RSE Meetup

Report of Contributions

https://events.hifis.net/e/rse-at-hzdr

Contribution ID: **1** Type: **not specified**

Welcome

Thursday 3 April 2025 15:00 (10 minutes)

Contribution ID: **2** Type: **not specified**

Using Jacamar for direct HPC access in a continuous validation pipeline in GitLab for CFD software

Thursday 3 April 2025 15:10 (10 minutes)

To increase the acceptance of open-source Computational Fluid Dynamics (CFD) software in industry, a continuous validation strategy is required to demonstrate robustness and reproducibility of the software package. HZDR has a long-term experience as a downstream developer for the most frequently used open-source CFD package released by the OpenFOAM Foundation. HZDR has established an active partnership with the core developers to further develop its capabilities for the simulation of multiphase flows, which require continuous validation.
To this end, HZDR utilizes the Helmholtz Cloud Services as a resource to implement a fully-automated validation database into the Helmholtz Codebase, using pipelines (Gitlab), containerization (Docker, Apptainer), workflow engines (Snakemake), templates (Copier) and direct access to HPC resources (Jacamar). In the talk we show the current status of the Jacamar installation on the HZDR cluster Hemera and its use for establishing a fully GitLab-integrated validation pipeline.

Presenters: LEHNIGK, Ronald; SUDHARSHNAM, Varun (HZDR)

Session Classification: Talks

Contribution ID: **4** Type: **not specified**

Introducing EVERSE - the European network for research software quality

Thursday 3 April 2025 15:20 (5 minutes)

The EU funded project EVERSE has been running for one year and has first outputs to show. This short talk is to introduce the project, its goals and current state as well as potentially interesting outcomes and further interactions for RSEs at HZDR.

Presenter: JUCKELAND, Guido (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Talks

Contribution ID: **5** Type: **not specified**

Discussion 1: Jacamar for HPC access

Thursday 3 April 2025 15:30 (25 minutes)

Session Classification: Talks

Contribution ID: **6** Type: **not specified**

Discussion 2: EVERSE and interactions for RSEs at HZDR

Thursday 3 April 2025 15:30 (25 minutes)

Session Classification: Talks

Contribution ID: **8** Type: **not specified**

Summary and Closing

Thursday 3 April 2025 15:55 (5 minutes)

Contribution ID: **9** Type: **not specified**

Testing different versions of Python dependencies

Thursday 3 April 2025 15:25 (5 minutes)

With PyPIConGPU[1] we support version ranges for certain dependencies. To check if the code works with different versions of a dependency and also combinations with other different versions of other dependencies, we generate a CI job[2] for each version combination (21 in total at the moment). Our test code relies on self-written scripts and the possibility to change the requirements.txt during the runtime of the CI job. Now we want to introduce a pyproject.toml[3] in PyPIConGPU and therefore need to rethink our CI test scripts. As part of this, we want to replace self-written code as much as possible with existing solutions to reduce the maintenance of the test code. The talk should be a starting point for a discussion to exchange ideas with other people on the topic.

[1] https://github.com/ComputationalRadiationPhysics/picongpu/tree/dev/lib/python/picongpu
[2] https://gitlab.com/hzdr/crp/picongpu/-/pipelines/1739861645
[3] https://github.com/ComputationalRadiationPhysics/picongpu/pull/5307

Presenter: EHRIG, Simeon

Session Classification: Talks

Contribution ID: **10** Type: **not specified**

Discussion 3: Testing different versions of Python dependencies

Thursday 3 April 2025 15:30 (25 minutes)

Session Classification: Talks