Karlsruher Institut für Technologie

18th HPC Café

03.09.2026

Agenda HPC Café – 03.09.2026

Topics for today:

- **Focus Topic: Using Containers with Apptainer as Software Environments on HoreKa 2, HoreKa and bwUniCluster 3.0**
- Transition to HoreKa 2: Status
- Discussion and open floor

As usual this format is meant to be interactive.
Don’t hesitate to ask questions!

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Using Containers with Apptainer as Software Environments on HoreKa 2, HoreKa and bwUniCluster 3.0

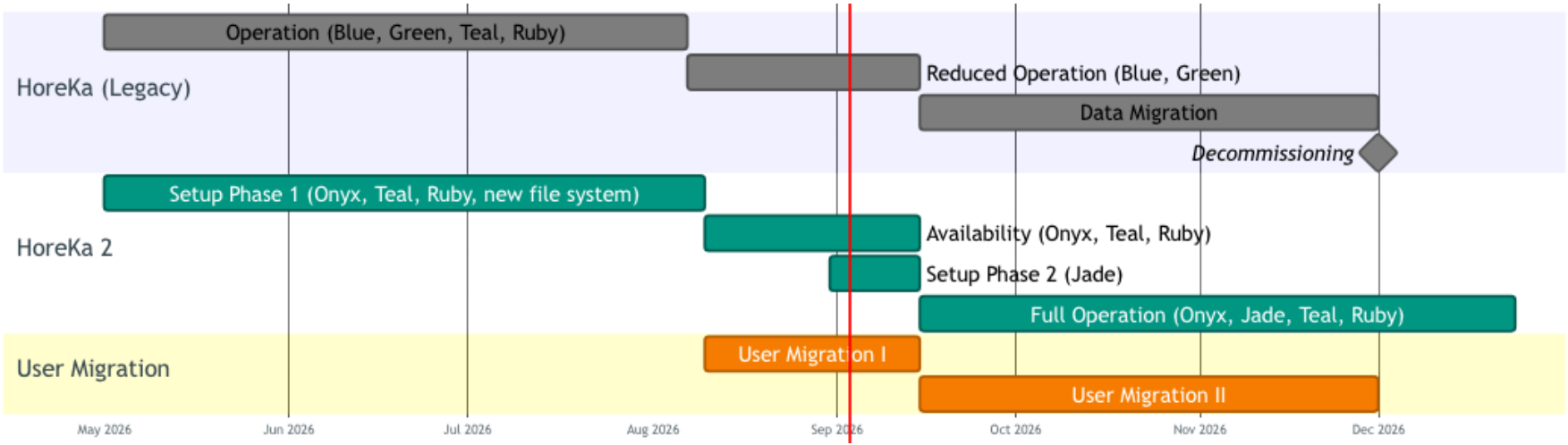
Holger Obermaier (SCC)

Karlsruher Institut für Technologie

Transition to HoreKa 2:

Status

Transition to HoreKa 2: Status



- New documentation under https://docs.nhr.kit.edu
- Transition of CPU projects currently ongoing

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Time for Discussion

Next HPC Café

- Next HPC Café planned for **1 October 2026, 10 am**
- Reminder: regular timeslot for the HPC Café
  - Every **first Thursday of the month 10:00 am**

- As always, open to hear ideas for topics and talks, from …
  - Yourself
  - Colleagues and collaborators
  - Also just expressions for “topics of interest”

Apptainer on HoreKa 2

Holger Obermaier | 3. Sept. 2026

Scientific Computing Center

Table of Contents

Motivation: Containerization

Containerization

- Application runs in an isolated user space
- Container provides a full and independent computing environment
  - Configurations, libraries, applications, dependencies
- OS kernel is shared by other containers and native applications

Motivation: Apptainer

Apptainer

- Tool for creating and running *containers*
- Tailored especially for *HPC* usage
- Allows unprivileged users to use containers
  $\Rightarrow$ *Fake root* can be used to build containers
- No *sub-UIDs* or *sub-GIDs* support required
  $\Rightarrow$ Only one user available in container environment
- Isolation with Linux User Namespaces
  $\Rightarrow$ Negligible performance impact
- Host directories can be mapped into the container
- CPU and GPU resources can be accessed from within the container

Video: Interactive container usage

Usage Pros

Reproducibility

- Identical environments across runs
- Consistent results
- Predictable performance

Portability

- Prepare container anywhere (e.g. on your personal laptop)
- Very complex software setups only need to be done once
- Deploy prebuilt container on the cluster

Usage Pros (continued)

Performance

- Build container optimized for the hardware
- **Note: This contradicts portability**

Convenience

- Use the same environment everywhere
- Share the environment within your scientific group
- Use containers prepared by the community
- Predefine your environment variables
- Have the necessary compiler and toolchain ready

Usage Cons

Drawbacks

- The *Easybuild modules* provided and optimized by the operational team are not used
  - Software updates are left to the user
  - Support for software issues is limited
  - Optimal performance requires hardware-matched container libraries
- One more layer of abstraction
  $\Rightarrow$ Debugging gets even more complex
- MPI setup is more complex

Apptainer - Building a Container

Definition Files

- Describe how to build a container
- Configure:
  - Base container image
  - Additional software (e.g. via package manager, or from source)
  - Runtime environment variables

Container Image Sources

- Docker Hub
- AMD ROCm Platform
- GNU Compiler Collection
- Intel oneAPI HPC Toolkit
- NVIDIA GPU Cloud (NGC)

Example: Building a GCC Container

Files and Resources

- Definition file: gcc.def
- GCC environment settings: env_GCC.sh
- OpenBLAS build script: build_OpenBLAS.sh

Video: Building a GCC container

Apptainer - Running an MPI Application

Problem: SLURM Software Package

Problem: `mpirun` invokes `srun` (SLURM) to launche processes
$\Rightarrow$ SLURM normally unavailable inside the container

Solution: Launch processes with `srun` outside the container

Problem: Resource Information

Problem: MPI needs resource allocation details

Solution: Use `srun -mpi=pmix` to pass resource info into container

Example: Running an MPI Application

Files and resources

- NVIDIA HPC SDK (includes NVIDIA HPC-X with latest MPI software stack)
  `apptainer pull docker://nvcr.io/nvidia/nvhpc:26.5-devel-cuda_multi-ubuntu24.04`
- MPI source code: hello_world.c
- Build script: build.sh
- Batch script: hello_world.sbatch

Output

```
Rank 1 of 2 (hk2n1004.localdomain)
Rank 0 of 2 (hk2n1003.localdomain)
```

Video: Running an MPI application