

SUSTAINABLE CODE DEVELOPMENT AND CASES MANAGEMENT WITH OPENFOAM FOUNDATION RELEASE

FREE OPENFOAM VKI SEMINAR





HELMHOLTZ ZENTRUM
DRESDEN-ROSSENDORF

SCANNING

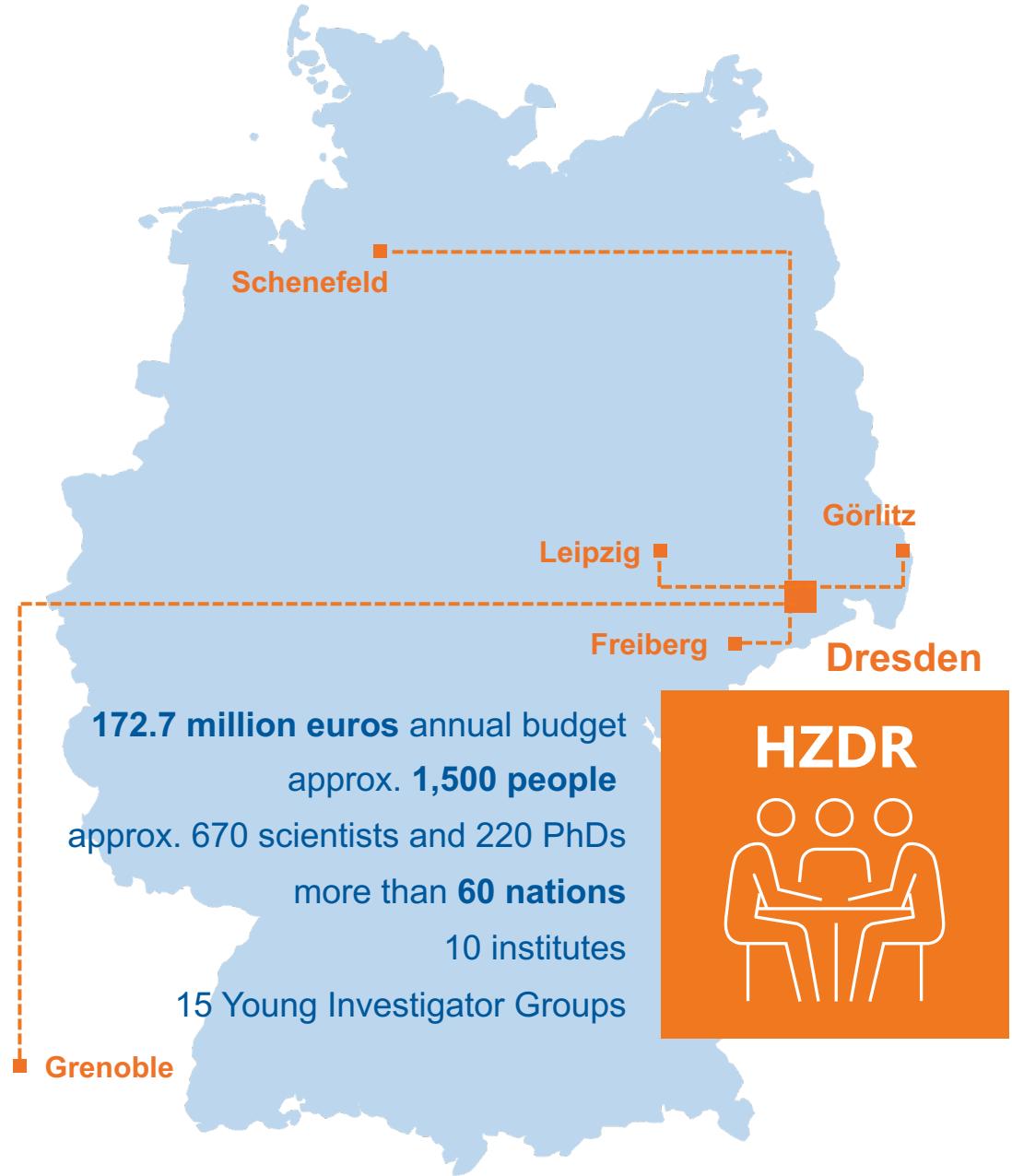
G17

Q11

L21

R12





WHO
ARE WE?

INSTITUTES AND CENTRAL DEPARTMENTS

Institute of Fluid Dynamics

Institute of Ion Beam Physics and Materials Research

Institute of Theoretical Physics

Institute of Radiopharmaceutical Cancer Research

Department of Information Services and Computing

Institute of Resource Ecology

Institute of Radiation Physics

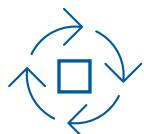
Dresden High Magnetic Field Laboratory

Institute of Radiooncology – OncoRay

Department of Research Technology

Helmholtz Institute Freiberg for Resource Technology

CASUS – Center for Advanced Systems Understanding



Energy



Matter



Health

INSTITUTE OF FLUID DYNAMICS

Departments in Institute of Fluid Dynamics

**Computational Fluid
Dynamics**

Dirk Lucas

**Experimental Thermal
Fluid Dynamics**

Uwe Hampel

**Magneto-
hydrodynamics**

Sven Eckert

**Transport Processes
at Interfaces**

Kerstin Eckert

Groups in Department of Computational Fluid Dynamics

**OpenFOAM modelling
of multiphase flows**

Fabian Schlegel

**Bubbles go with the
turbulent flows**

Tian Ma

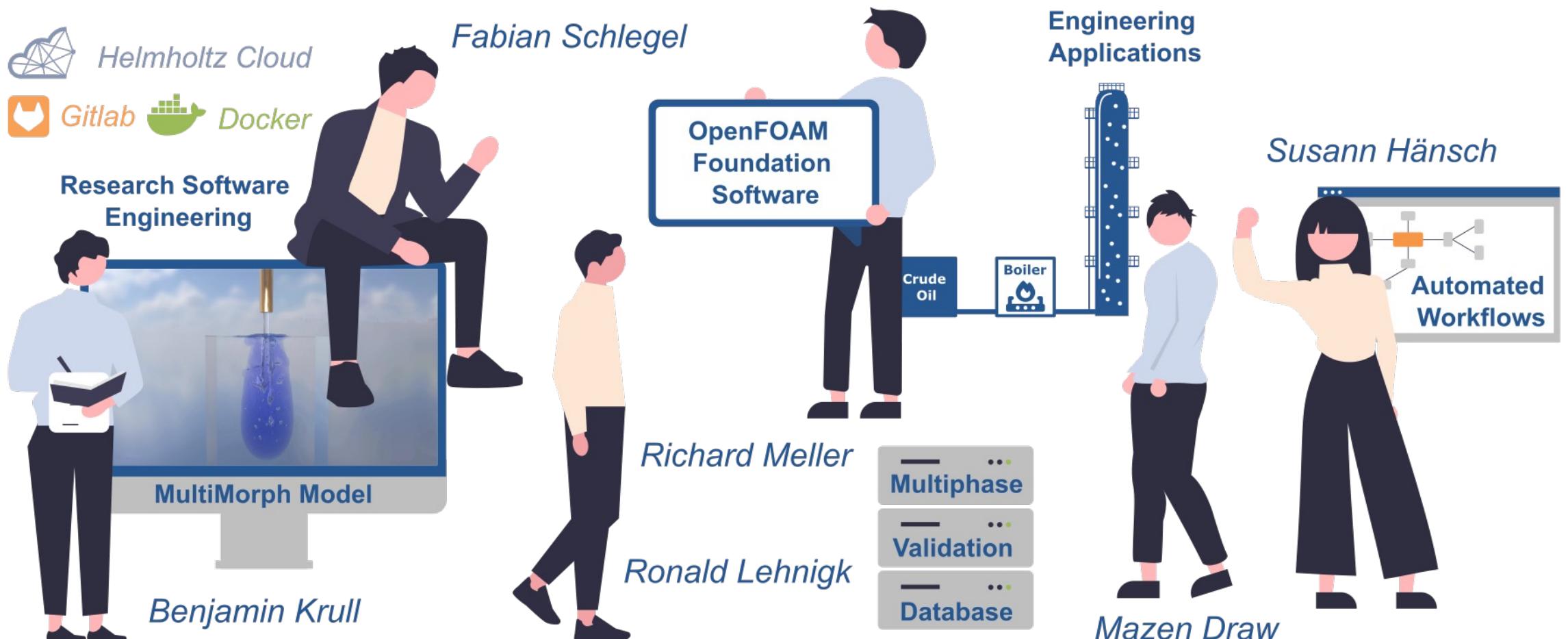
**Flotation and reactive
multiphase flows**

