Retrospect, Status and Perspective of the Development of containmentFOAM

S. Kelm, M. Kampili, G. Vijaya Kumar, X. Liu, A. George, R. Ji,
L.M.F. Cammiade, K. Arul Prakash, H.-J. Allelein

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containmentFOAM

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Federal Ministry
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Nuclear Safety and Consumer Protection

based on a decision of
the German Bundestag
Project No. 150 1633B

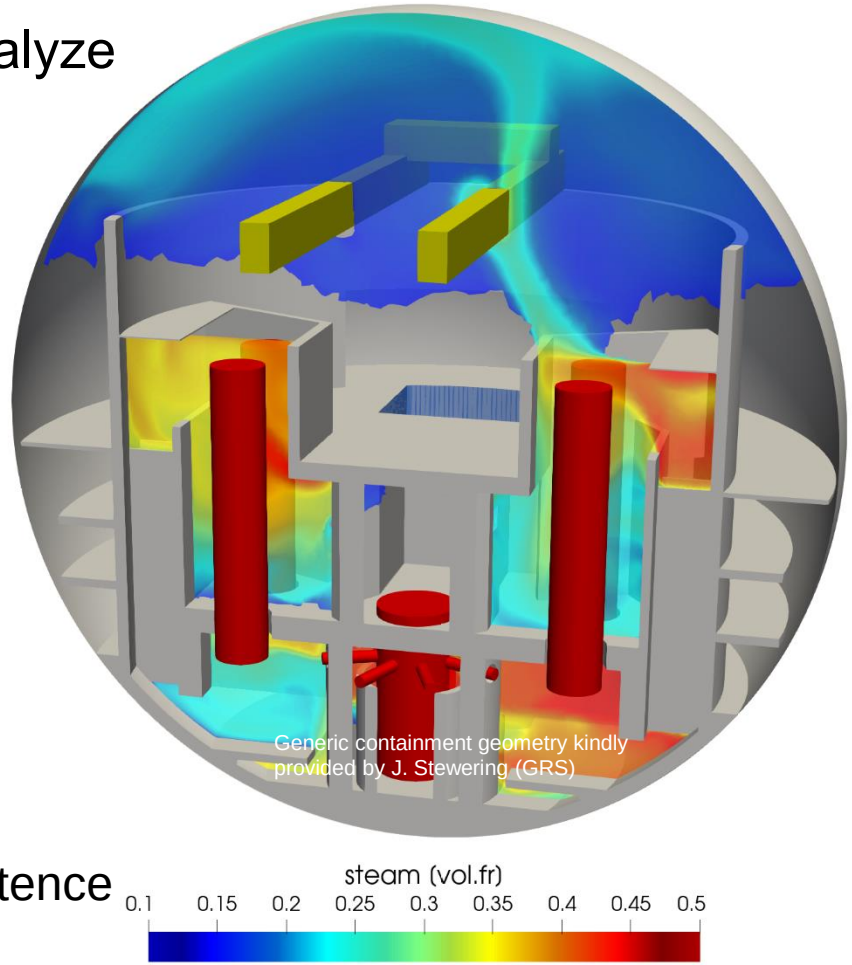
JÜLICH
Forschungszentrum
Mitglied der Helmholtz-Gemeinschaft

OUTLINE

- Introduction
  - Background and Motivation
  - Strategy and General Considerations
  - Status of containment∇FOAM
- Open-source challenges
  - Maintenance, distribution
  - User-Developer interaction
- Best practices
- Summary and Perspective

BACKGROUND

- Development of containment∇FOAM [1] as an open basis to analyze containment pressurization, flows, H_2/CO and aerosol behavior:
  - Basis for our research within the Helmholtz Nusafe program:
    - Replacement of previous commercial code basis & legacy code
    - Support experiments & transfer of experimental results to plant scale
    - Investigate interaction of physical phenomena and safety systems under representative conditions
    - Assess effectiveness of (passive) safety systems and measures
    - Contribution to national CFD reference package for NRS
  - Carrier to disseminate our research and ensure its application
  - International cooperation (e.g. IITM, IAEA-ONCORE, OECD/NEA)
  - Attractive platform for education, training and maintenance of competence



Generic containment geometry kindly provided by J. Stewering (GRS)

[1] Kelm, S. et al. "The Tailored CFD Package 'containmentFOAM' for Analysis of Containment Atmosphere Mixing, H_2/CO Mitigation and Aerosol Transport" *Fluids* (2021) 6, no. 3: 100. https://doi.org/10.3390/fluids6030100

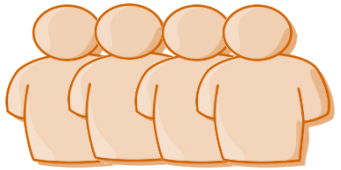
CONTAINMENTFOAM ENVIRONMENT

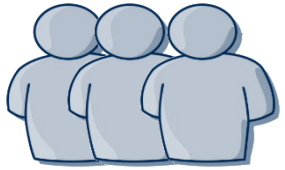
JÜLICH Forschungszentrum

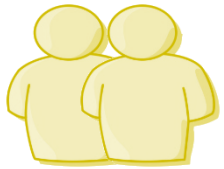
- Active developers team


PI
(permanent)


PostDoc


PhD students


students & trainees


technical staff
(permanent)


former
PhD students

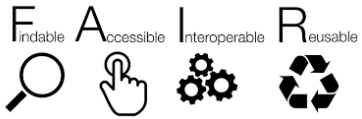
  - ➢ Mostly temporary contributors with different levels of qualification!

- Current collaborators, users & beta-testers:

GRS global research for safety
der Bundeswehr Universität München
KIT
POLITÉCNICA UNIVERSIDAD POLITÉCNICA DE MADRID
PAUL SCHERRER INSTITUT PSI
INDIAN INSTITUTE OF TECHNOLOGY MADRAS
RWTH AACHEN UNIVERSITY
FH AACHEN UNIVERSITY OF APPLIED SCIENCES
framatome
JAEA
KAERI

MOTIVATION TO USE THE OS APPROACH

- Obviously:
  - FAIR is the way to do meaningful publicly funded research!



- Many further benefits:
  - Visibility of the individual's work and the project:
    - ➢ Motivation for contributors and new applicants to join
  - Reusability of the research output by others:
    - ➢ Increases impact and KPI (citations)
    - ➢ In-line with Helmholtz digitalization strategy
  - Involvement of temporary staff at different education levels:
    - ➢ Possibility to keep them involved beyond their contract
  - International collaboration:
    - ➢ No troubles with license agreements but maybe contributors agreements needed

DEVELOPMENT OF CONTAINMENTFOAM

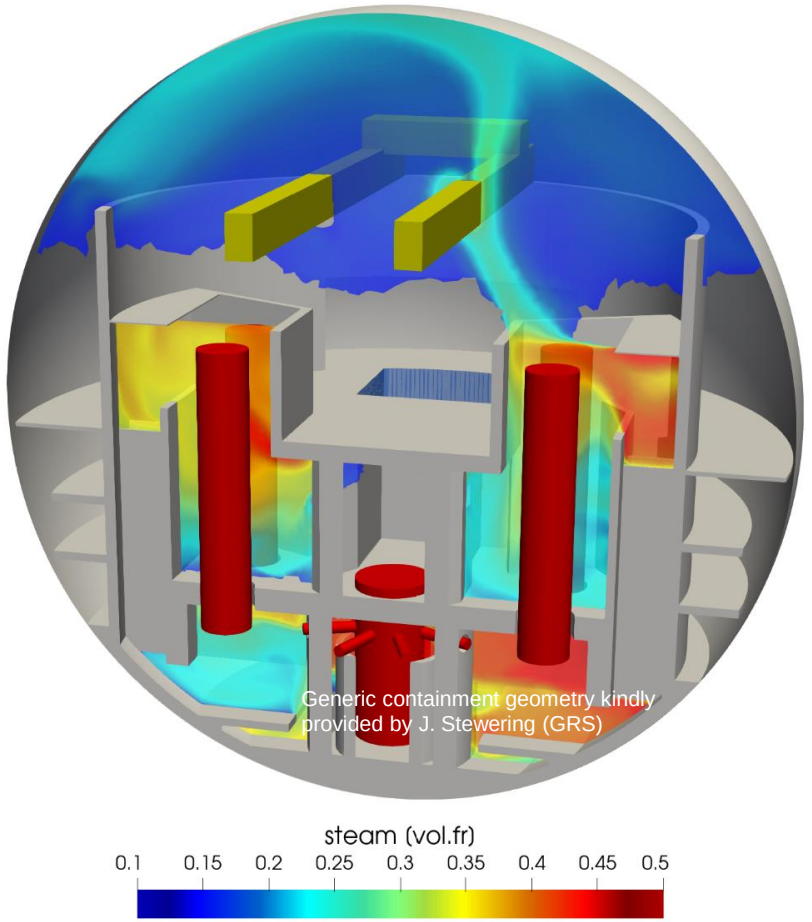
Strategy and General Considerations

- Coordinated R&D effort (currently 14 active contributors, cumulative > 25 person years R&D)
  - Multi-scale and Multi-physics application:
    - All physical phenomena and their interaction need to be considered to be representative of a accident progression
      - No separate effect consideration possible, models have to be robustly coupled
      - Model basis has to be well balanced in terms of accuracy and efficiency
    - Baseline set of models
      - Model set with known limitations rather than optimal model for a specific condition
      - User guidance for consistent application of the baseline model
      - Limit maintenance effort
  - Framework / quality assurance
    - Guided case setup and solution monitoring
    - Common post processing (functionObjects), data handling and minimum I/O
    - Software framework for uncertainty quantification

