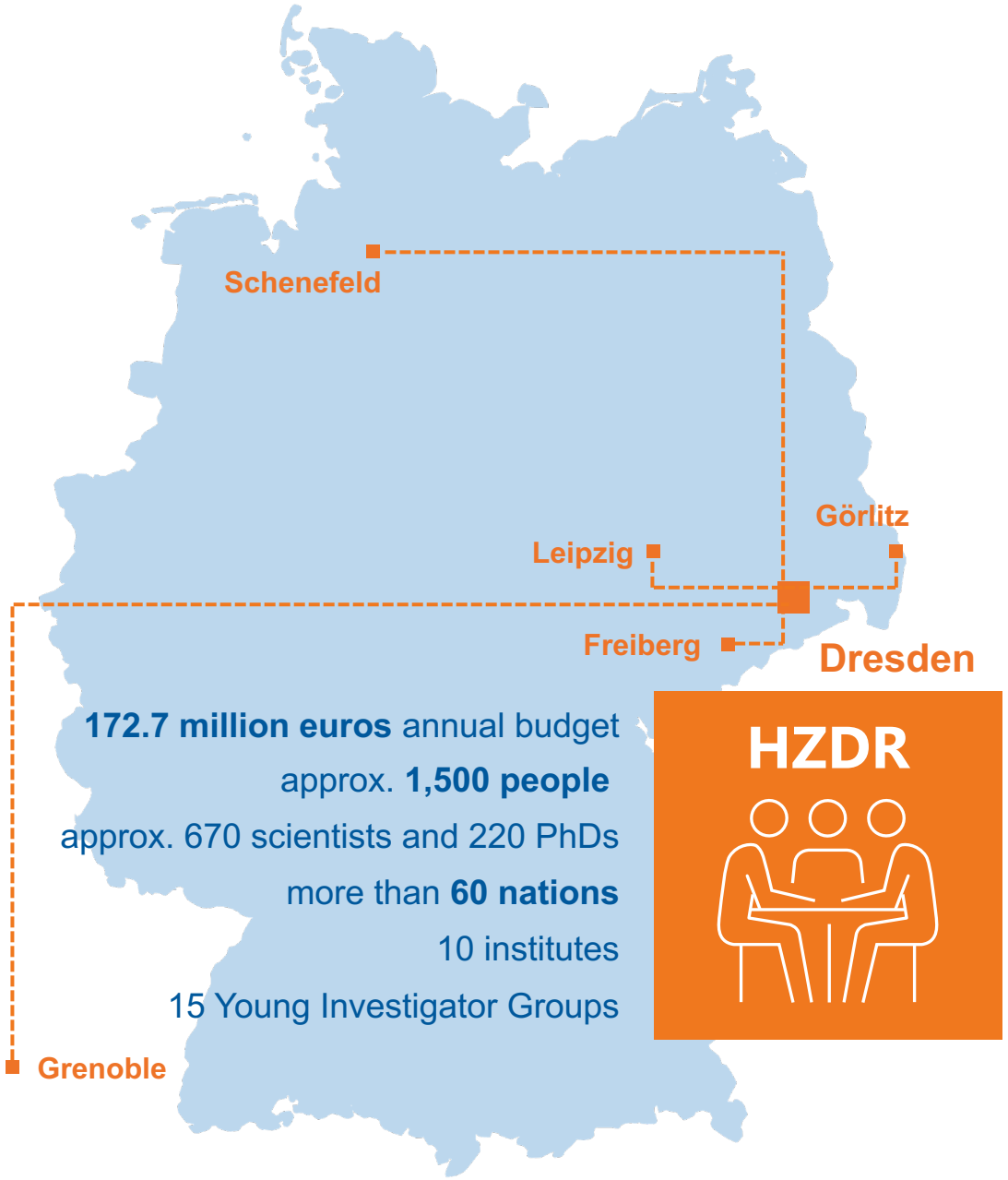
HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

# Sustainable Code Development and Cases Management with OpenFOAM Foundation Release

## Free OpenFoam VKI Seminar

Institute of Fluid Dynamics – Department of Computational Fluid Dynamics – Dr. Fabian Schlegel – www.hzdr.de/multimorph


HZDR
HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF
SCANNING
G17
Q11
L21
R12
X1
X2
X3
X4




**172.7 million euros** annual budget

approx. **1,500 people**

approx. 670 scientists and 220 PhDs

more than **60 nations**

10 institutes

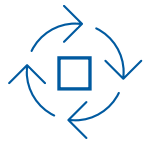
15 Young Investigator Groups

**HZDR**

# 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



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# 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



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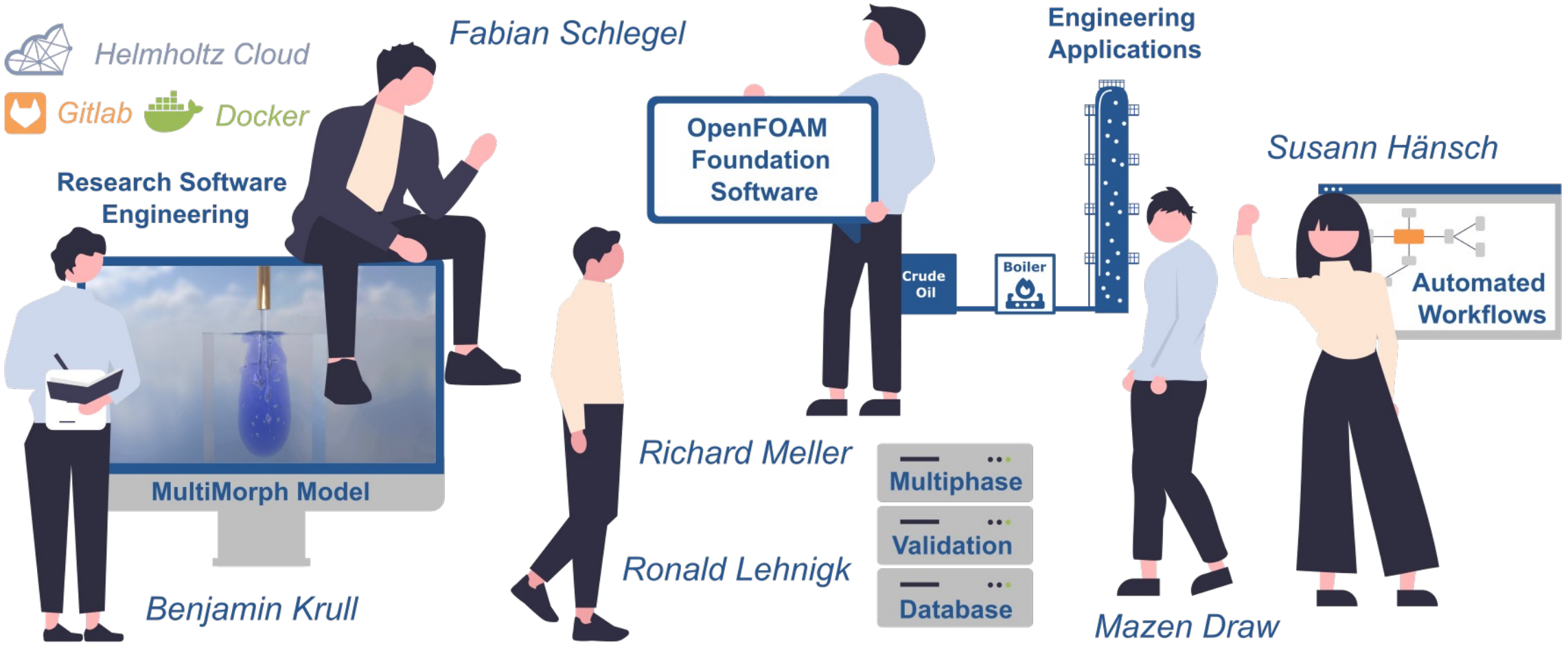
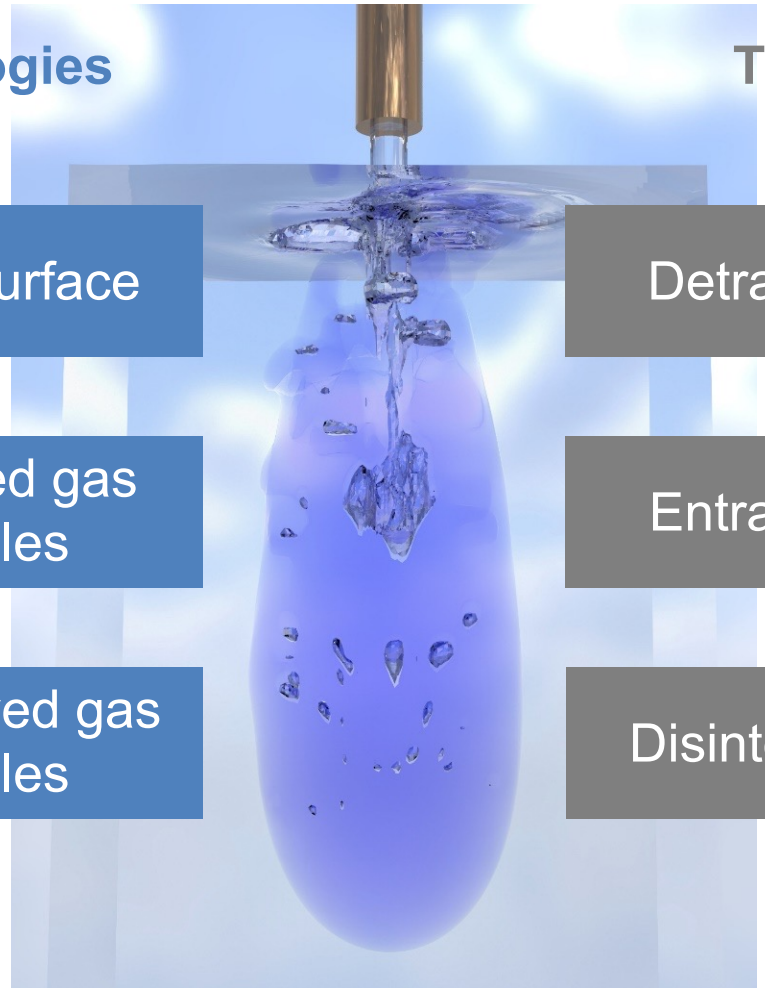
# The OpenFOAM Group and our Interests

## Numerical simulation of multiphase flows in engineering applications



## Modern simulation methods at HZDR

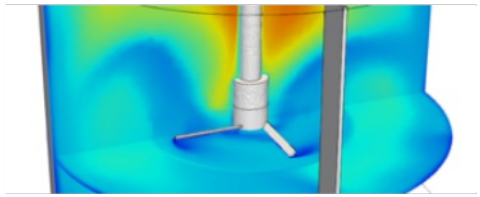



Simulation of a plunging jet with **MultiMorph model**

# WHAT ARE **WE DOING?**

# Scales and Accuracy in numerical simulations

efficiency,
grid spacing



System-scale simulation

Engineering-scale simulation

Reynolds-Averaged Navier-Stokes (RANS)

