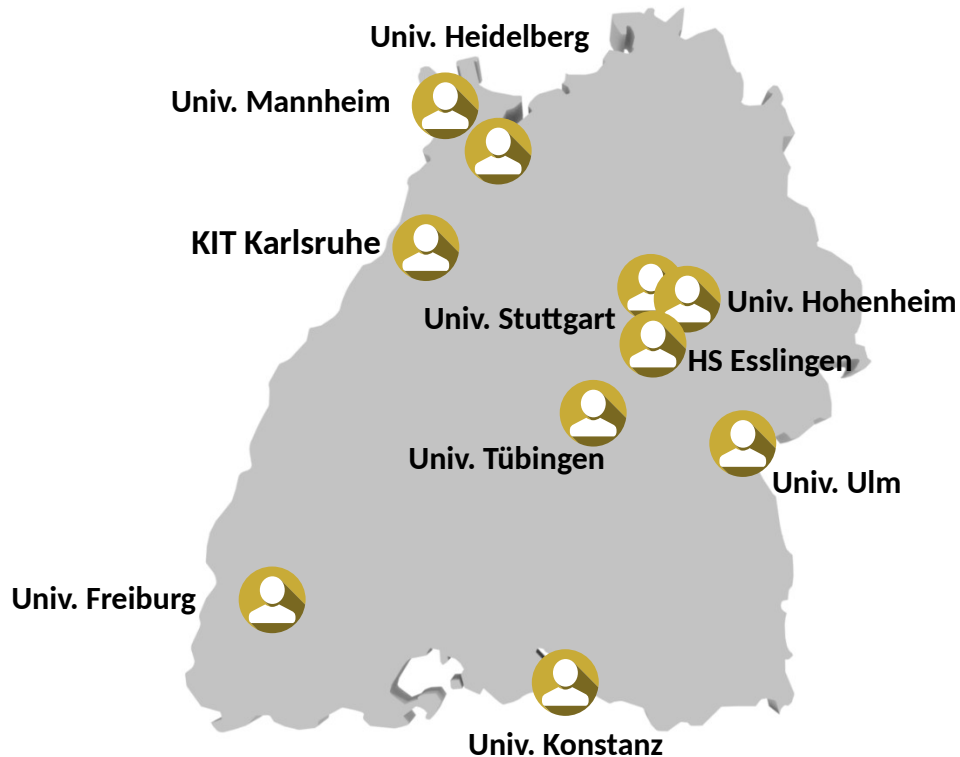# bwHPC-S5:
Scientific Simulation and Storage Support Services
as part of bwHPC

Robert Barthel, **Project Office bwHPC-S5**

9th bwHPC Symposium 2023, 23.10.2023

www.bwhpc.de

bwHPC Consortium and Funding

- Universities in the state of Baden-Württemberg, Germany
  - since **2013**
    state-wide infrastructure for HPC and Data Facilities and User Support

Background & Motivation

- Typical HPC / Data Facilities:
    - Many entry level systems at different location
    - Or state-wide systems but local administraion/identity management
    - Shortage of local expertice to fully support all scientific domains

- Solutions: **Coordination and state-wide policies** to simpify usage for users

    → establishing „federated" services

Approach (1/2)

- (IT) framework of universities (by ALWR-BW) & (to be) approved by DFG

  In Baden-Württemberg:
  2013-2018, 2018-2024, 2025-2032 :

  - bwHPC =   **H**igh **P**erformance **C**omputing (HPC) & **D**ata **I**ntensive **C**omputing (DIC) … in **B**aden-**W**ürttemberg

  - Defining:
    - policies for shared infrastructure and support structures
    - locations for infrastructure
    - governance
    - implementation and coordination platforms,
      e.g. state-wide IT support projects **bwHPC-S5** …

Federated IT services
and
science support

bw|HPC

Approach (2/2)

- (IT) framework of universities (by ALWR-BW)

  In Baden-Württemberg:
 **2025-2032** :

- Key topics for bwHPC-S5:
  - Integration in NHR, (GCS, EuroHPC) + NFDI
  - Integration of new system and method concepts (**AI, ML or quantum computing**) in support structures
  - More comprehensive needs analyses
  - Increase **energy efficiency**
  - Flexible integration of new system components and architectures
  - Software strategies towards **sustainability**
  - Expand functionalities of BaWü data federation
 - Strategies handling **sensitive data** and **digital sovereignty**

Federated IT services
and
science support

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Federation by bwHPC (1/2)

