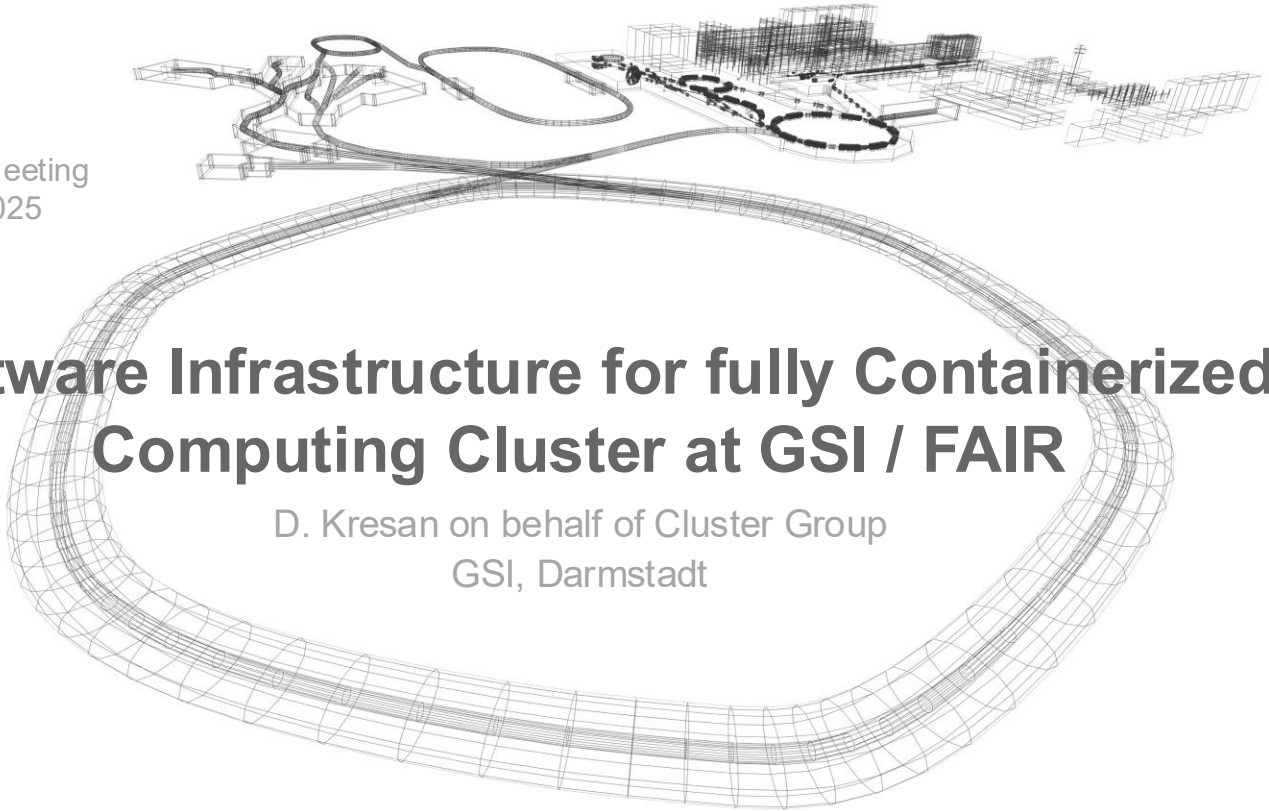


11-th MT Annual Meeting
3 – 6 November 2025
GSI, Darmstadt

A detailed wireframe model of a particle accelerator, likely the FAIR facility. It shows a large, oval-shaped ring structure with a complex internal lattice of beams and supports. The model is rendered in a light gray wireframe style, highlighting the intricate geometry of the facility.

Software Infrastructure for fully Containerized Computing Cluster at GSI / FAIR

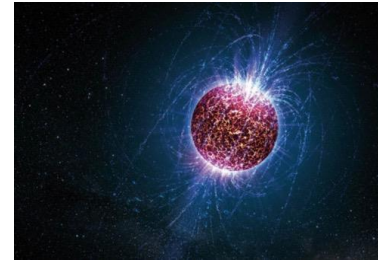
D. Kresan on behalf of Cluster Group
GSI, Darmstadt

4 Scientific Pillars of FAIR



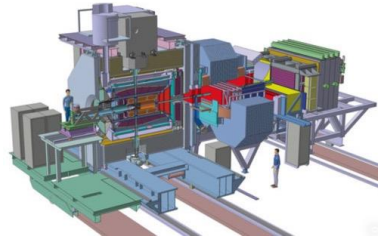
NUSTAR

Nuclear Structure
Astrophysics and
Reactions. Experiments
with atomic nuclei are the
key to understanding stars



CBM

Compressed Baryonic
Matter. The collision of
atomic nuclei at high
speeds can simulate the
conditions inside
supermassive objects for
a split second



PANDA

Antiproton Annihilation at
Darmstadt. How can
antimatter help us
understand the mass of
matter and the strong
force?

