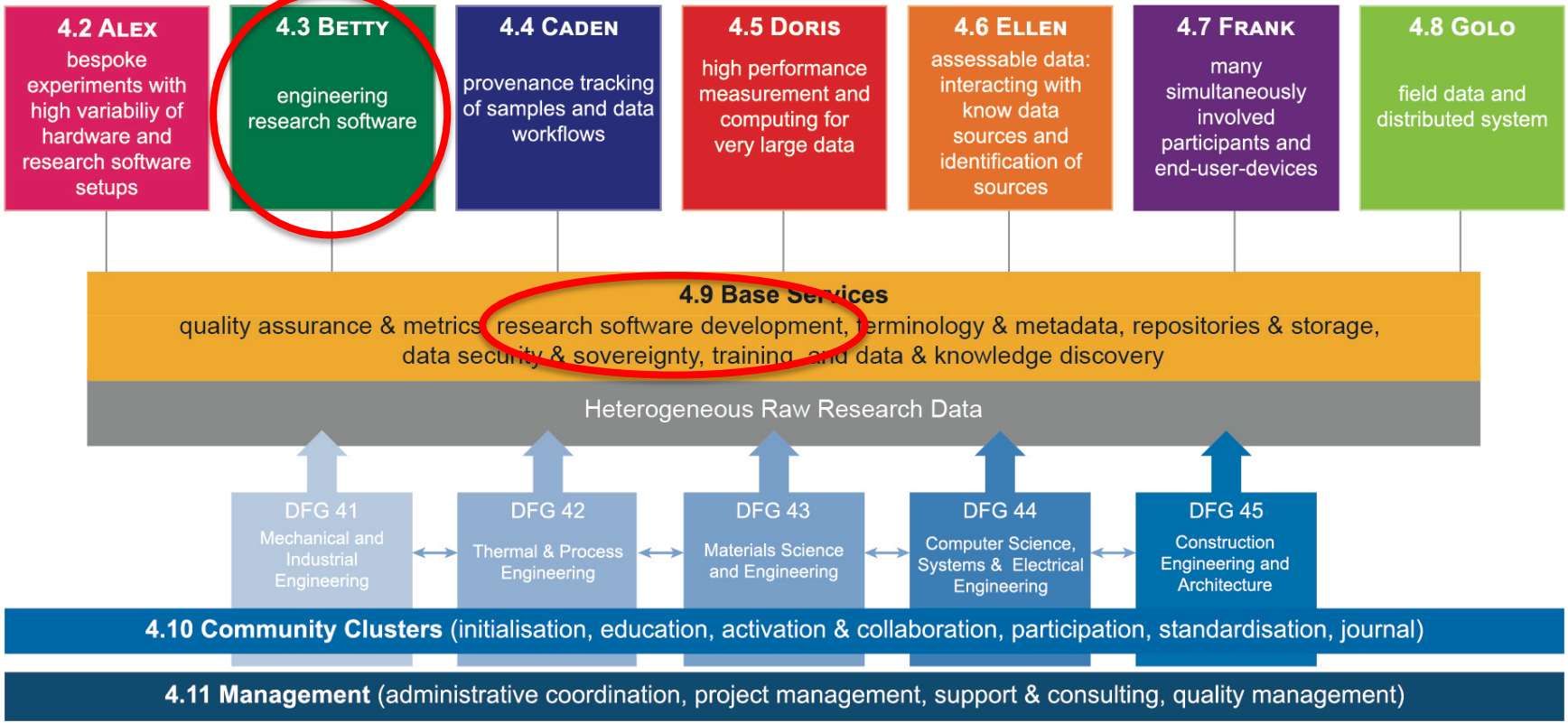
NFDI4Ing Community Meeting
04. Oktober 2021
Vorstellung Betty

BETTY within NFDI4Ing



Key objectives

Each engineer…

- … is equipped with tools and knowledge for the development of validated quality-assured research software
- … is able to guarantee reproducibility or at least transparency of computational results obtained with research software
- … can equip his research with standardised metadata and find relevant software and data of other researchers

Key objectives

Each engineer…

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Quality assurance

- … is able to guarantee t transparency of computational results obtained with re

Reproducibility

- … can equip his research with standardised meta software and data of other researchers

Findability

Betty sub-archetypes

The two ends of the spectrum

Developer

- publishes tools or libraries
- ensures portability
- uses automated testing
- provides documentation/manual

User

- applies research software
- uses a GUI or input file(s)
- publishes research results as produced by the software

Betty sub-archetypes

… and its wide interior…

?

