TRIGGERING HPC JOBS VIA GITLAB

R. LEHNIGK, F. SCHLEGEL

Institute of Fluid Dynamics · Computational Fluid Dynamics · Dr. Ronald Lehnigk · r.lehnigk@hzdr.de · www.hzdr.de

OUR RESEARCH INTEREST: SIMULATION OF MULTIPHASE FLOWS
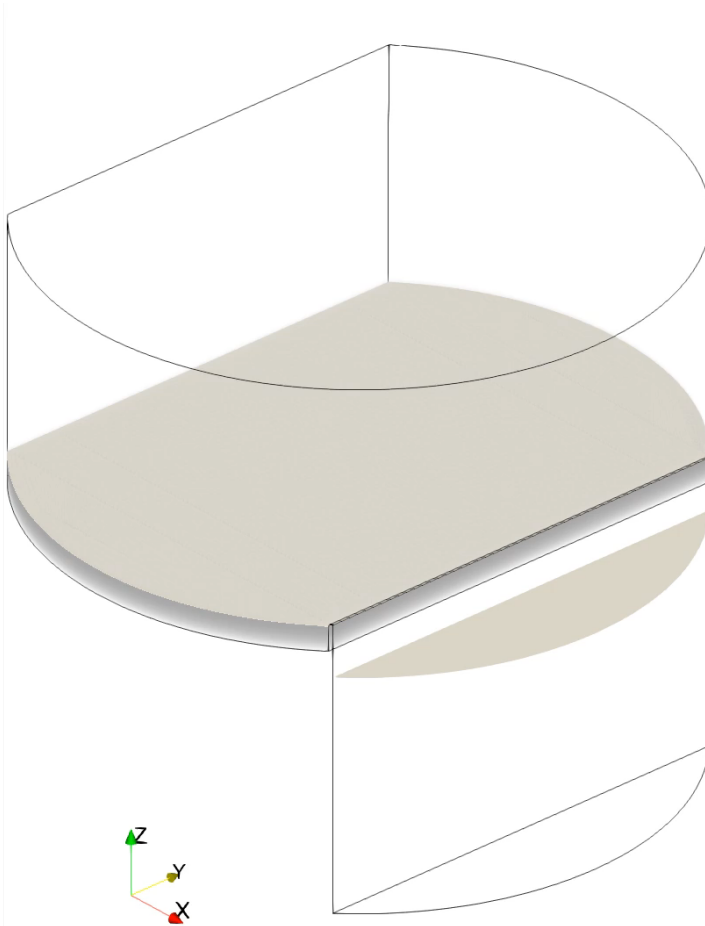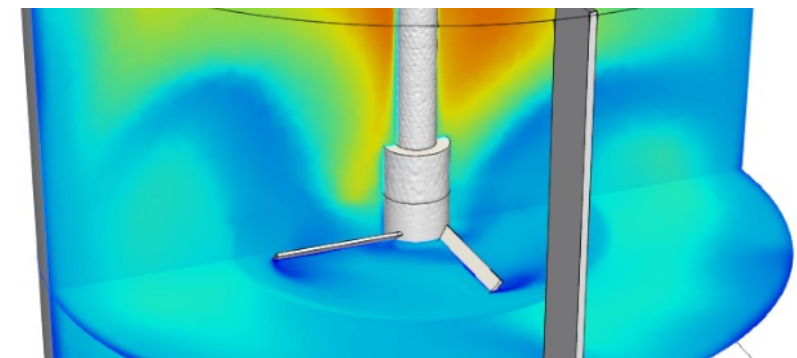

Distillation column tray
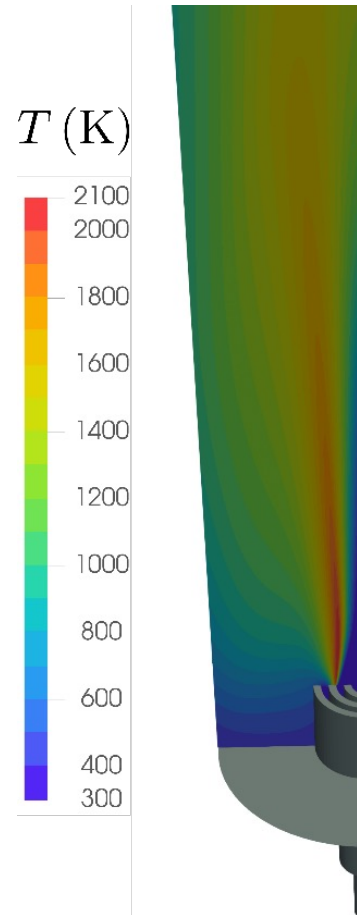
Flame synthesis of nano particles