- Federation of HPC enabling sytems being part of a state-wide data federation
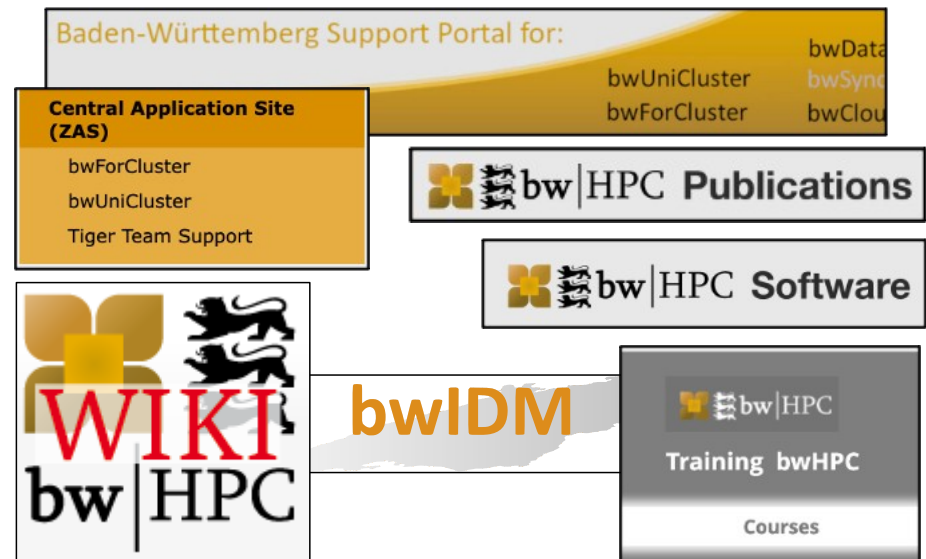 - both tailored to the needs of defined scientific domains