Roland Rzehak

approx. 25 people including approx. 12 scientists and 8 PhDs

THE OPENFOAM GROUP AND OUR INTERESTS

NUMERICAL SIMULATION OF MULTIPHASE FLOWS IN ENGINEERING APPLICATIONS



Modern simulation methods at HZDR

Morphologies

Water surface

Resolved gas bubbles

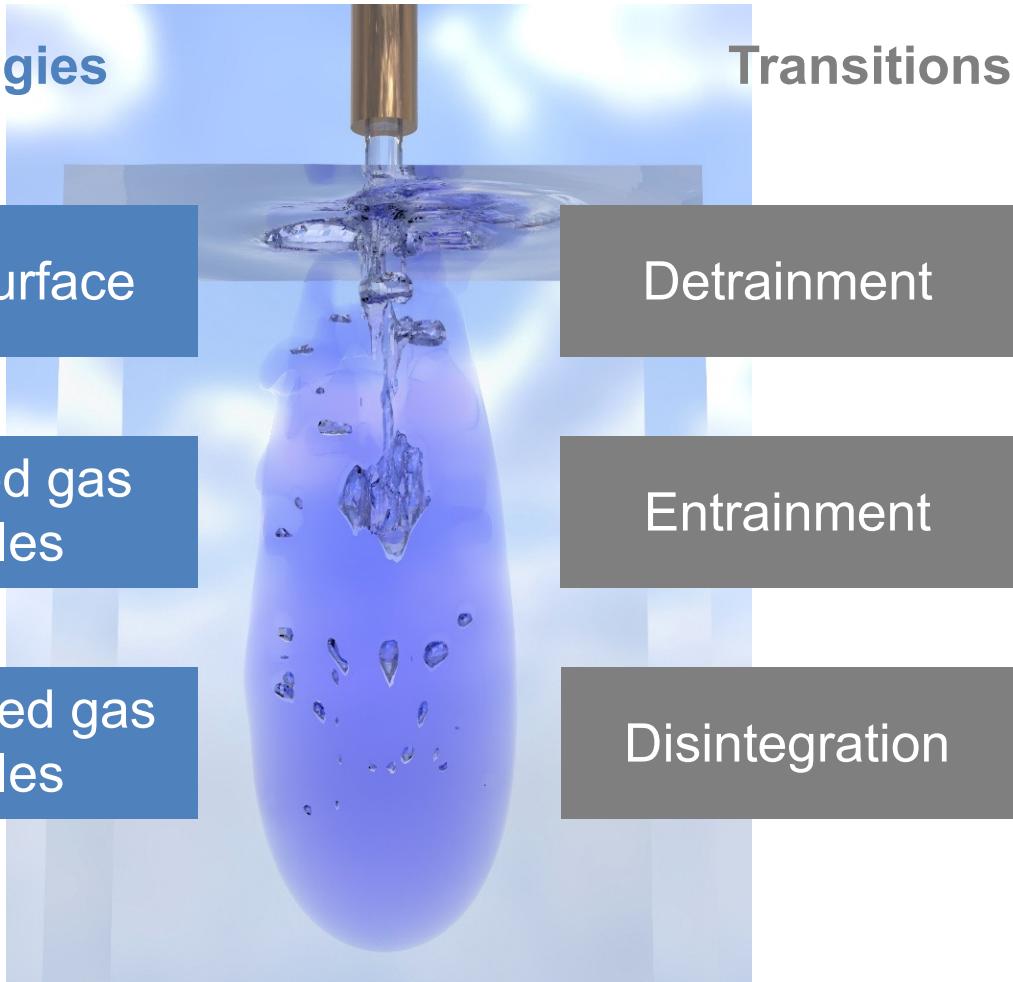
Unresolved gas bubbles

Transitions

Detrainment

Entrainment

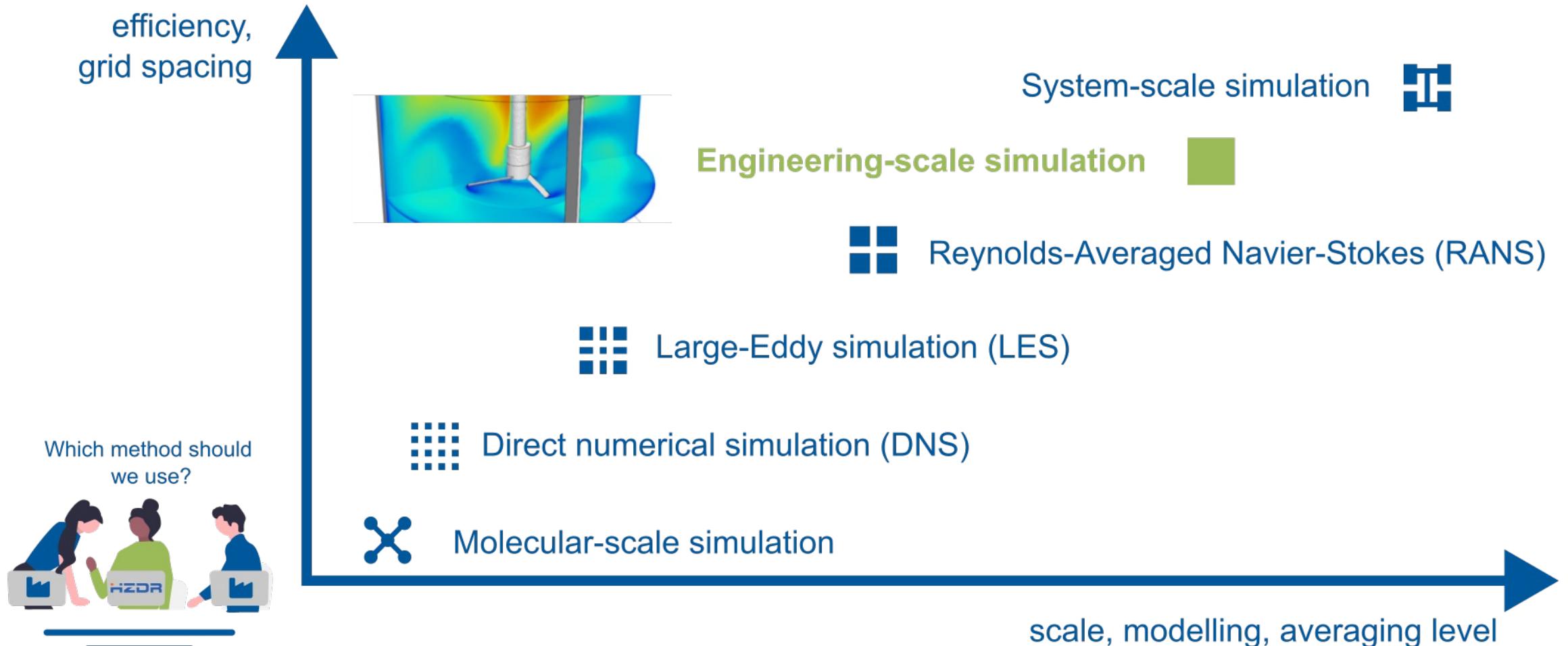
Disintegration



Simulation of a plunging jet with **MultiMorph model**

WHAT ARE
WE DOING?

SCALES AND ACCURACY IN NUMERICAL SIMULATIONS



MULTIPHASE FLOWS CHARACTERISED BY BROAD RANGE OF SCALES

Swirl separator for separating gas from liquid

Industrial applications contain **all morphologies**

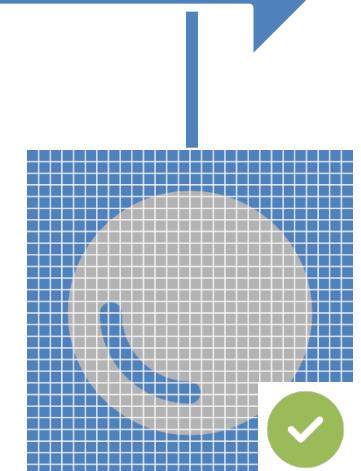
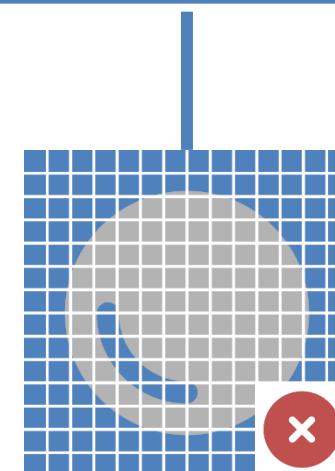
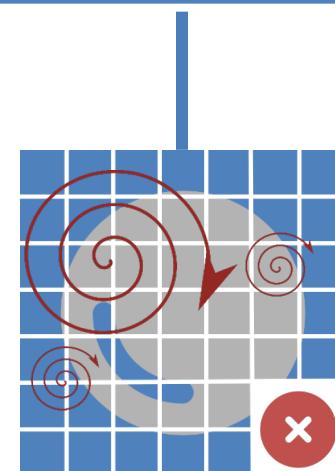
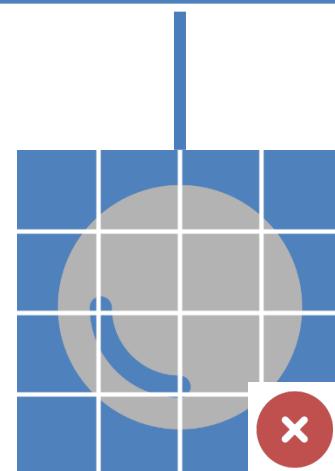
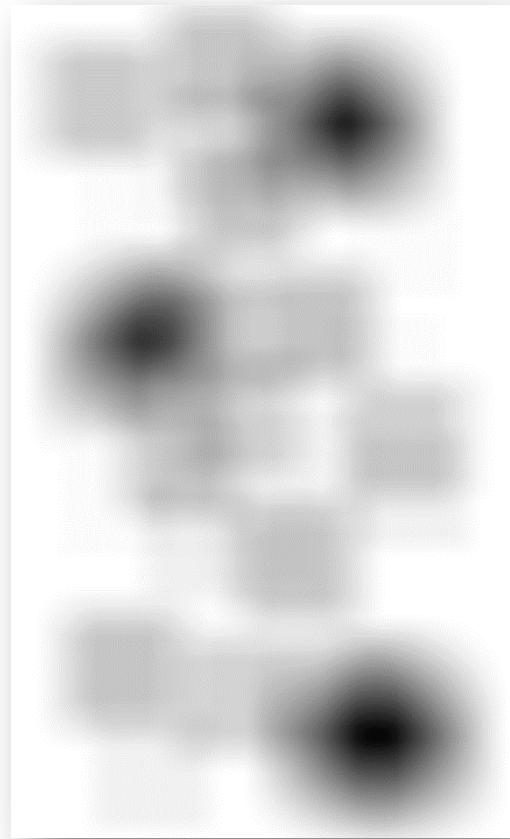
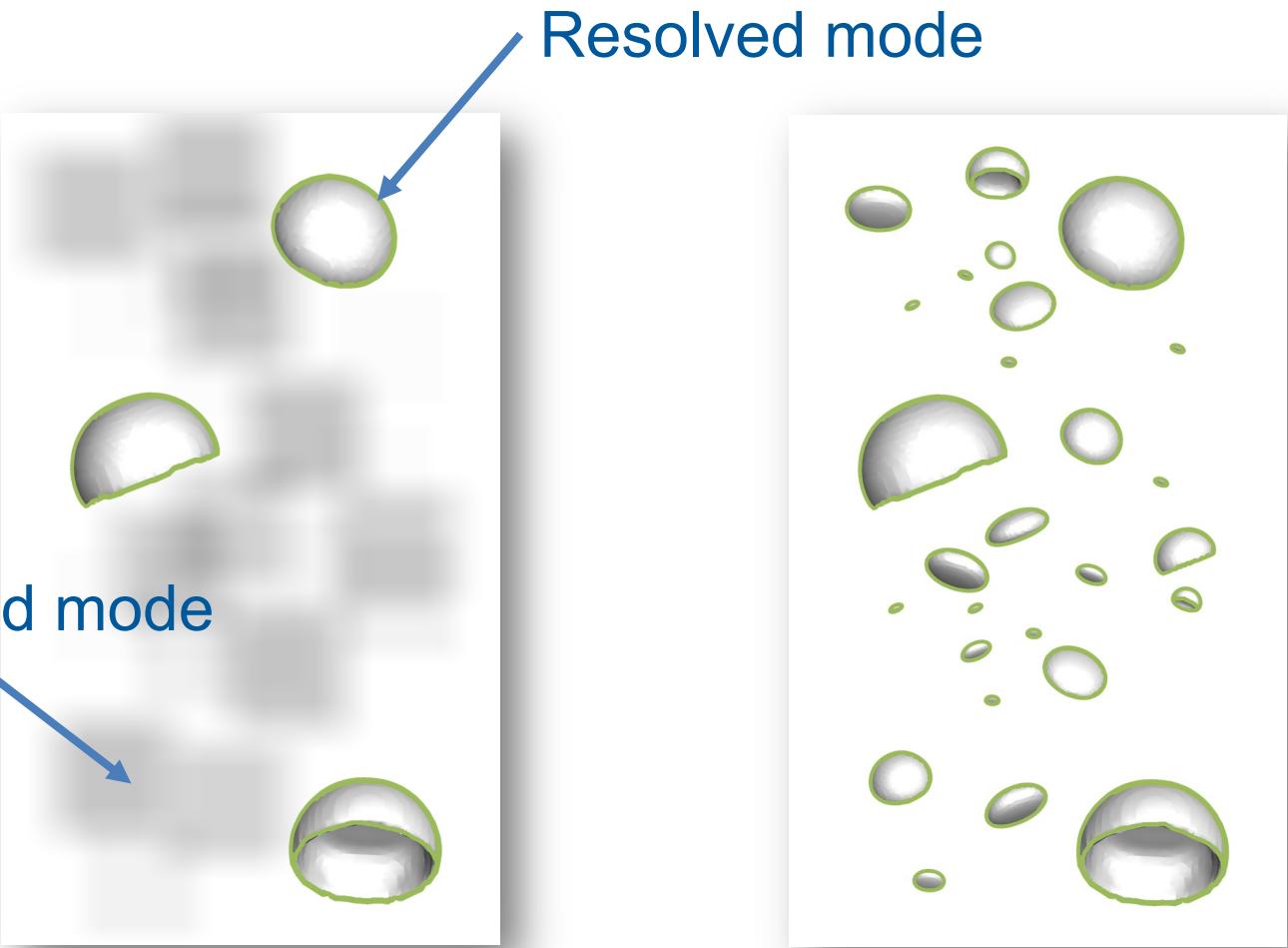