Large-Eddy simulation (LES)

Direct numerical simulation (DNS)

Molecular-scale simulation

Which method should
we use?


scale, modelling, averaging level



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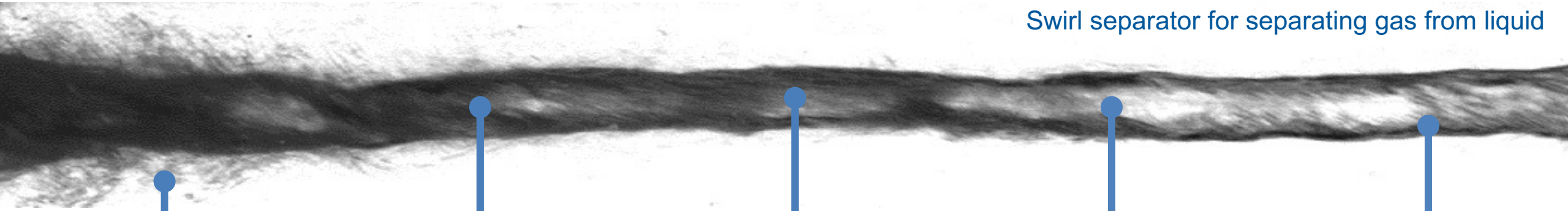
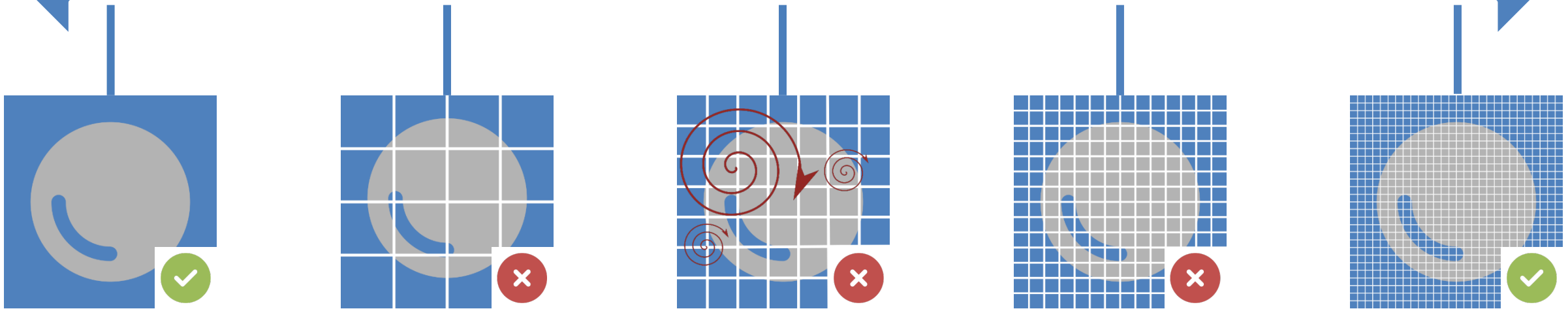
# MULTIPHASE FLOWS CHARACTERISED BY BROAD RANGE OF SCALES



Swirl separator for separating gas from liquid

Industrial applications contain **all morphologies**





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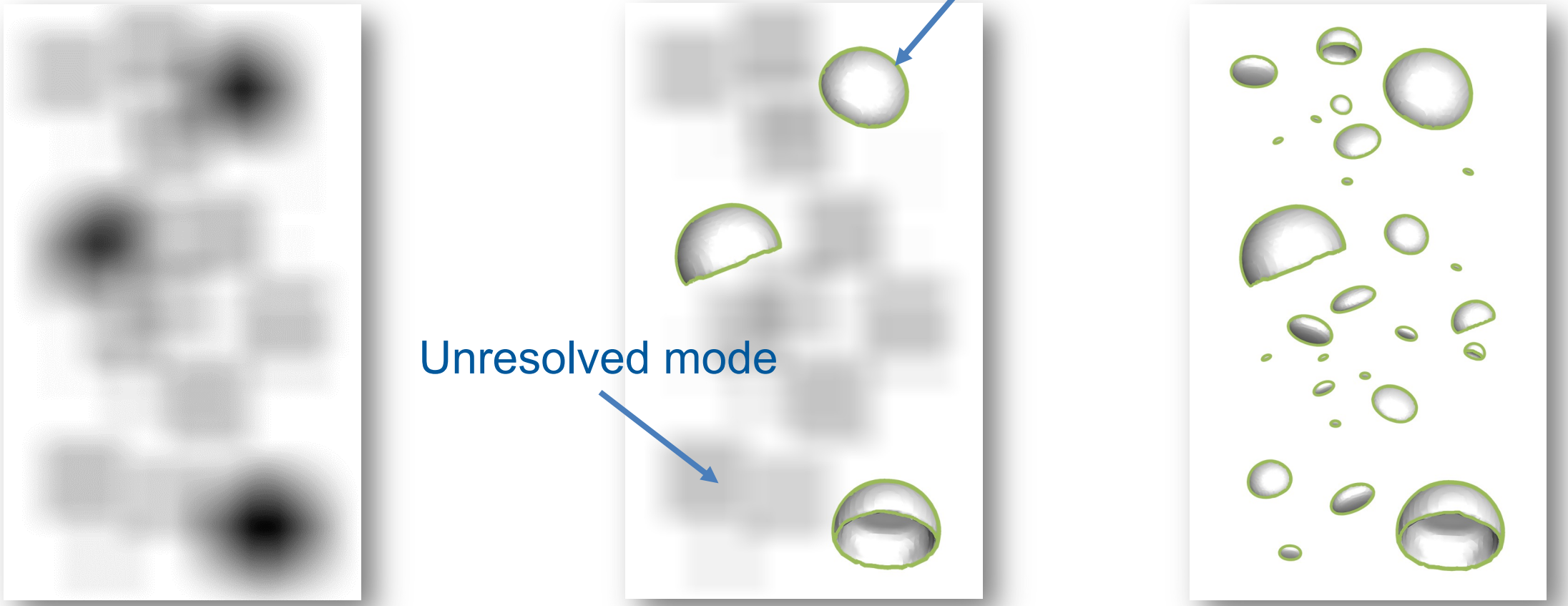
# ILLUSTRATION OF INTERFACE TREATMENT




Euler-Euler Model

**MultiMorph**

Volume-of-Fluid



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# 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

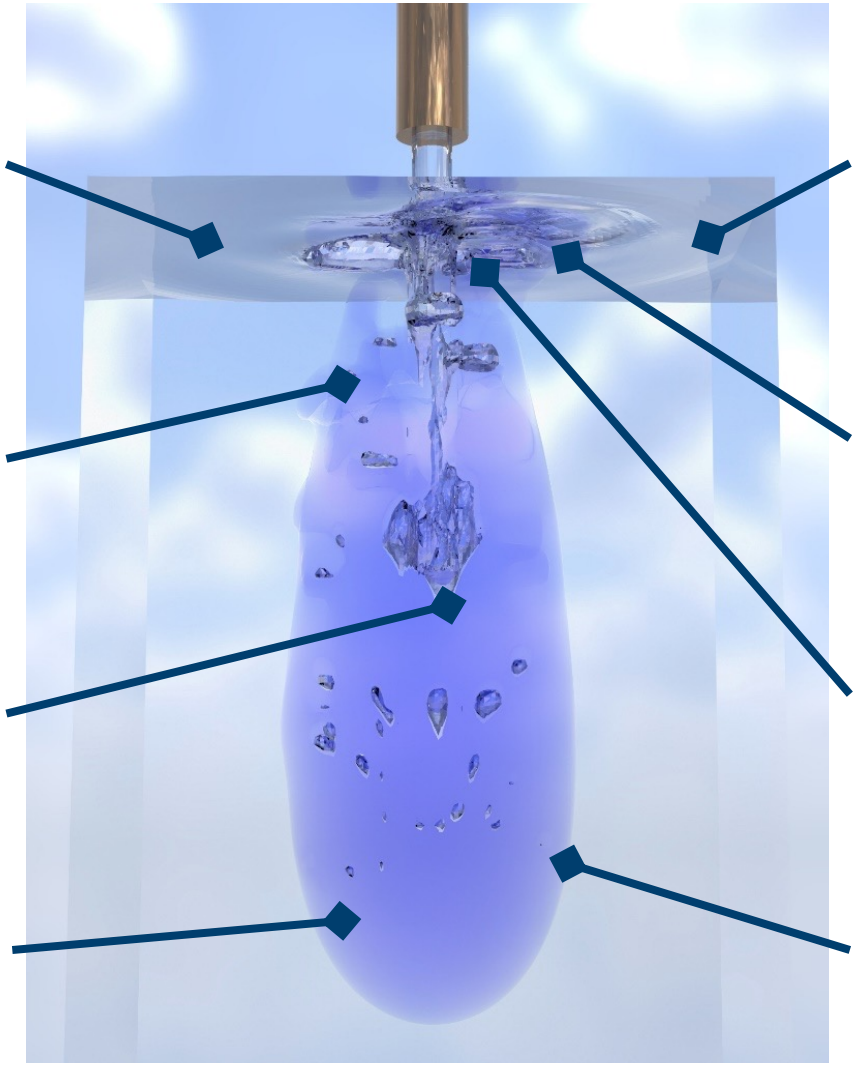
Meller et al. (2023). **Momentum exchange modeling for coarsely resolved interfaces in a multifield two-fluid model.** *Int J Num Method Fluid*, *95*(9), 1521-1545.