STATUS OF CONTAINMENTFOAM

Modeling Pressurization, Aerosol Transport and H_2/CO Gas Mixing and Mitigation

- Flows and Transport Phenomena
  - **Efficient Multi-Species Solver:** effective binary diffusion; Wilke mixture ✓
  - **Turbulence transport**: k-ω SST model with buoyancy terms, ✓ simple and generalized gradient diffusion hypothesis formulation ✓
  - **Conjugate heat transfer** ✓
  - **Wall condensation**: single phase diffusion layer model, ✓ implemented as face fluxes, ✓ dedicated wall treatment ✓
  - **Fog formation**: drift flux model with PBM ✓, two phase formulation ✓
  - **Gas radiation**: Emission-based Reciprocity Monte Carlo Method, ✓ SNBCK and LBL spectral models ✓
  - **Aerosol transport**: LPT with Continuous Random Walk model for turbulent dispersion, ✓ Eulerian drift flux model including hygroscopic growth ✓
- Technical Systems and Components
  - **PARs**: Code coupling with mechanistic model *REKODIREKT* ✓
  - **Burst discs, flaps, doors**: conditional mesh interfaces ✓
  - **Heat exchangers**: porous media ✓ 🕮



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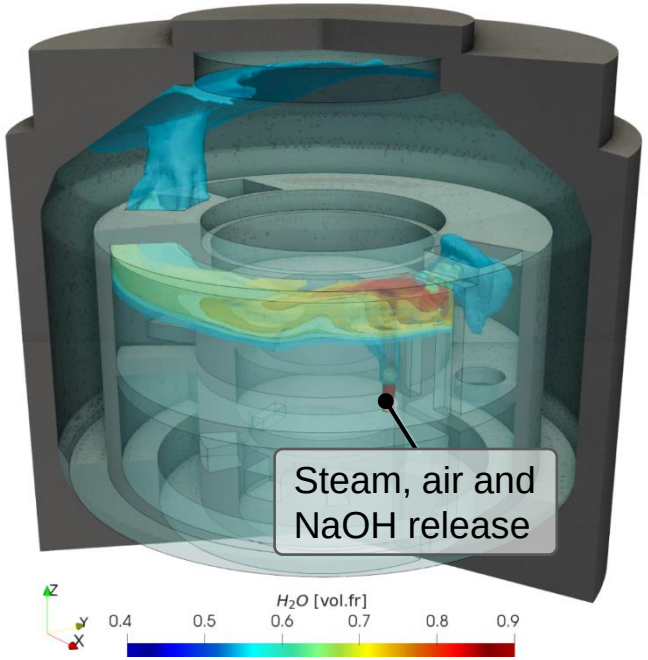
STATUS OF CONTAINMENTFOAM

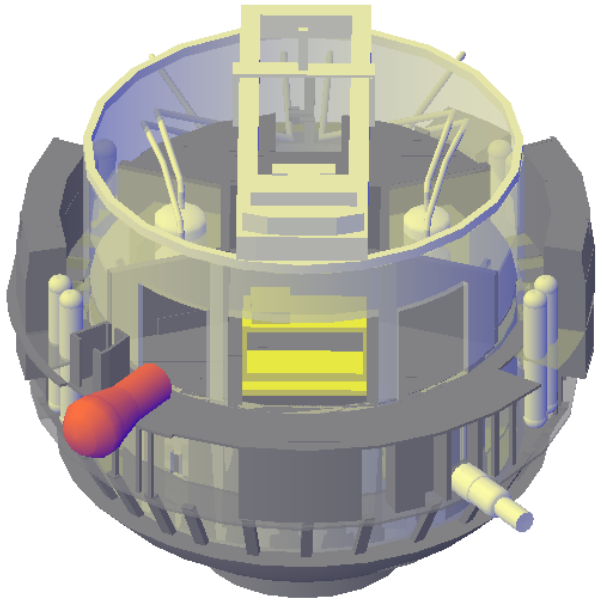
Applications

- ISP-37 VANAM M3
  – thermo-fluid dvnamics and aerosol distribution



  - 600 m³, 20.000 s
  - ~ 400 ..1100 s / day @ 128 CPU

- German KONVOI PWR (1400 MW_{el})
  – flammable gas distribution, combustion risk and mitigation



AMHYCO

UNIVERSIDAD POLITÉCNICA DE MADRID

  - Work-in-Progress (CAD model by UPM)
  - ~ 70000 m³, $\mathcal{O}$ ~ 1000 s

🕮 S. Kelm et al., „Technical Scale CFD Analysis of the Pressurization and Transport Processes in the Battelle Model Containment during the ISP 37 VANAM M3 Test “, accepted for publication at NUTHOS 13, Taichung, Taiwan, September 5-10, 2022
🕮 L. S. Lopez et al., *Development of a detailed 3D CAD model of a generic PWR-KWU containment as a basis for a better assessment of H2/CO combustion risk,* Proc. ENYGF'21

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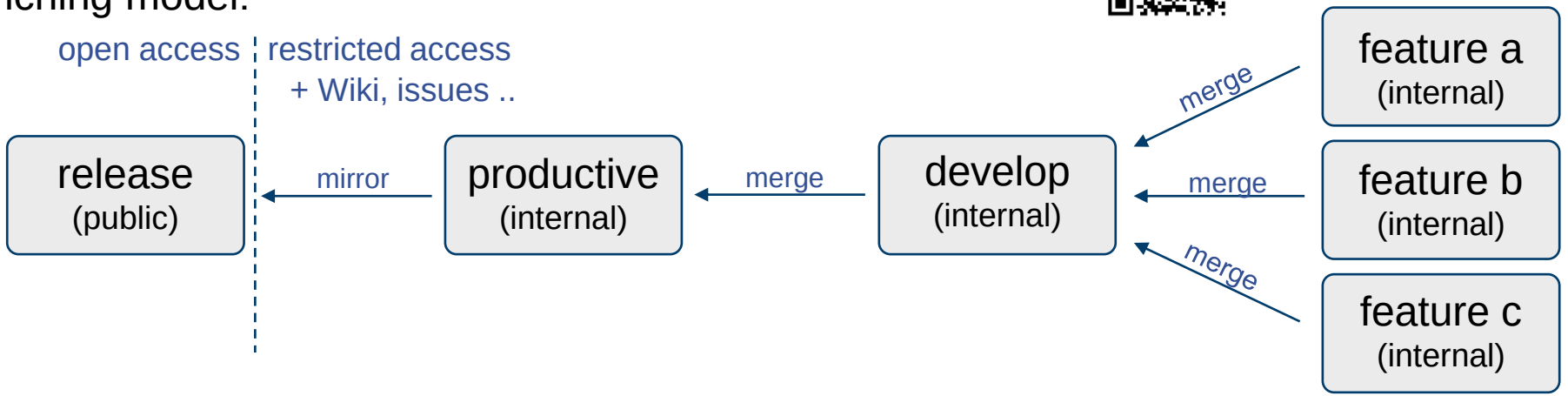
UNIQUE OPEN SOURCE ISSUES

- Licensing: derived from the original code basis OpenFOAM The OpenFOAM Foundation : GNU public license v 3.0
- Distribution: via gitlab *https://go.fzj.de/containmentFOAM*
  - Branching model:



- long-term maintenance (supported by BMUV, Project No. 150 1633B in collaboration with GRS, Project No. RS1603A)
  - mostly a ‘non-scientific’ work (implications on funding or visible research output)
  - but requires skilled scientists who know the models and their numerical implementation peculiarities
  - comprehensive efforts to follow refactoring of of the original code basis (OpenFOAM)