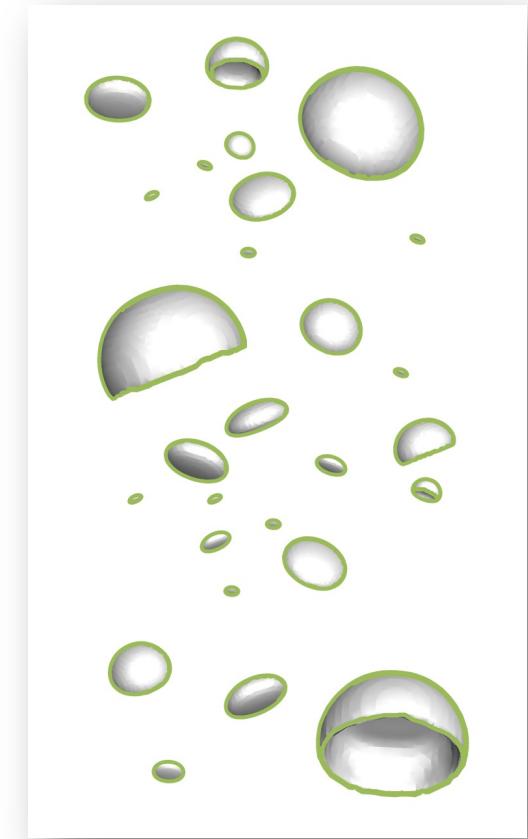
ILLUSTRATION OF INTERFACE TREATMENT



Euler-Euler Model



MultiMorph



Volume-of-Fluid

DEVELOPMENT STATUS OF MULTIMORPH MODEL

Resolved interface

Meller et al. (2021). Basic verification of a numerical framework applied to a morphology adaptive multifield two-fluid model considering bubble motions. *Int J Num Method Fluid*, 93(3), 748-773.

Under-resolved bubbles

Meller et al. (2023). Momentum exchange modeling for coarsely resolved interfaces in a multifield two-fluid model. *Int J Num Method Fluid*, 95(9), 1521-1545.

Disintegration

Meller et al. (2024). Numerical Transfer Towards Unresolved Morphology Representation in the MultiMorph Model. *Nucl Eng Design*, 428, 113470.

Over-resolved bubbles

Krull et al. (2024). A filtering approach for applying the two-fluid model to gas-liquid flows on high resolution grids. *Chem Eng Sci*, 119909.



Interface turbulence

Tekavčič et al. (2021). Validation of a morphology adaptive multi-field two-fluid model considering counter-current stratified flow with interfacial turbulence damping. *Nucl Eng Design*, 379, 111223.

Accumulation

Yin et al. (2023). A CFD approach for the flow regime transition in a vane-type gas-liquid separator. *Int J Multiphase Flow*, 159, 104320.

Empirical entrainment

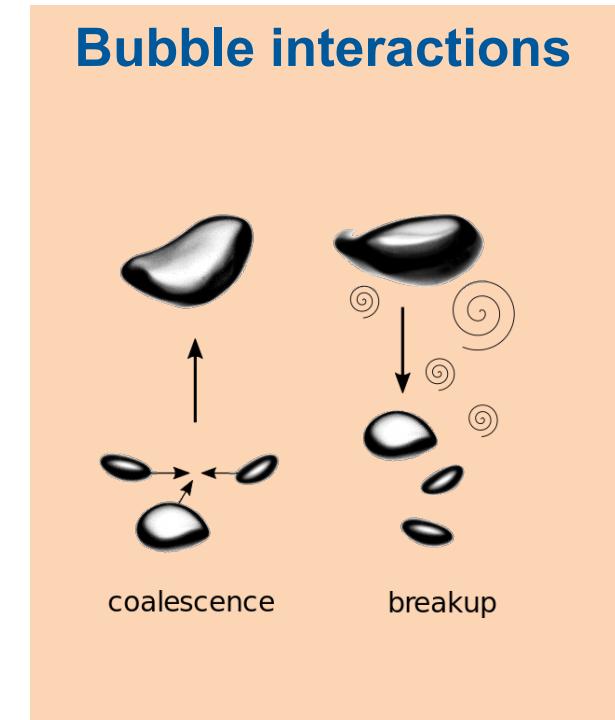
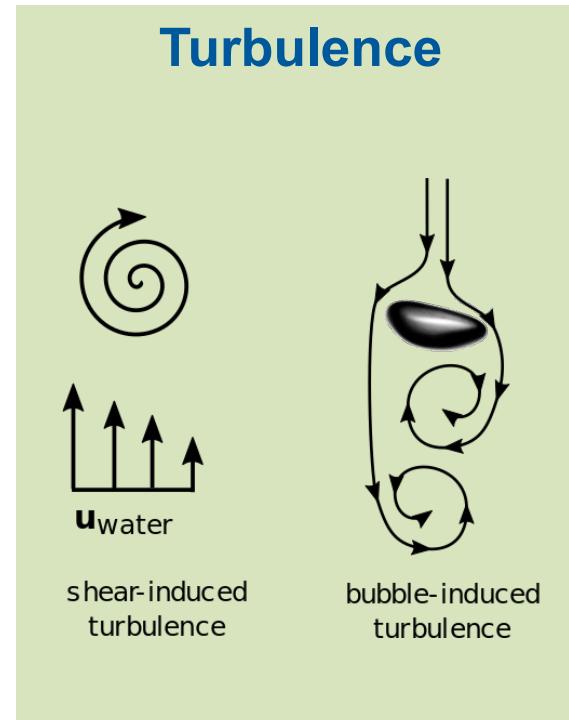
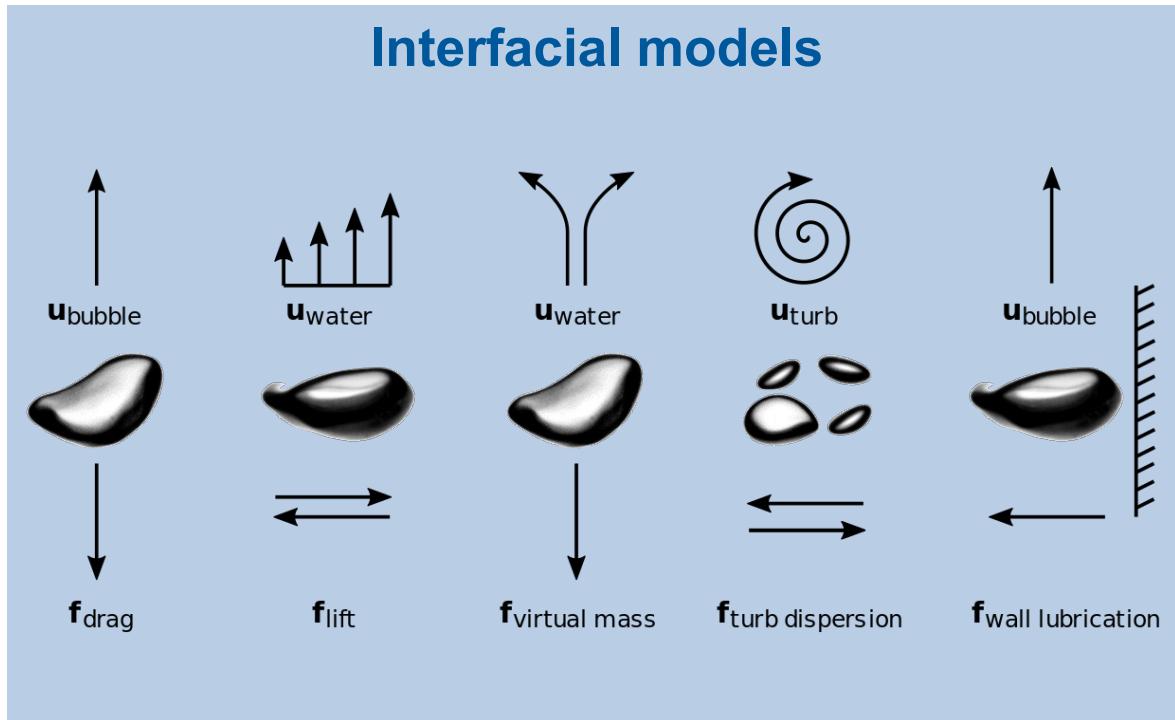
Wang et al. (2023). Simulation of droplet entrainment in annular flow with a morphology adaptive multifield two-fluid model. *Phys Fluid*, 35(10).

General concept

Schlegel et al. (2023). Openfoam-hybrid: A morphology adaptive multifield two-fluid model. *Nucl Sci Eng*, 197(10), 2620-2633.

