# bwHPC:
# Hardware and Storage Architecture

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Universität Konstanz

Universität Mannheim

Universität Stuttgart

Eberhard Karls Universität Tübingen

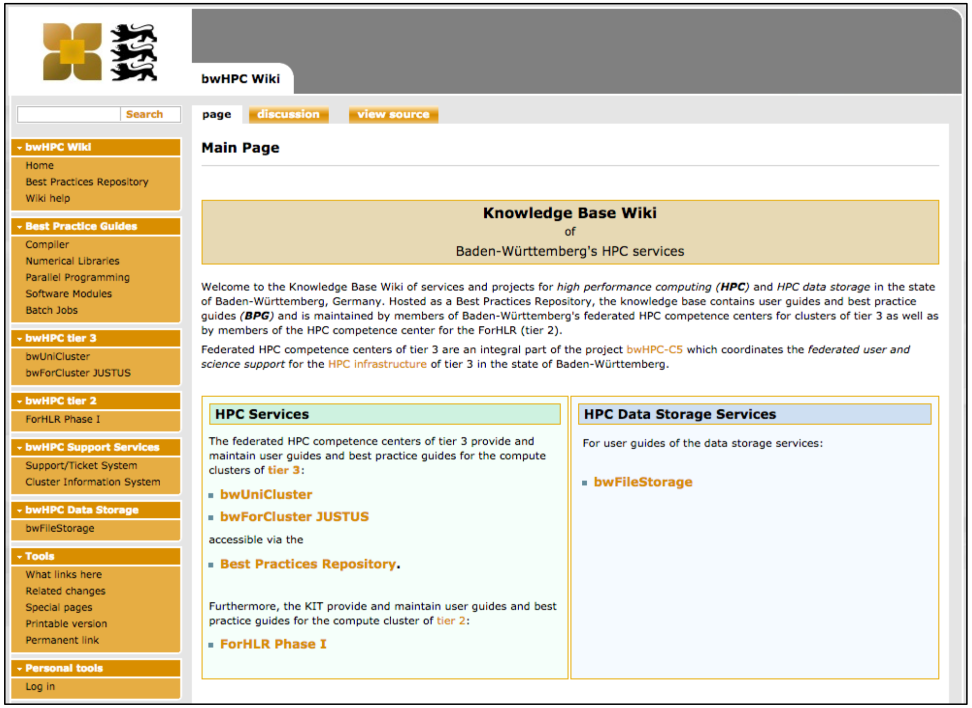
KIT Karlsruher Institut für Technologie

ulm university universität uulm

Funding: Baden-Württemberg
MINISTERIUM FÜR WISSENSCHAFT, FORSCHUNG UND KUNST

# Reference: bwHPC-C5 Best Practices Repository

- Most information given by this talk can be found at http://bwhpc-c5.de/wiki:
    - Category:Hardware_and_Architecture
    - Or choose the cluster, then „Hardware and Architecture“ or „File Systems“



Main Page

**Knowledge Base Wiki**
of
Baden-Württemberg's HPC services

Welcome to the Knowledge Base Wiki of services and projects for *high performance computing* (***HPC***) and *HPC data storage* in the state of Baden-Württemberg, Germany. Hosted as a Best Practices Repository, the knowledge base contains user guides and best practice guides (***BPG***) and is maintained by members of Baden-Württemberg's federated HPC competence centers for clusters of tier 3 as well as by members of the HPC competence center for the ForHLR (tier 2).

Federated HPC competence centers of tier 3 are an integral part of the project bwHPC-C5 which coordinates the *federated user and science support* for the HPC infrastructure of tier 3 in the state of Baden-Württemberg.

**HPC Services**

The federated HPC competence centers of tier 3 provide and maintain user guides and best practice guides for the compute clusters of tier 3:

- **bwUniCluster**
- **bwForCluster JUSTUS**

accessible via the

- **Best Practices Repository.**

Furthermore, the KIT provide and maintain user guides and best practice guides for the compute cluster of tier 2:

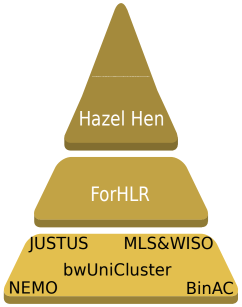
- **ForHLR Phase I**

**HPC Data Storage Services**

For user guides of the data storage services:

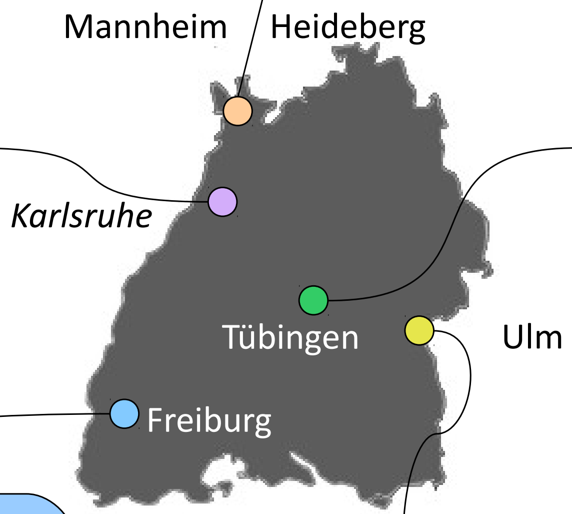
- **bwFileStorage**

# Clusters @ Tier 2+3



***bwForCluster MLS& WISO***
***(10/2015):***
Economics & Social Science,
Molecular Life Science

***bwUniCluster***
***(02/2014):***
General purpose,
Teaching & Education
***ForHLR I+II***
***(09/2014),(03/2016):***
Research, high scalability



***bwForCluster BinAC***
***(11/2016):***
Bioinformatis,
Astrophysics

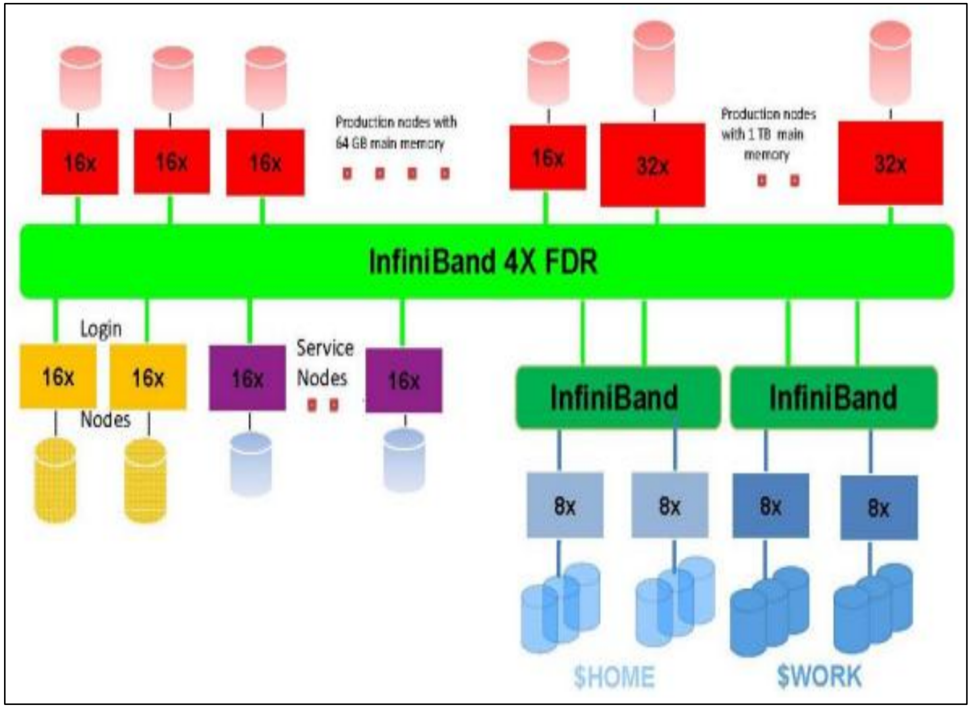
***bwForCluster NEMO***
***(09/2016):***
Neurosciences,
Micro Systems Engineering,
Elementary Particle Physics