- configures and customizes software to serve certain needs
- writes application code on the basis of libraries
- writes scripts for pre- and post-processing
- combines self-written and imported software solutions in a unique toolchain

Betty sub-archetypes

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- configures and customizes software to serve certain needs
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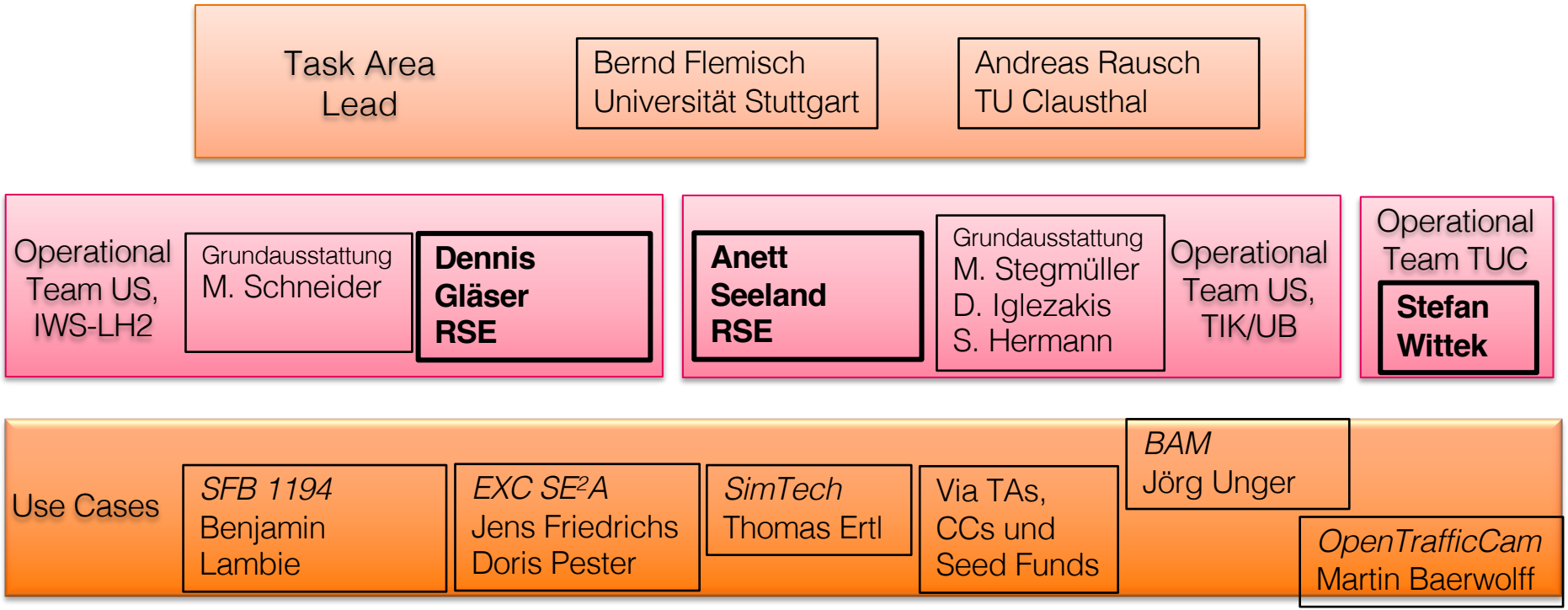
- combines self-written and imported software solutions in a unique toolchain (workflow)

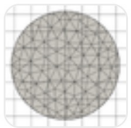
Organisation



Use Cases

SFB 1194, TU Darmstadt

- **Project context:** SFB 1194 “Interaction between Transport and Wetting Processes”.
- **Software project: Argo** (OpenFOAM plugin for two-phase flow simulations)
- **Goals:**
  - CI pipeline with unit, system & physical tests **Quality assurance**
  - Separate storage of secondary test data (for interpretation & tracking)?
  - Separate public storage of test reference data (e.g. for benchmarking)?
  - Git-Workflow that integrates reproducibility measures related to publications **Reproducibility** **Findability**