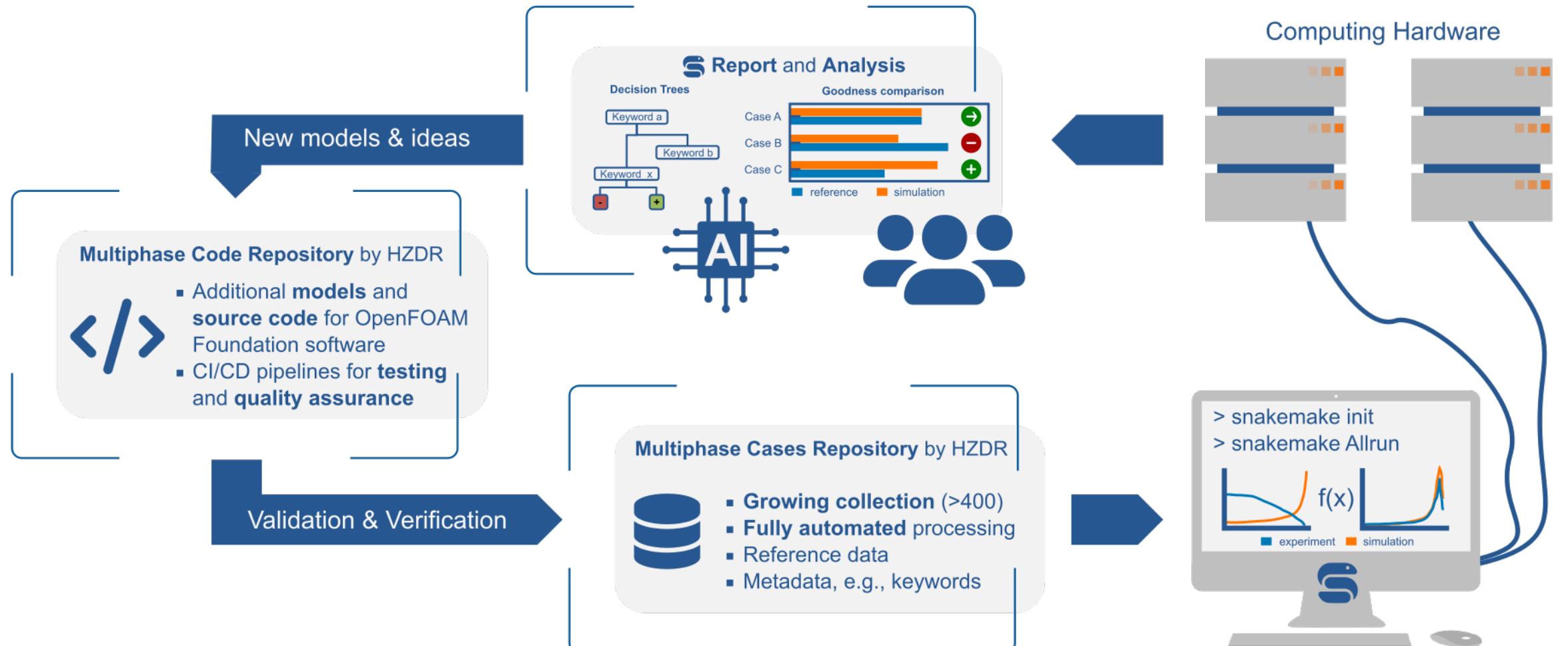
BASELINE MODEL FOR POLY-DISPERSE GAS LIQUID FLOWS

CLOSURE MODELS NEEDED FOR EULER-EULER SIMULATIONS



► Lecture on Multiphase Flows planned for 2025

VALIDATION STRATEGY FOR MULTIPHASE FLOWS



SOFTWARE PUBLICATIONS

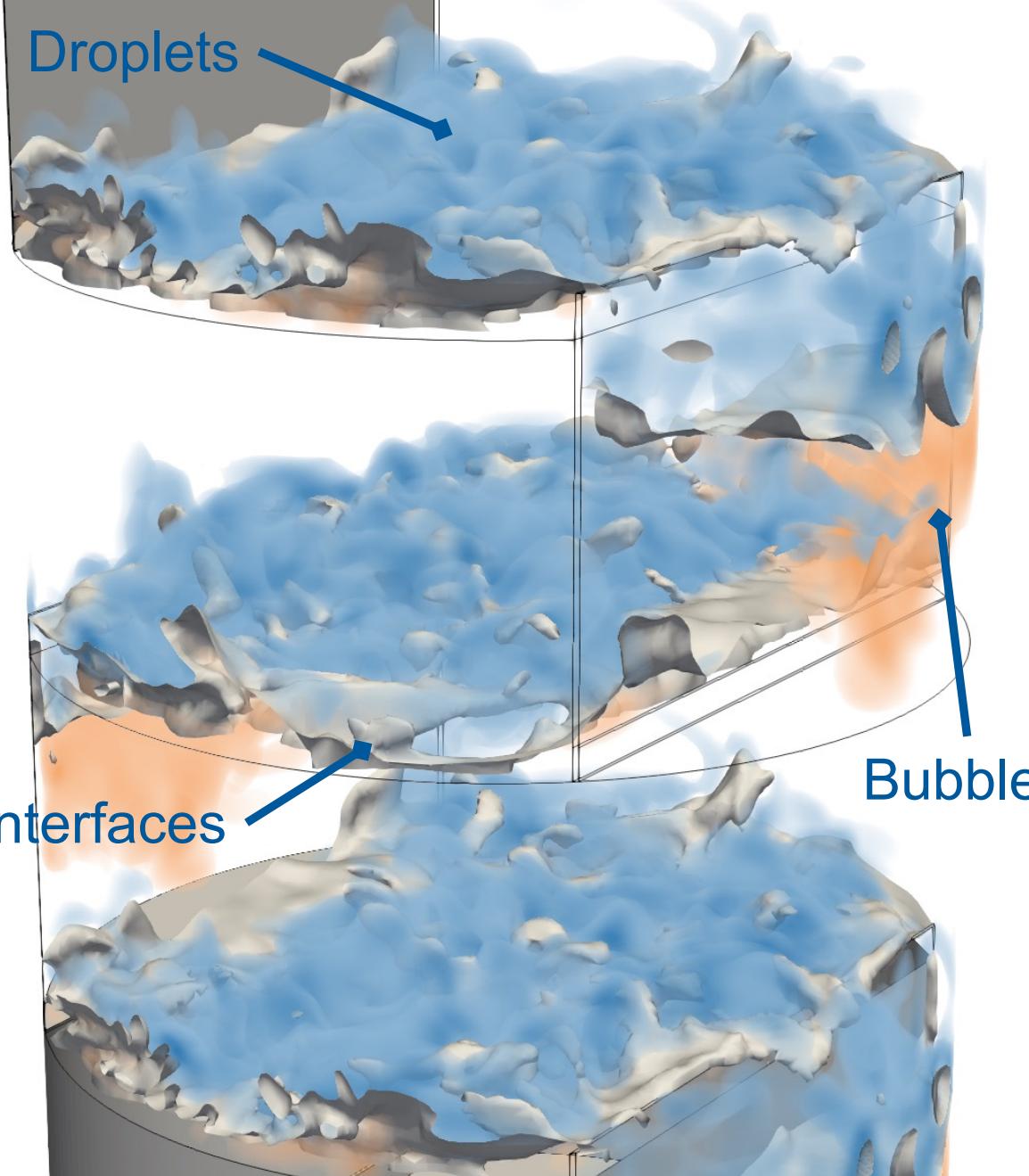
Schlegel et al. (2024, August 22). **Multiphase Code Repository by HZDR for OpenFOAM Foundation Software** (Version 11-s.1-hzdr.1). Rodare.
<http://doi.org/10.14278/rodare.3105>



<https://hzdr.de/multimorph>

Hänsch et al. (2024, August 22). **Multiphase Cases Repository by HZDR for OpenFOAM Foundation Software** (Version 11-s.1-hzdr.1-cases.1). Rodare.
<http://doi.org/10.14278/rodare.3104>

Schlegel et al. (2024, October 10). **Multiphase Python Repository by HZDR** (Version 1.3.1). Rodare.
<http://doi.org/10.14278/rodare.3191>