Plunging jet

Mixer vessel

DRESDEN concept

OUR TOOL: OPENFOAM

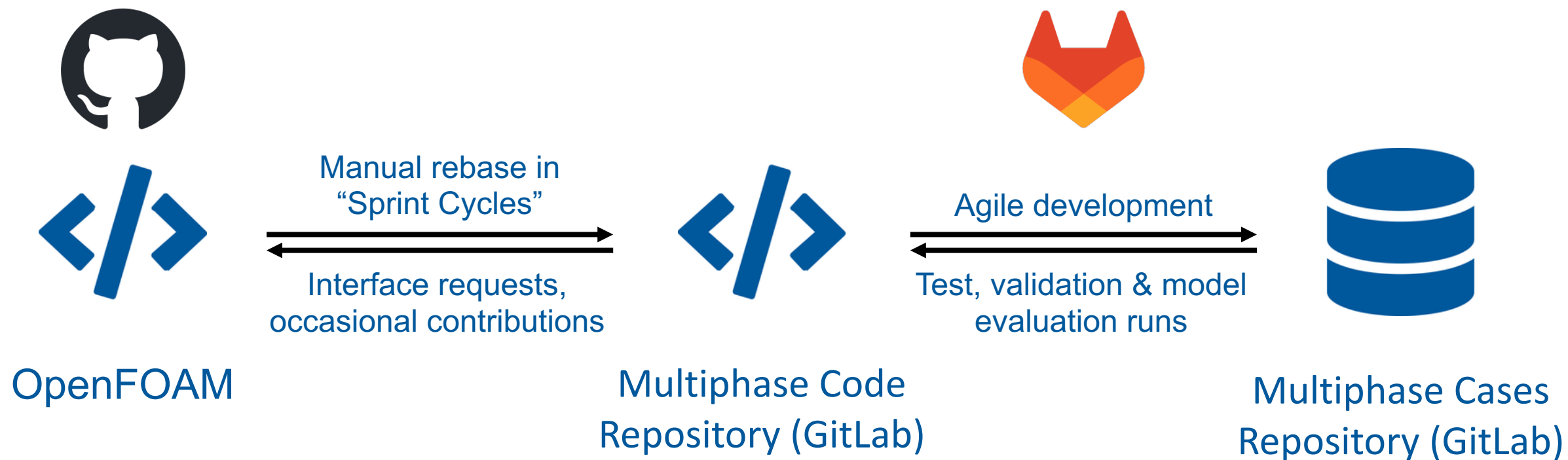## AN OPEN-SOURCE COMPUTATIONAL FLUID DYNAMICS (CFD) LIBRARY

- Based on Finite Volume Method (FVM)
- Written in C++ by Engineers
- Domain specific language – data structures and operators tailored for CFD

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} \quad \longrightarrow \quad \text{fvm::ddt(U) + fvm::div(phi, U)}$$

- Object-oriented and extendable design facilitates addon development

25.01.24   Triggering HPC Jobs via GitLab

DRESDEN concept   **HZDR**

OUR APPROACH: ADDON DEVELOPMENT

CENTERED AROUND CODEBASE.HELMHOLTZ.CLOUD

Manual rebase in "Sprint Cycles"

Interface requests, occasional contributions

Agile development

Test, validation & model evaluation runs

OpenFOAM

Multiphase Code Repository (GitLab)

Multiphase Cases Repository (GitLab)

RO DARE
ROSSENDORF DATA REPOSITORY

framatome EVONIK Leading Beyond Chemistry ALFA LAVAL BASF We create chemistry GRS KIT sunfire

(among others)