## 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.



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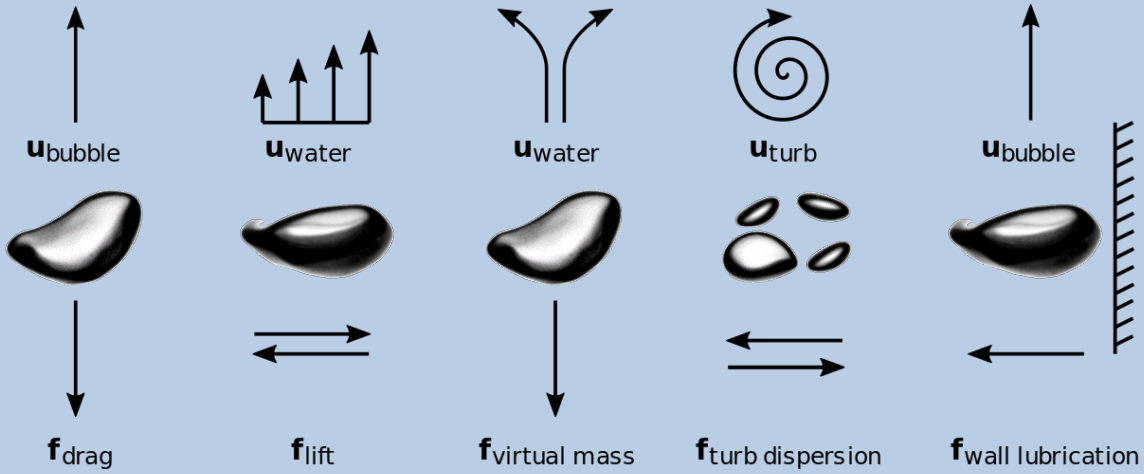
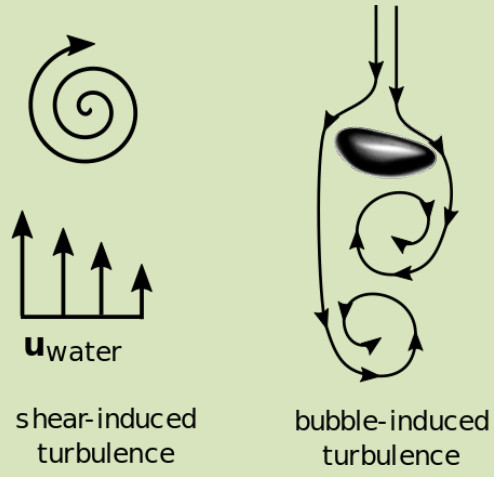
# BASELINE MODEL FOR POLY-DISPERSE GAS LIQUID FLOWS