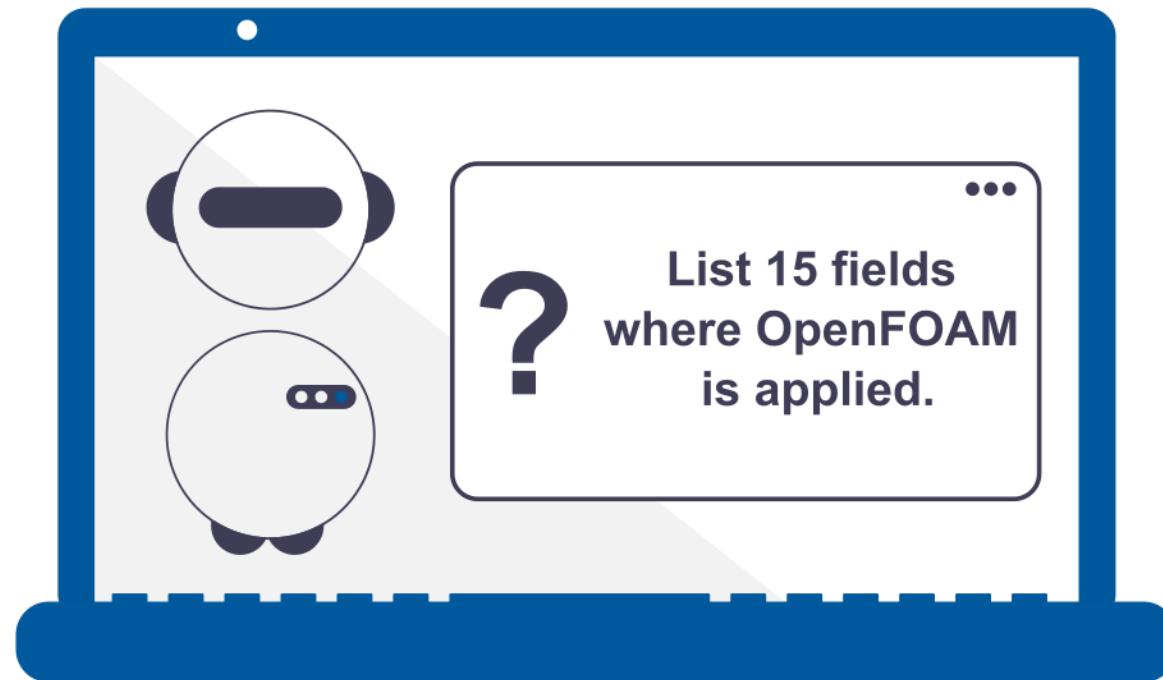


Simulated two-phase flow in a tray column

DIVING INTO OPENFOAM FOUNDATION SOFTWARE

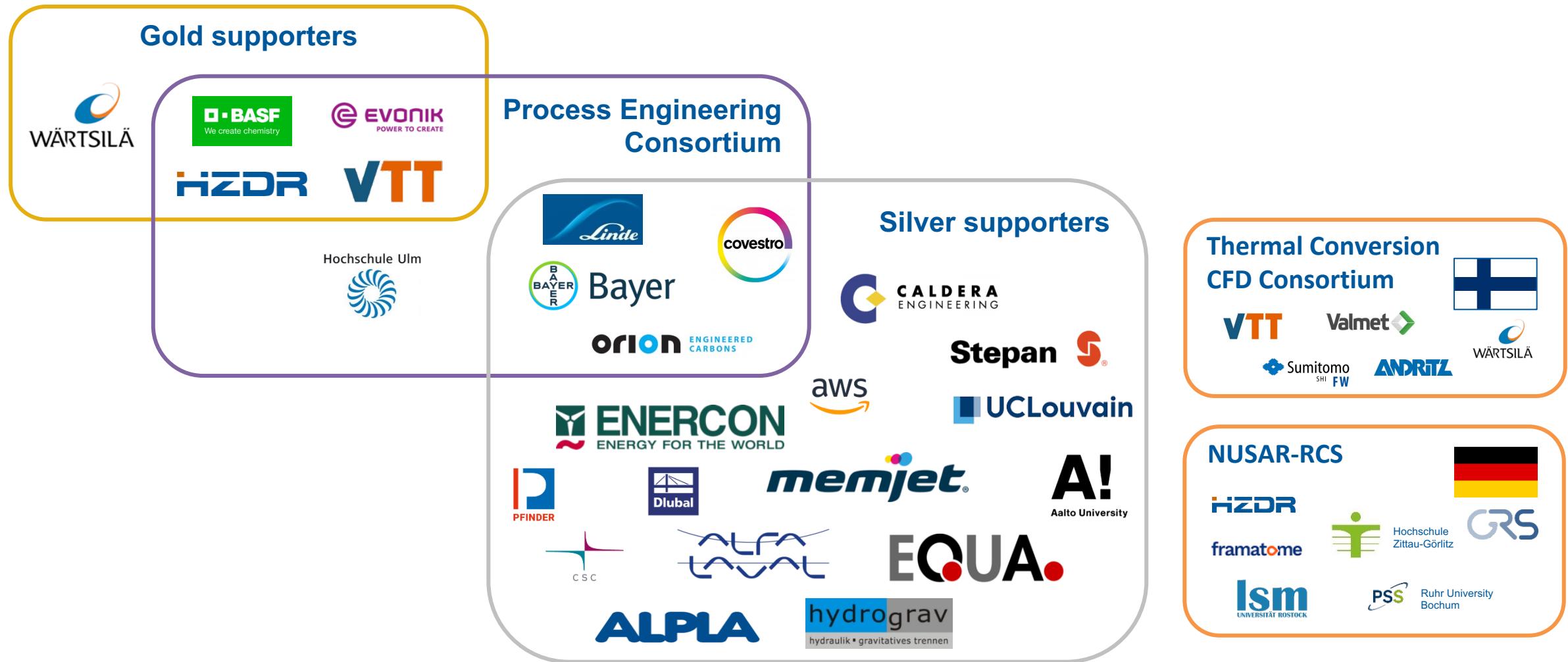


FIELD OF APPLICATIONS FOR OPENFOAM FOUNDATION SOFTWARE

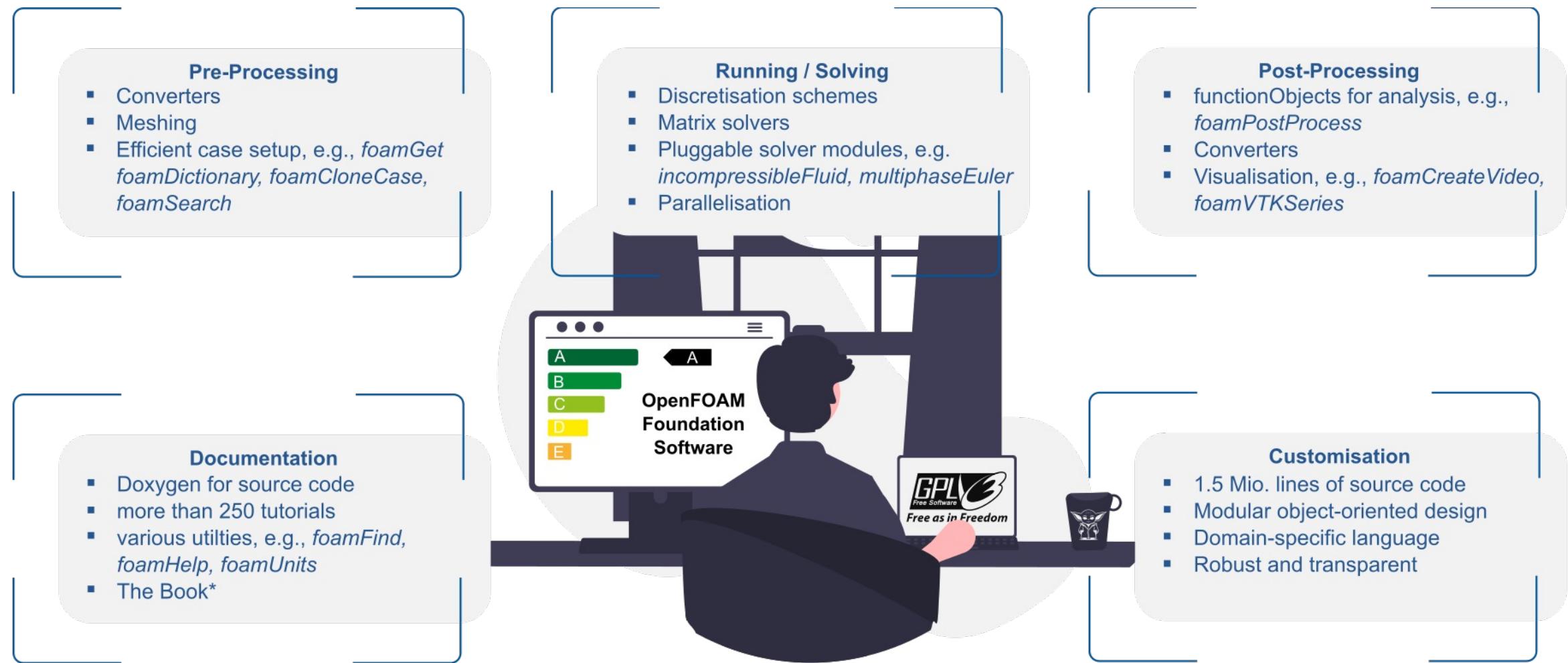


Generated by ChatGPT

COMMUNITY FOR OPENFOAM FOUNDATION SOFTWARE

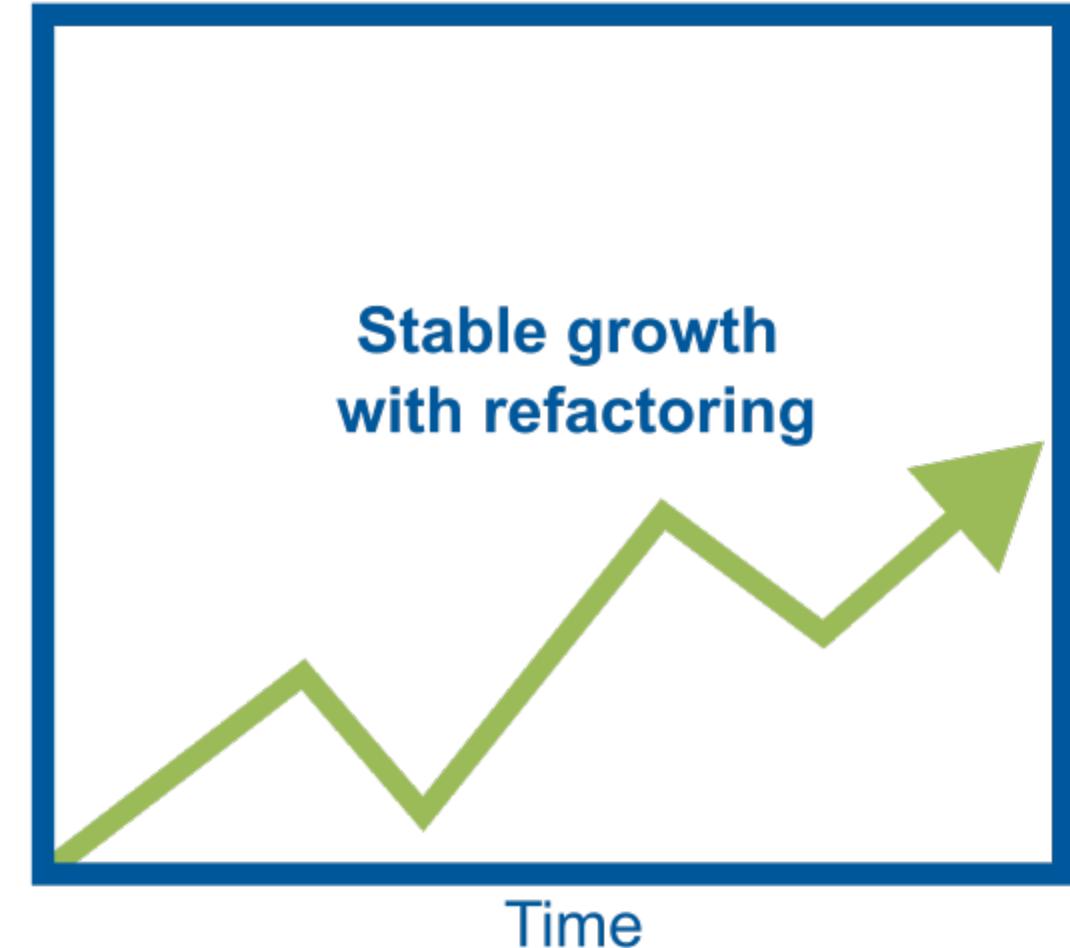
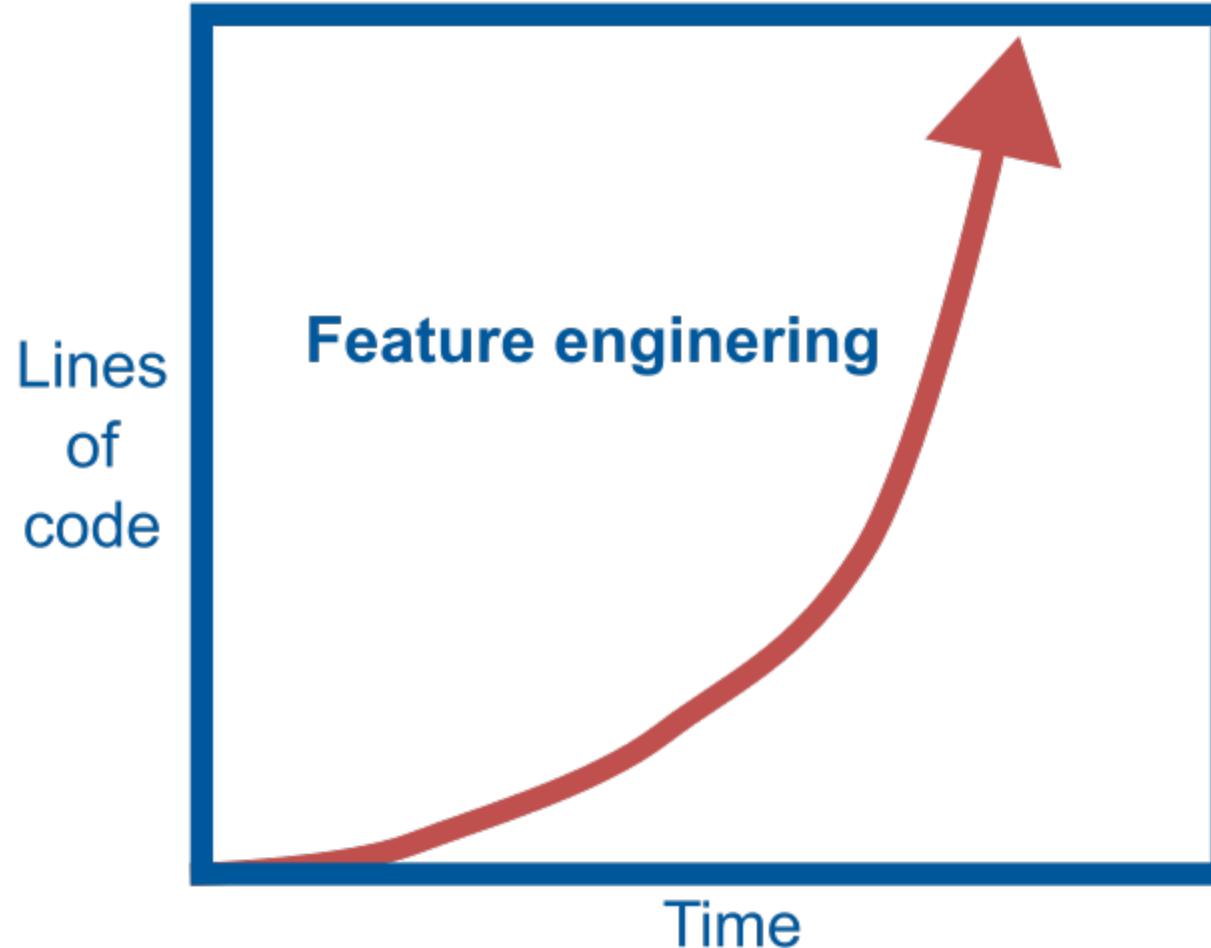