***bwForCluster JUSTUS***
***(12/2014):***
Computational Chemistry

# System Architecture

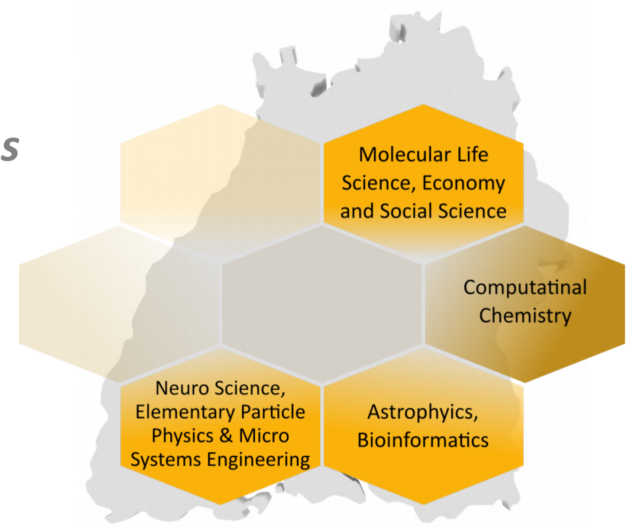
# System and Storage Architecture (bwUniCluster)

- each (compute/login) node has sixteen Intel Xeon processors, local memory, disks and network adapters, connected by fast InfiniBand 4X FDR interconnect
- Roles:
  - Login Nodes
  - Compute Nodes
  - File Server Nodes
  - Administrative Server Nodes



# bwUniCluster

*Federated HPC tier 3 resources*


Molecular Life Science, Economy and Social Science
Computatinal Chemistry
Neuro Science, Elementary Particle Physics & Micro Systems Engineering
Astrophyics, Bioinformatics

Selected characteristics:

- General purpose HPC entry level incl. education
- Universities are Shareholders
- Federated operations, multilevel fairsharing

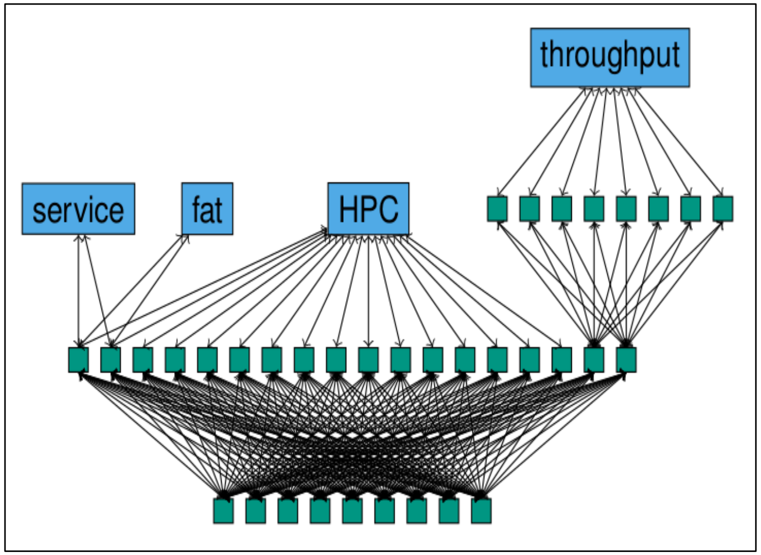
| | Thin | Fat | *In Preparation* |
|---|---|---|---|
| # nodes | 512 | 8 | *352* |
| Core/node | 16 | 32 | *28* |
| Processor | 2.6 GHz (Sandy Br.) | 2.4 GHz (Sandy Br.) | *2.0 GHz (Broadwell)* |
| Main Mem | 64 GiB | 1024 GiB | *128 GiB* |
| Local Storage | 2 TB HDD | 7 TB HDD | *480 GB SSD* |
| Interconnect | InfiniBand 4x FDR | | *InfiniBand FDR/EDR* |
| Blocking | 1:1 (50%), 1:8 (50%) | | *1:1* |
| PFS – HOME | 427 TB Lustre | | |
| PFS – Workspaces | 853 TB Lustre | | |

# System Properties (1)

- Compute node types:
  - Thin: for applications using high number of processors, distributed memory, communication over InfiniBand (MPI)
  - Fat: for shared memory applications (OpenMP or explicit multithreading)
  - Other types exist on some clusters
- Processor types:
  - (older ← → newer)
    … – Sandy Bridge – Ivy Bridge – Haswell – Broadwell – ...
- Main memory:
  - Useful to know when requesting resources (pmem, mem) during batch job submission

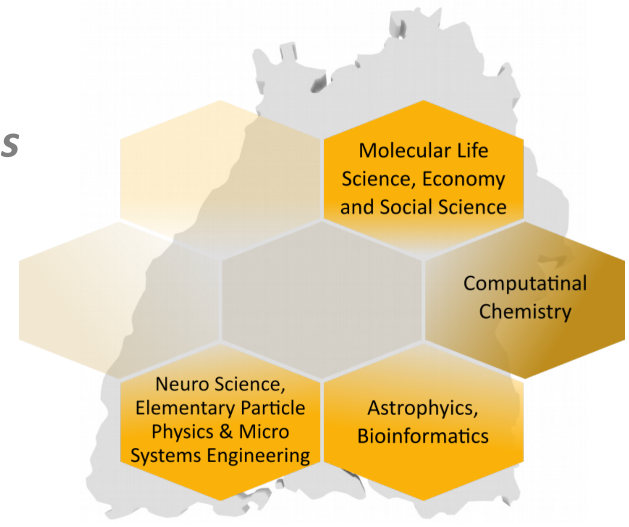
# System Properties (2)

- Local Storage:
  - Size and read/write performance interesting when using local file system ($TMP / $TMPDIR)
- InfiniBand:
  - (older ← → newer, higher speed, lower latency)
    … – QDR – FDR – EDR – …
  - Or Omni-Path instead
- Blocking:
  - Ratio of uplink and downlink bandwidth
  - Non-blocking if equal
  - Example bwUnicluster:
    both blocking and „fat tree“ area



# bwUniCluster

*Federated HPC tier 3 resources*



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Computatinal Chemistry

Neuro Science, Elementary Particle Physics & Micro Systems Engineering

Astrophyics, Bioinformatics

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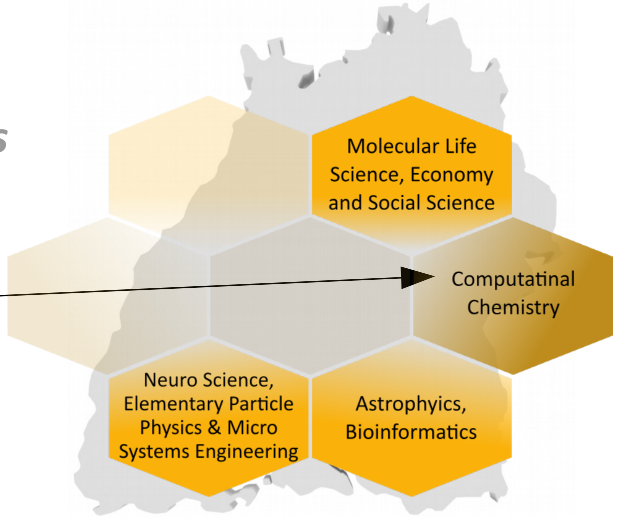
# bwForCluster JUSTUS

*Federated HPC tier 3 resources*



Molecular Life Science, Economy and Social Science
Computatinal Chemistry
Neuro Science, Elementary Particle Physics & Micro Systems Engineering
Astrophyics, Bioinformatics

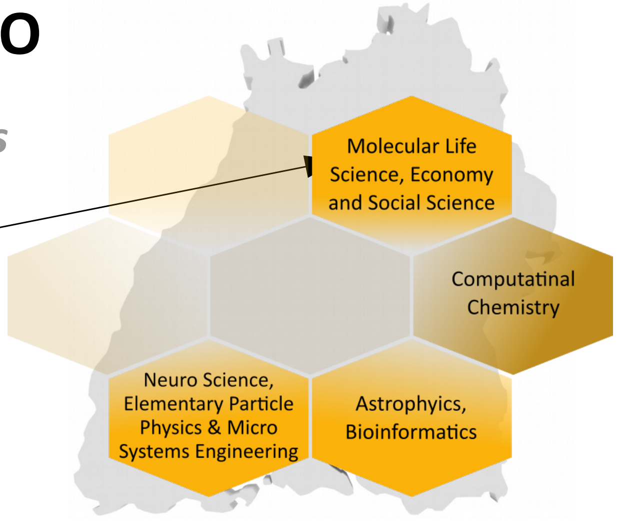
Selected characteristics:

- Dedicated to **computational chemistry**
  - High I/O, large MEM jobs
- User and software support by *bwHPC competence center*

| | Diskless | SSD | Big SSD | Large Mem SSD | Visual |
|---|---|---|---|---|---|
| # nodes | 202 | 204 | 22 | 16 | 2 |
| Core/node | 16 | 16 | 16 | 16 | 16 |
| Processor | 2,4 GHz (Xeon E5-2630v3, Haswell) | | | | |
| Main Mem | 128 GiB | | 256 GiB | 512 GiB | 512 GiB |
| Local Storage | - | 1 TB SSD | 2 TB SSD | | 4 TB HDD |
| Interconnect | InfiniBand QDR | | | | |
| Blocking | 1:8 | | | | |
| HOME | 200 TB NFS | | | | |
| PFS – Workspaces | 200 TB Lustre | | | | |
| Block storage | 480 TB (local mount via RDMA) | | | | |
| Special feature | | | | | NVIDIA K6000 |

# bwForCluster MLS&WISO

*Federated HPC tier 3 resources*


Molecular Life Science, Economy and Social Science
Computatinal Chemistry
Neuro Science, Elementary Particle Physics & Micro Systems Engineering
Astrophysics, Bioinformatics

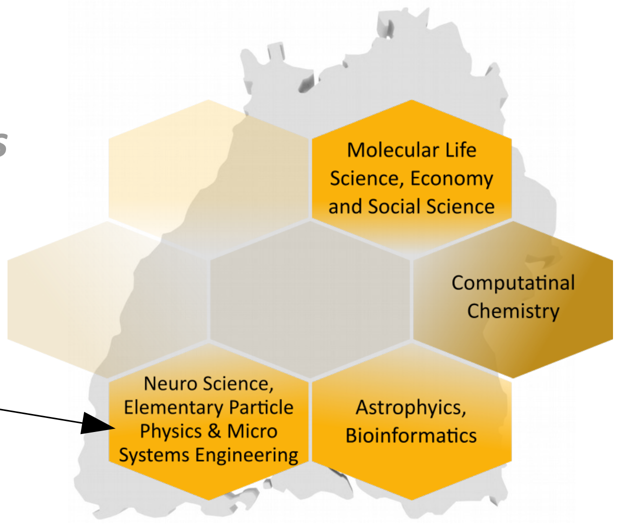
Selected characteristics:

- Dedicated to **molecular life science, economics and social science + cluster for method development**
- User and software support by *bwHPC competence center*

| | Standard | Best | Coprocessor (GPU) | Coprocessor (MIC) | Fat | Fat (Ivy Bridge) |
|---|---|---|---|---|---|---|
| **Node Feature** | standard | best | gpu | mic | fat | fat-ivy |
| **Quantity** | 476 | 148 | 18 | 12 | 8 | 4 |
| **Processors** | 2 x Intel Xeon E5-2630v3 (Haswell) | 2 x Intel Xeon E5-2640v3 (Haswell) | 2 x Intel Xeon E5-2630v3 (Haswell) | 2 x Intel Xeon E5-2630v3 (Haswell) | 4 x Intel Xeon E5-4620v3 (Haswell) | 4 x Intel Xeon E4-4020v2 (Ivy Bridge) |
| **Processor Frequency (GHz)** | 2.4 | 2.6 | 2.4 | 2.4 | 2.0 | 2.6 |
| **Number of Cores** | 16 | 16 | 16 | 16 | 40 | 32 |
| **Working Memory (GB)** | 64 | 128 | 64 | 64 | 1536 | 1024 |
| **Local Disk (GB)** | 128 (SSD) | 128 (SSD) | 128 (SSD) | 128 (SSD) | 9000 (SATA) | 128 (SSD) |
| **Interconnect** | QDR | FDR | FDR | FDR | FDR | FDR |
| **Coprocessors** | – | – | 1 x Nvidia Tesla K80 | 2 x Intel Xeon Phi 5110P | – | – |

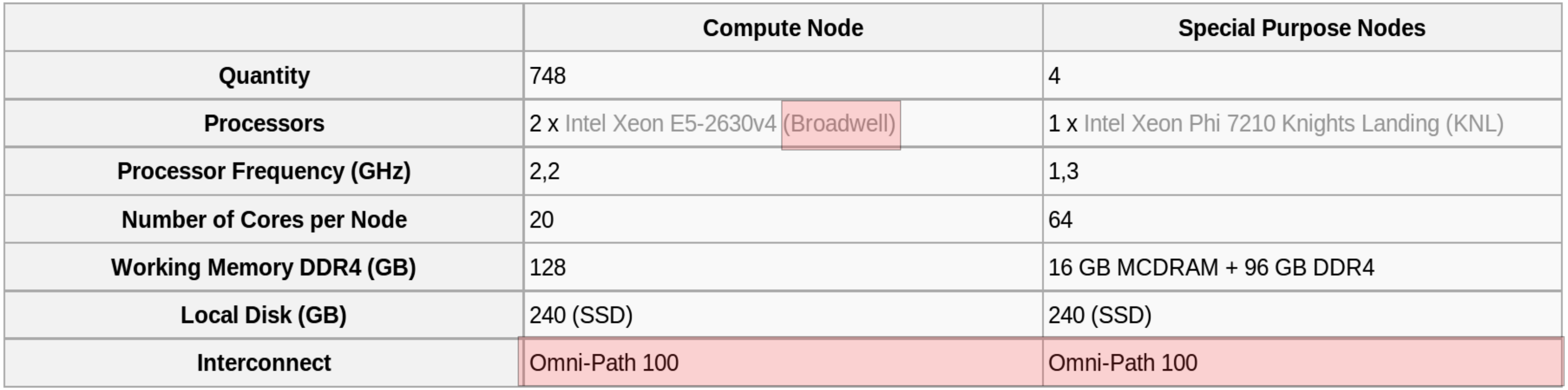
# bwForCluster NEMO

*Federated HPC tier 3 resources*


Molecular Life Science, Economy and Social Science
Computatinal Chemistry
Neuro Science, Elementary Particle Physics & Micro Systems Engineering
Astrophyics, Bioinformatics

Selected characteristics:

- Dedicated to **neuro science, elementary particle physics, micro systems engineering**
  - Virtual machine images deployable
- User and software support by *bwHPC competence center*



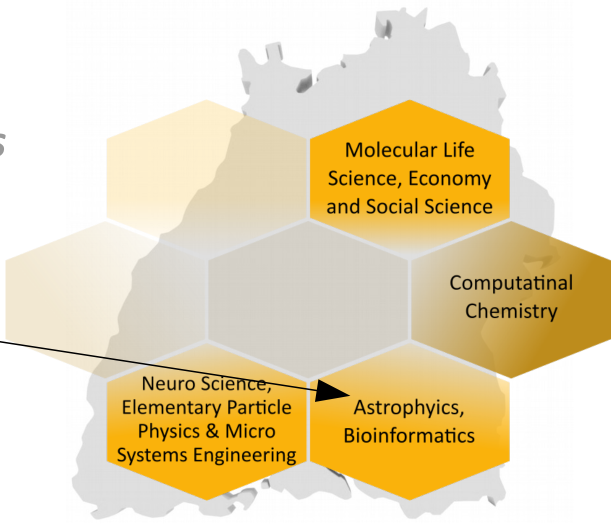
| | Compute Node | Special Purpose Nodes |
|---|---|---|
| **Quantity** | 748 | 4 |
| **Processors** | 2 x Intel Xeon E5-2630v4 (Broadwell) | 1 x Intel Xeon Phi 7210 Knights Landing (KNL) |
| **Processor Frequency (GHz)** | 2,2 | 1,3 |
| **Number of Cores per Node** | 20 | 64 |
| **Working Memory DDR4 (GB)** | 128 | 16 GB MCDRAM + 96 GB DDR4 |
| **Local Disk (GB)** | 240 (SSD) | 240 (SSD) |
| **Interconnect** | Omni-Path 100 | Omni-Path 100 |

