

# Model optimization using Snakemake workflows

# Who am I?

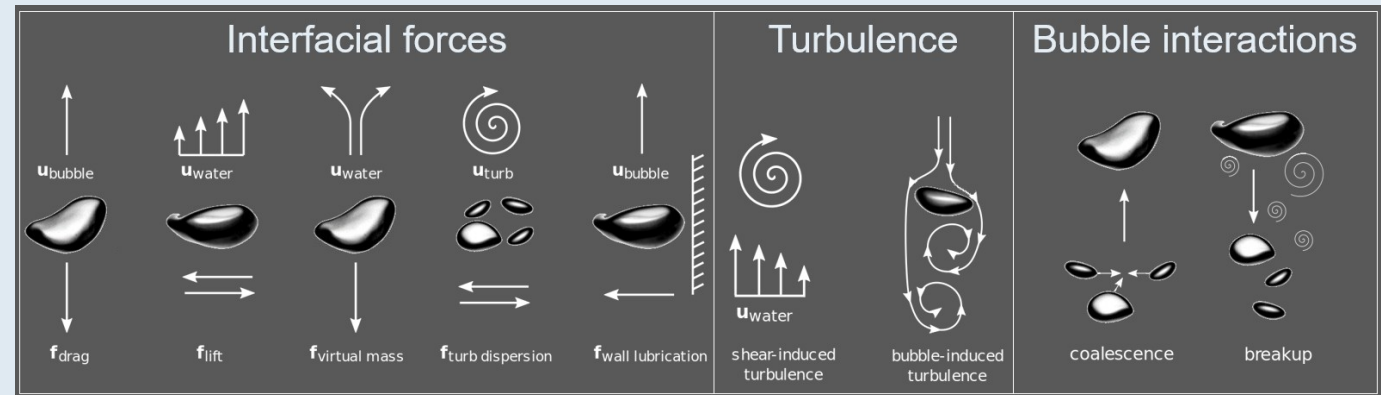
## Post-Doc at CFD department

- Euler-Euler modeling of polydisperse flows
- Development of state-of-the-art closures
- Since 2017 OpenFOAM contributors agreement
- Multiphase Code Repository by HZDR for OpenFOAM software



## Model development strategy

Dozen closure models needed for E-E CFD:



Numerous possible model combinations and parameters to choose from and no consensus in the multiphase community

Our vision: A fixed set of closure models („Baseline models“) with predictive abilities for all types of bubbly flows in an geometry

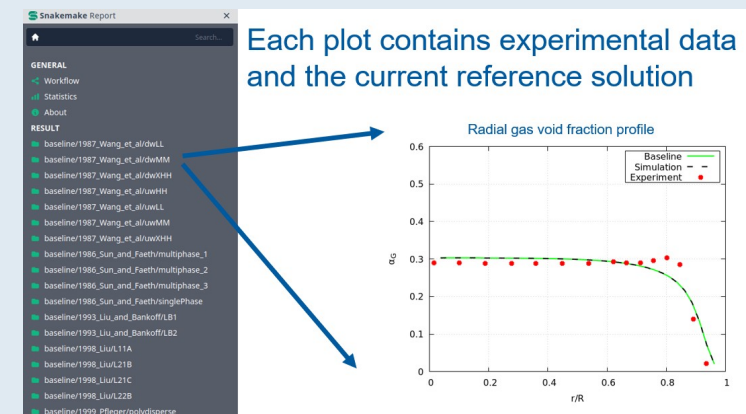
# What is my Framework?