UNIQUE OPEN SOURCE ISSUES

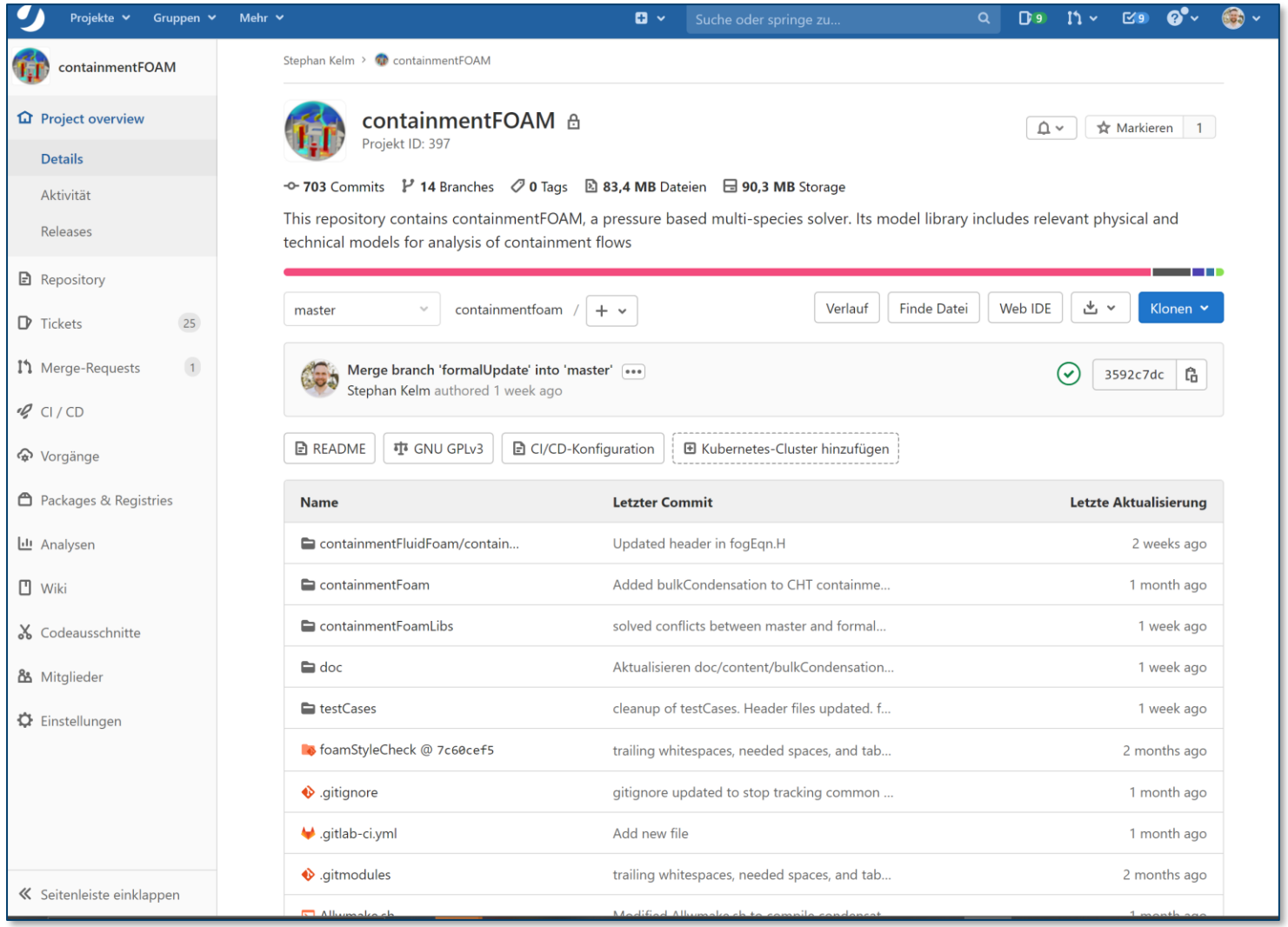
Developer - User Interaction

- Challenges:
  - Derivation from / add-on to a famous OS-CFD package enables a broad distribution and usage
    - Known and unknown users → different channels for communication
    - Users with different applications, background and experience (e.g., meshing, CFD, OpenFOAM, containment phenomenology & modeling etc.)
      - Skilled OpenFOAM users may have different established, but ‘incompatible’ workflows, modeling approaches etc.
      - Different applications may exceed the models’ validity range targeted by the developers
      - How to prevent user errors (inconsistent setups, misunderstanding)
  - Specific developments are highly complex (product of 4 years PhD projects)
    - How to enable best ‘usability’ of new developments to provide user feedback to the developers ?
    - How to transfer the developers experience to the user?
  - ➢ Provide and maintain a useful documentation and user guidance
    - Successful usage is important to keep the user's group active
    - Limit time for support

UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

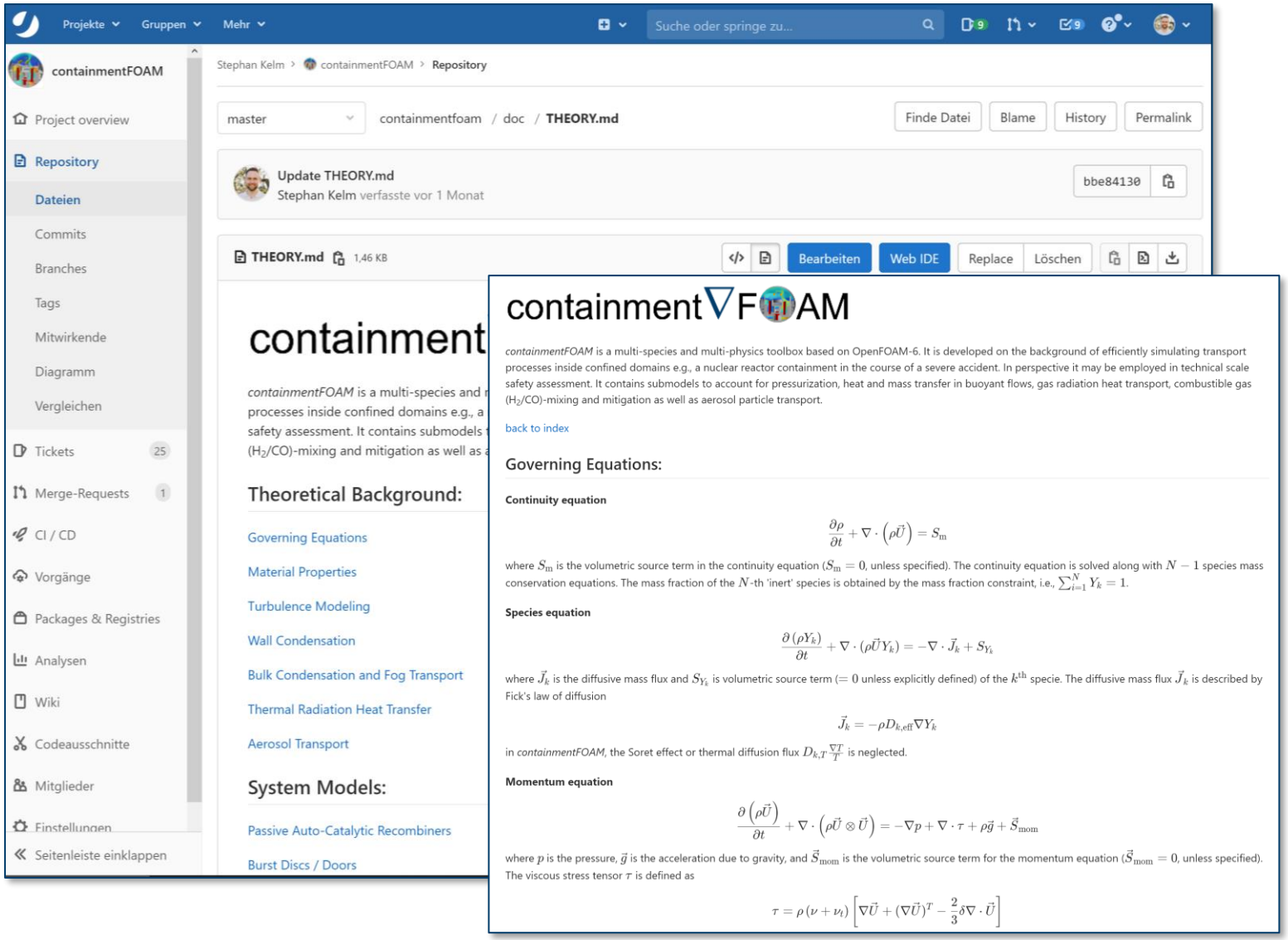
- GitLab platform at FZJ
  - Version management
  - CI/CD Environment
  - Ticket system
  - Wiki (only internal)
  - flexible account management via ‚github accounts‘



UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

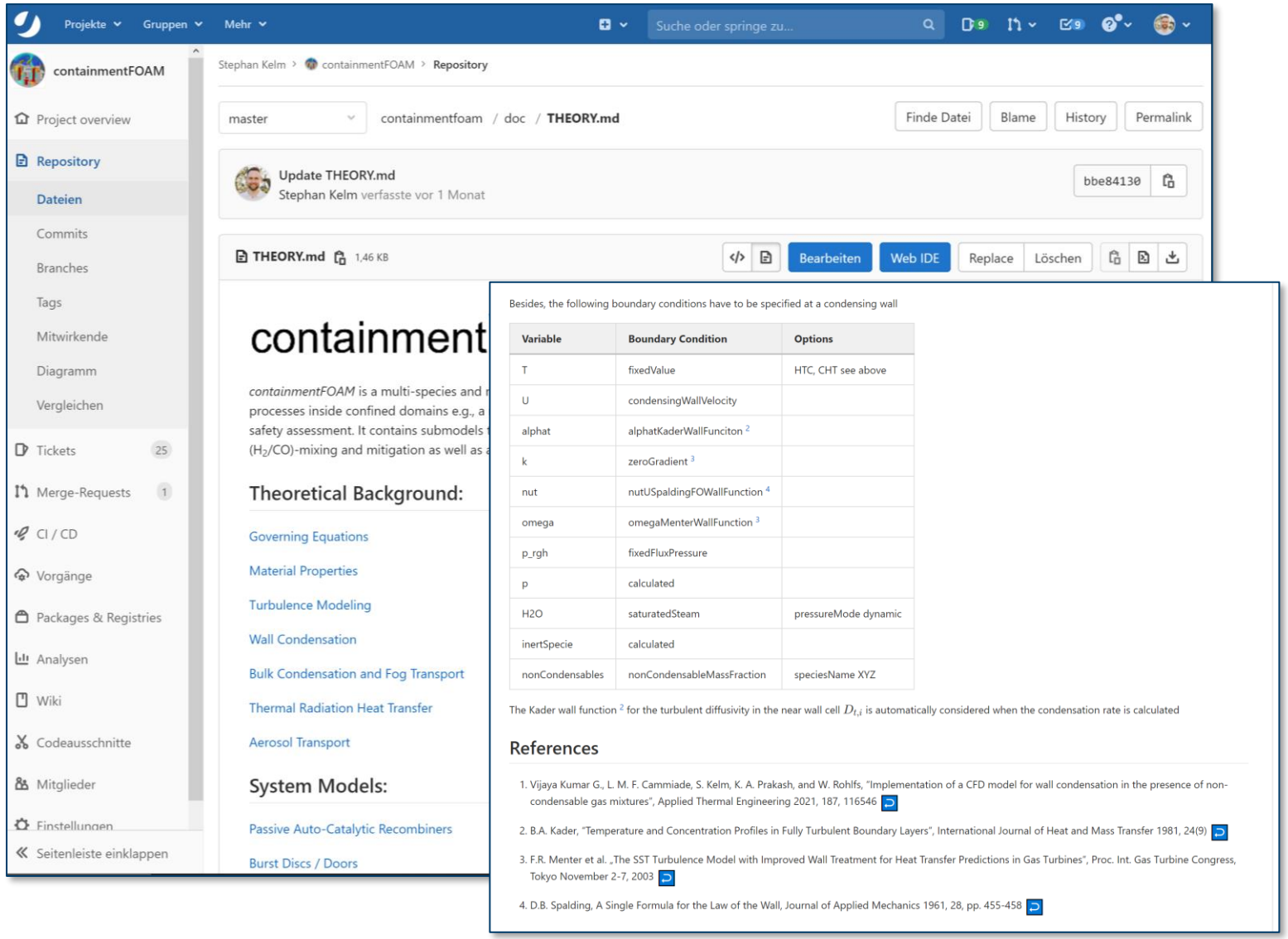
- GitLab platform at FZJ
  - Version management
  - CI/CD Environment
  - Ticket system
  - Wiki
  - flexible account management
  - GitLab flavored Markdown files
    - Model details



UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

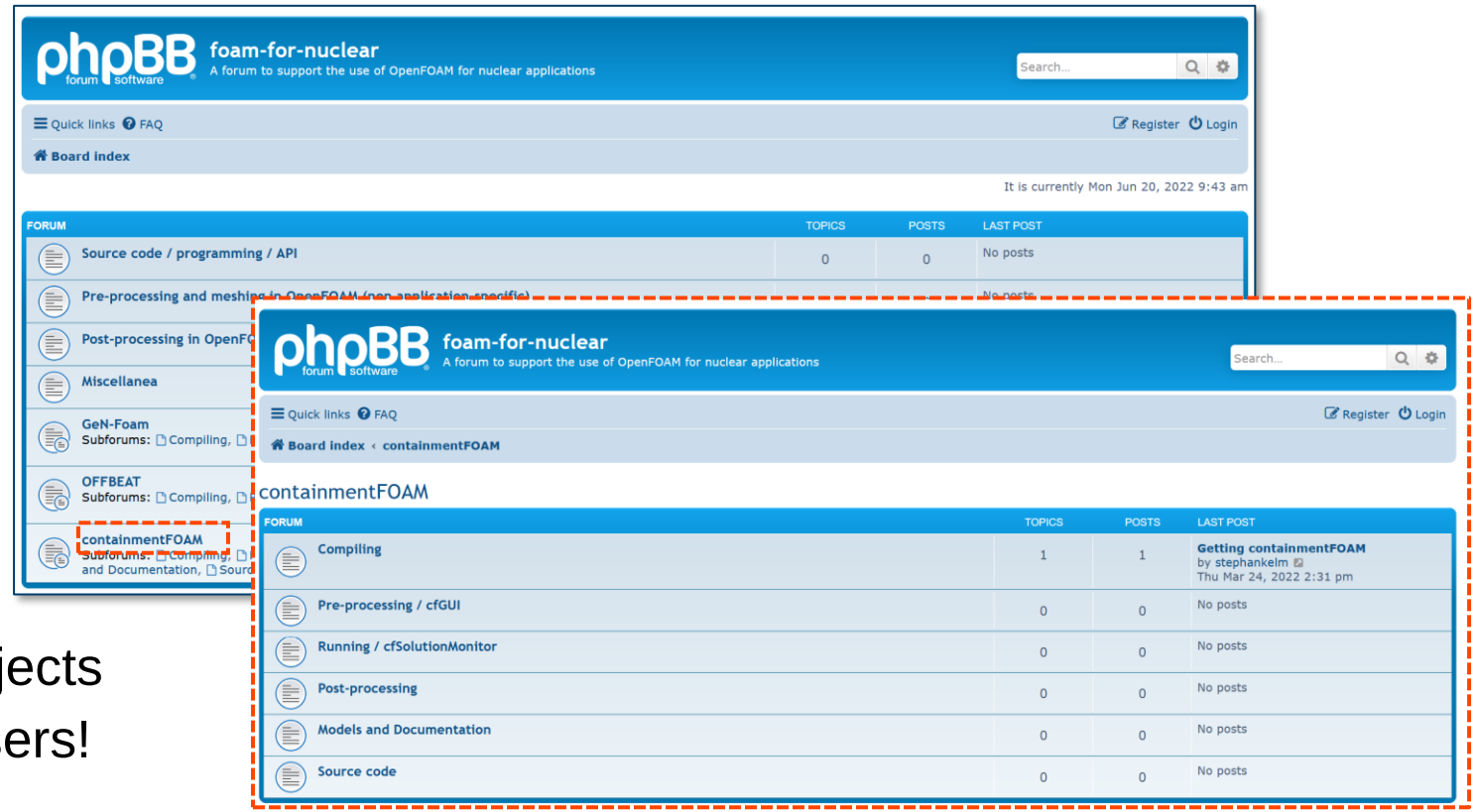
- GitLab platform at FZJ
  - Version management
  - CI/CD Environment
  - Ticket system
  - Wiki
  - flexible account management
  - GitLab flavored Markdown files
    - Model details
    - Recommended usage
    - Link to source files
    - References



UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

- Communication channels:
  - Mattermost chat system (upon request / invitation)
  - Discussion forum
    - https://foam-for-nuclear.org/phpBB/
      thanks to Carlo Fiorina for hosting it !
  - containmentfoam@fz-juelich.de



➢ User support is mandatory, as the projects success depends on the number of users!

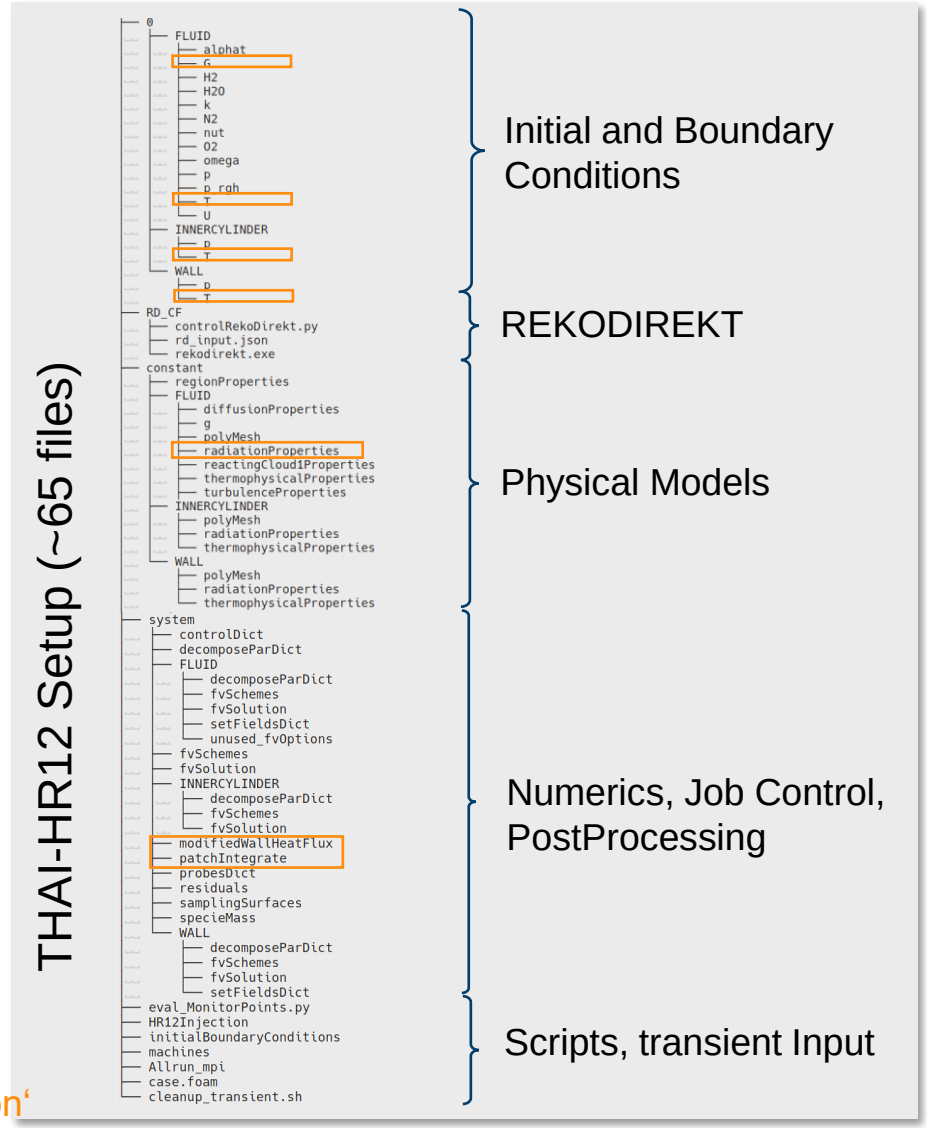
UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

- Containment analysis comprises interaction of multiple physical phenomena and safety systems:
  - Definition in separate files (‚dictionary‘)
  - Dependencies among dictionaries (and models)
  - Inconsistent definitions possible, which may not cause a crash
  - Broad variety of numerical methods and schemes

➢ ‚Standard‘ & Best Practice required:

  - Prevent input errors
  - Ensure consistent model application
  - Enable comparable and reproducible analysis
  - Support / bug identification and fixing.

