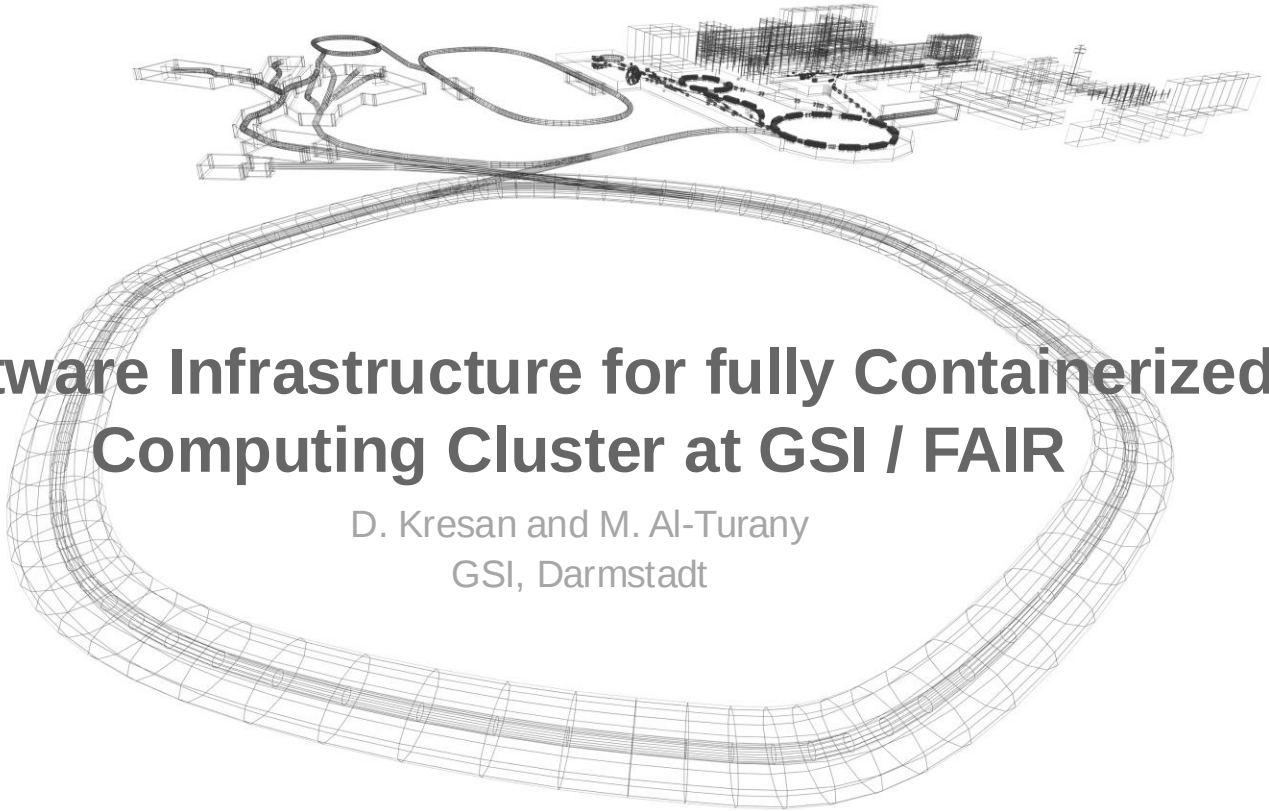


A detailed wireframe model of a particle accelerator, likely the FAIR facility. It shows a large, roughly circular main ring with several smaller, more complex structures and connecting paths. The model is rendered in a light gray wireframe style, showing the internal structure and layout of the facility.