Supporting **Users / Science**
by federated competence centers & services
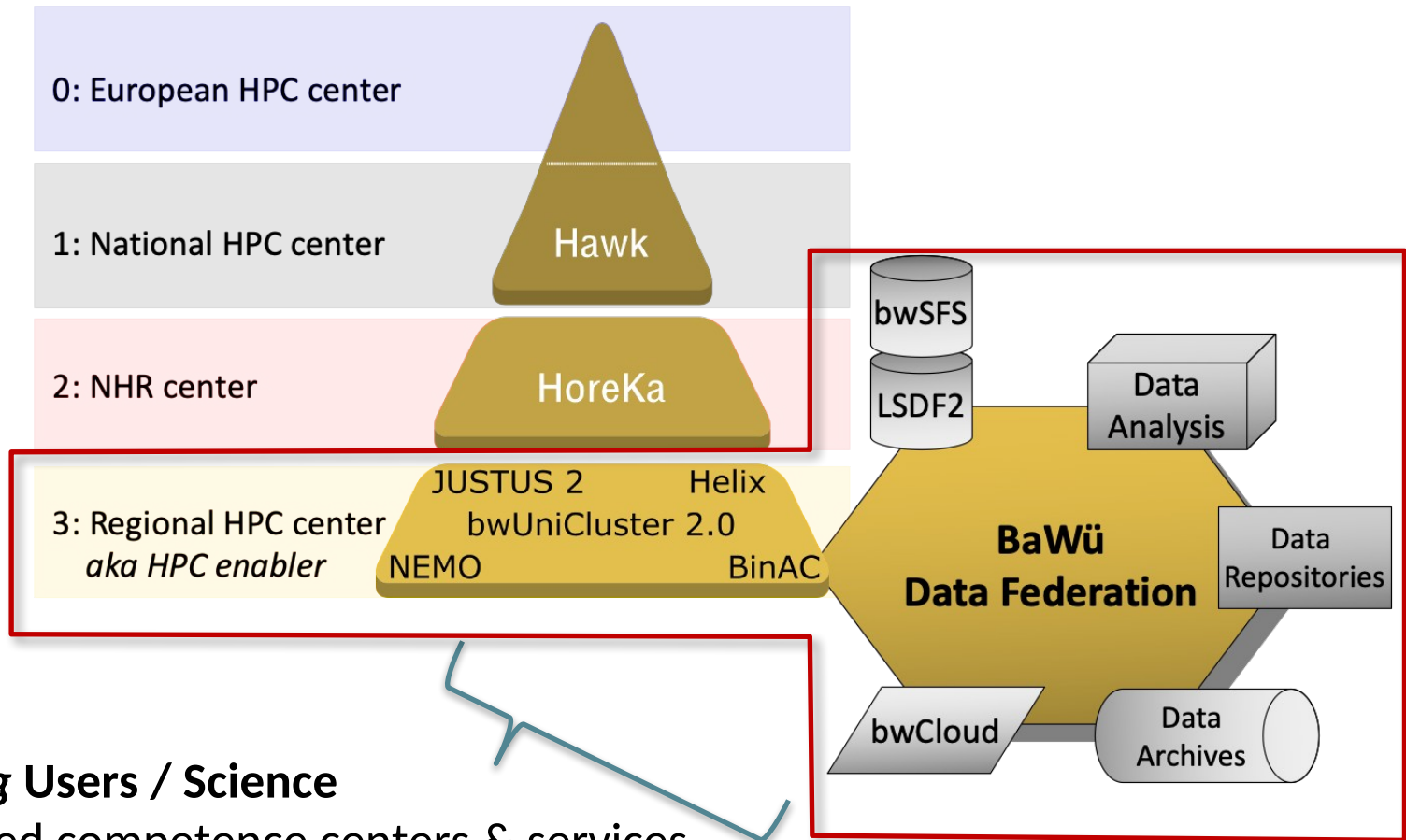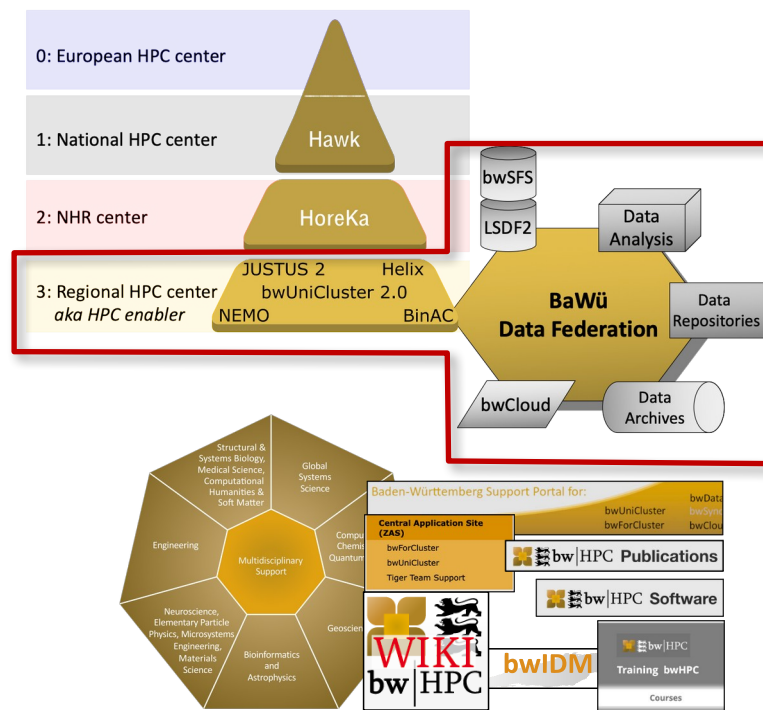
