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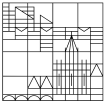
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HPC Workflows

- Introduction -

Samuel Braun, KIT, SCC

References

-  bwHPC Wiki
<https://wiki.bwhpc.de>
-  NHR@KIT User Documentation
<https://docs.nhr.kit.edu/>

■ Material: Slides & Scripts

■ <https://indico.kit.edu/event/5741/>

■ Outline

- What is a supercomputer? Do I need one?
- What are typical **workflows**?
- What else should be kept in mind?

Goal of this lesson

- Thematic mapping of course content

What is a supercomputer?

■ What is a supercomputer? Do I need one?

■ Supercomputer alias HPC Cluster

- Compute nodes
- Interconnect
- Storage
- Infrastructure

■ Exact definition?

- No. Performance relative to current personal compute devices
- Expensive

■ When to use HPC Clusters, when NOT

HPC: yes

- Many separate calculations in parallel (HTC)
- Software can efficiently divide problem into many smaller problems that run in parallel
- Need more RAM (memory) than normal computer can provide
- Need many/big GPUs
- Need to process large amounts of data that do not fit on normal computer

HPC: no

- Calculation runs in serial , only few calculations
- Workflow: run one calculation, analyze data locally, then run the next calculation
- Other computational needs than raw computing power
- Services (well, AI ...), webservers, ...

■ When to use HPC Clusters, when NOT

Misconceptions

- The performance of a single HPC compute core is not higher than that of your typical desktop computer. The main things HPC offers:
 - Many compute cores / nodes
 - Much RAM (memory)
 - GPUs

Requirements

- Linux shell knowledge
- HPC-specific knowledge
 - Software module system
 - How to use the scheduler / job scripts: how to send calculations to a computer
 - ...
- Expect waiting times between 1h and 2 days until calculation(s) start

What are typical workflows?

■ Workflow: User centric view

- Registration
- Login, file transfer
- Software
- Storage, data lifecycle
- Compute resources, scheduler
- Pre-processing, computation, and post-processing

■ Registration

■ bwUniCluster

- no project description
- entitlement for self-registration is sufficient
- questionnaire within 14 days

■ bwForClusters

- project description
- entitlement

■ HoreKa / HoreKa 2

- project proposal

Details here:

bwHPC and NHR: Concepts,
Infrastructure and User Support

■ Login, file transfer

■ Login

- SSH (Port 22)
- JupyterHub (HTTPS)
- IDEs: VS Code, ... (SSH)

■ File transfer

- SCP, RSYNC, SFTP, ... (SSH)
- WebDAV

■ Login node

- No compute here

Details here:

Technical Access and Data Transfer

■ Software

■ Most software provided by HPC team

- software modules (lmod)

■ Own software

- pre-compiled
- self-compiled
- EasyBuild
- Containers: Apptainer, Enroot
- Python, ... - Packages

Details here:

- Software Modules
- Software II

■ Storage, data lifecycle

■ Different storage options

- HOME
- Workspaces
- TMPDIR, BeeOND
- LSDF, ...

■ Performance, lifetime, backup, ...

■ Lifecycle your data

Details here:

- File Systems
- File Systems II

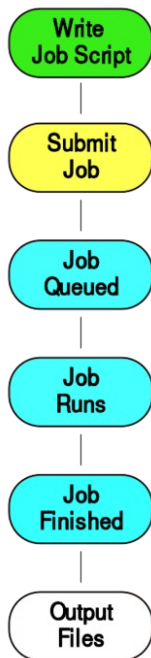
■ Compute resources, scheduler

- Compute on Compute Nodes (only!)
- Which of the available hardware fits your needs?
- How to access the compute nodes:
 - Batch
 - Interactive
- How to choose the (right amount of) resources

Details here:

- Batch System - Introduction
- Batch System - Best practices and parallel Jobs

■ Pre-processing, computation, and post-processing



- Compute intensive tasks only on compute nodes
- Automate job-lifecycle (as much as possible)
- Pre- and post-processing
 - Remote visualization?
 - GUI (?)
 - Data transfers

Details here:

- Batch System - Introduction
- Additional Topics: Usage of bwHPC & HoreKa Clusters (incl. JARDS)

What else should be kept in mind?

■ Policies & Use of AI Helpers

■ Growing use of AI assistants (since ~1 year)

- Massive impact on login nodes
- High CPU- and IOPS-loads

■ Policy: AI on login nodes

- **HK2: Forbidden**
- UC3, HK: under evaluation, likely to be forbidden

■ General Note

- Try to acquire or maintain the ability to operate the systems yourself
- Do not interact with our HPC systems exclusively via LLM and prompting

■ The lay of the land / Aktuelle Großwetterlage

■ Frequent lockdowns of the login nodes

- AI is good in finding security holes...
- **Massive** increase in necessary security-related actions on our part since ~1year
- **Every one to two weeks, we're on the verge of a server shutdown**

■ We need to decide

- Are we affected?
- How serious is the situation?
- How to mitigate?
- Are there less severe mitigation measures than a lockdown?

■ We must ensure the **integrity of our system and your data!**

■ Email Communication and Support Tickets

■ All HPC users are subscribed to **mailing lists**

- These are used to communicate current events
- Despite clear announcements, we still receive many support tickets
- **Please read and pay attention to these emails!**

■ Ticket system

- <https://nhr-helpdesk.scc.kit.edu> or <https://bw-support.scc.kit.edu/>
- Assign the ticket to the respective HPC-Cluster

■ Wiki

- Currently, the user documentation is spread across three websites

- <https://wiki.bwhpc.de> **bwUniCluster, bwForCluster**
- <https://www.nhr.kit.edu/userdocs/> **HoreKa , HAICORE, Future Technologies Partition DEPRECATED**, will be taken out of service with the HoreKa decommissioning
- <https://docs.nhr.kit.edu/> **HoreKa 2, HAICORE 3.0, Future Technologies Partition Under construction**, not yet complete; will be complete upon the launch of HoreKa 2

■ Contribution

- bwHPC Wiki: via ticket in support portal
- NHR user documentation: via GitLab issue

■ Current Status of HK2 Commissioning

- GPU Partition "Jade": Currently in the integration phase. Commissioning is delayed due to external supplier and service provider dependencies
- HoreKa 2 Launch: Regular operation is expected to start in mid-November 2026
- Migration Phase 2: The launch of Jade will officially trigger the second, mandatory phase of the migration to HoreKa 2
- Current HoreKa Status: Operating with significantly reduced hardware capacity. Available CPU resources are already strictly limited → Limits of the computer building
- Action Required: Users are strongly recommended to prepare their migration to HoreKa 2 as early as possible

■ Facility & Infrastructure Update

- Required electrical inspection necessitates downtime of **ALL** HPC systems in calendar week 48
- We will combine this forced downtime with our own maintenance work, building updates, and commissioning of HoreKa 2 to minimize downtime as much as possible
- Thank you for your understanding

Thank you for your attention.

Questions?