## CLOSURE MODELS NEEDED FOR EULER-EULER SIMULATIONS

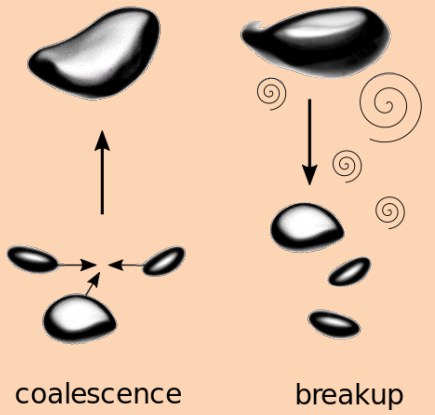
### Interfacial models




### Turbulence

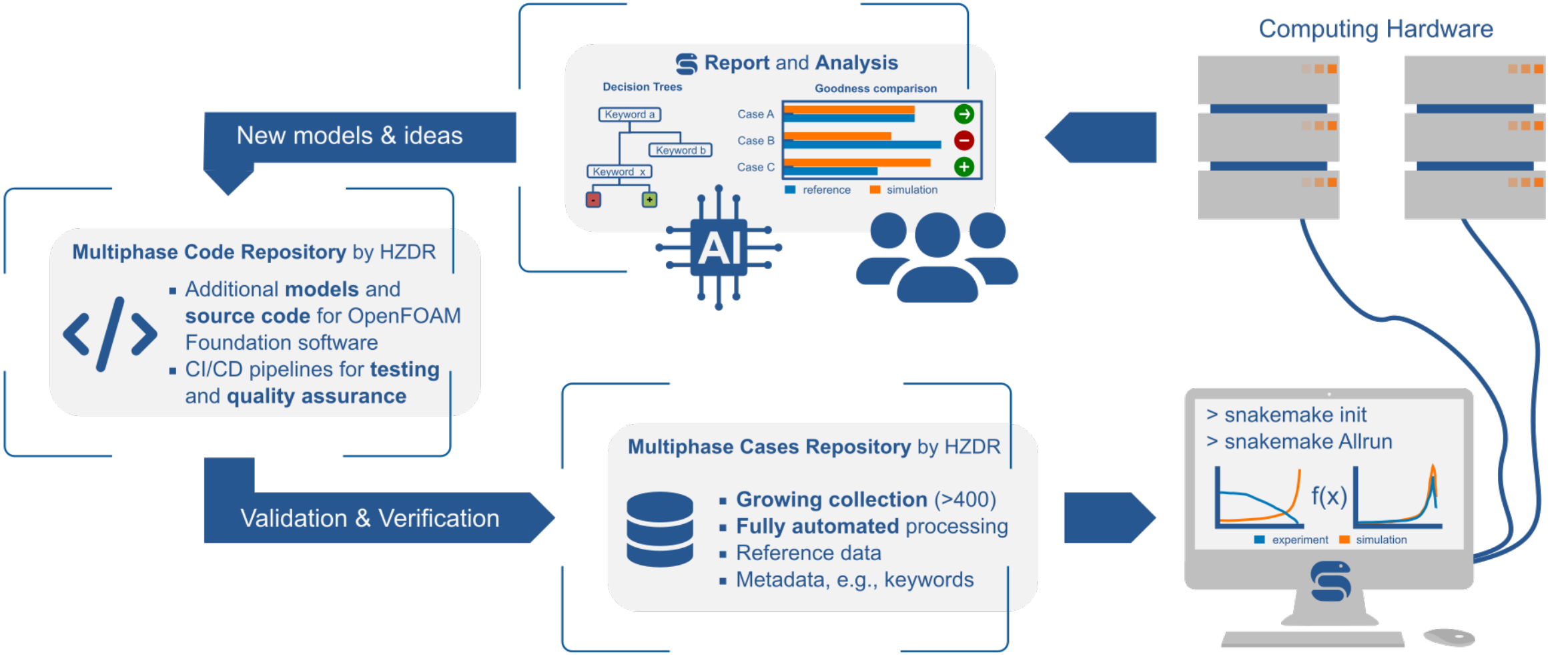



### Bubble interactions




► Lecture on Multiphase Flows planned for 2025

# VALIDATION STRATEGY FOR MULTIPHASE FLOWS



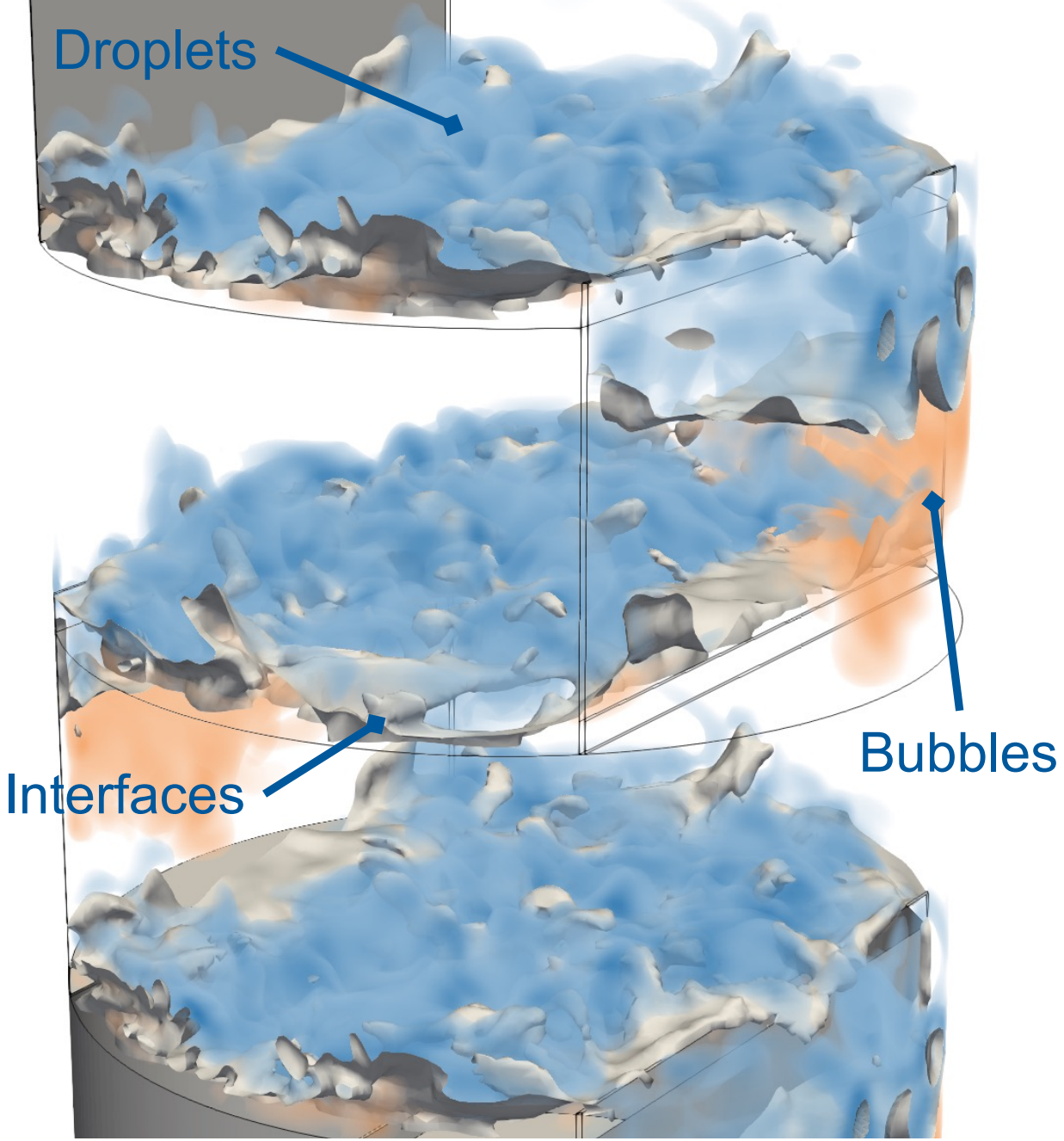
# SOFTWARE PUBLICATIONS

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

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

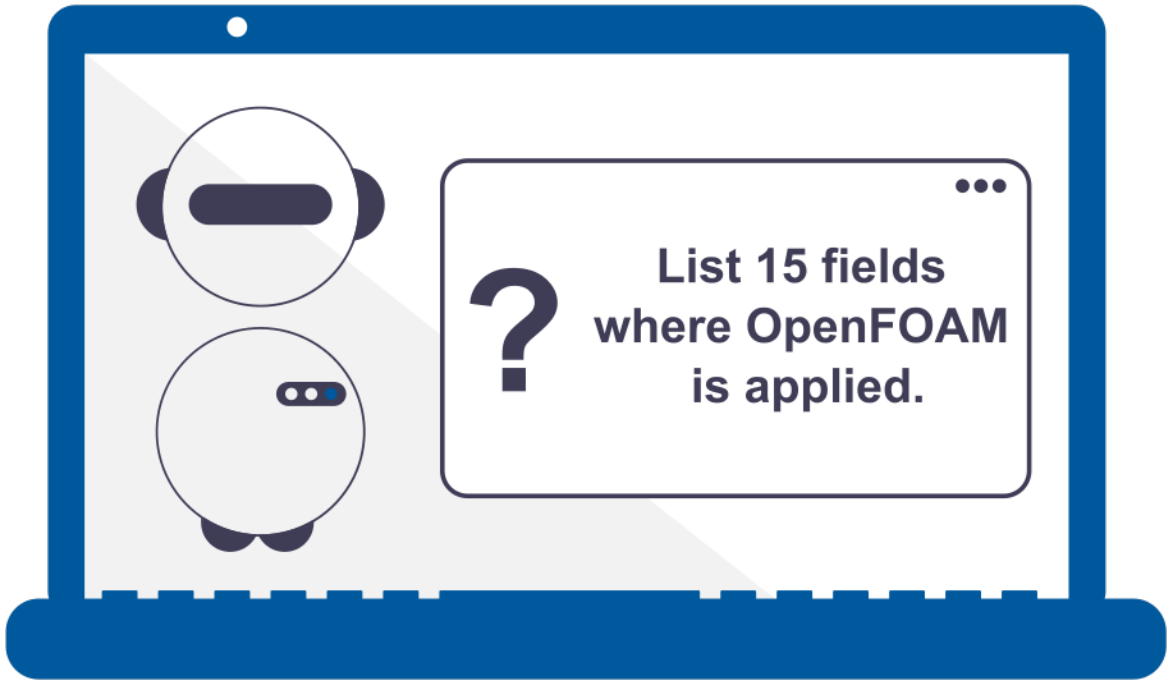
https://hzdr.de/multimorph




Simulated two-phase flow in a tray column

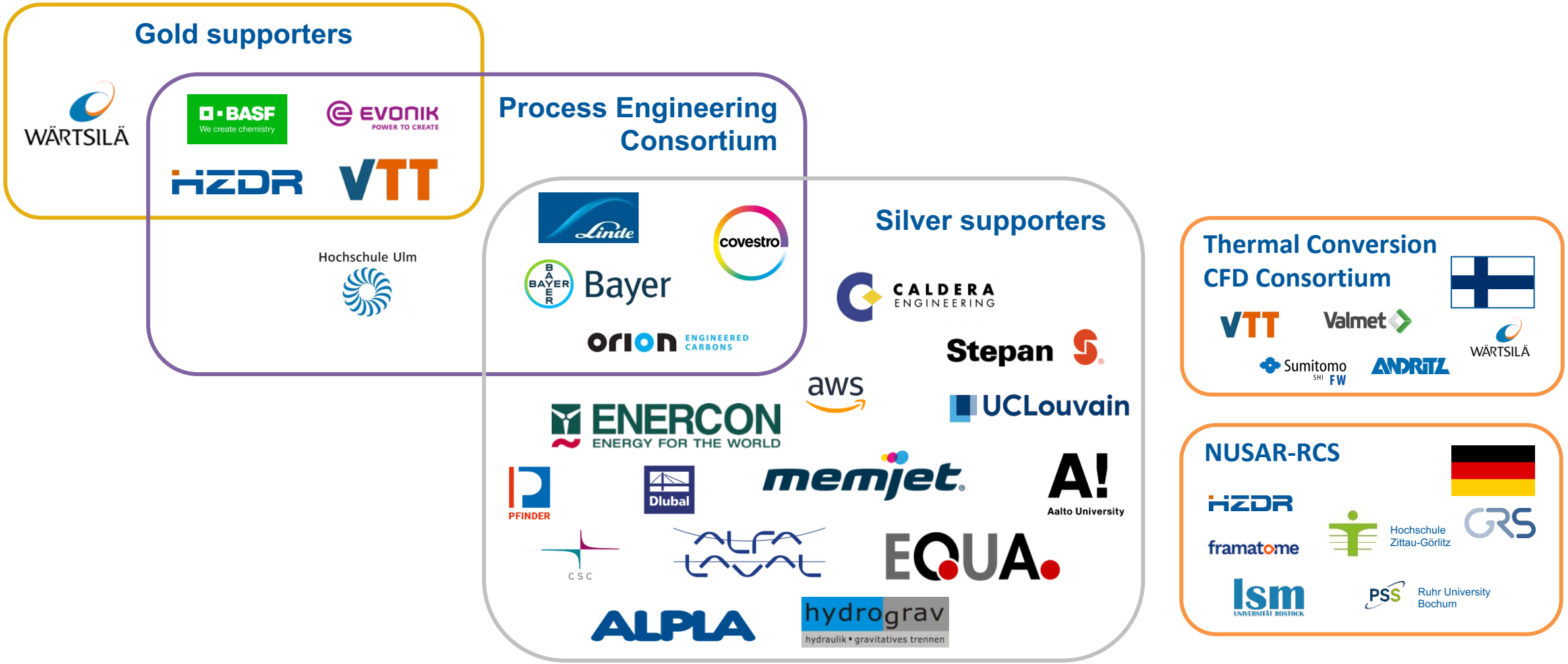
# DIVING INTO OPENFOAM FOUNDATION SOFTWARE

# Field of Applications for OpenFOAM Foundation Software




Generated by ChatGPT

# COMMUNITY FOR OPENFOAM FOUNDATION SOFTWARE



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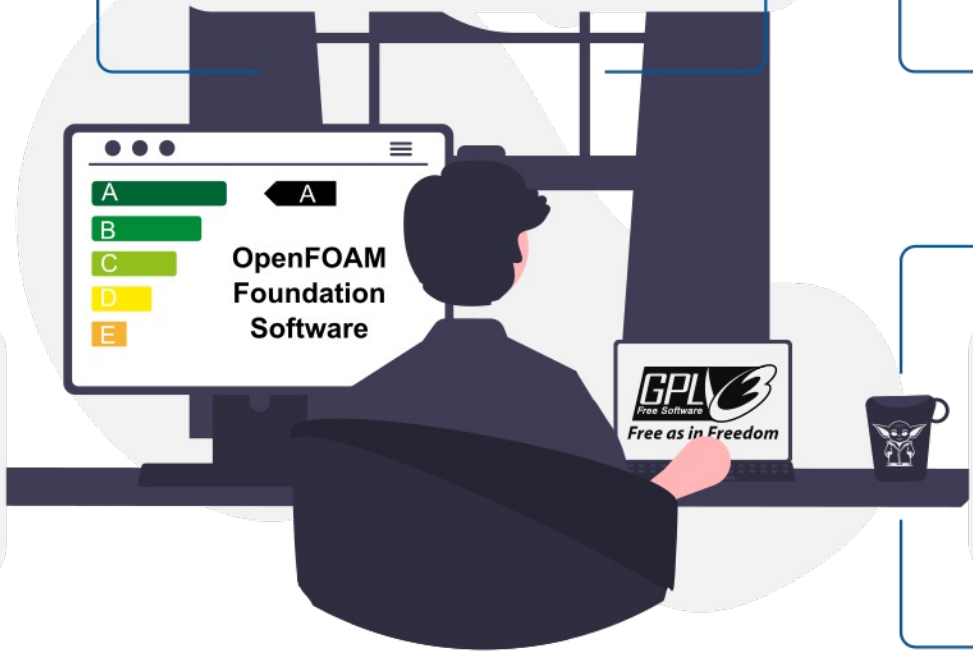
# THE PACKAGE BY OPENFOAM FOUNDATION SOFTWARE

**Pre-Processing**
- Converters
- Meshing
- Efficient case setup, e.g., *foamGet foamDictionary, foamCloneCase, foamSearch*

**Running / Solving**
- Discretisation schemes
- Matrix solvers
- Pluggable solver modules, e.g. *incompressibleFluid, multiphaseEuler*
- Parallelisation

**Post-Processing**
- functionObjects for analysis, e.g., *foamPostProcess*
- Converters
- Visualisation, e.g., *foamCreateVideo, foamVTKSeries*

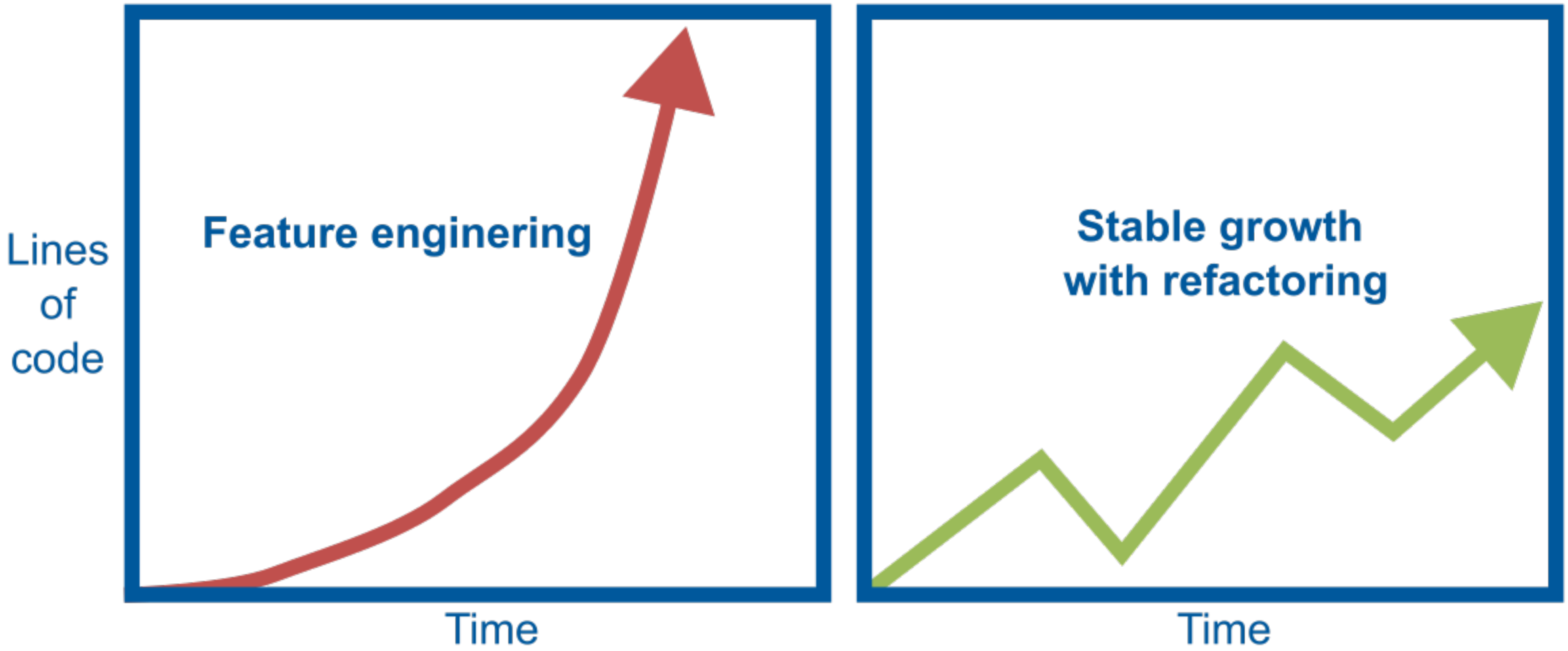



**Documentation**
- Doxygen for source code
- more than 250 tutorials
- various utilties, e.g., *foamFind, foamHelp, foamUnits*
- The Book*