Federation by bwHPC (2/2)
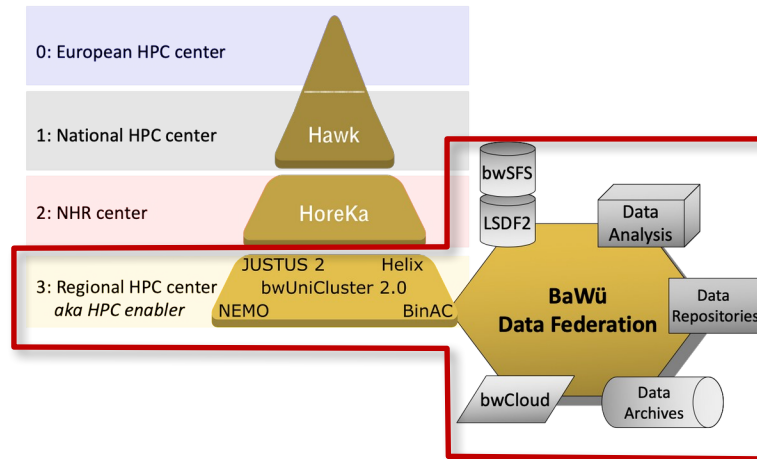
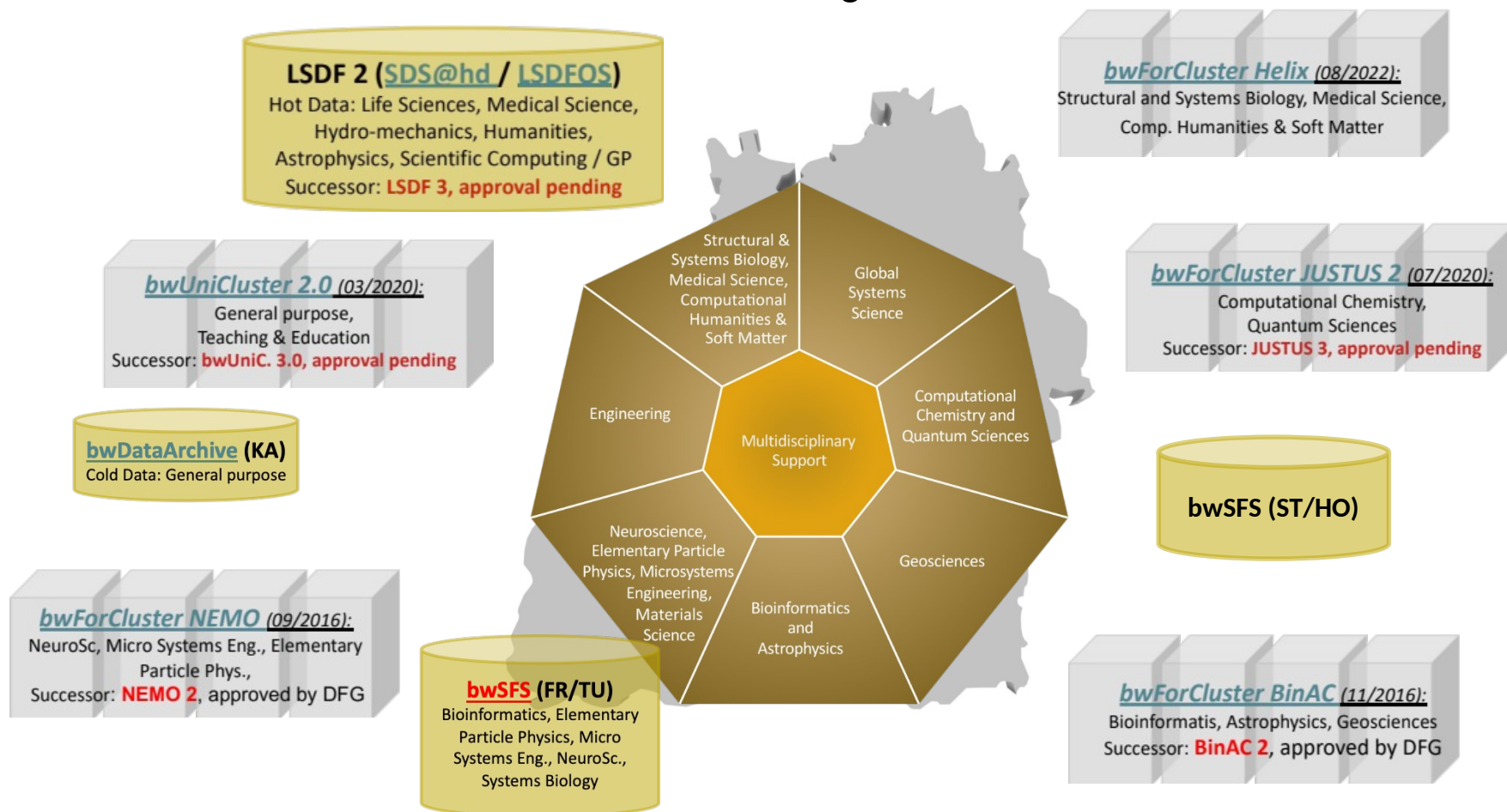## bwHPC competence centers / portals and services