# bwForCluster BinAC

*Federated HPC tier 3 resources*

<u>Selected characteristics:</u>

- Dedicated to **astrophysics, bioinformatics**
  - Dual GPU systems
- User and software support by *bwHPC competence center*

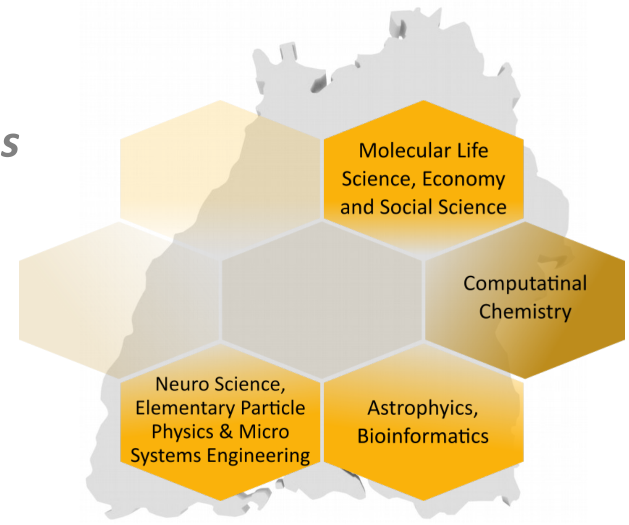


Molecular Life Science, Economy and Social Science
Computatinal Chemistry
Neuro Science, Elementary Particle Physics & Micro Systems Engineering
Astrophycis, Bioinformatics

| | Standard | Fat | GPU |
|---|---|---|---|
| **Quantity** | 236 | 4 | 60 |
| **Processors** | 2 x Intel Xeon E5-2630v4 (Broadwell) | 4 x Intel Xeon E5-4620v3 (Haswell) | 2 x Intel Xeon E5-2630v4 (Broadwell) |
| **Processor Frequency (GHz)** | 2.4 | 2.0 | 2.4 |
| **Number of Cores** | 28 | 40 | 28 |
| **Working Memory (GB)** | 128 | 1024 | 128 |
| **Local Disk (GB)** | 256 (SSD) | 256 (SSD) | 256 (SSD) |
| **Interconnect** | FDR | FDR | FDR |
| **Coprocessors** | – | – | 2 x Nvidia Tesla K80 |

# ForHLR I

*Federated HPC tier 2 resources*


Molecular Life Science, Economy and Social Science
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Neuro Science, Elementary Particle Physics & Micro Systems Engineering
Astrophysics, Bioinformatics

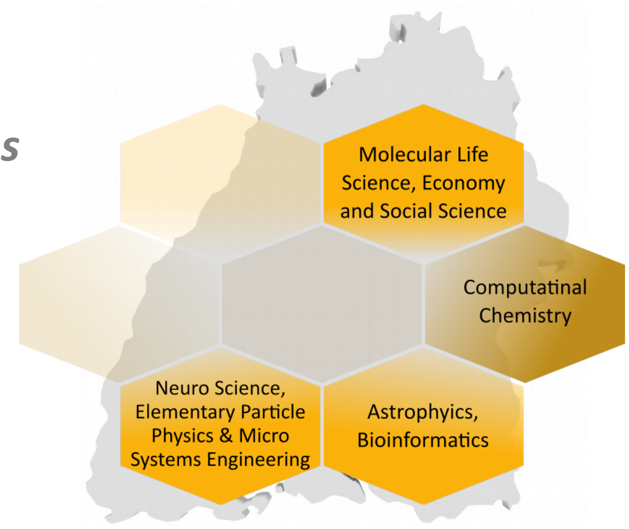
Selected characteristics:

- Next level for advanced HPC users
- Research, high scalability

| | Thin | Fat |
|---|---|---|
| # nodes | 512 | 16 |
| Core/node | 20 | 32 |
| Processor | 2.5 GHz (Sandy Br.) | 2.6 GHz (Sandy Br.) |
| Main Mem | 64 GiB | 512 GiB |
| Local Storage | 2 TB HDD | 8 TB HDD |
| Interconnect | InfiniBand 4x FDR | |
| Blocking | Non-blocking | |
| PFS – HOME | 427 TB Lustre | |
| PFS – Workspaces | PROJECT 427 TB Lustre, WORK/workspace 853 TB Lustre | |

# ForHLR II

*Federated HPC tier 2 resources*


Molecular Life Science, Economy and Social Science
Computatinal Chemistry
Neuro Science, Elementary Particle Physics & Micro Systems Engineering
Astrophysics, Bioinformatics

Selected characteristics:

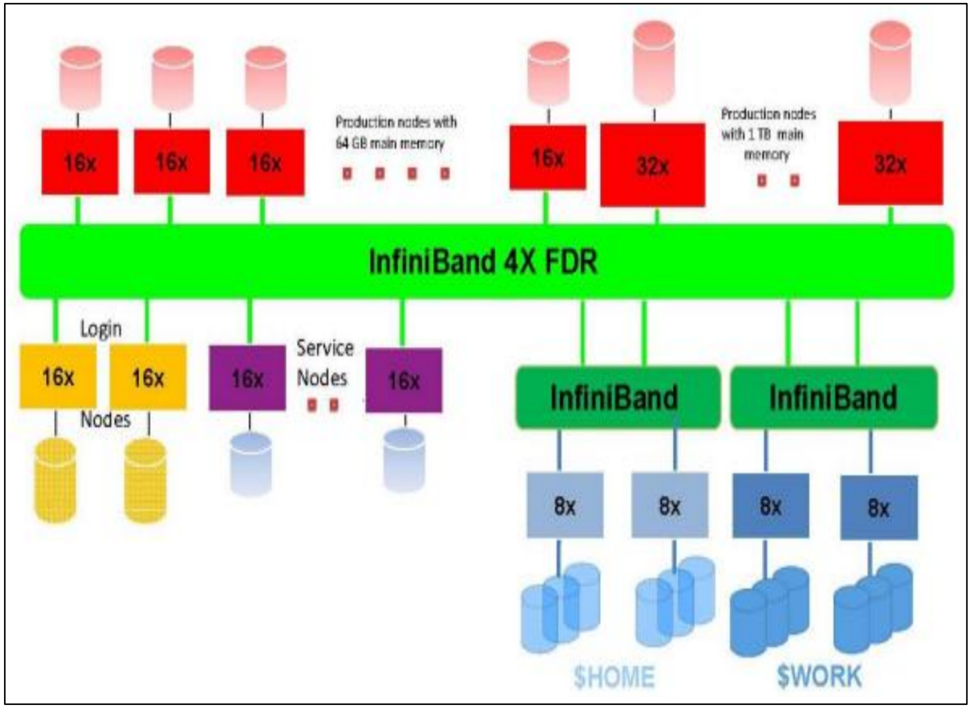
- Next level for advanced HPC users
- Research, high scalability

| | Thin | Fat |
|---|---|---|
| # nodes | 1152 | 21 |
| Core/node | 20 | 48 |
| Processor | 2.6 GHz (Haswell) | 2.1 GHz (Haswell) |
| Main Mem | 64 GiB | 1024 GiB |
| Local Storage | 480 GB SSD | 3840 GB SSD |
| Interconnect | InfiniBand 4x EDR | |
| Blocking | Non-blocking | |
| Graphic cards | | 4 NVIDIA GeForce GTX980 Ti |
| PFS – HOME | 427 TB Lustre | |
| PFS – Workspaces | PROJECT 610 TB Lustre, WORK 1220 TB Lustre, workspace 3050 TB Lustre | |

# Storage Architecture

# System and Storage Architecture (bwUniCluster)

- File Systems:
  - Local ($TMP or $TMPDIR): each node has its own file system
  - Global ($HOME, $PROJECT, $WORK, workspaces): all nodes access the same file system; located in parallel file system