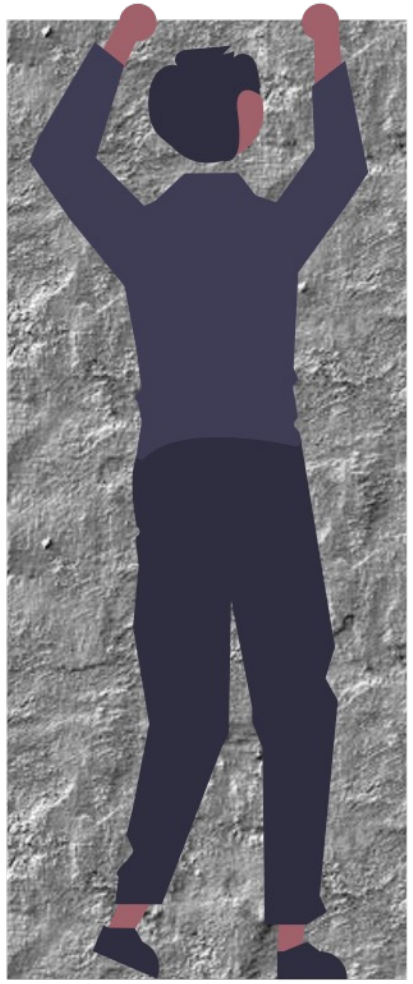
**Customisation**
- 1.5 Mio. lines of source code
- Modular object-oriented design
- Domain-specific language
- Robust and transparent

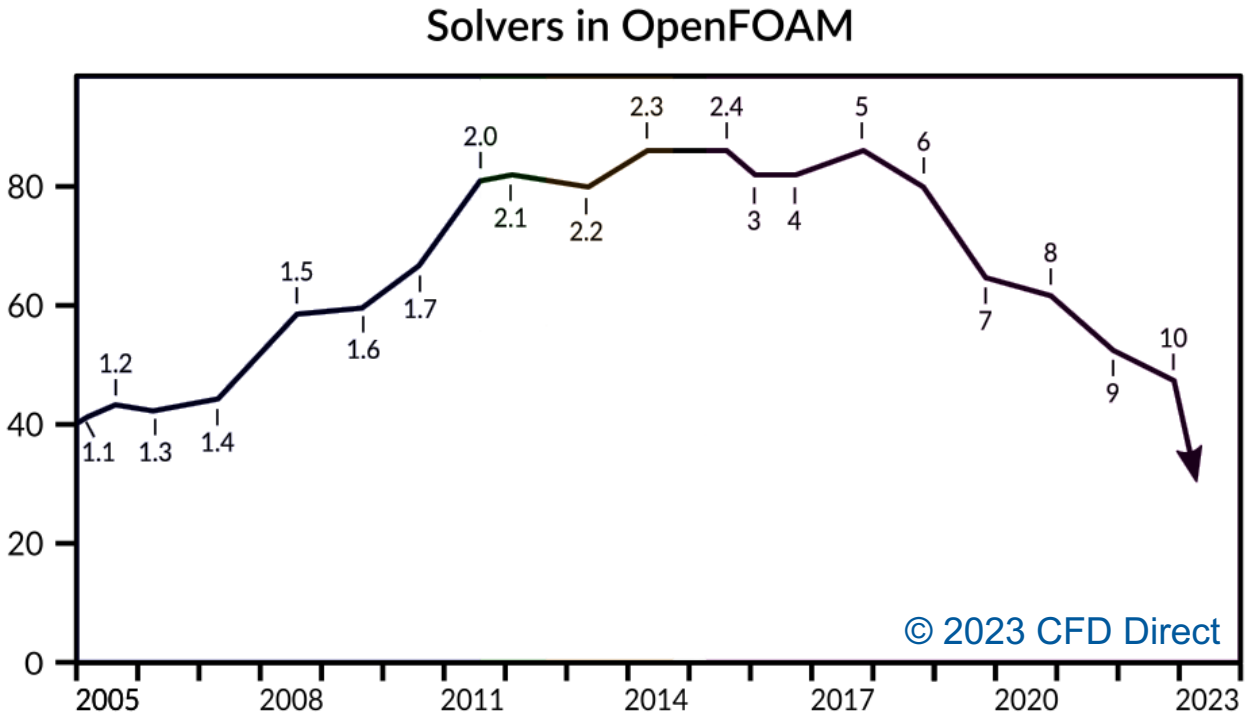
*Greenshields and Weller, Notes on Computational Fluid Dynamics: General Principles, CFD Direct Limited

# Feature engineering vs stable growth



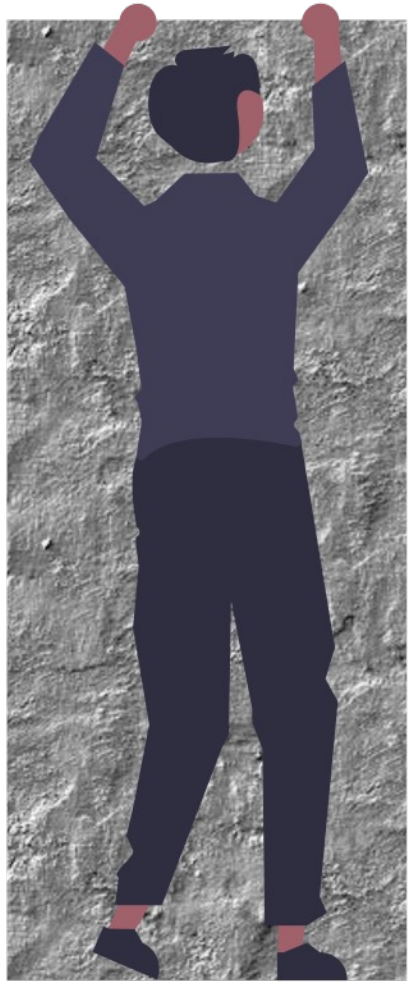
# LOOK ACROSS THE WALL – SOLVER MODULES






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

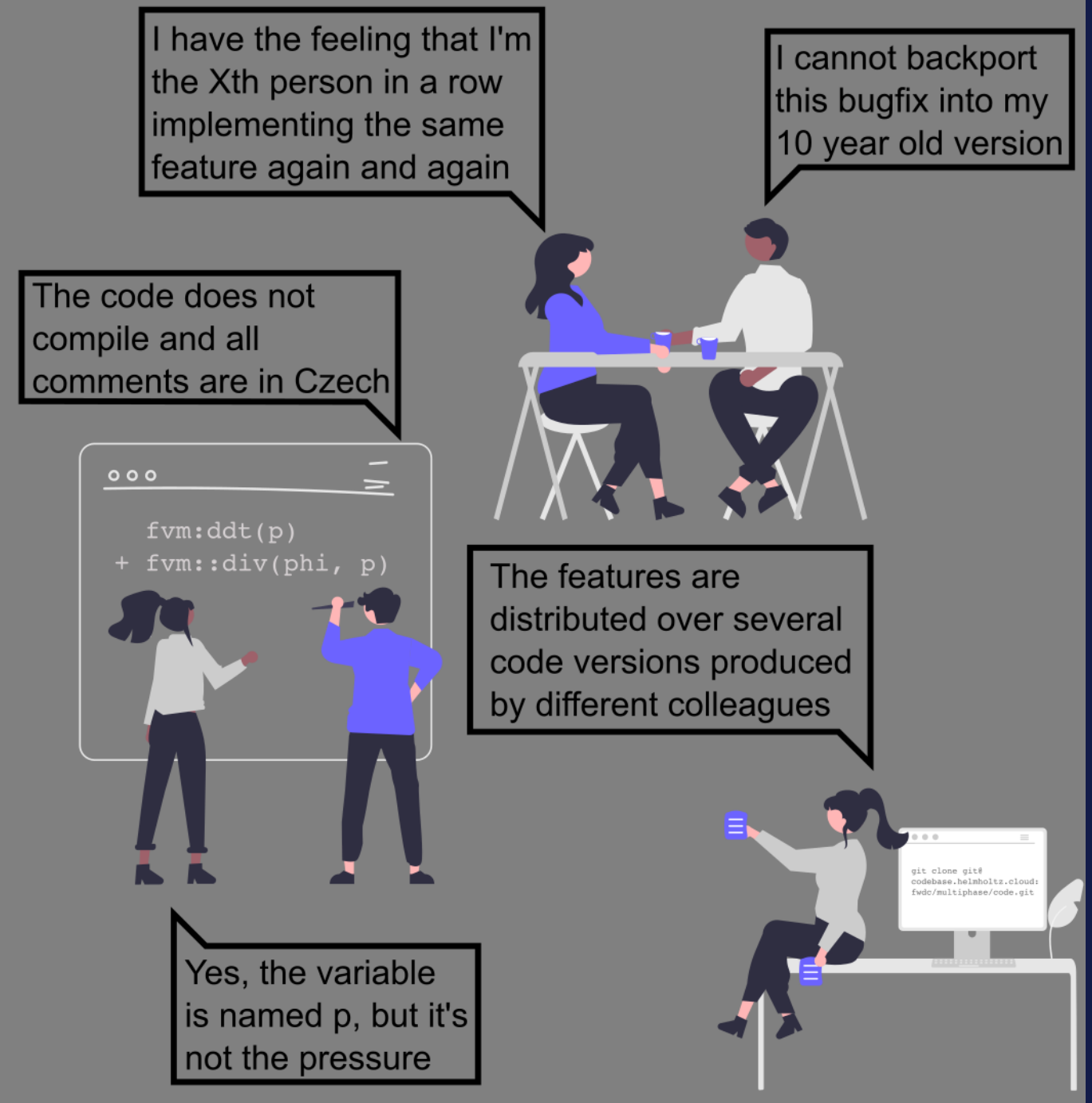
# LOOK ACROSS THE WALL – NEW UNIT SYSTEM



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 [l/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