DRESDEN concept HZDR
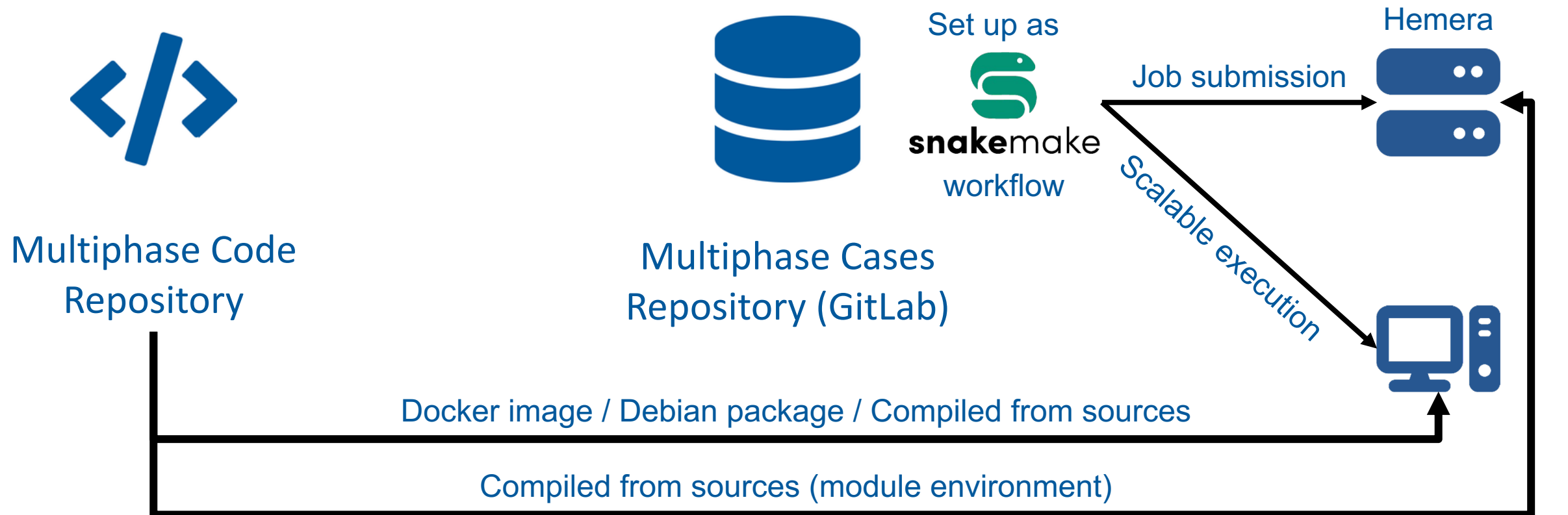
OUR STATUS: VALIDATION/MODEL EVALUATION RUNS

USING SNAKEMAKE WORKFLOW MANAGEMENT SYSTEM

Multiphase Code Repository

Set up as **snake**make workflow

Multiphase Cases Repository (GitLab)

Hemera

Job submission

Scalable execution

Docker image / Debian package / Compiled from sources

Compiled from sources (module environment)

DRESDEN concept   HZDR

OUR STATUS: MERGE REQUEST TEST PIPELINE

SINGLE TIMESTEP RUNS FOR TESTING CASE INPUT SYNTAX COMPATIBILITY WITH CODE
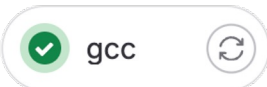
User-defined Variables for Pipeline

Variable	Value	Remark
DOWNSTREAM_BRANCH	main	Branch name in Cases Repository

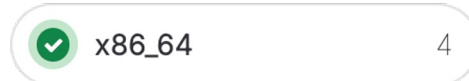Triggers test run in downstream project

GitLab "performance" runners

Scalable execution

Multiphase Code Repository

Multiphase Cases Repository (GitLab)

snakemake

build

✓ gcc

test

✓ downstream
  Trigger job

✓ x86_64   4

Downstream

✓ Cases
  #339154
  Multi-project

test

✓ snakemake

DRESDEN concept
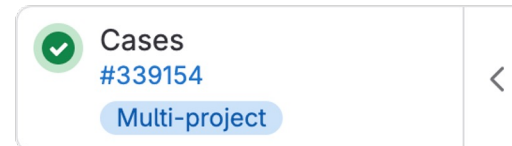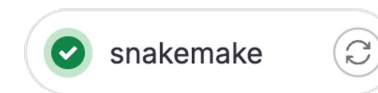
HZDR
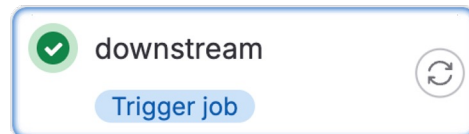
OUR STATUS: VALIDATION/MODEL EVALUATION PIPELINE