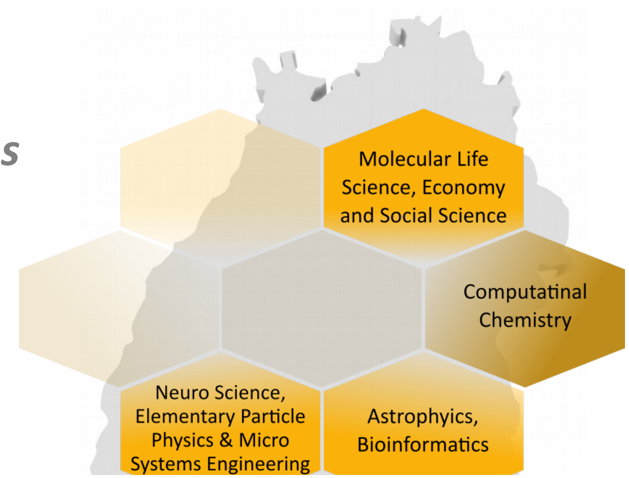


# File Systems

- All Clusters:
  - $TMP or $TMPDIR: local, files are removed at end of batch job, no backup
  - $HOME: global, permanent, backup on most clusters, quota,
    same home directories on ForHLR I+II, bwUniCluster
  - workspaces: global, entire workspace expires after fixed period, no backup, no quota, higher throughput
    HowTo: http://www.bwhpc-c5.de/wiki/index.php/Workspace
- ForHLR I+II, bwUniCluster:
  - $WORK: global, no backup, no quota, higher throughput,
    file lifetime 28 days (1 week guaranteed)
- ForHLR I+II:
  - $PROJECT: global, permanent, backup, quota
    use $PROJECT instead because $HOME quota for project group very small

# bwUniCluster

*Federated HPC tier 3 resources*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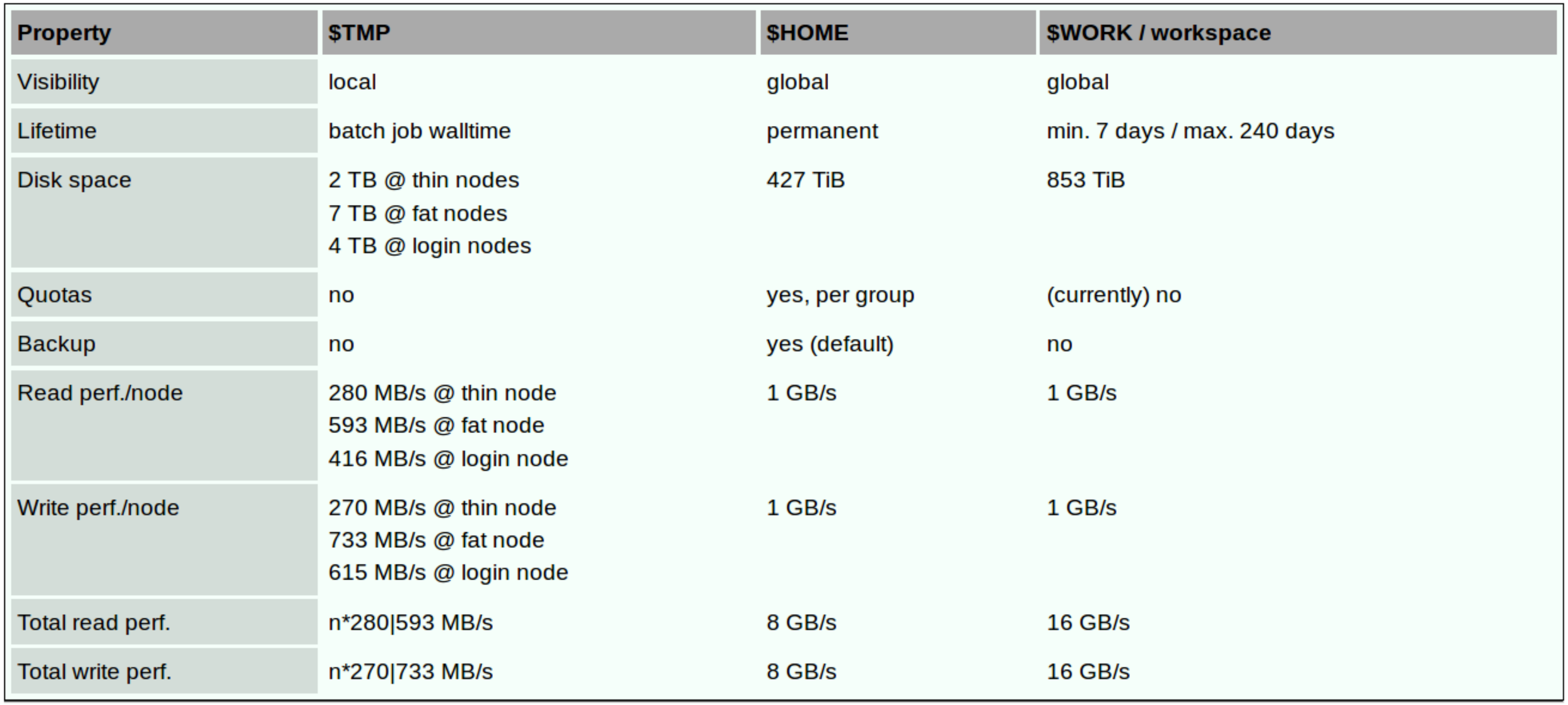
## Selected characteristics:

- General purpose HPC entry level incl. education
- Universities are Shareholders
- Federated operations, multilevel fairsharing



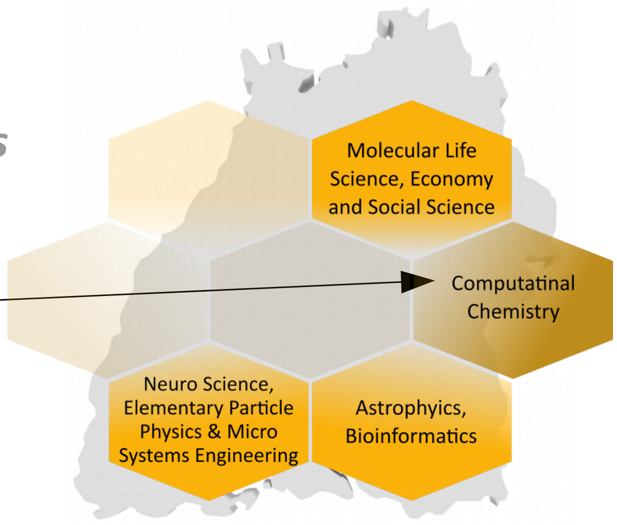
| Property | $TMP | $HOME | $WORK / workspace |
|---|---|---|---|
| Visibility | local | global | global |
| Lifetime | batch job walltime | permanent | min. 7 days / max. 240 days |
| Disk space | 2 TB @ thin nodes<br>7 TB @ fat nodes<br>4 TB @ login nodes | 427 TiB | 853 TiB |
| Quotas | no | yes, per group | (currently) no |
| Backup | no | yes (default) | no |
| Read perf./node | 280 MB/s @ thin node<br>593 MB/s @ fat node<br>416 MB/s @ login node | 1 GB/s | 1 GB/s |
| Write perf./node | 270 MB/s @ thin node<br>733 MB/s @ fat node<br>615 MB/s @ login node | 1 GB/s | 1 GB/s |
| Total read perf. | n*280\|593 MB/s | 8 GB/s | 16 GB/s |
| Total write perf. | n*270\|733 MB/s | 8 GB/s | 16 GB/s |

# bwForCluster JUSTUS

*Federated HPC tier 3 resources*

Selected characteristics:

- Dedicated to **computational chemistry**
  - High I/O, large MEM jobs
- User and software support by *bwHPC competence center*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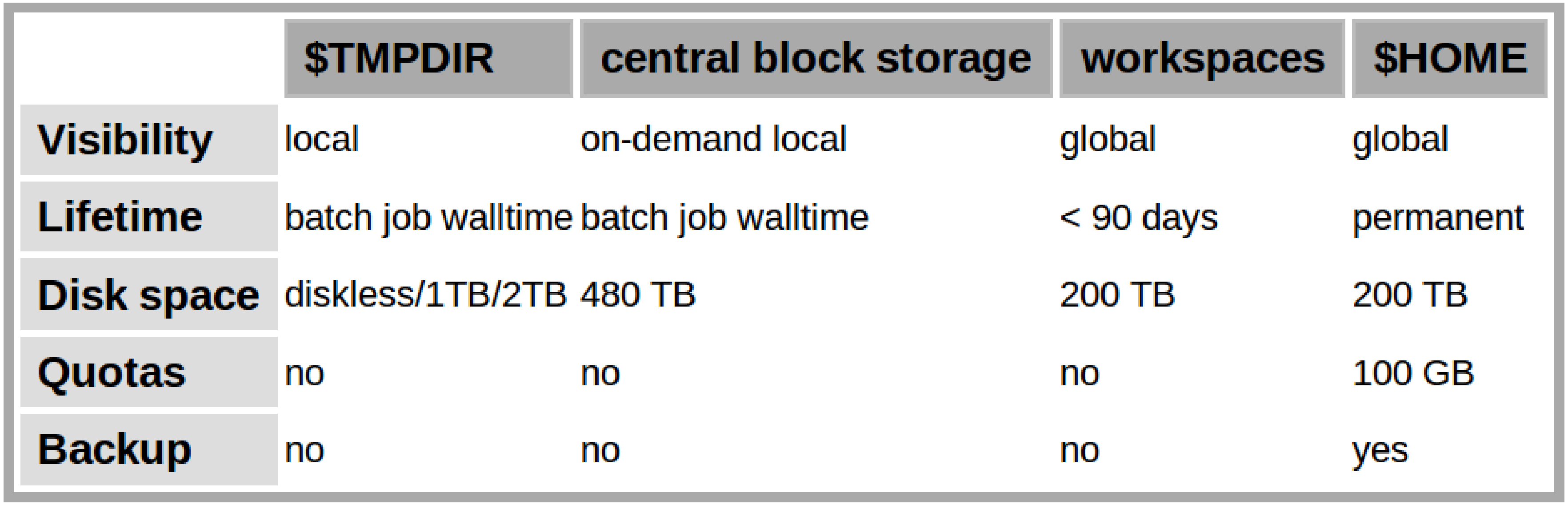
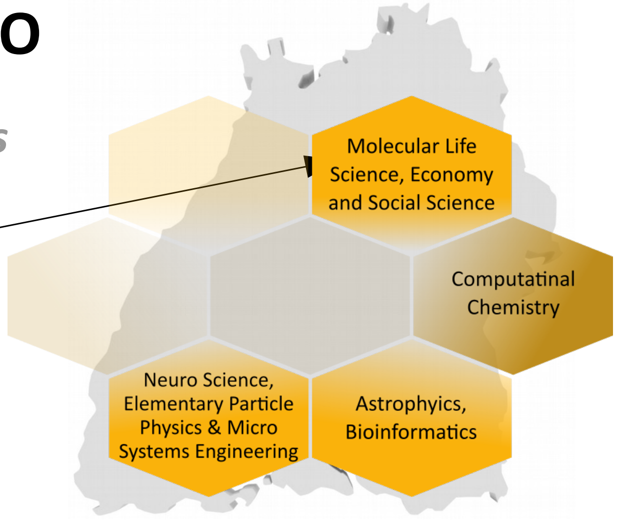


| | $TMPDIR | central block storage | workspaces | $HOME |
|---|---|---|---|---|
| **Visibility** | local | on-demand local | global | global |
| **Lifetime** | batch job walltime | batch job walltime | < 90 days | permanent |
| **Disk space** | diskless/1TB/2TB | 480 TB | 200 TB | 200 TB |
| **Quotas** | no | no | no | 100 GB |
| **Backup** | no | no | no | yes |

# bwForCluster MLS&WISO

*Federated HPC tier 3 resources*


Molecular Life Science, Economy and Social Science
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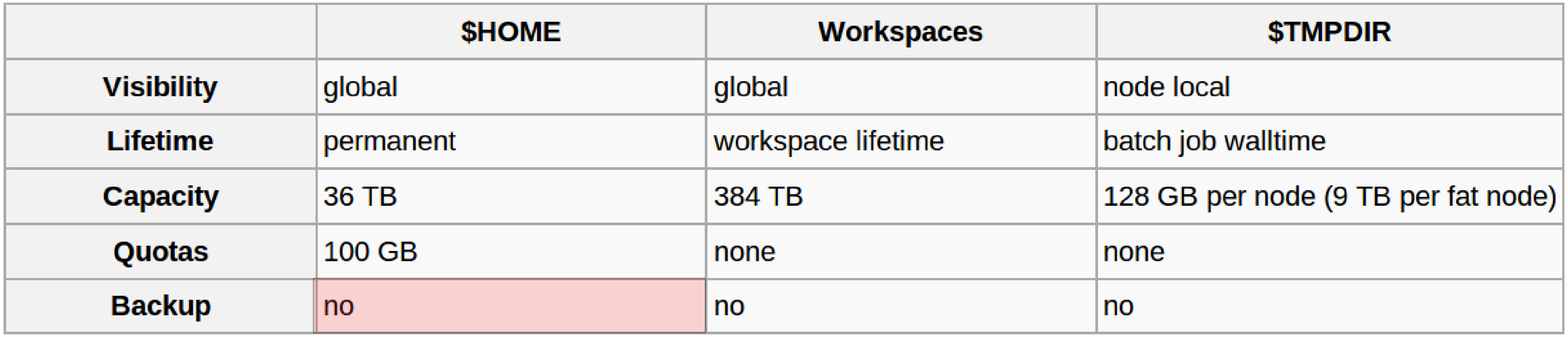
Astrophyics, Bioinformatics

Selected characteristics:

- Dedicated to **molecular life science, economics and social science**

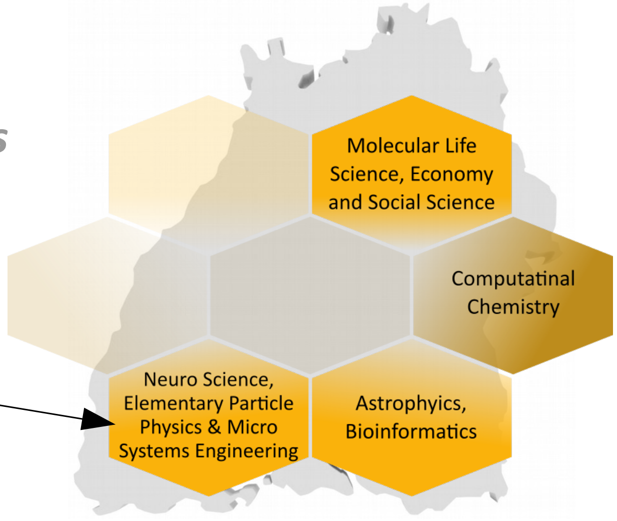
  **+ cluster for method development**
- User and software support by *bwHPC competence center*



| | $HOME | Workspaces | $TMPDIR |
|---|---|---|---|
| **Visibility** | global | global | node local |
| **Lifetime** | permanent | workspace lifetime | batch job walltime |
| **Capacity** | 36 TB | 384 TB | 128 GB per node (9 TB per fat node) |
| **Quotas** | 100 GB | none | none |
| **Backup** | no | no | no |