THE PACKAGE BY OPENFOAM FOUNDATION SOFTWARE

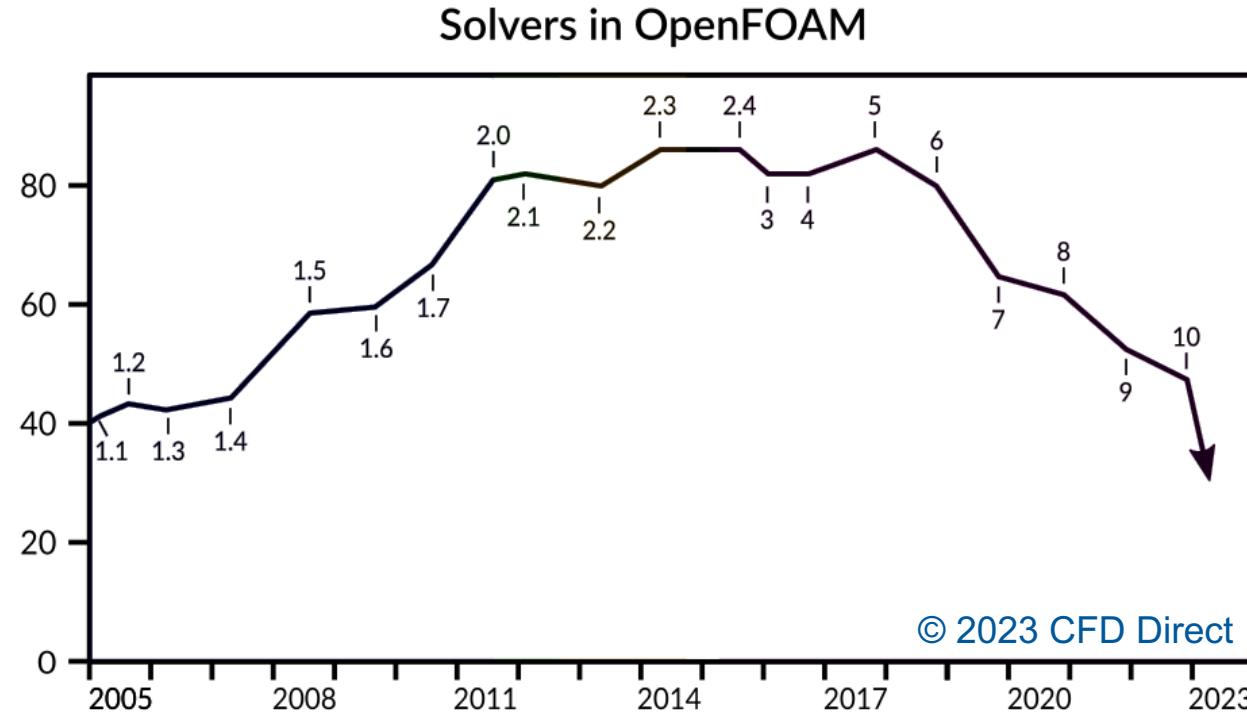
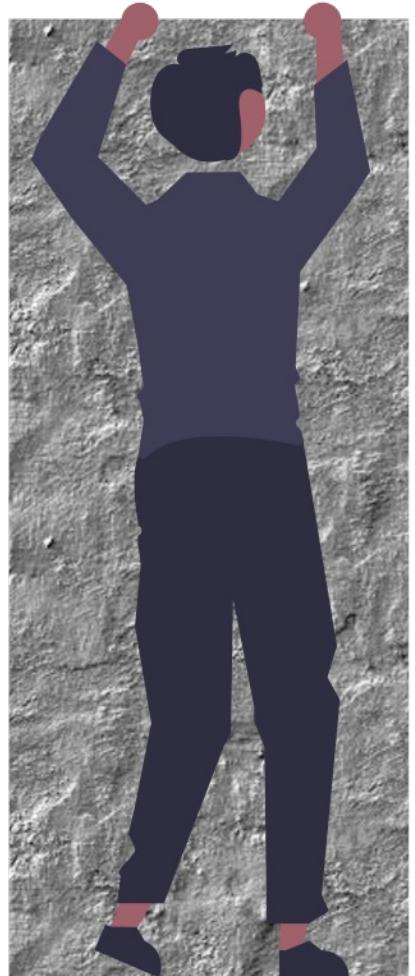


*Greenshields and Weller, Notes on Computational Fluid Dynamics: General Principles, CFD Direct Limited

FEATURE ENGINEERING VS STABLE GROWTH

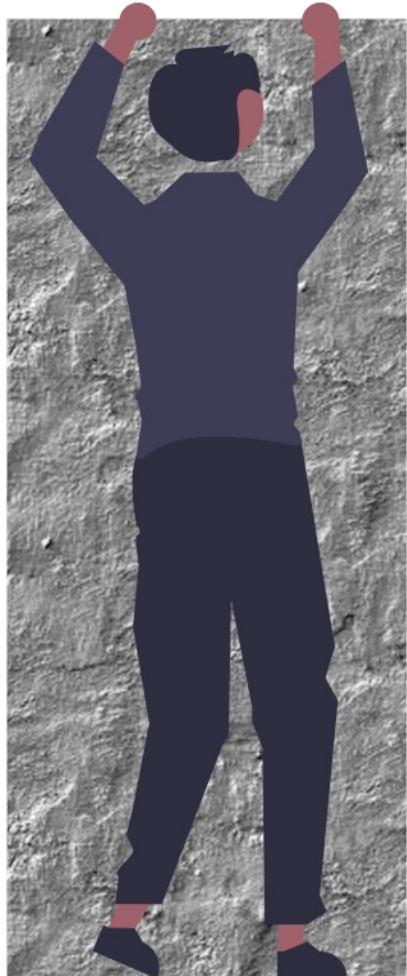


LOOK ACROSS THE WALL – SOLVER MODULES



- Reduce complexity and need for customisation
- Enabling multi-region simulations, e.g. conjugate heat transfer

LOOK ACROSS THE WALL – NEW UNIT SYSTEM

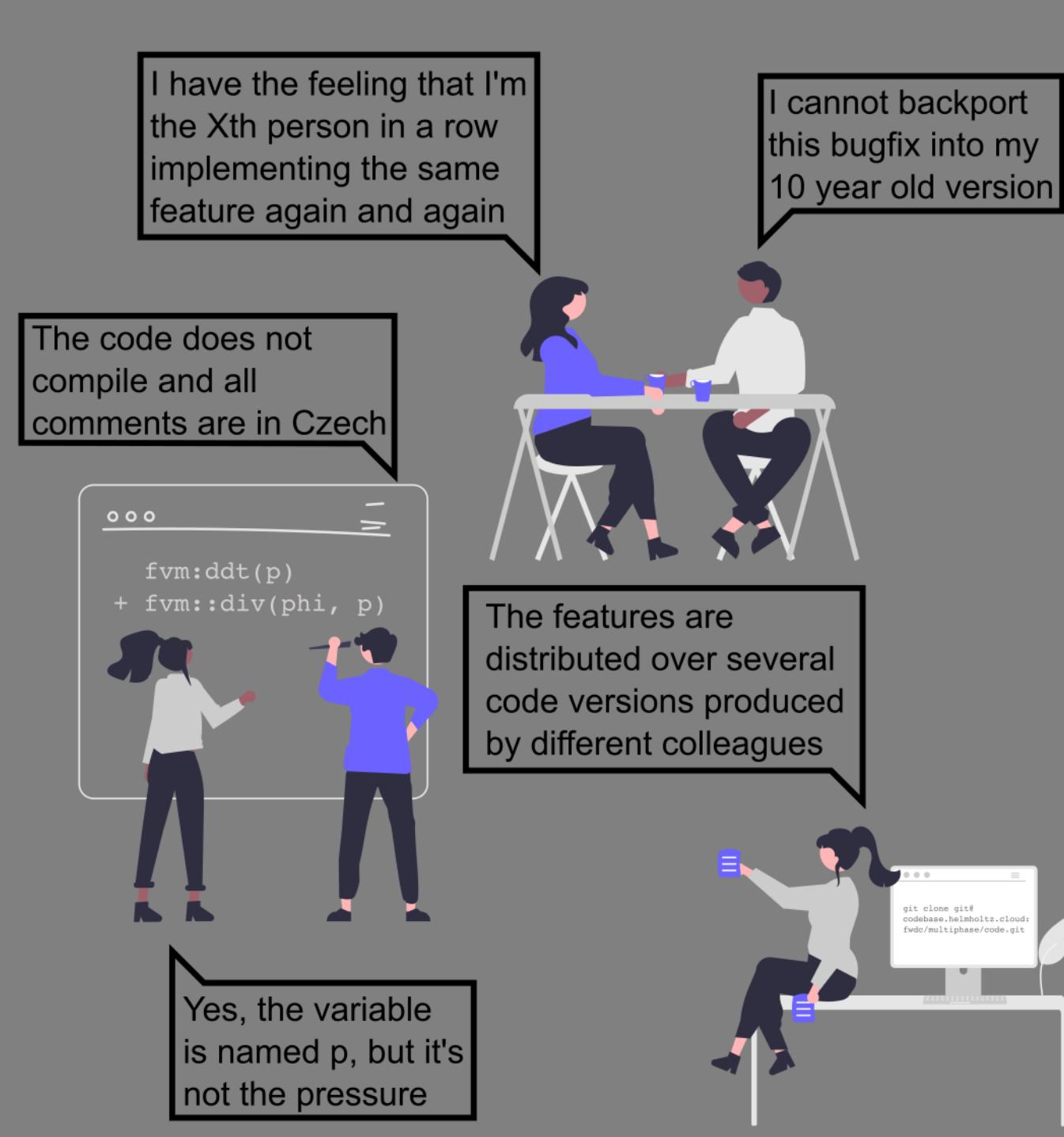


Now possible to specify units for majority of input parameters
(automatically converted to SI units by OpenFOAM Fundation software)

```
boundaryField
{
    inlet
    {
        type flowRateInletVelocity;
        volumetricFlowRate 0.1 [1/s];
        value $internalField;
    }
}
```

Standard: kg, m, s, K, kmol, A, Cd

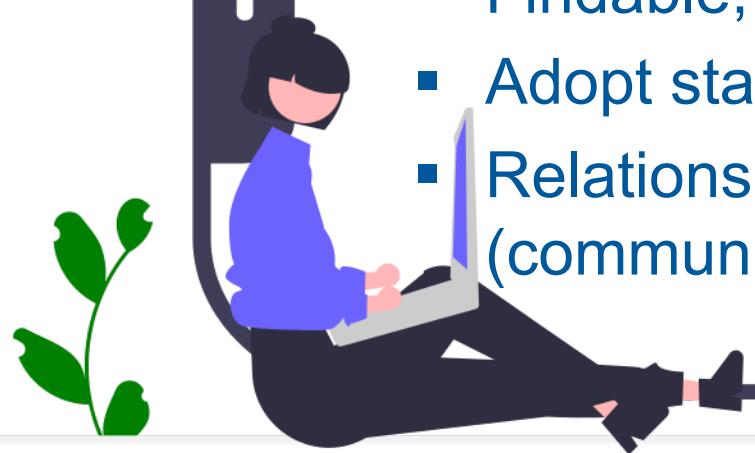
Derived: Hz, N, Pa, J, W, g, um, mm, cm, km, l, ml, us, ms, min, hr, mol, rpm, bar,
atm, kPa, Mpa, cal, kcal, cSt, cP, %, rad, rot, deg