Software Infrastructure for fully Containerized Computing Cluster at GSI / FAIR

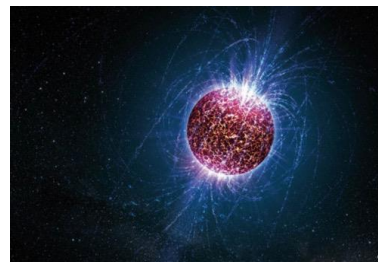
D. Kresan and M. Al-Turany
GSI, Darmstadt

4 Scientific Pillars of FAIR



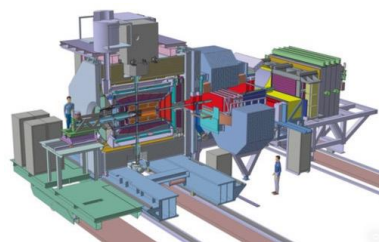
NUSTAR

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?

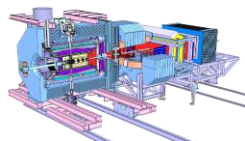
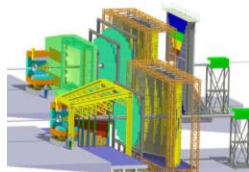


APPA

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

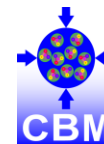


ALICE



No sperate hardware for the online clusters of CBM and PANDA

Generic batch farm for GSI/FAIR Users



R³B

panda



BIOMAT

APPA

...

- Heavy-Ion Collisions and Hadron Physics:
 - Online event processing, HTC, MC Simulations
- Nuclear Physics:
 - mostly offline batch processing
- Bio-physics, Med-physics:
 - MC simulations, AI with GPUs
- Plasma physics:
 - large scale MPI
- Theory:
 - large scale MPI, memory-bound
- All 6 communities need different software tools