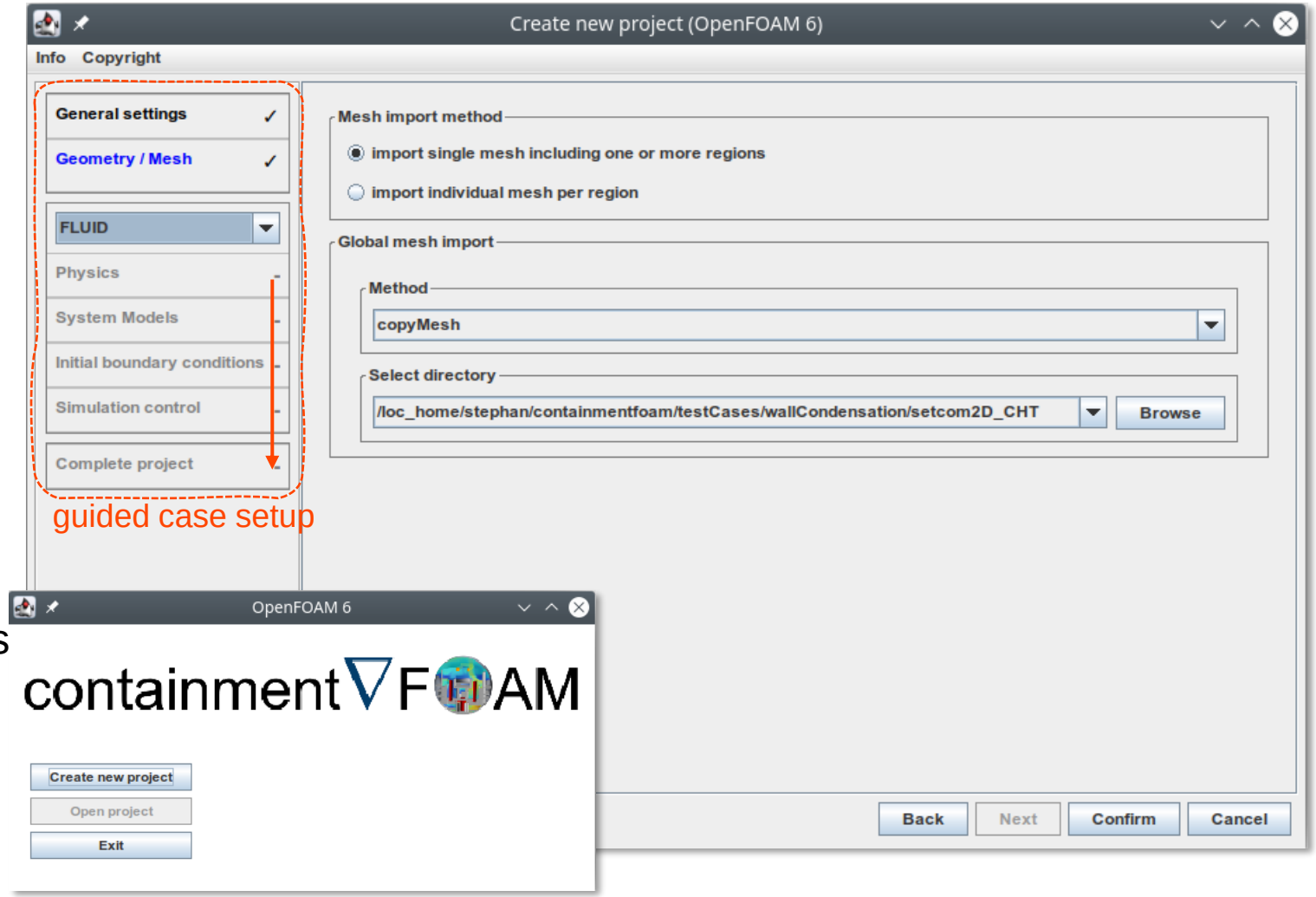


Definition ‚gas radiation‘

UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

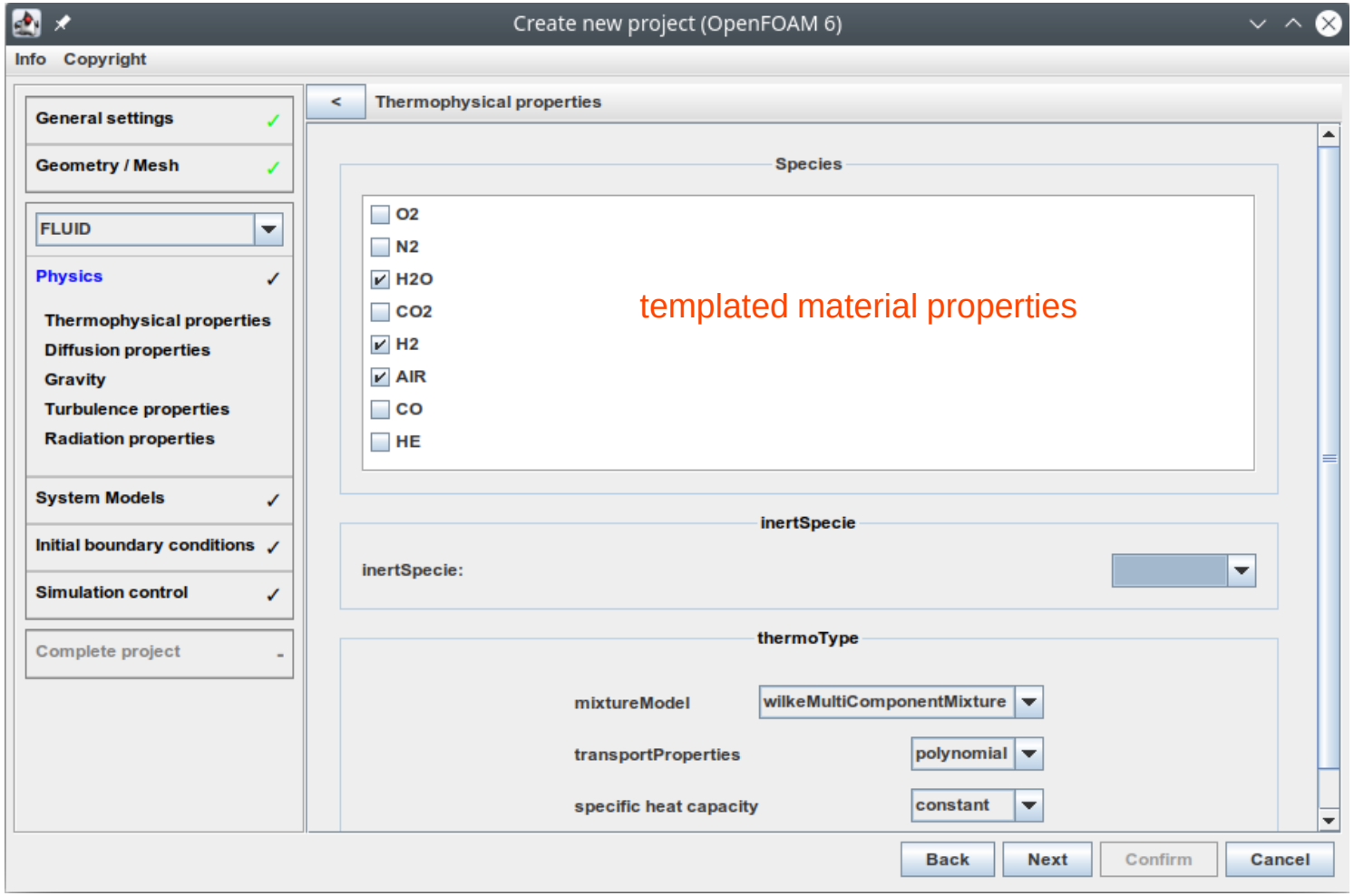
- General idea:
  - Workflow, structure and syntax close to OpenFOAM
  - limit functionality to baseline model and fundamental functions
  - ➢ Enable easy entry for new users (only a mesh is needed)
  - ➢ Enable fallback for bug tracking
- Mesh import
  - Using OpenFOAM® utilities and libraries
  - Reads mesh quality metrics for further use (e.g. numerics settings)



UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

- Mesh import
- Templated material properties
  - Calculator
  - Polynomial fits (NIST data)