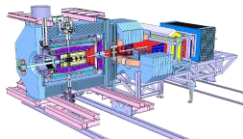
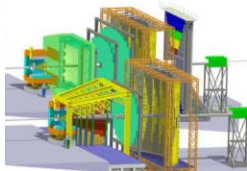


APPA

Atomic, Plasma Physics
and Applications. From the
investigation of atoms and
macroscopic effects in
materials or tissues all the
way to engineering and
medical applications

Computing at FAIR: The resources in the Green Cube will be shared between the different FAIR/GSI Partners

Dynamically allocated resources for exclusive usage and limited time



Analysis Facilities

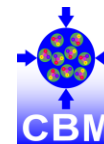


ALICE



No sperate hardware for the online clusters of CBM and PANDA

Generic batch farm for GSI/FAIR Users



R³B

panda



BIOMAT

APPA

■ ■ ■ ■ ■

- Requirements for the computing cluster
 - Highly scalable
 - Easily maintainable
 - Portability of user applications
- Separate user application space from host system
- Jobs are executed in a container
- **Minimal host system:** HW drivers + Slurm and Apptainer

- All-in-One solution for containerized environment:
 - Container image
 - Software Stack
 - Interactive session
 - Job submission
- Covers majority of use cases
- Developed and supported by GSI / IT

Task	Based on	Language
Login into container	OpenSSH	Bash
Job submission	SPANK Plugin	C
Building / testing of container images	GitLab CI/CD	Makefile
Managing software stack	Spack	Python / Bash

Self-developed, self-maintained and based on Free Software

Login into container

- Start container session on a submitter node upon login
- Fully transparent to user
- Customizable: also use your own container
- <https://doi.org/10.5281/zenodo.16752892>



Slurm Cluster – Virgo 3.0 Submit Node – Manual: <https://hpc.gsi.de/virgo>

Container launched: `/cvmfs/vae.gsi.de/vae24/containers/vae24-user_container_20240418T1037.sif`

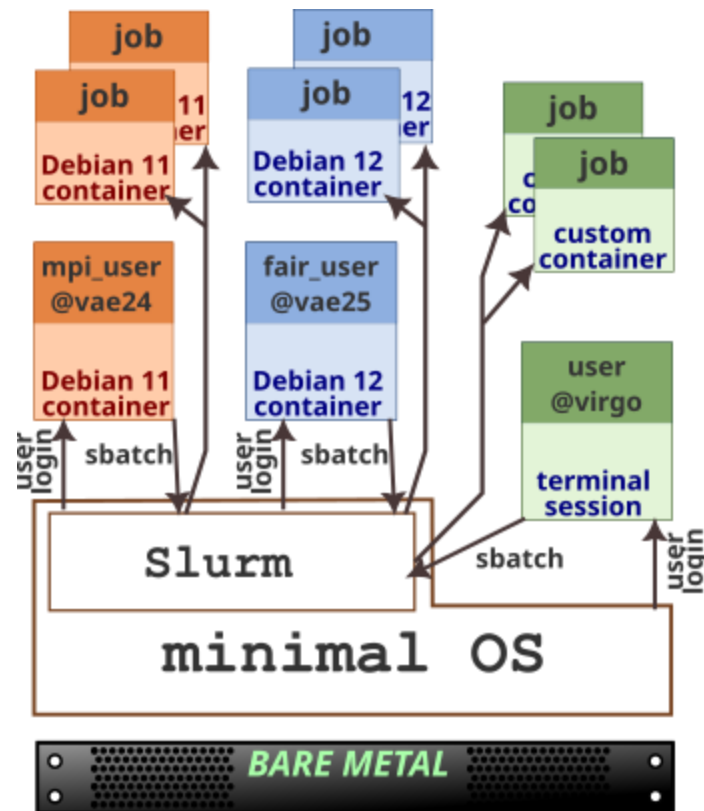
`kresan@lxbk1135:~ > realpath $(echo $APPTAINER_CONTAINER)`

`/cvmfs/vae.gsi.de/vae24/containers/vae24-user_container_20240418T1037.sif`

`kresan@lxbk1135:~ >`

Job submission

- VAE has Slurm client installed – submit jobs from container
- Job runs with the same Apptainer image
- Based on SPANK plugin
- Customizable with environment variable
- <https://doi.org/10.5281/zenodo.17431440>





- Apptainer definition files in git repository
- 3 Stages of a pipeline:
 - Commit triggers build of container images with dependency tracking
 - Perform tests
 - Deploy images on CVMFS → production

SDGroup / confd / Pipelines

All 672 Finished Branches Tags [View analytics](#) [Clear runner caches](#) [New pipeline](#)

Filter pipelines [Show Pipeline ID](#)

