of science communities to science clusters and data facilities
- Representation of HPC users interests concerning:
resource demands, HPC technologies and software licences, adjustment of 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 (www.bwhpc.de/wiki)
- 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?