SUSTAINABLE DOWNSTREAM DEVELOPMENT

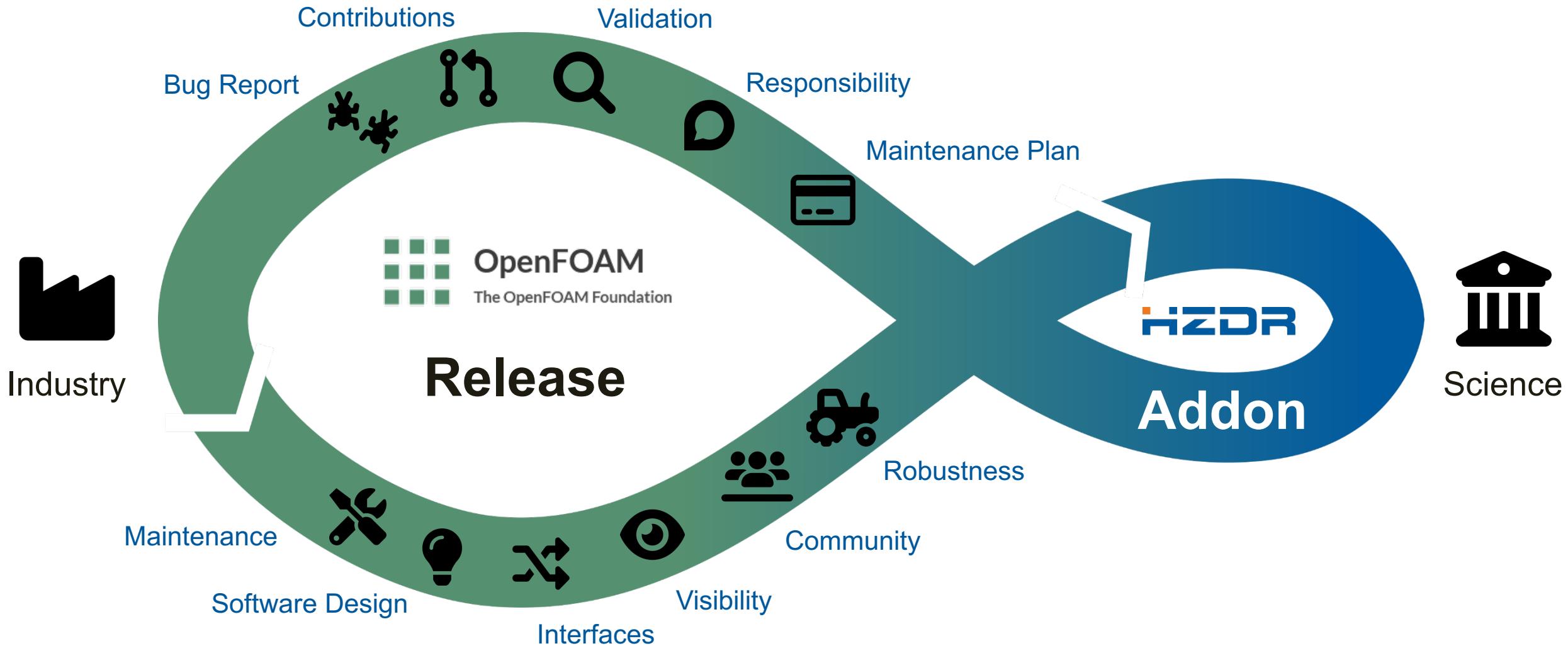
OUR DEVELOPMENT PHILOSOPHY

- Use OpenFOAM Foundation utilities whenever possible
- Provide templates for cases including documentation
- Automate everything possible (Gitlab CI/CD, Snakemake)
- Pre-installed working environment (Docker, VSCode)
- Findable, Accessible, Interoperable, Reproducable (FAIR)
- Adopt standards by OpenFOAM Foundation
- Relationship to core developers
(communication, maintenance & project funding)



CONTRIBUTION TO OPENFOAM

CONTRIBUTOR WITH ADDON



HELMHOLTZ CLOUD BY HIFIS

BACKBONE



GitLab
Helmholtz Codebase

Doxxygen

and beyond

MegaLinter

Docker

Debian packages

Apptainer

Pip

Jupyter Notebook

Snakemake

Rodare

Visual Studio Code

OUR REPOSITORIES

 Infrastructure Templates, e.g., for documentation, CI/CD configuration, and scripts	 Includes for CI/CD  Jinja Templates	 Megalinter for Static Code Analysis  Copier for Template Rendering
---	---	--

	 Multiphase	 NUSAR		Other
 Python Utilities for pre- and post-processing, workflow, and daily usage	 Code Modified solvers, models, tests, and tutorials	 Cases Setups, for scalable workflow with Snakemake	 Code 	 Cases 

Multiphase Python Repository by HZDR
10.14278/rodare.3093

Multiphase Code Repository by HZDR
10.14278/rodare.767

Multiphase Cases Repository by HZDR
10.14278/rodare.811

 **Helmholtz Login & Helmholtz AAI**

<https://rodare.hzdr.de>



PORTABLE WORKFLOW WITH GITLAB



Apptainer + Snakemake = Portability

apptainer pull docker://<image>

Merge Request Pipeline

Project information

Source code for Multiphase Code Repository by HZDR for OpenFOAM Foundation Software.

Multiphase Flow Numerical Si... OpenFOAM + 9 more

pipeline passed chat mattermost documentation wiki license GPL v3 validation report main documentation doxygen Downloads 4268.0 Views 16052.0 Latest Release 11-s.1-hzdr.1 Made with Copier pre-commit enabled

1,409 Commits 111 Branches 29 Tags 10.7 GiB Project Storage 18 Releases

README GNU General Public License v3.0 or later CHANGELOG CONTRIBUTING CI/CD configuration GitLab Pages Configure Integrations

Created on November 06, 2018

A HIFIS Service | Privacy | Imprint | Support | Documentation | Changelog | Status

SUMMARY

- Development of a morphology-adaptive Euler-Euler method for engineering scale simulations
 - Validation strategy for numerical simulations of multiphase flows
 - OpenFOAM Foundation software is the perfect package for us
 - Applying modern IT-tools and CI/CD strategies to allow sustainable research
- Demo on selected tools to organize simulation setups by Ronald Lehnigk

ACKNOWLEDGEMENT

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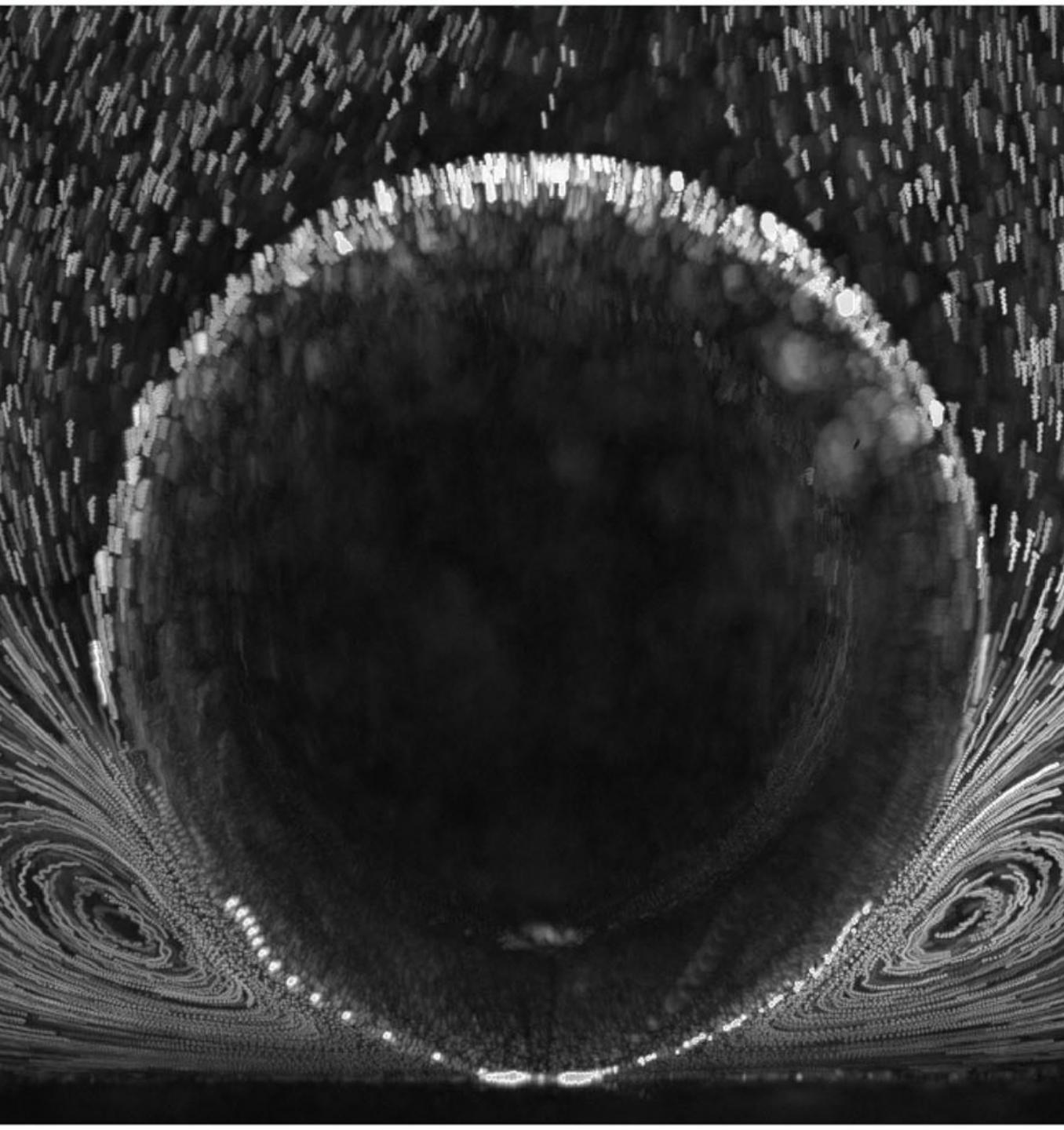
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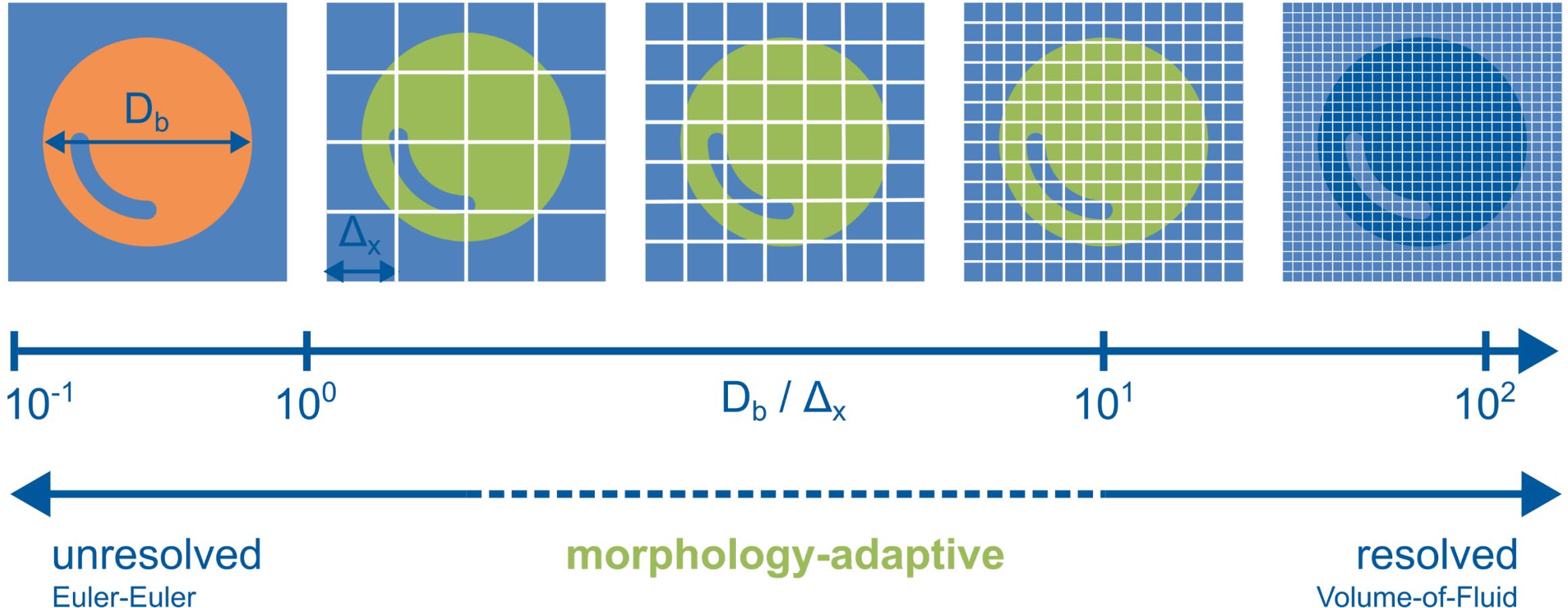
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SLIDES AS
BACKUP