## Continuous testing with the Multiphase Cases Repository by HZDR for OpenFOAM Foundation

- Growing number of validation cases
- Standardised case setups
- Cases under Git version control
- Managed in Gitlab
- Keywords allow categorisation of cases
- Selection of cases for closure model testing

## Automation via Snakemake workflow

- Workflow management system for scalable and reproducible data analysis
- Fully-automated pre-processing, solving and post-processing of validation cases
- Integration into existing Gitlab environment
- Automated production of hundreds of plots in well-structured reports:



# What is my Framework?

## Analysing new closure models

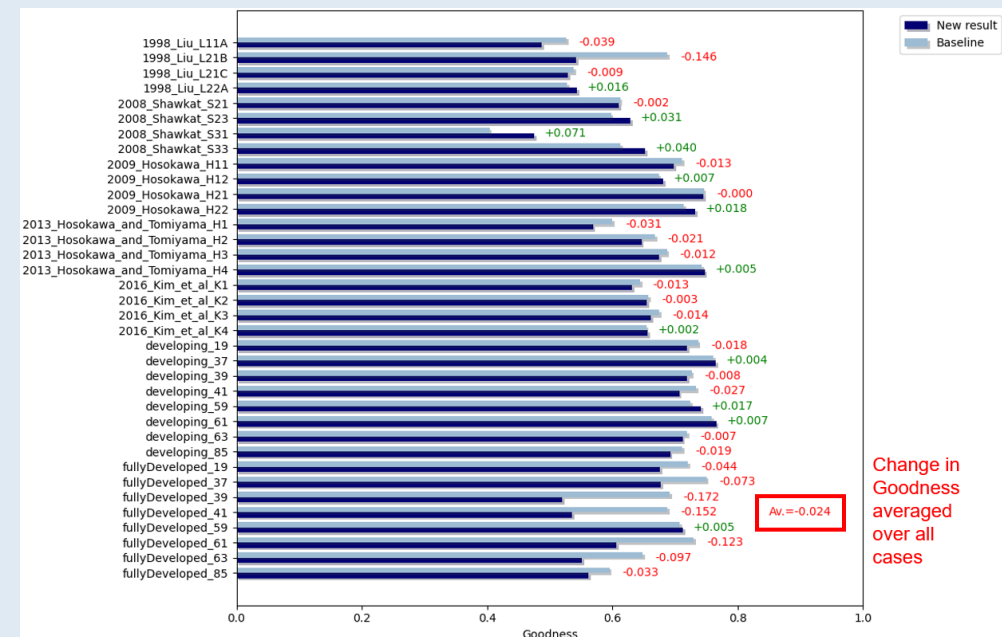
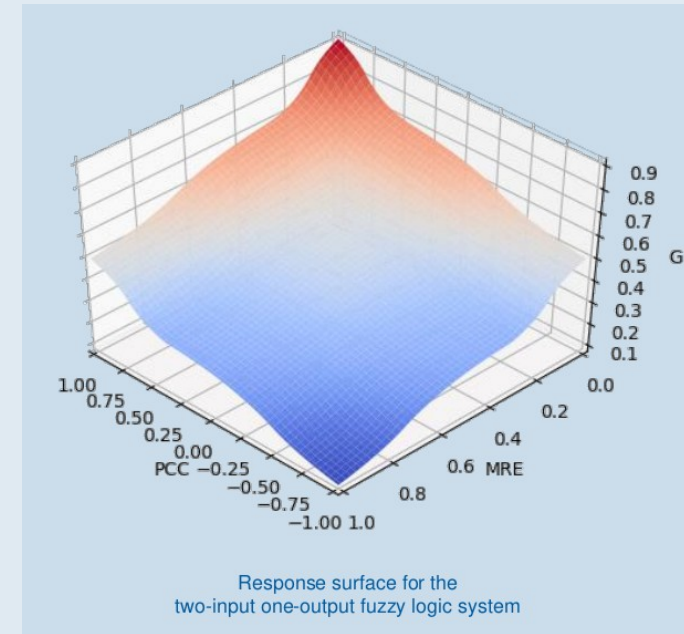
- Integrated Fuzzy-Logic system
- Input:

Error metrics comparing CFD vs. validation plots  
(e.g. Mean relative error MRE, Pearson correlation coefficient PCC)

- Output:

„Goodness“ value G between 0 and 1

- Quantification of the agreement of the CFD prediction with the validation data



# What is my Challenge?

## Model development aided by data science „experiments“

- Identify the optimal model set by running consecutive workflows on cluster + result evaluation
- Optimizing model parameters ~
- What are suitable optimization algorithms for an efficient use of ressources?
- Is it possible to integrate such tests into Gitlab for documentation? Model experiments feature?