- 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



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

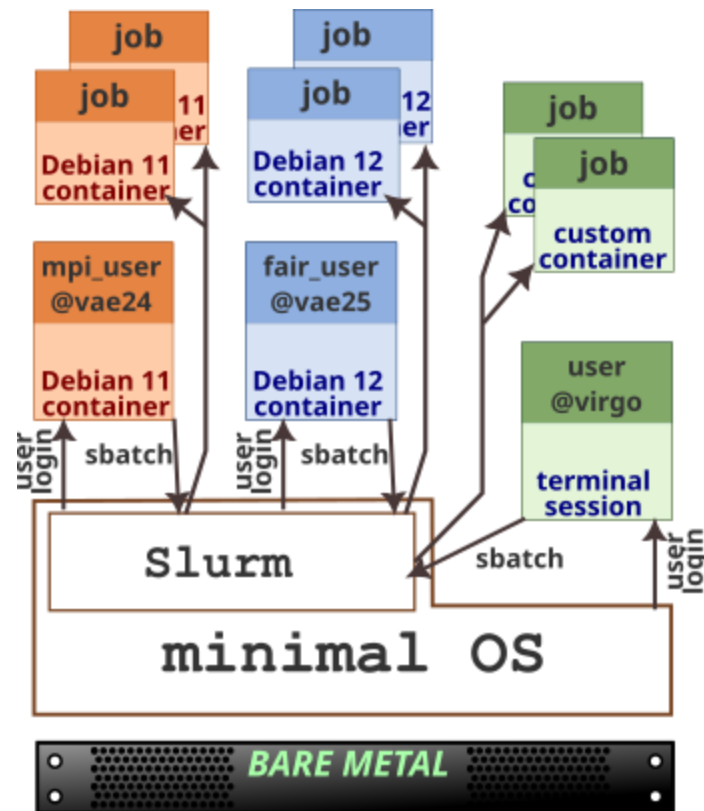
```
kresan@lxbk1135:~ > realpath $(echo $APPTAINER_CONTAINER)
```

```
/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





- 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](#)

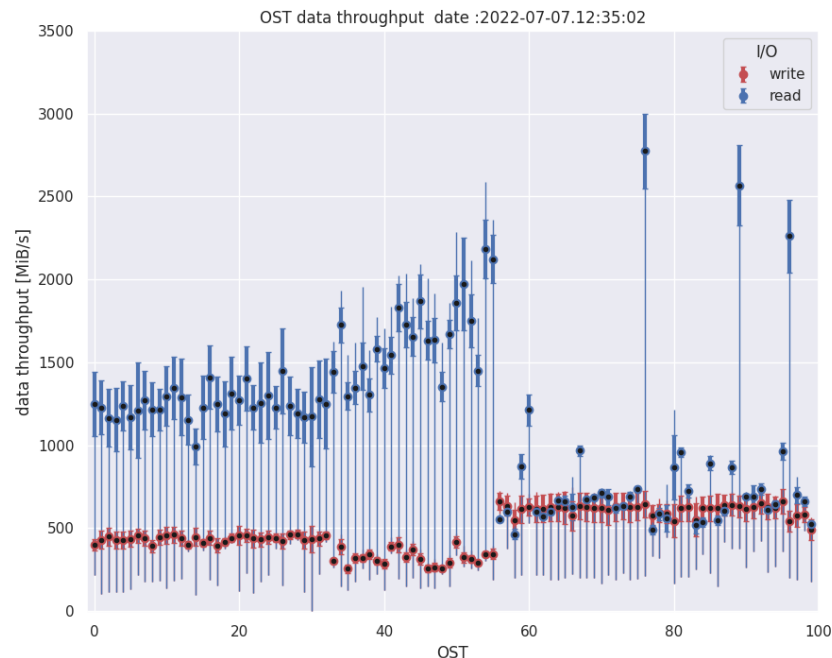
Status	Pipeline	Created by	Stages	Actions
Passed 0 00:22:02 9 months ago	[vae24] Remove /bin/bash command. #10827 3 develop → ddc6473d latest		✓ ✓ ✓	Download
Cancelled 0 00:00:51 9 months ago	Use /etc/profile in zahnuv. #10826 3 develop → a1375a32		✗ ✗ ✗	Refresh Download
Passed 0 00:20:57 9 months ago	[vae24] Set /etc/profile in BASH_ENV. #10802 3 develop → a1375a32		✓ ✓ ✓	Download
Passed 0 00:23:26 9 months ago	[vae24] Prepend /bin to PATH. #10724 3 develop → 9eaa893		✓ ✓ ✓	Download
Passed 0 00:21:52 9 months ago	[vae24] Use bash.bashrc #10723 3 develop → 2495f152		✓ ✓ ✓	Download
Passed 0 00:21:28 9 months ago	[vae24] Use runscript section. #10722 3 develop → 258a2ef8		✓ ✓ ✓	Download
Passed 0 00:32:49 9 months ago	[vae24] Call Spack login script directly. #10721 3 develop → 13f4342e		✓ ✓ ✓	Download
Passed 0 00:30:52 10 months ago	[vae23] Change uri for buster-backport #10427 3 master → 918b138e latest		✓ ✓ ✓	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



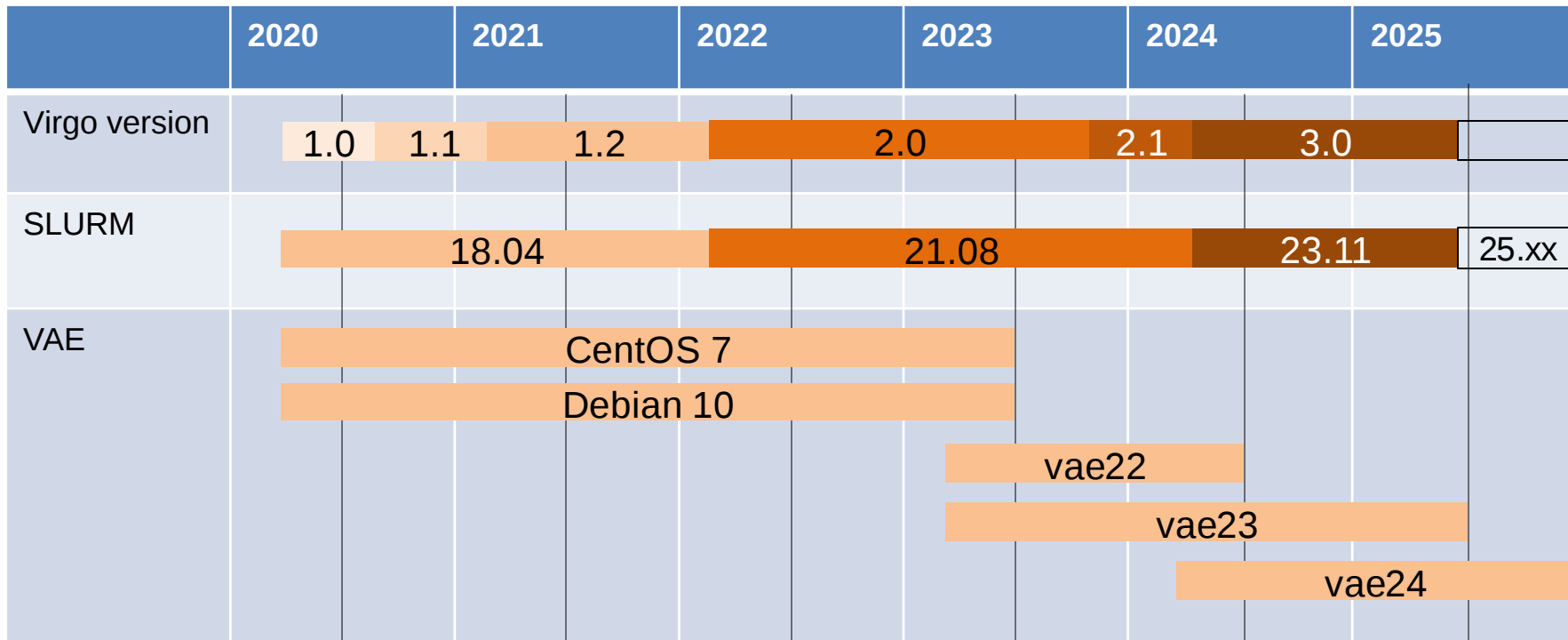
- Large software stack + dependencies in each version of VAE
- Use package manager Spack
 - Multiple versions of packages
 - Multiple build targets
 - Dependency tracking and resolving
 - Environments
 - Multiple compilers and mixed toolchains
- <https://github.com/spack/spack>