bwHPC at a larger scale

Governance: *Policy making and assessment procedures to (re)define federation*

- Baden-Württemberg:
  - Steering Committee for digital research infrastructure
  - User Steering Committee + Computer center directors committee
  - Implementation tasks and its evaluation in „phases"

Structing bwHPC federation

- Federated bwHPC Competence Centers
  - Coordinate, channel and provide expertise in defined science and research areas for HPC clusters of tier 3 and storage facilities

LSDF 2 (SDS@hd / LSDFOS)
Hot Data: Life Sciences, Medical Science, Hydro-mechanics, Humanities, Astrophysics, Scientific Computing / GP
Successor: **LSDF 3, approval pending**

bwForCluster Helix (08/2022):
Structural and Systems Biology, Medical Science, Comp. Humanities & Soft Matter

bwUniCluster 2.0 (03/2020):
General purpose, Teaching & Education
Successor: **bwUniC. 3.0, approval pending**

bwForCluster JUSTUS 2 (07/2020):
Computational Chemistry, Quantum Sciences
Successor: **JUSTUS 3, approval pending**

bwDataArchive (KA)
Cold Data: General purpose

bwSFS (ST/HO)

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):
Bioinformatis, Astrophysics, Geosciences
Successor: **BinAC 2**, approved by DFG

Heptagon sections:
- Structural & Systems Biology, Medical Science, Computational Humanities & Soft Matter
- Global Systems Science
- Engineering
- Multidisciplinary Support
- Computational Chemistry and Quantum Sciences
- Neuroscience, Elementary Particle Physics, Microsystems Engineering, Materials Science
- Bioinformatics and Astrophysics
- Geosciences

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Highlights of bwHPC-S5 (1/3)

- 7 bwHPC competence centers +1 „cross-sectional" team
  - Covering 33+ DFG scientific domains (2nd level)
- Supporting 5500+ Users:
  - State-wide support portal

    Baden-Württemberg Support Portal for:
    bwUniCluster   bwData
    bwForCluster   bwSync
                          bwClou

    - 700+ Support anwers quarterly
  - Community specific software:

    bw|HPC **Software**

    - https://www.bwhpc.de/software.php
    - 680+ Software modules
  - Categorization of publications

    bw|HPC **Publications**

    - 2100+, https://www.bwhpc.de/user_publications.php

Tiger Team projects:
https://zas.bwhpc.de/shib/call4tt.php

110+ projects

- ☐ Porting of applications to bwUniCluster/bwForCluster
- ☐ Optimization of batch job scripts
- ☐ Parallelization of sequential parts of code
- ☐ Build configuration
- ☐ Usage/Linkage of performance-optimized libraries
- ☐ Implementation and optimization of workflows
- ☐ Checkpointing/restart functions of applications
- ☐ Implementation and optimization of data management
- ☐ I/O performance optimization

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Highlights of bwHPC-S5 (2/3)

- Supporting 5500+ Users:
  - Training: State-wide coordination & program
    - training.bwhpc.de
    - 400-500 training course participants per semester
      - Incl. Web seminars, e-learning coures
  - ZAS: State-wide cluster assignment portal
    - zas.bwhpc.de
    - 450+ Compute Projects (since 2013)
  - Wiki: State-wide information portal
    - 165+ user guides …
    - 65 authors

  - Surveys: annually since 2018
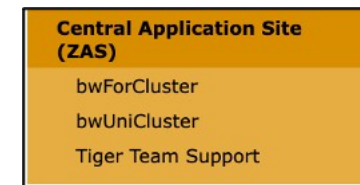
Highlights of bwHPC-S5 (3/3)

- Supporting 5500+ Users:
  - Annual state-wide results workshops (= bwHPC symposia)

- Under the „hood" activities
  - State-wide processing of KPIs

  - Techology evaluation
    & implementation to enhance services

  - Aiding procurement processes &
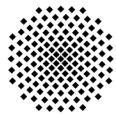   defining operating models
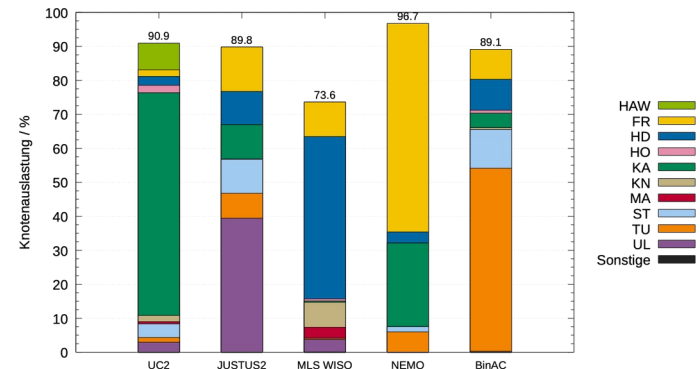
Acknowledgement
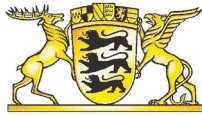
- And all contributors and members of bwHPC-S5:
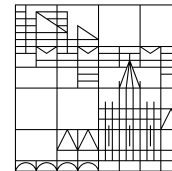
Thank you for your attention!

- https://www.bwhpc.de
- office@bwhpc.de