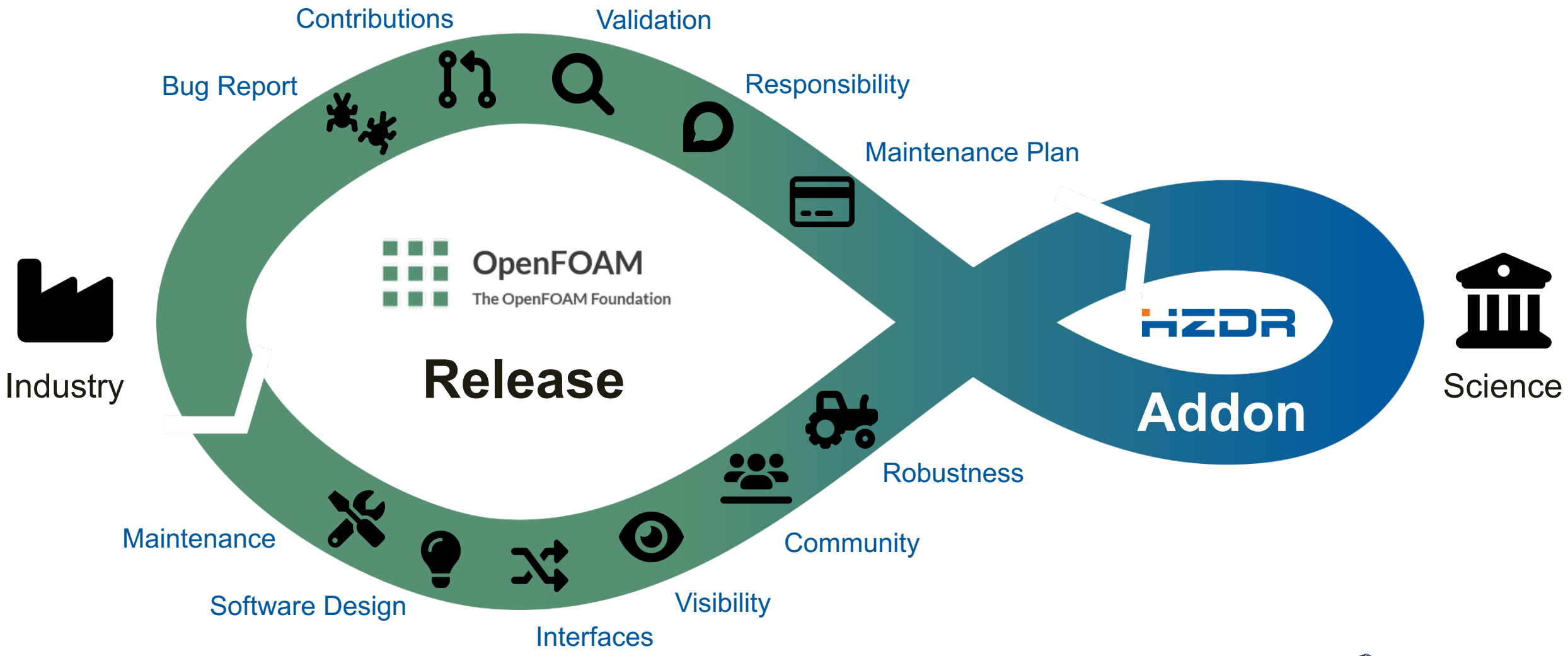

# SUTAINABLE DOWNSTREAM DEVELOPMENT

# 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)

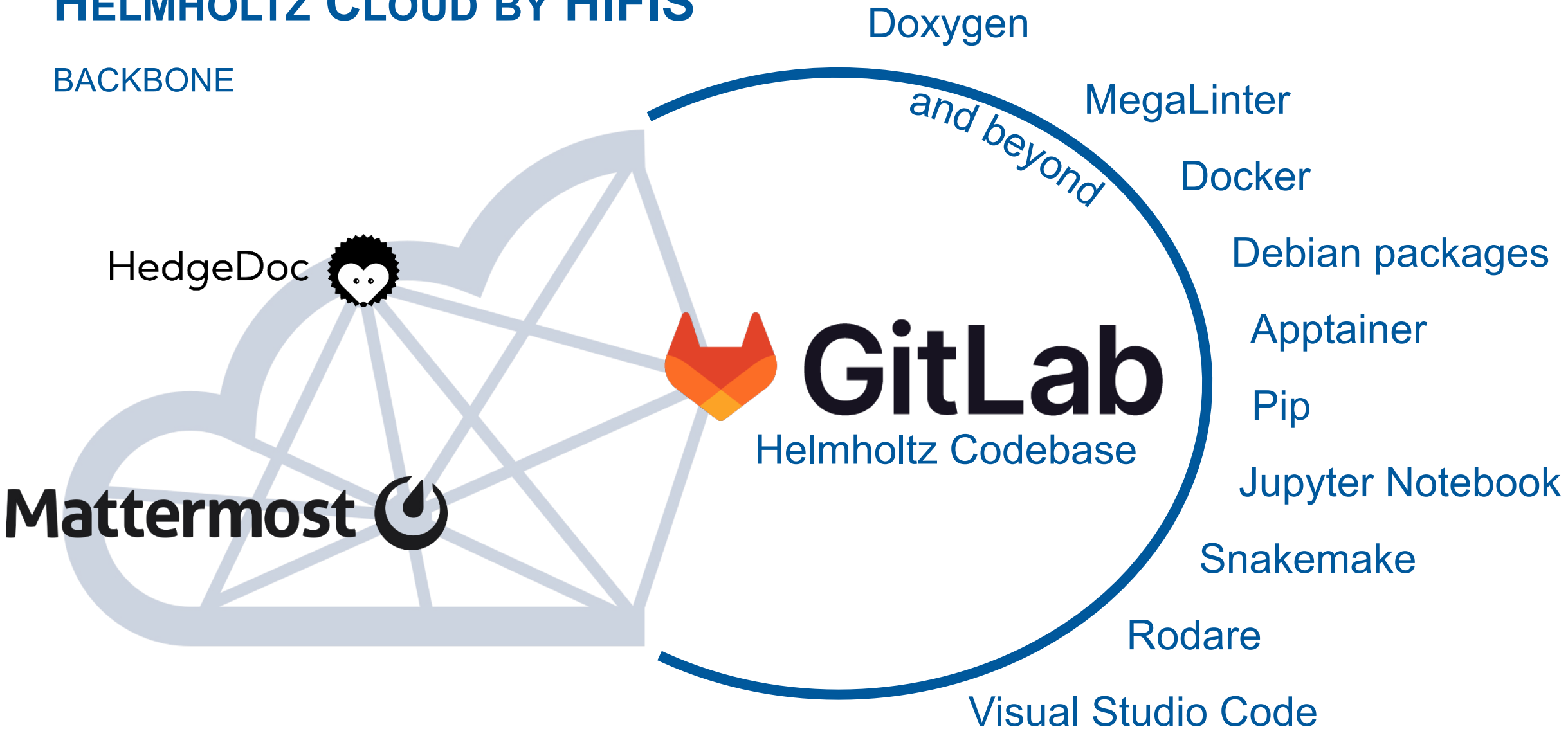
# Contribution to OpenFOAM

## Contributor with addon

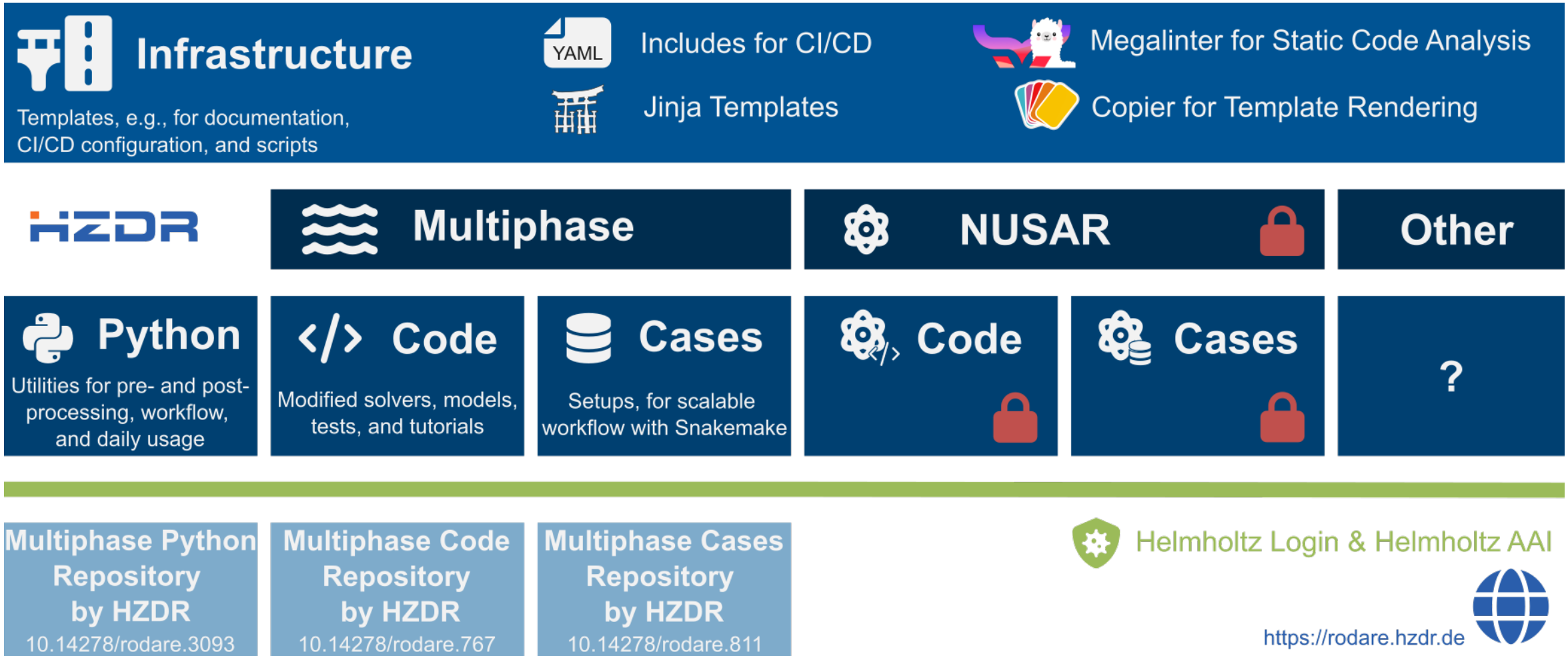


# HELMHOLTZ CLOUD BY HIFIS

BACKBONE



# Our Repositories



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# PORTABLE WORKFLOW WITH GITLAB