BRANCH-SPECIFIC, WEB-TRIGGERED FROM GITLAB

Workflow commands are sent
to Hemera as
➤ user "ofuser"
from
➤ "internal"-tagged GitLab runners
using
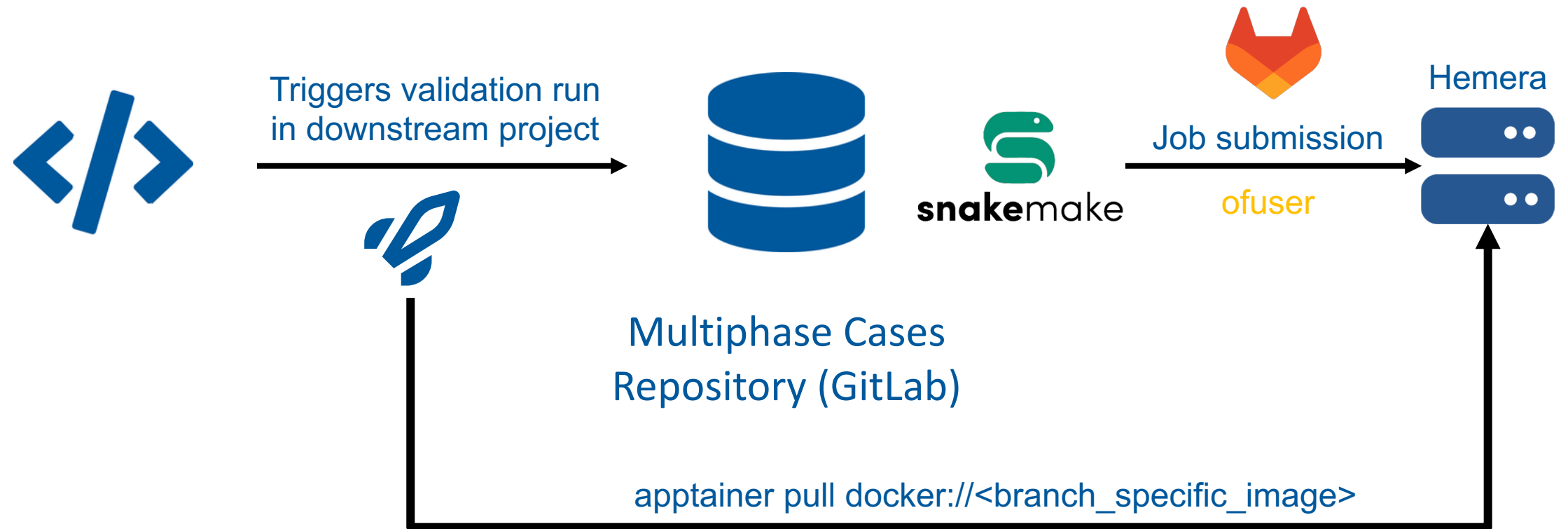➤ Python Fabric library for ssh communication

Job submission

ofuser

Hemera

Multiphase Cases
Repository (GitLab)

We'd like it to be the user triggering the pipeline.

DRESDEN concept

HZDR

Mid term goal: Merge request validation pipeline

Branch-specific, triggered from GitLab

Triggers validation run
in downstream project

Job submission

ofuser

Hemera

Multiphase Cases
Repository (GitLab)

apptainer pull docker://<branch_specific_image>

We'd like it to be the commit author.

Triggering HPC Jobs via GitLab

DRESDEN
concept

HZDR

BACKUP SLIDES

OUR STATUS: VALIDATION/MODEL EVALUATION PIPELINE

USER INTERFACE (USING GITLAB'S PREFILLED VARIABLES)

Run for branch name or tag

[main ⌄]

Variables

| Variable ⌄ | PROJECT_DIRECTORY | /bigdata/openfoam/workflow/multiphase/cases |

Project directory wherein the working directory for this pipeline is created. 'ofuser' must have access.

| Variable ⌄ | WORKING_DIRECTORY | ${GITLAB_USER_LOGIN}-${CI_COMMIT_BRANCH}-${CI_COMMIT_SHORT_SHA}-${CI_PIPELINE_ID} |

Name of the working directory created by this pipeline. For better identification, keep the default setting.

| Variable ⌄ | JOBS | 10 |

The maximum number of jobs submitted in parallel to the hemera cluster.

| Variable ⌄ | PARTITION | defq ⌄ |

Hemera partition to run jobs on. Overrides setting in Slurm profile.

| Variable ⌄ | TIME | 5760 |

Hemera wall time per job in minutes. Overrides setting in Slurm profile.

DRESDEN concept   HZDR

OUR STATUS: VALIDATION/MODEL EVALUATION PIPELINE

VALIDATION REPORT (DEPLOYED TO GITLAB PAGES)

25.01.24   Triggering HPC Jobs via GitLab