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



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

Requesting new software packages

- Templated form
- Gather enough information
- Each request is reviewed carefully

New Issue

Title (required)

Type



Issue

Description

Software Installation Request

Preview B I       

I hereby request the installation of software on the [GSI virgo cluster](https://hpc.gsi.de/virgo/) as described in the following:

```
(fields marked with * are mandatory)
* **Name***: (e.g. ROOT)
* **Version***: (e.g. 6.20.04)
* **Homepage***: (e.g. https://root.cern)
* **License***: (e.g. LGPL)
* **Known packages***: (e.g. unknown / `root` in Fedora 32 / `root@6.20.04` in Spack)
* **Flags***: (e.g. optimized release build and development headers / with optional module ... enabled)
* **Integration with other software***: (e.g. no built-in lib... / needs to work with given openmpi on virgo )
* **Virtual Application Environment(s) (VAE)**: (e.g. debian8 / centos7)
* **Considered alternatives which are already installed** (e.g. I need the exact software specified here because ... / I do not know alternatives, but I welcome suggestions / I considered alternative ... but it does not work because ...)
```

I need the above software for my work:

```
* **Collaboration***: (e.g. ALICE / CBM / Panda / Theory / ...)
* **Use case***: (e.g. sim / reco / analysis / productivity / software development / testing ...)
* **Users***: (e.g. myself / my group / ...)
```

```
**Additional information** (e.g. none / anything else you want us to know but did not fit the above questionnaire)
```

Switch to rich text editing



Thank you!



d.kresan@gsi.de