**Code**
with Apptainer images

Test runs for downstream project

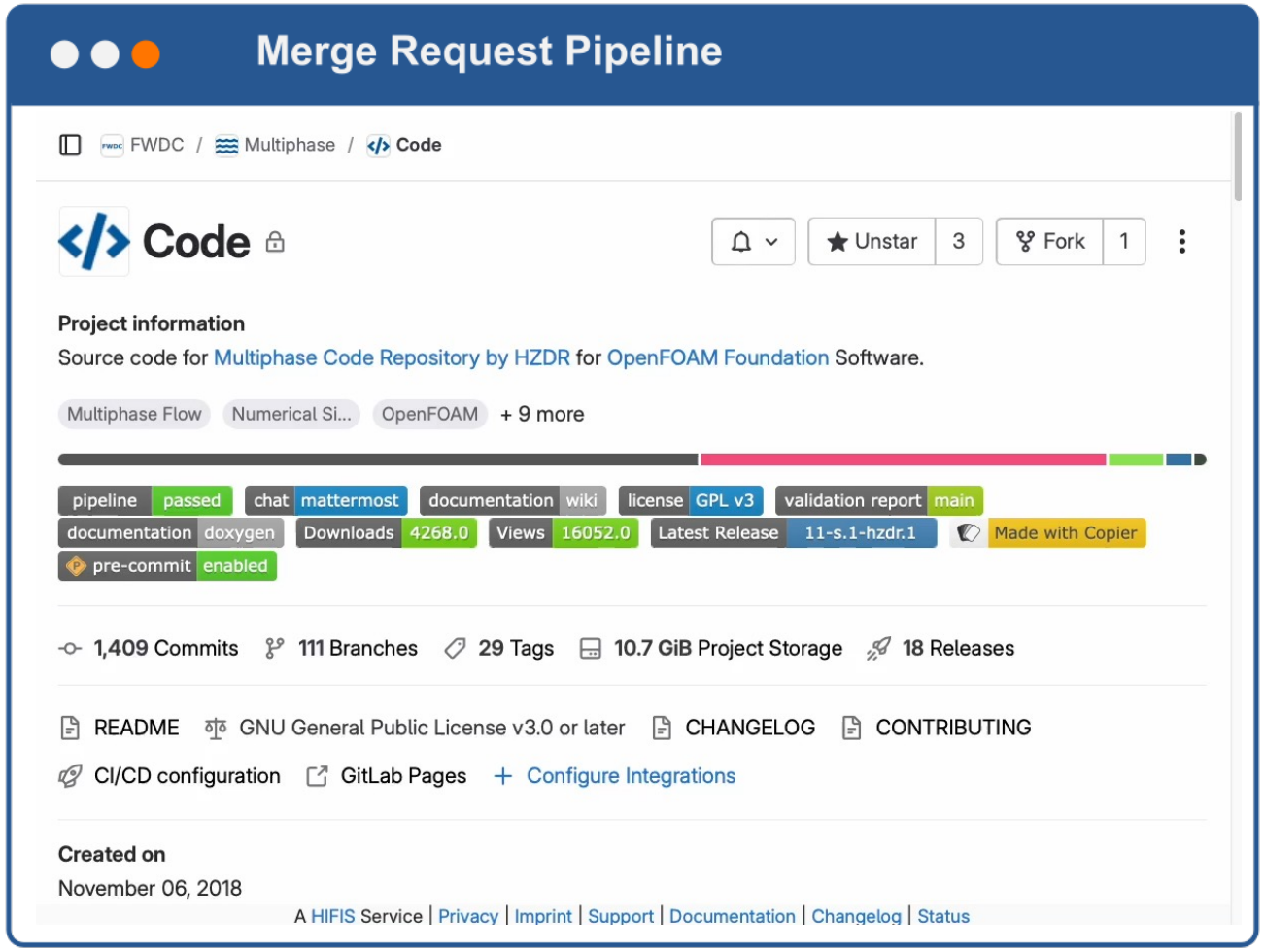
**Cases**
with Snakemake workflow

Scalable execution

**Gitlab Runner**

**Apptainer**
**+**
**Snakemake**
**=**
**Portability**

```
apptainer pull docker://<image>
```



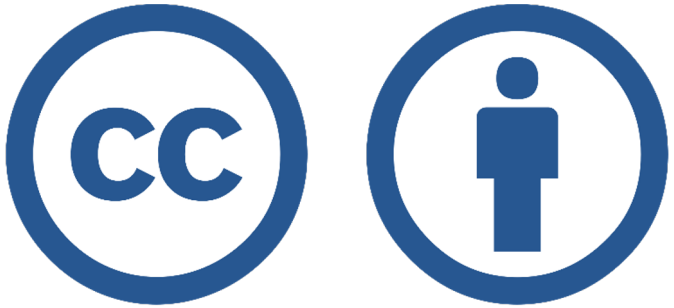
# SUMMARY

- 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

## LICENSE



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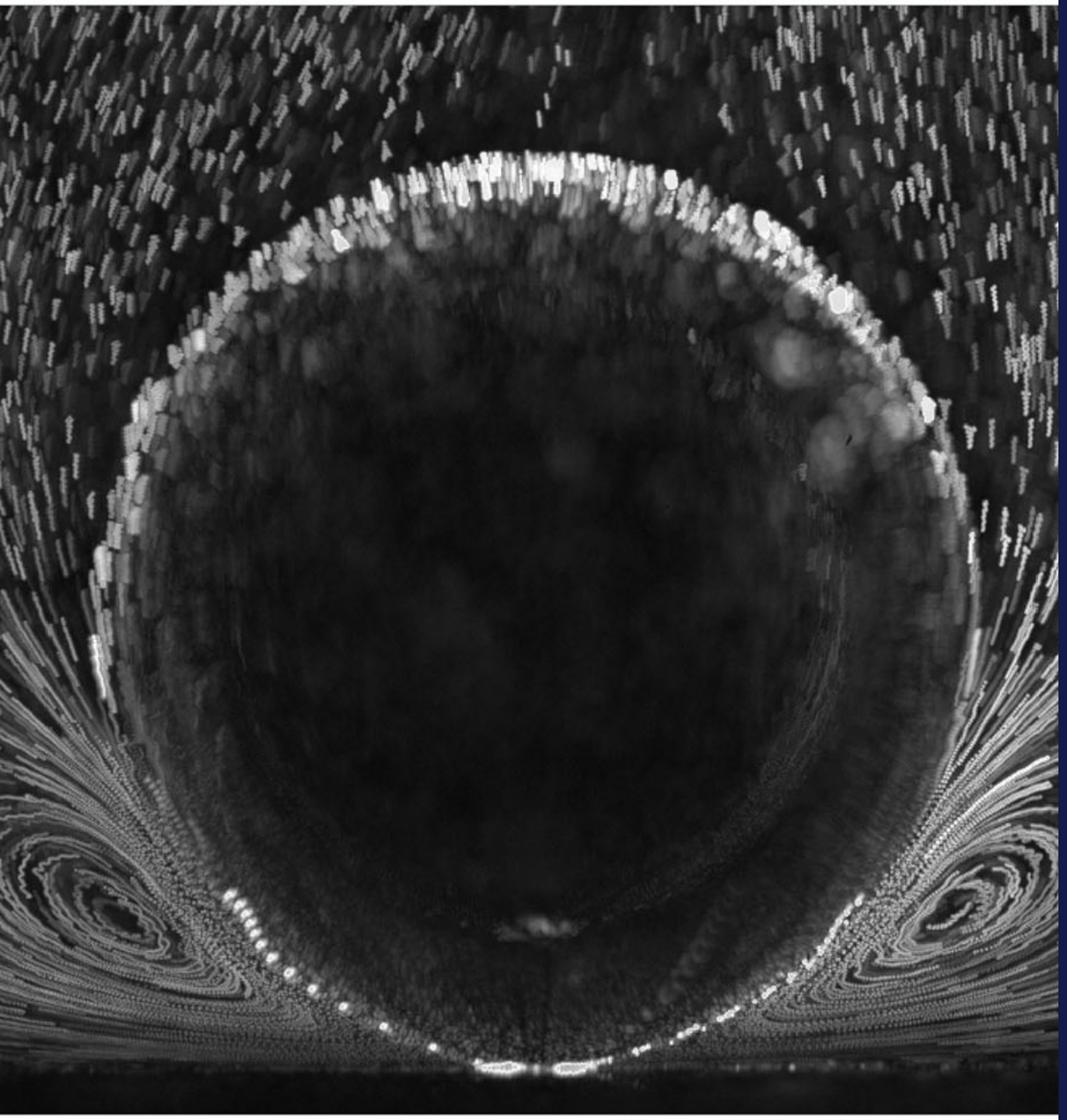
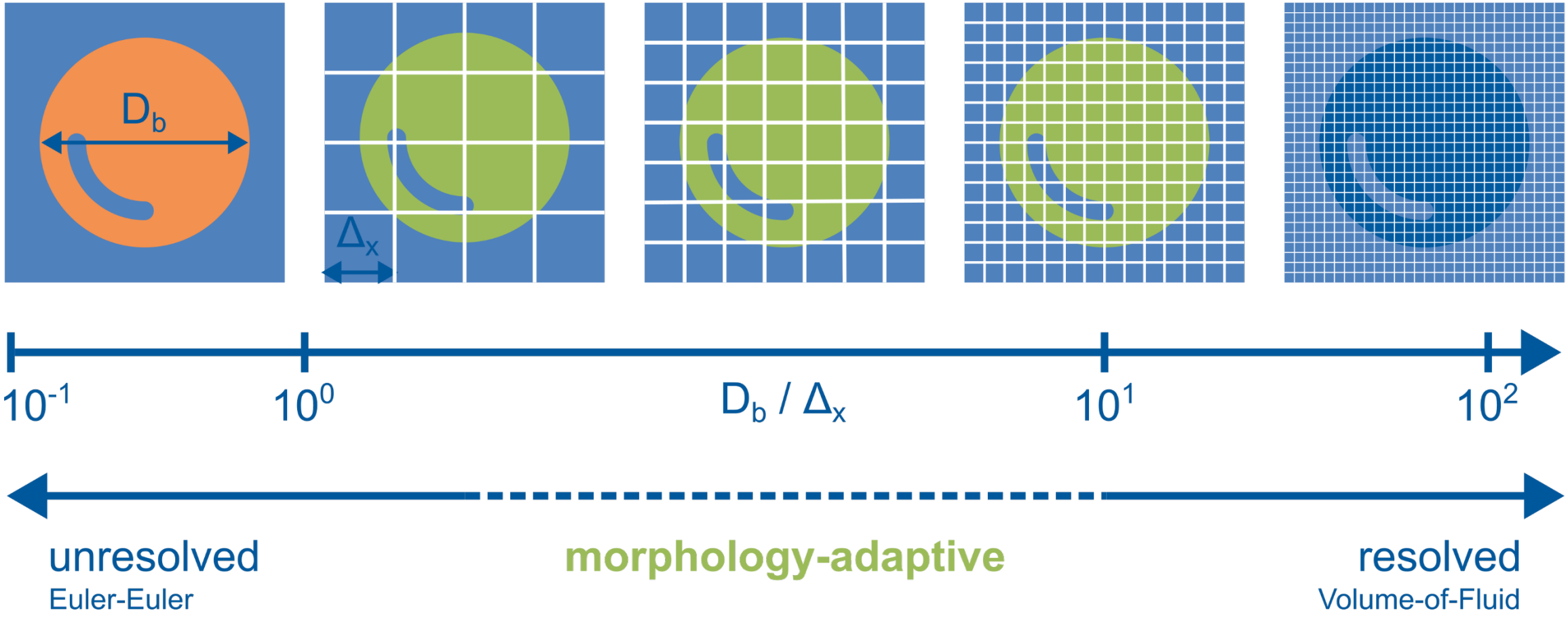
You may do so in any reasonable manner, but not in any way that suggests the licensor endorses you or your use.