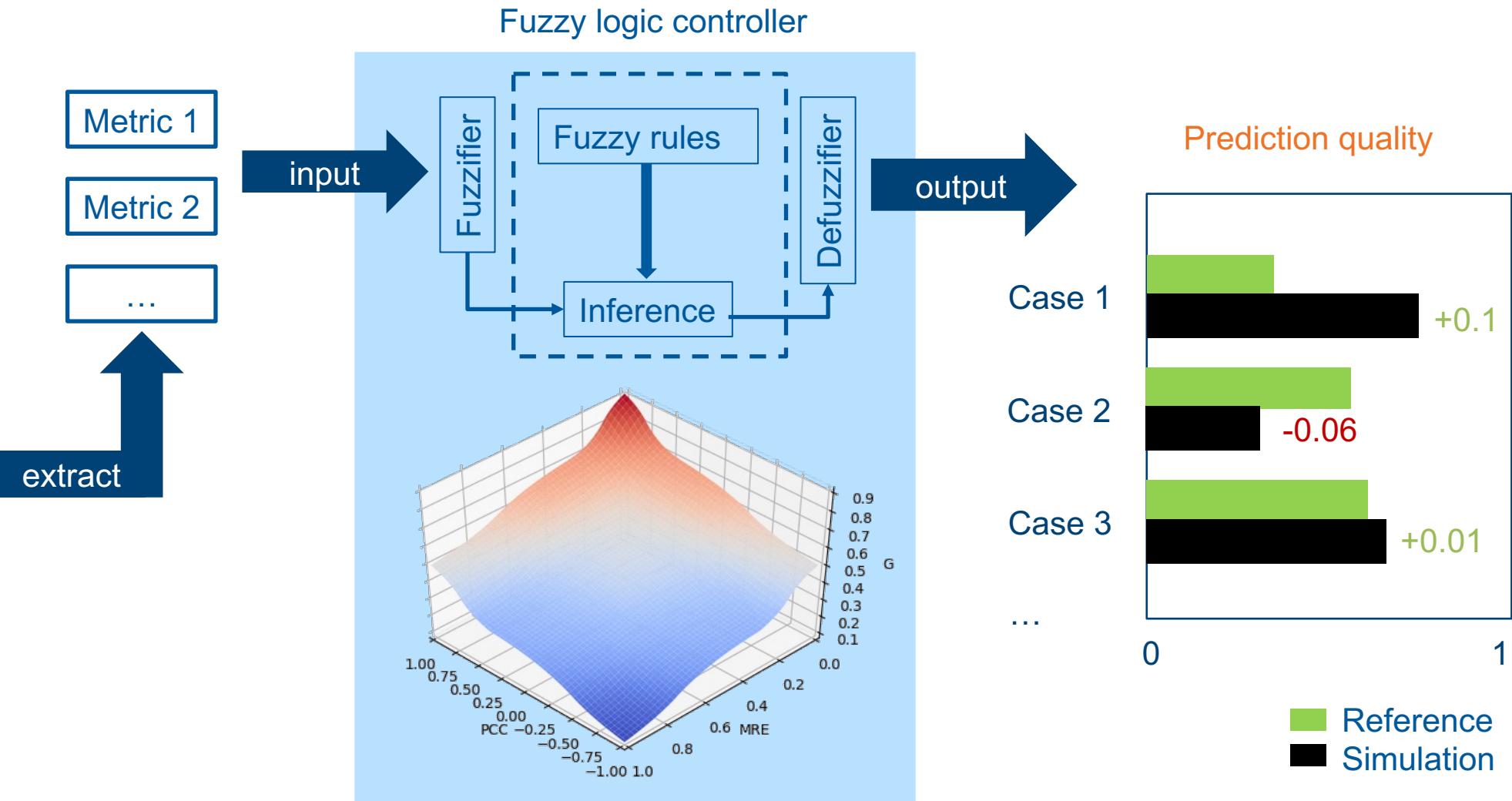
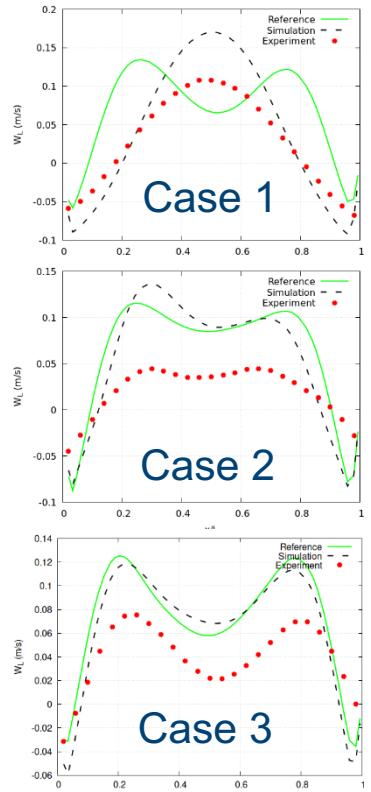


A MORPHOLOGY-ADAPTIVE MULTIFIELD Two-FLUID MODEL



QUANTIFYING THE CFD PREDICTION QUALITY

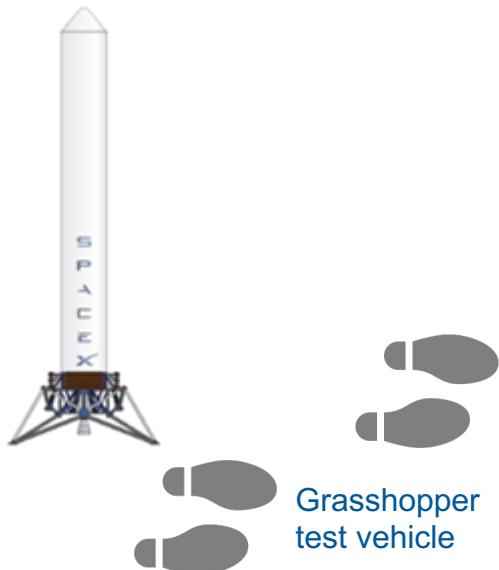
Do results improve
with a new
model/setup/code?



QUALITY OF SOFTWARE ENGINEERING

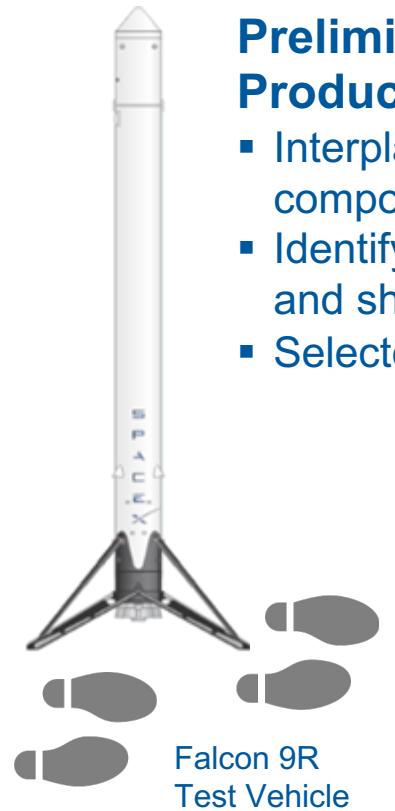
Feasibility Prototype

- Validate individual features
- Check feasibility
- Extremely important



Preliminary Product Prototype

- Interplay of components
- Identify limitations and shortcomings
- Selected features



Falcon 9 FT

Demonstration Prototype

- Most of the features and functions
- Start user testing

Core Maintainers



- ## Production Software
- All features
 - Fully optimized
 - Production ready

Visual Studio Code for Developers

The screenshot displays the Visual Studio Code interface with several tabs open, each showing a different file from the OpenFOAM codebase:

- cellPressureCorrectorC**: Shows the implementation of the `cellPressureCorrector()` function.
- ResolvedPhaseSystem.C**: Shows the `~ResolvedPhaseSystem()` destructor and other member functions.
- segregatedPhaseInterface.C** (Working Tree): Shows the implementation of the `gradAlphaf()` function for the `segregatedPhaseInterface`.
- segregatedPhaseInterface.C** (Working Tree) (Details): A detailed view of the `gradAlphaf()` implementation.
- PROBLEMS**: Shows one error related to the declaration of `phase3`.
- OUTPUT**: Shows the terminal output of a build command, indicating an error due to undeclared variable `phase3`.
- TERMINAL**: An integrated terminal window showing the same error message.

Key features highlighted in the interface include:

- SOURCE CONTROL**: A sidebar for managing Git operations like committing changes.
- Track source code changes**: A sidebar for monitoring code modifications.
- Attach to docker containers**: A sidebar for connecting to Docker environments.
- Interact with Gitlab instance**: A sidebar for managing Gitlab projects.
- Source code with syntax highlighting**: A tooltip for the code editor.
- Analyse and jump through source code**: A tooltip for the code navigation feature.
- Integrated terminal**: A tooltip for the terminal window.

Visual Studio Code for Users

The screenshot shows a dark-themed instance of Visual Studio Code with the following panels:

- EXPLORER**: Shows a tree view of the project structure under "11-s.1 (WORKSPACE) [CONTAINER REGISTRY.HZDR..]".
- EDITOR**: Displays two files: "controlDict" and "createGraphs". "controlDict" contains configuration for a solver, start time, stop time, and output. "createGraphs" contains shell commands for plotting reference and simulation data.
- PROBLEMS**: Shows 12 errors related to Docker command execution.
- TERMINAL**: Displays a terminal session with Docker commands and file listing.
- PORTS**: Shows a preview of a plot titled "velocity.png" comparing Reference, Simulation, and Benchmark data.
- Integrated terminal**: Located at the bottom right, showing a git log and file listing.
- Gitlab project information**: Located at the bottom left, showing a link to Container registry.hzdr.de/fwdc/multiph...

Built-in preview of graphs and plots

Edit case configuration with syntax highlighting