UNIQUE OPEN SOURCE ISSUES

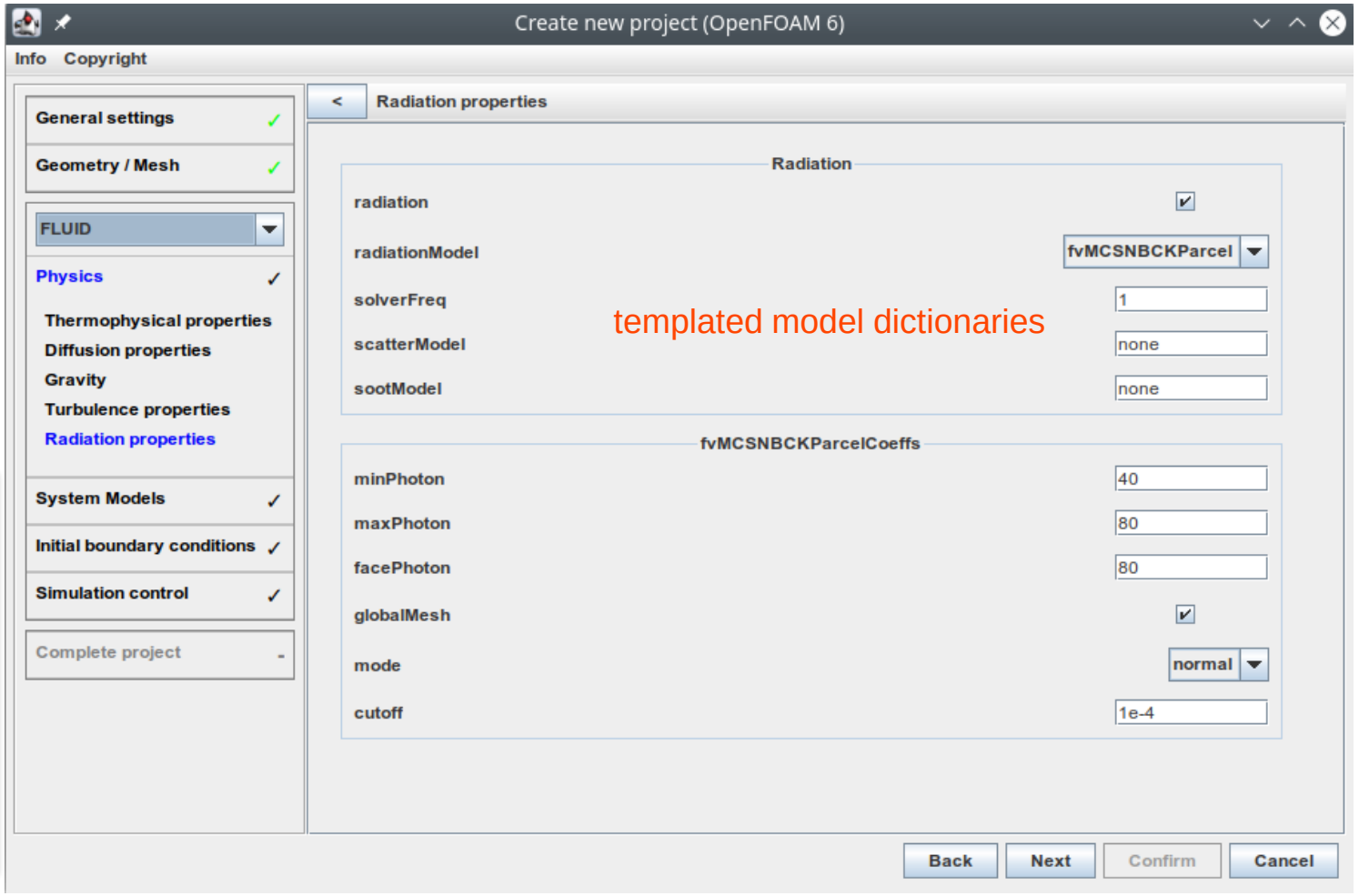
Developer - User Interaction

- Mesh import
- Templated material properties
- Flexible model templates based on JSON, logical rules and tooltips by the containmentFOAM developers (no Java skills needed)

```
"fvMCMParcelCoeffs":{
      "__settings__":["type=oneLineValue"],

      "__values__":
      [
      ["_show_{Label(text=minPhoton)}","_show_{TextField(text=4)};"],
      ["_show_{Label(text=maxPhoton)}","_show_{TextField(text=50)};"],
      ["_show_{Label(text=facePhoton)}","_show_{TextField(text=1)};"],
      ["_show_{Label(text=cutoff)}","_show_{TextField(text=1e-2)};"]
      ]
},

  "absorptionEmissionModel":{
      "__settings__":["type=oneLineValue"],

      "__values__":
      [
      ["_show_{Label(text=absorptionEmissionModel)}","_show
      {ChoiceBox(text=[constantAbsorptionEmission,nongreyMeanAbsorptionEmission])};"]
      ]
  },
```

default parameters

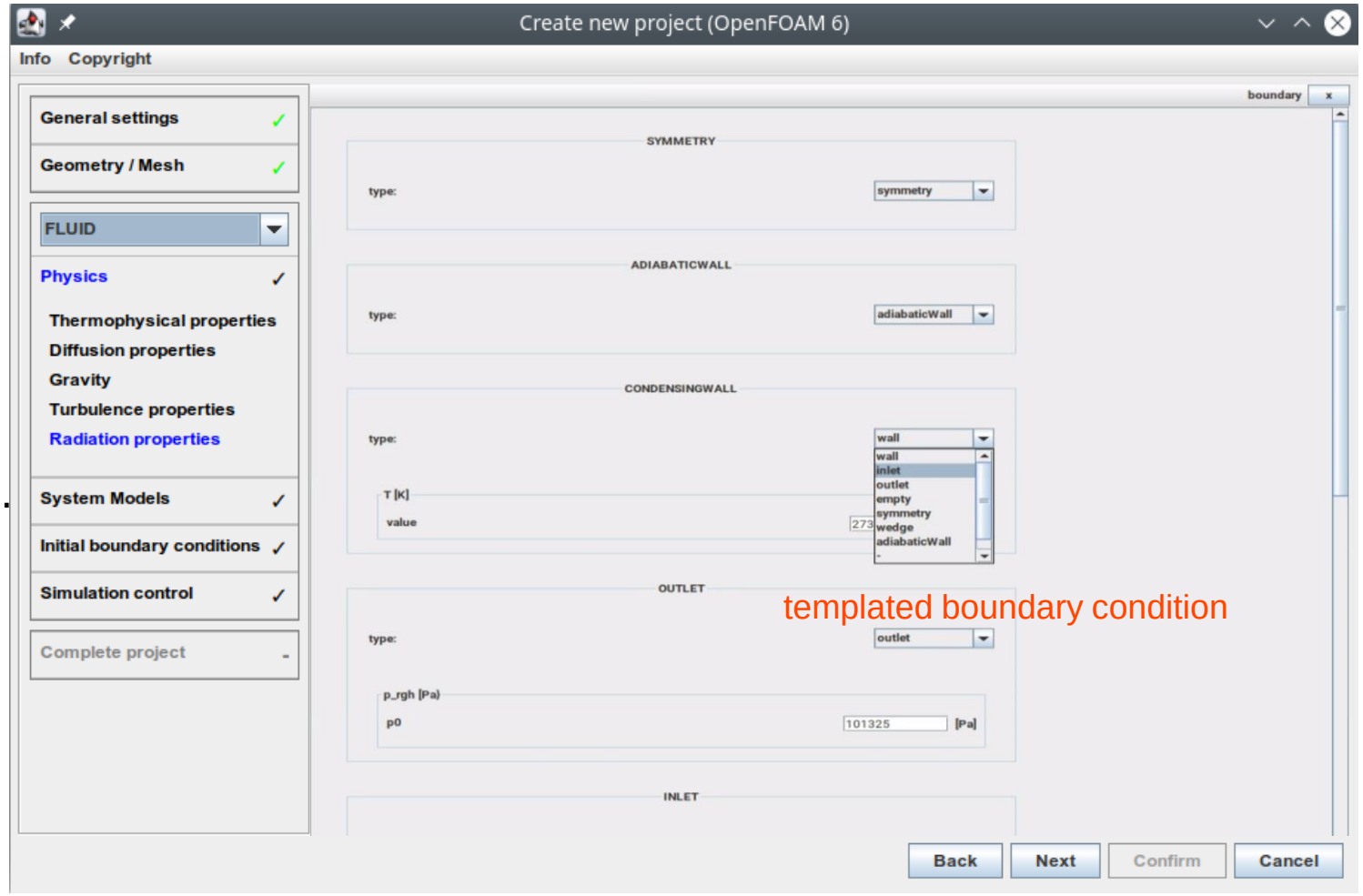
model selection



UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

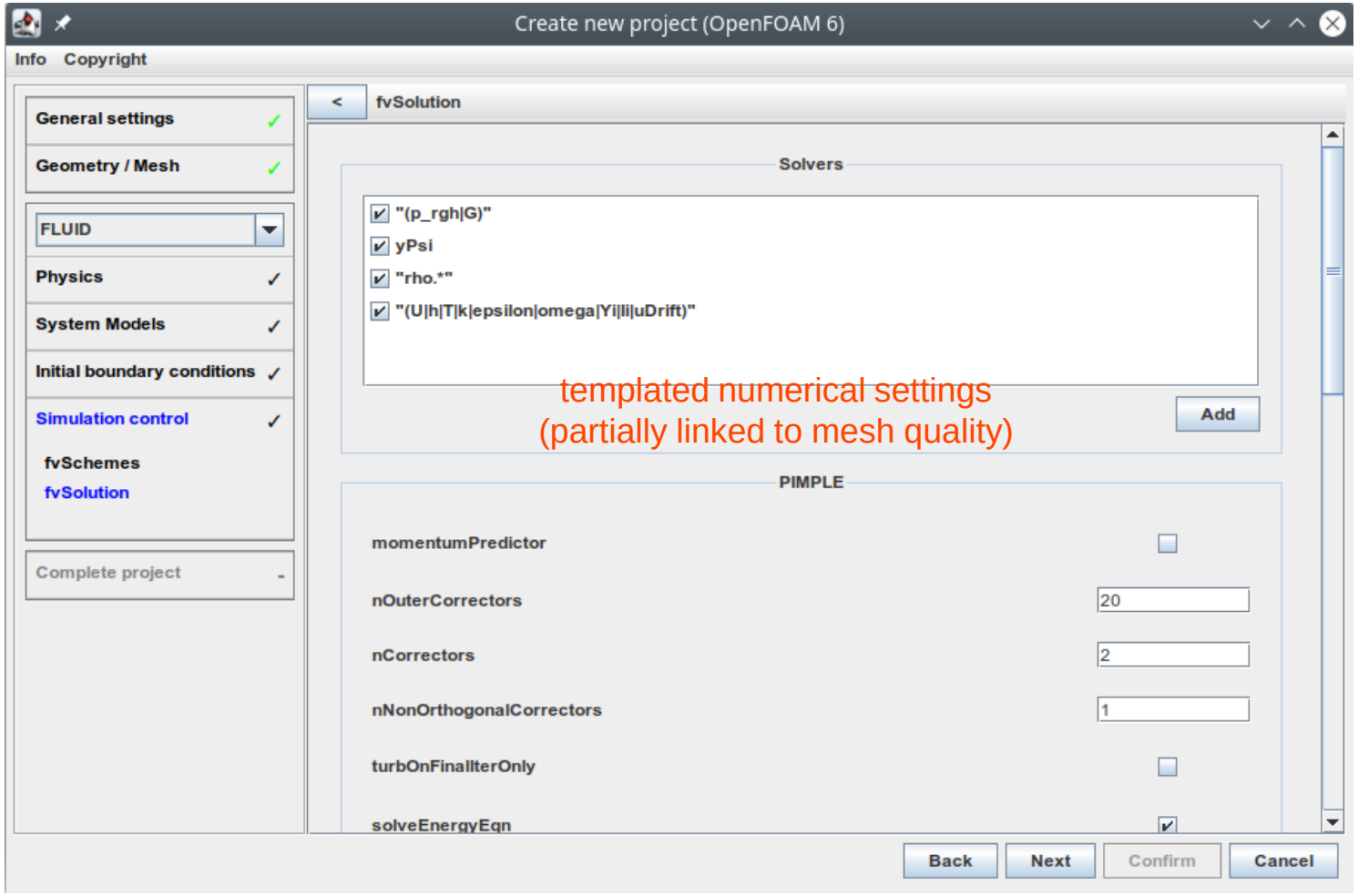
- Mesh import
- Templated material properties
- Flexible extension
- Consistent IC & BC specification
  - Predefined boundary types (‚condensing wall', ‚inlet' etc.)
  - csv import, table editor, global variables..



UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

- Mesh import
- Templated material properties
- Flexible extension
- Consistent IC & BC specification
- Numerics and simulation control
  - Best practice for numerical settings (fvSchemes and fvSolution)

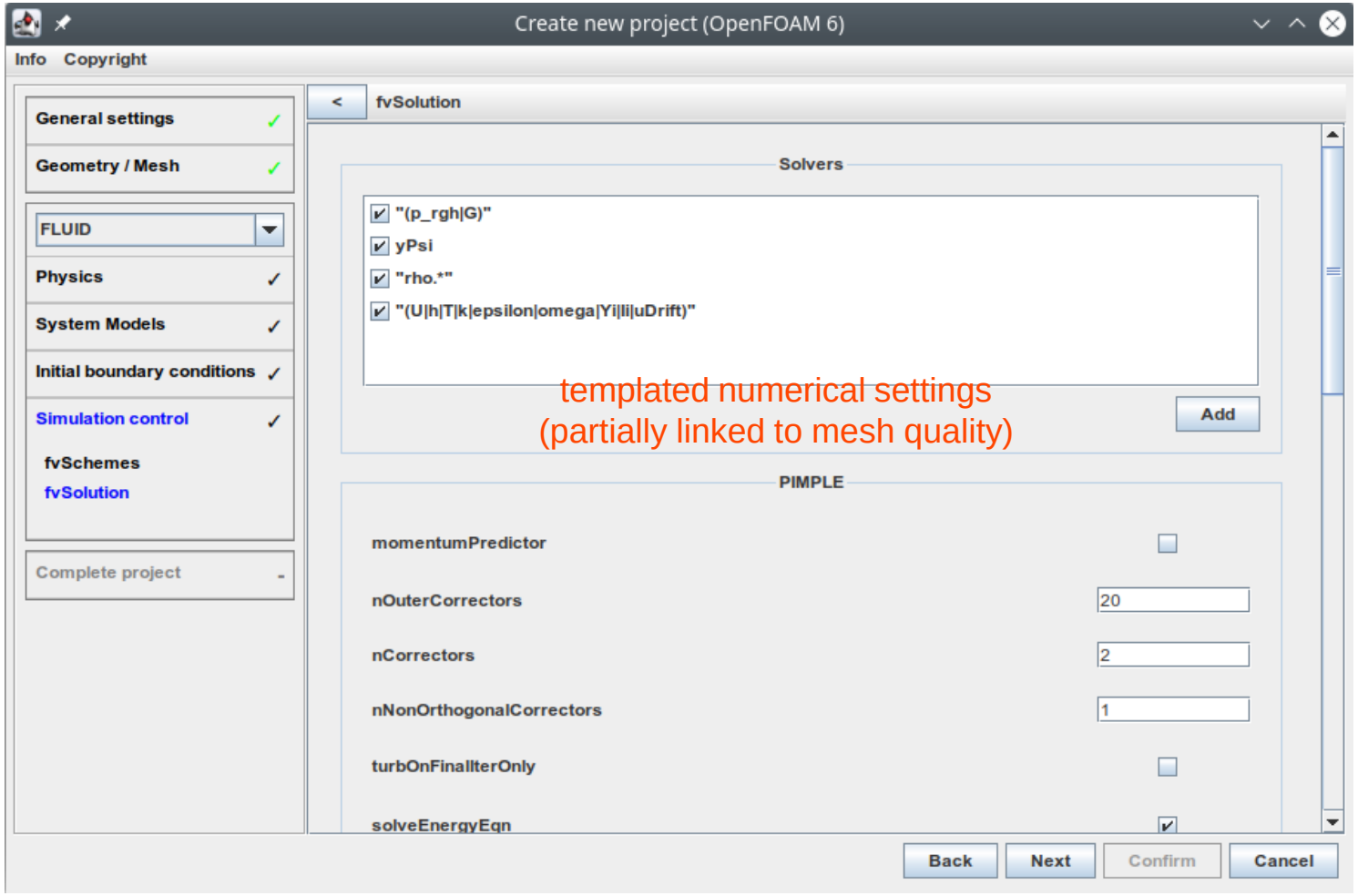


UNIQUE OPEN SOURCE ISSUES

Developer - User Interaction

- Mesh import
- Templated material properties
- Flexible extension
- Consistent IC & BC specification
- Numerics and simulation control
  - Best practice for numerical settings (fvSchemes and fvSolution)
  - Include predefined functionObjects (e.g. mass/energy Balance)

➢ Fast, reproducible and verified case setup is fundamental requirement for code use, support and trustful analysis

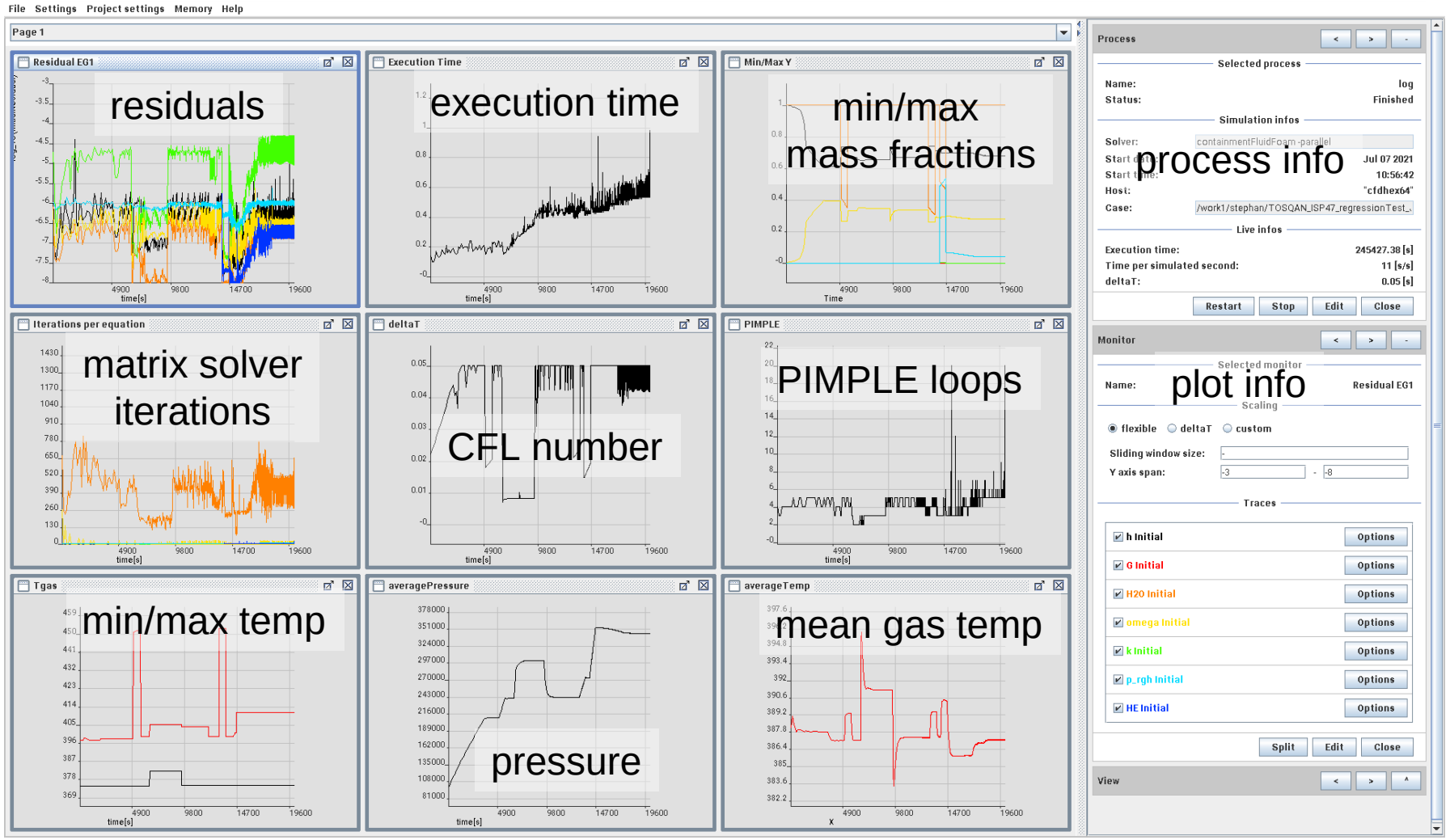


UNIQUE OPEN SOURCE ISSUES

Solution Monitor

- Good setup an then ?
  - ➢ Solution Monitoring!