Status	Pipeline	Created by	Stages	Actions
Passed 0 00:22:02 9 months ago	[vae24] Remove /bin/bash command. #10827 jf develop → dcc6473d Logs		✓ ✓ ✓	Download
Cancelled 0 00:00:51 9 months ago	Use /etc/profile in zahnu. #10826 jf develop → a1375a32		✗ ✗ ✗	Refresh Download
Passed 0 00:20:57 9 months ago	[vae24] Set /etc/profile in BASH_ENV. #10802 jf develop → a1375a32		✓ ✓ ✓	Download
Passed 0 00:23:26 9 months ago	[vae24] Prepend /bin to PATH. #10724 jf develop → 9ea8e9f3		✓ ✓ ✓	Download
Passed 0 00:21:52 9 months ago	[vae24] Use bash.bashrc #10723 jf develop → 2495f152		✓ ✓ ✓	Download
Passed 0 00:21:28 9 months ago	[vae24] Use runscript section. #10722 jf develop → 258a2ef8		✓ ✓ ✓	Download
Passed 0 00:32:49 9 months ago	[vae24] Call Spack login script directly. #10721 jf develop → 13f4342e		✓ ✓ ✓	Download
Passed 0 00:30:52 10 months ago	[vae23] Change uri for buster-backport #10427 jf master → 918b138e Logs		✓ ✓ ✓	Download

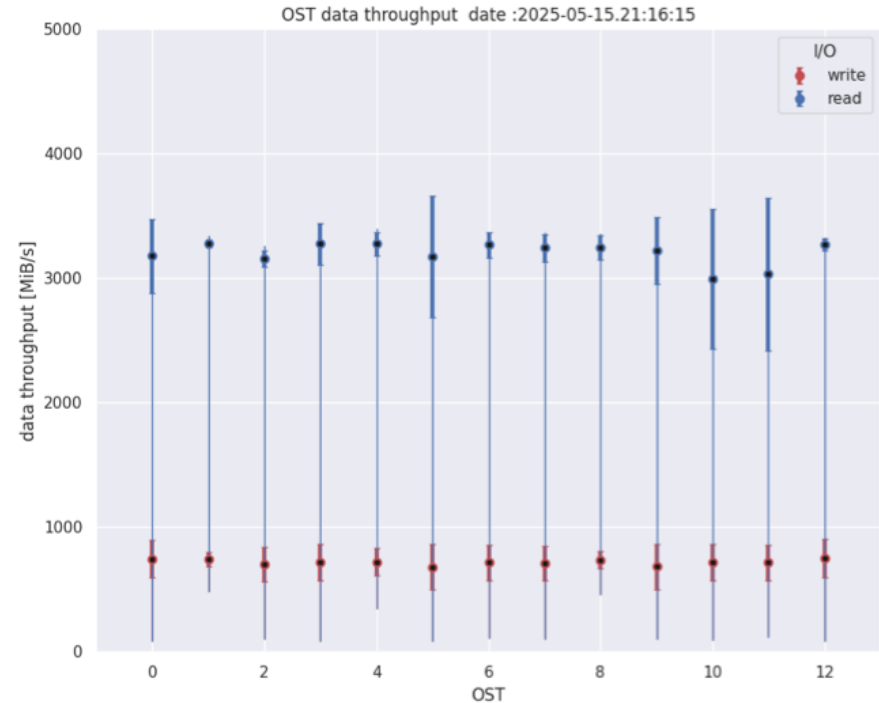
CI test 1: simple use case



- MPI test program with just initialization
- Launch container, load software stack
- Compile the test binary
- Submit job with test program

CI test 2: MPI based parallel I/O

- Self-developed parallel I/O benchmark
- Launch container, load software stack
- Compile the binaries
- Launch the benchmark using Slurm, write to shared Lustre storage
- Test passed if certain I/O throughput achieved



- Large software stack + dependencies in each version of VAE
- Use package manager Spack
 - Multiple versions of packages
 - Multiple build targets
 - Dependency tracking and resolving
 - Environments
 - Multiple compilers and mixed toolchains
- <https://github.com/spack/spack>



Spack

- Packages are built on a dedicated server within containers (install path matters!)
- Deploy on CVMFS
- When VAE image is launched – bind-mount CVMFS
- Make available within VAE: configure as Spack “upstream”

VAE timeline

	2020	2021	2022	2023	2024	2025	2026
Slurm version	18.04		21.08		23.11		25.xx
VAE	CentOS 7						
	Debian 10						
				vae22 (Deb. 10)			
				vae23 (Debian 10)			
					vae24 (Debian 11)		
						vae25 (Debian 12)	

- Release new version every year
- Bump major version of Spack, GCC, OpenMPI, Python, etc.. + update dependencies
- Support for 2 years

Thank you!



d.kresan@gsi.de