# bwForCluster NEMO

*Federated HPC tier 3 resources*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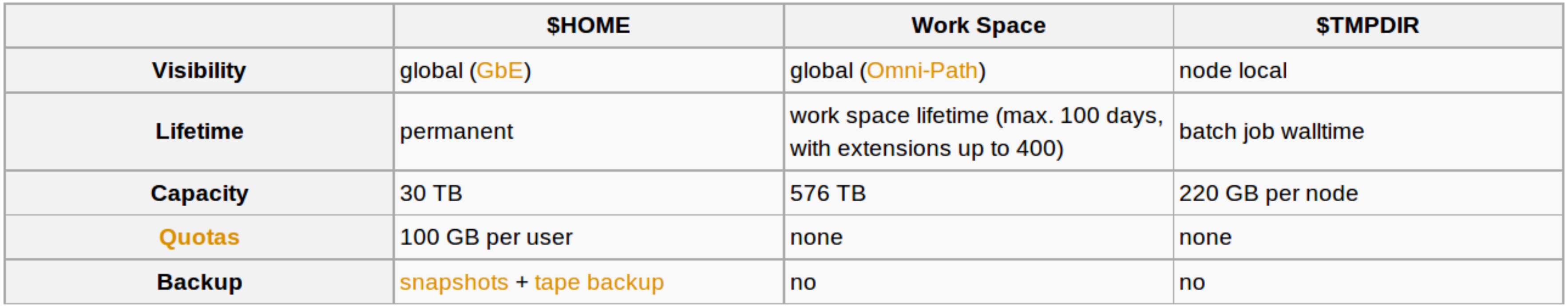
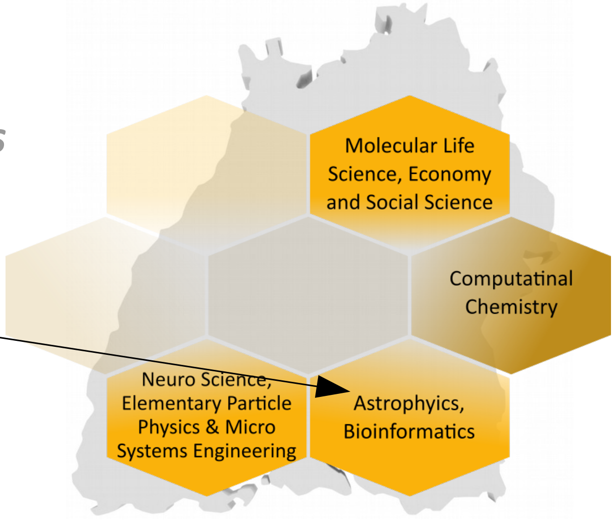


| | $HOME | Work Space | $TMPDIR |
|---|---|---|---|
| **Visibility** | global (GbE) | global (Omni-Path) | node local |
| **Lifetime** | permanent | work space lifetime (max. 100 days, with extensions up to 400) | batch job walltime |
| **Capacity** | 30 TB | 576 TB | 220 GB per node |
| **Quotas** | 100 GB per user | none | none |
| **Backup** | snapshots + tape backup | no | no |

# bwForCluster BinAC

*Federated HPC tier 3 resources*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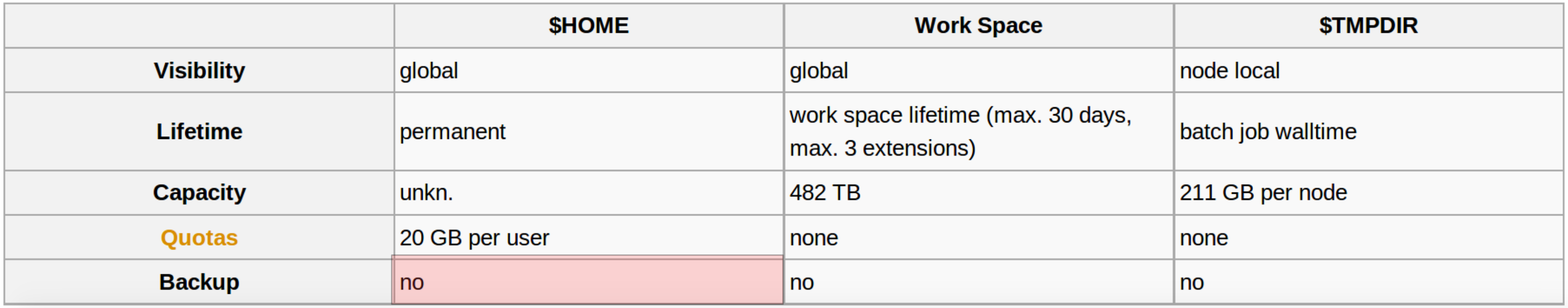
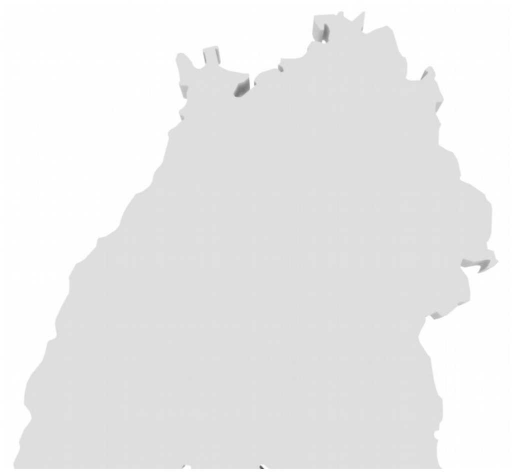


| | $HOME | Work Space | $TMPDIR |
|---|---|---|---|
| **Visibility** | global | global | node local |
| **Lifetime** | permanent | work space lifetime (max. 30 days, max. 3 extensions) | batch job walltime |
| **Capacity** | unkn. | 482 TB | 211 GB per node |
| **Quotas** | 20 GB per user | none | none |
| **Backup** | no | no | no |

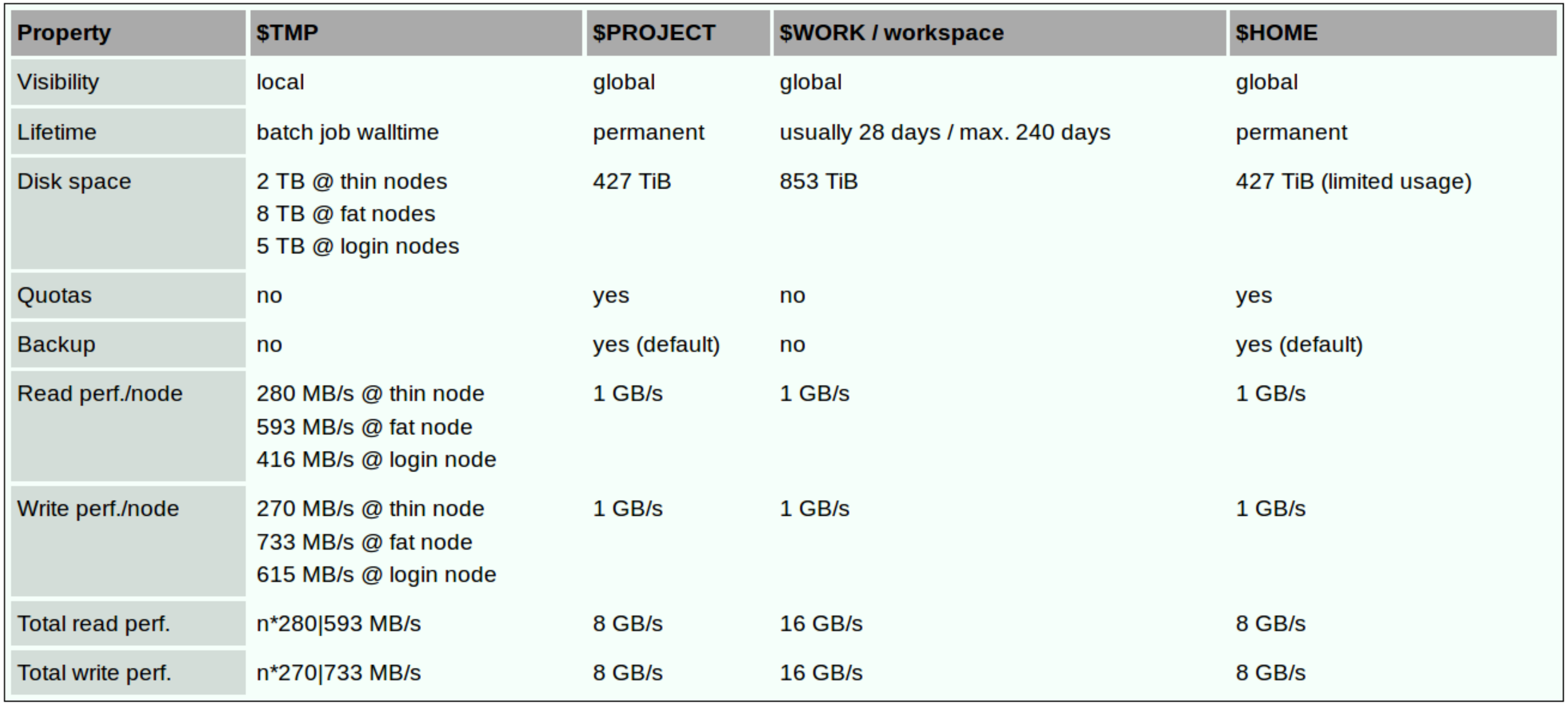
# ForHLR I

*Federated HPC tier 2 resources*



Selected characteristics:

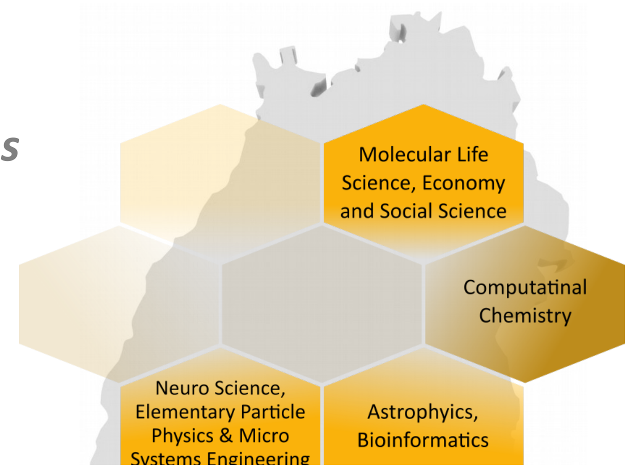
- Next level for advanced HPC users
- Research, high scalability



| Property | $TMP | $PROJECT | $WORK / workspace | $HOME |
|---|---|---|---|---|
| Visibility | local | global | global | global |
| Lifetime | batch job walltime | permanent | usually 28 days / max. 240 days | permanent |
| Disk space | 2 TB @ thin nodes<br>8 TB @ fat nodes<br>5 TB @ login nodes | 427 TiB | 853 TiB | 427 TiB (limited usage) |
| Quotas | no | yes | no | yes |
| Backup | no | yes (default) | no | yes (default) |
| Read perf./node | 280 MB/s @ thin node<br>593 MB/s @ fat node<br>416 MB/s @ login node | 1 GB/s | 1 GB/s | 1 GB/s |
| Write perf./node | 270 MB/s @ thin node<br>733 MB/s @ fat node<br>615 MB/s @ login node | 1 GB/s | 1 GB/s | 1 GB/s |
| Total read perf. | n*280\|593 MB/s | 8 GB/s | 16 GB/s | 8 GB/s |
| Total write perf. | n*270\|733 MB/s | 8 GB/s | 16 GB/s | 8 GB/s |

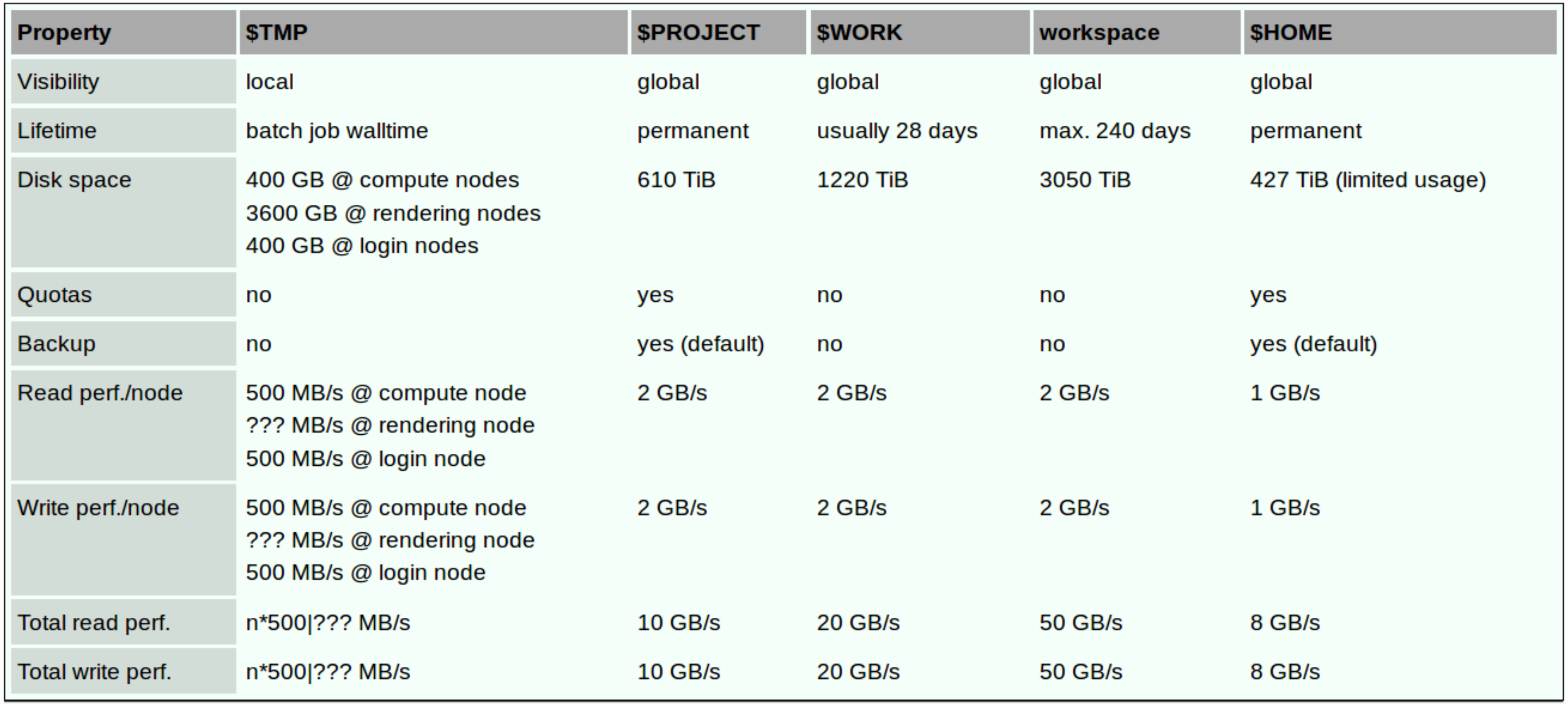
# ForHLR II

*Federated HPC tier 2 resources*


Molecular Life Science, Economy and Social Science
Computatinal Chemistry
Neuro Science, Elementary Particle Physics & Micro Systems Engineering
Astrophyics, Bioinformatics

Selected characteristics:

- Next level for advanced HPC users
- Research, high scalability



| Property | $TMP | $PROJECT | $WORK | workspace | $HOME |
|---|---|---|---|---|---|
| Visibility | local | global | global | global | global |
| Lifetime | batch job walltime | permanent | usually 28 days | max. 240 days | permanent |
| Disk space | 400 GB @ compute nodes<br>3600 GB @ rendering nodes<br>400 GB @ login nodes | 610 TiB | 1220 TiB | 3050 TiB | 427 TiB (limited usage) |
| Quotas | no | yes | no | no | yes |
| Backup | no | yes (default) | no | no | yes (default) |
| Read perf./node | 500 MB/s @ compute node<br>??? MB/s @ rendering node<br>500 MB/s @ login node | 2 GB/s | 2 GB/s | 2 GB/s | 1 GB/s |
| Write perf./node | 500 MB/s @ compute node<br>??? MB/s @ rendering node<br>500 MB/s @ login node | 2 GB/s | 2 GB/s | 2 GB/s | 1 GB/s |
| Total read perf. | n*500\|??? MB/s | 10 GB/s | 20 GB/s | 50 GB/s | 8 GB/s |
| Total write perf. | n*500\|??? MB/s | 10 GB/s | 20 GB/s | 50 GB/s | 8 GB/s |

# Thank you for your attention!

# Questions?