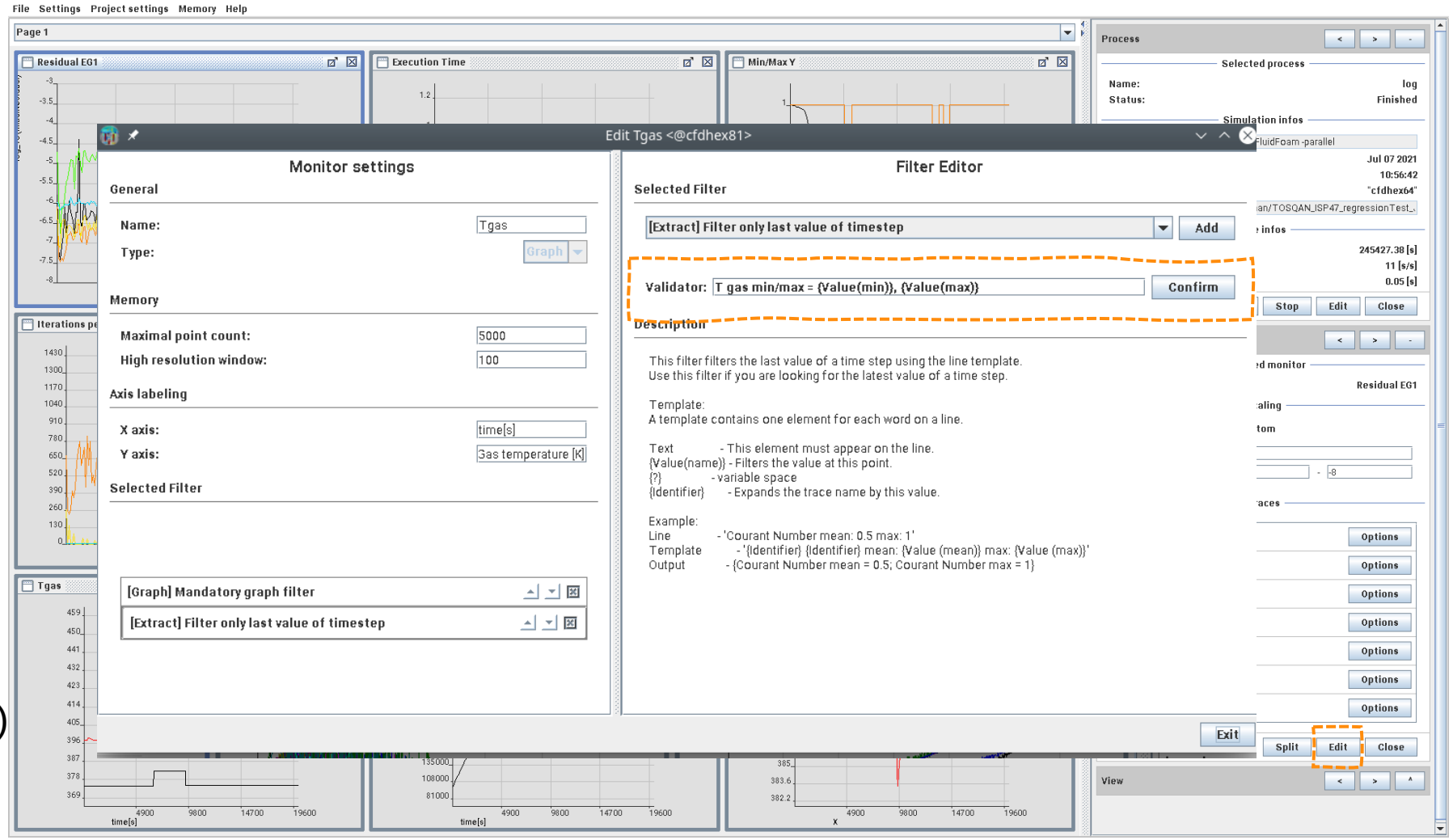
- Based on OpenJDK and jchart2D
  (http://jchart2d.sourceforge.net/)
  - Streams OpenFOAM logs and functionObject output
  - Grid and tabbed view



CONTAINMENTFOAM FRAMEWORK

Solution Monitor

- Based on OpenJDK and jchart2D
  (http://jchart2d.sourceforge.net/)
  - Steams OpenFOAM logs and functionObject output
  - Tab and Grid view
  - Flexible Regular Expression syntax
  - Filters, e.g. floating average, exponential smoothing, FFT..
  - Edit setup at runtime (selected dictionaries only)



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BEST PRACTICES IN NUCLEAR OS-PROJECTS

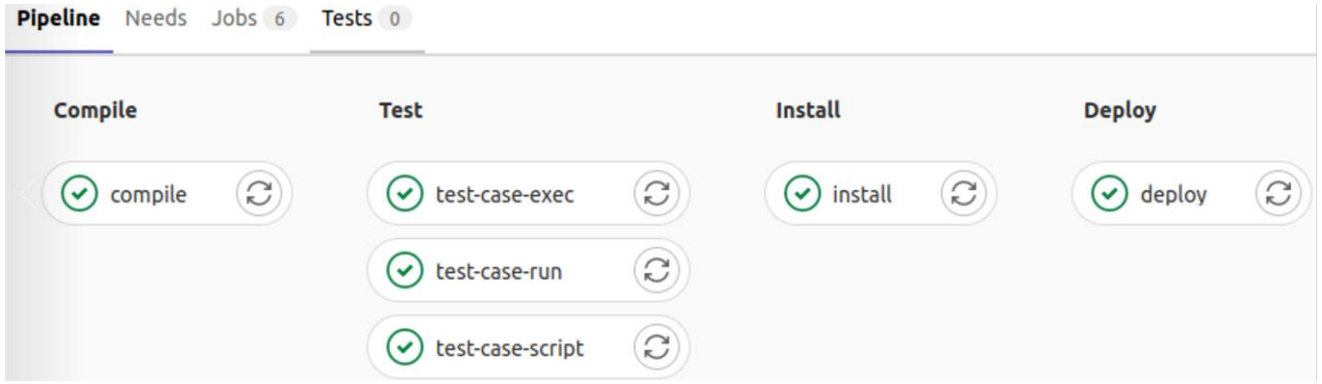
Our experiences

- Documentation:
  - Do it in parallel to code development, e.g. using gitlab flavored markdown.
- Requirements:
  - Export control & dual use: needs time and careful argumentation with non-technical persons
  - Think of (internal and external) users!
  - Think of maintainability: aim for code-quality, harmonized code style, best practices etc.

BEST PRACTICES IN NUCLEAR OS-PROJECTS

Our experiences

- Management:
  - Currently, in personal union with group lead
  - Future, group of (internal and external) contributors
- Testing / CI:
  - Build test + simple test cases via CI pipeline; complex (costly) cases executed manually
  - Merge from ‘feature’ to ‘development branch’ only after independent review and testing (git ’approval’)



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SUMMARY AND CONCLUSIONS

- Development of containment∇FOAM as an OpenFOAM add-on for containment flows since 2017
- Coordinated effort to enable integration and balance of individual sub models and maintenance under the different time horizon of the individual contributors
- Productive version was released in 2021 – https://go.fzj.de/containmentFOAM, currently small & known users group
- Measures taken to enable a productive user-experience and promoting a larger users group
  - Parallel development of Java based tools to assist users:
    - cfGUI – templated workflow to create new simulation setups
    - cfSolutionMonitor – graphical visualization of simulation logs for run-time verification and analysis
  - Communication via Mattermost chat, discussion forum
- Several best practices for software development employed, but limits exist due to manpower
- Applications: PWR flammable gas control (EU-AMHYCO), iPWR containment cooling (EU-SASPAM)

ACKNOWLEDGEMENTS

- German Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection for funding code maintenance and integration to the national CFD reference package CF2REF (Fkz **150 1633B**) as well as the ongoing projects UQ4CFD (Fkz **150 1595**) and SETCOM-2 on wall condensation modeling (Fkz **150 1591**)
- Former German Federal Ministry of Economic Affairs and Energy (BMWi) and for funding projects related to further development of CFD for reactor safety application (Fkz **150 1407)** and the REKO experimental and model development program (Fkz **150 1308 / 150 1394 / 150 1470**) as well as the SETCOM projects (Fkz **1501404 / 1501489**)
- **H**elmholtz **I**nterdisciplinary Doctoral **T**raining in **E**nergy and **C**limate Research (HITEC) Graduate School, the German Academic Exchange Service (DAAD) and the Chinese Scholarship Council (CSC) for funding PhD positions and student exchange
- Prof. K. Arul Prakash, **I**ndian **I**nstitute of **T**echnology **M**adras, India (IITM) for collaborating under IITM-RWTH Joint Doctoral Programme, DAAD IIT-MSP Programmes.
- Our contributors, partners and colleagues and beta testers
- The original developers, maintainers an contributors of OpenFOAM®

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Federal Ministry
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based on a decision of
the German Bundestag

Supported by:

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for Economic Affairs
and Climate Action

on the basis of a decision
by the German Bundestag

HITEC
Graduate School
for energy & climate

Bundesministerium
für Bildung
und Forschung

DAAD

- BACKUP

MAINTENANCE

- Design of containmentFOAM
  - Not a stand-alone software, but add-on to OpenFOAM
  - new functionality is added via
    - cloned and modified code (minor extensions)
    - separate base/derived classes (e.g., condensation)
      - Access information from OpenFOAM
      - Conducting plausibility checks during instantiation
      - Doing the math
      - Provide access functions to solvers/models
      - Encapsulated for better maintainability

```
FatalErrorInFunction
<< " Illegal boundary condition for " << U.name() << " field boundary = "
<< mesh.boundaryMesh()[patchi].name()
<< " . Select 'condensingWallVelocity' boundary condition"
<< " .Wall condensation error "
<< exit(FatalError);
```

plausibility check for model use and defined boundary conditions

```
//- Update fog velocity
condensation->bulkUFogCorrect();

//- Compute sum of uFog and uDrift volumetric flux fields
phiFog = fvc::flux(condensation->bulkUFog()) + fvc::flux(condensation->bulkUDrift(g));

fvScalarMatrix fogEqn
(
    fvm::ddt(fog)
  + fvm::div(phiFog, fog, "div(phi,fog)")
  ==
    fvm::laplacian((massDiffusion->Dt(0) + condensation->bulkDBrownian()), fog)
  + condensation->bulkMassTransferRate()
);
```

access functions used in the solver. Here fogEqn.H