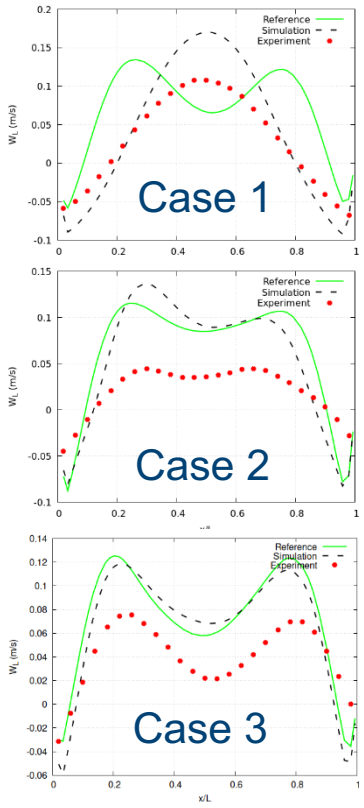
# Slides as **Backup**

# A Morphology-Adaptive Multifield Two-Fluid Model



# QUANTIFYING THE CFD PREDICTION QUALITY

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




Metric 1

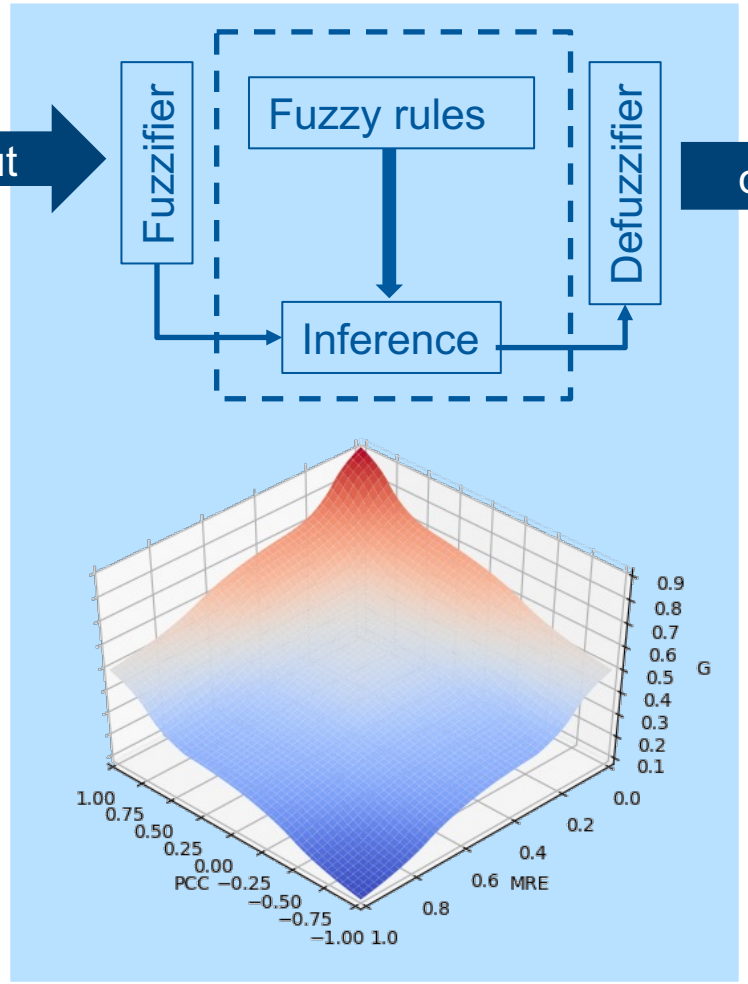
Metric 2

…

extract

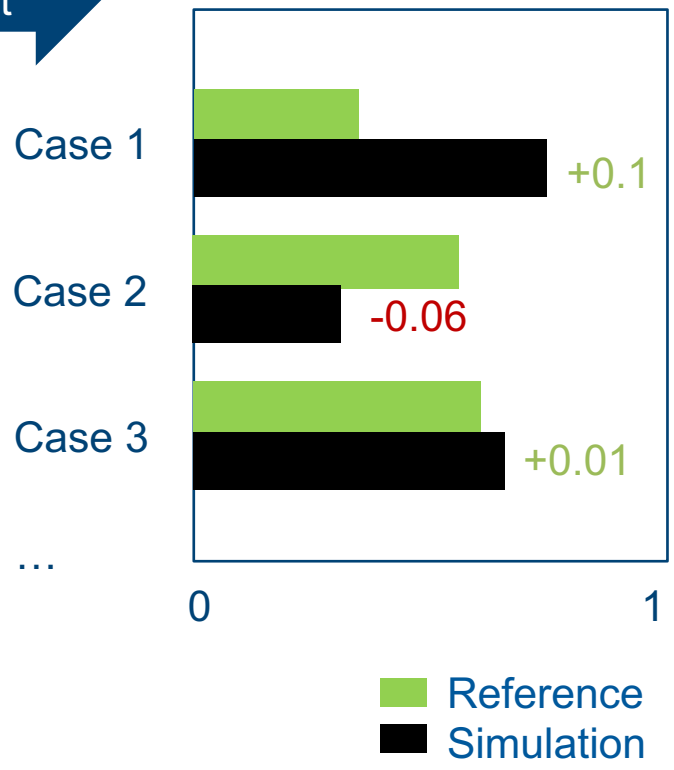
input

Fuzzy logic controller



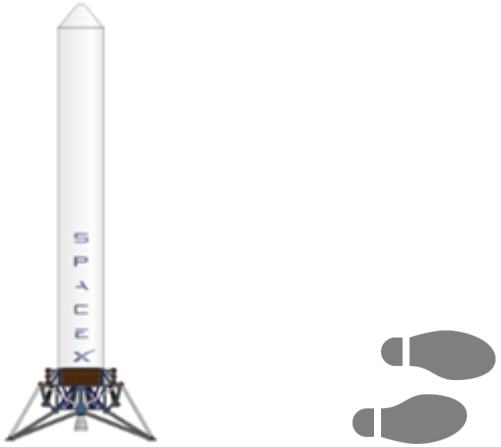

output

Prediction quality



# Quality of Software Engineering

**Feasibility Prototype**
- Validate individual features
- Check feasibility
- Extremely important



Grasshopper test vehicle

**Preliminary Product Prototype**
- Interplay of components
- Identify limitations and shortcomings
- Selected features

Falcon 9R Test Vehicle

Falcon 9 FT

**Demonstration Prototype**
- Most of the features and functions
- Start user testing

Core Maintainers

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



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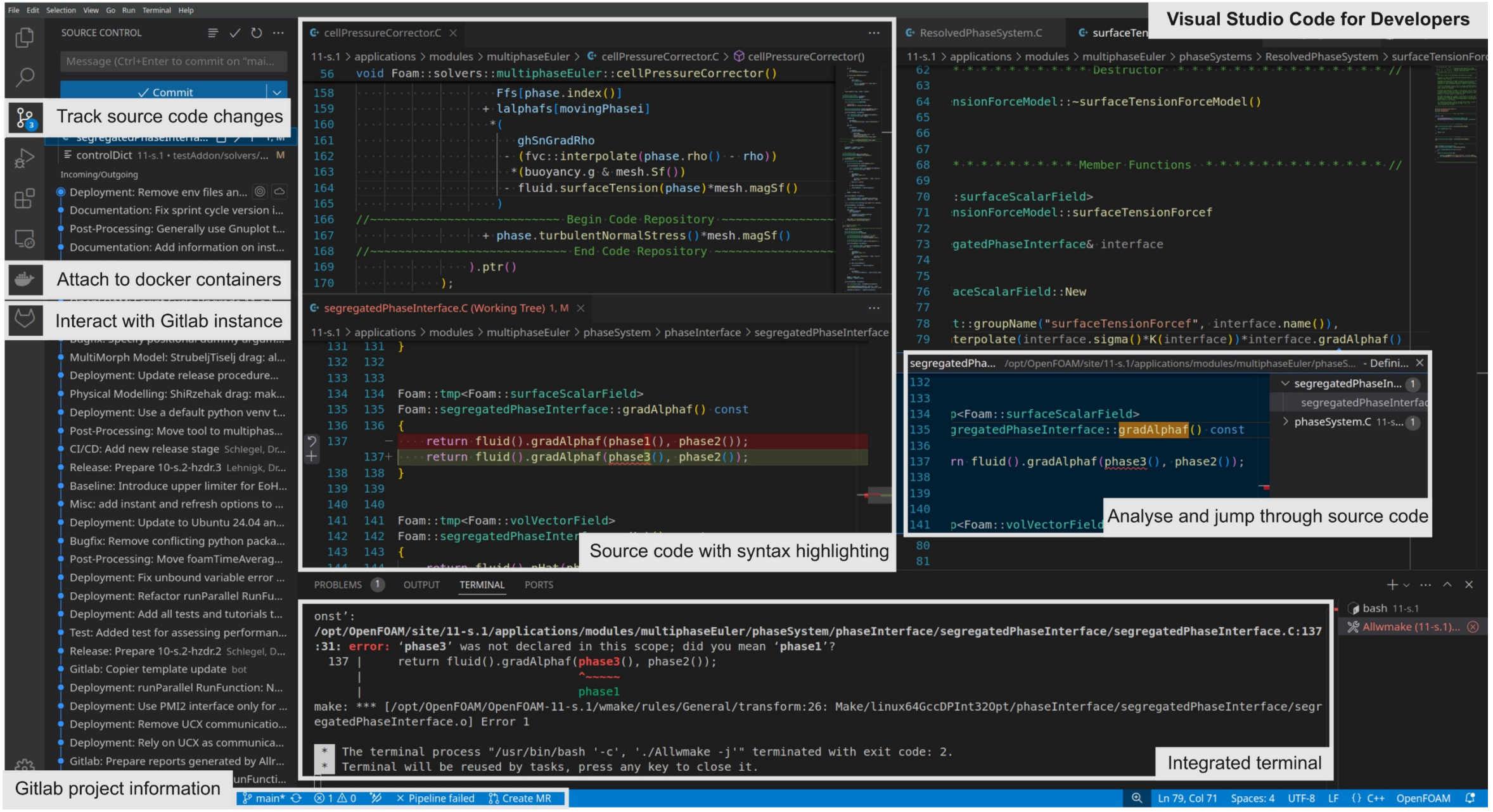
# Visual Studio Code for Developers



# Visual Studio Code for Users