argo

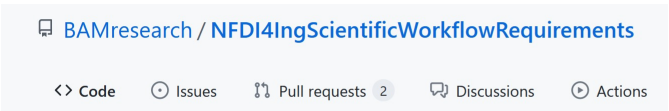
Project ID: 23940628

Use Cases

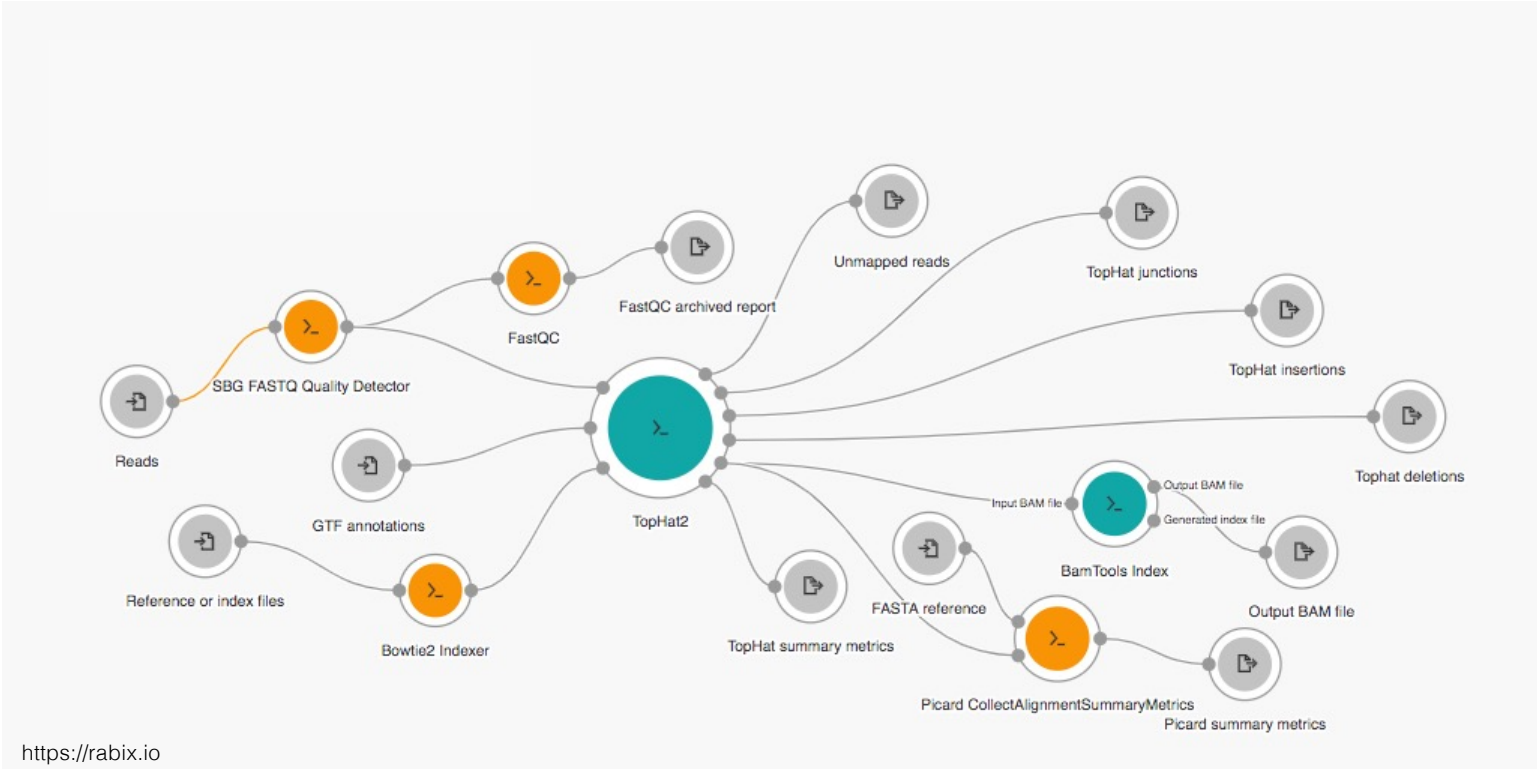
BAM , Division 7.7 „Modelling and Simulation“

Reproducibility

- **Title:** Aufbau eines Portfolios von Tools für die Erstellung und Dokumentation reproduzierbarer **Simulationsworkflows.**



Software-driven scientific workflows



https://rabix.io

Software-driven scientific workflows

Characteristics

- highly customized orchestration of a variety of software solutions
- tools in the workflow…
  - … mutually depend on each other via input/output data & parameters
  - … may themselves depend on a number of third-party software packages
  - … at the time of a publication: specific package versions used

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Challenges:

- **Transparency/Documentation**
- **Reproducibility/Reusability**

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Challenges:

- **Transparency/Documentation**
- **Reproducibility/Reusability**
- **Usable on HPC systems?**

Use Cases

BAM , Division 7.7 „Modelling and Simulation“

Reproducibility

- **Title:** Aufbau eines Portfolios von Tools für die Erstellung und Dokumentation reproduzierbarer **Simulationsworkflows.**
- **Goals:**
  - Definition of aspects of „FAIR“ research workflows
  - Definition of requirements on workflow tools to fulfill those aspects
  - Evaluation & discussion of pros and cons of existing tools
  - Initiation of a SIG for discussion
  - Implementation of representative use cases with existing tools, documentation & evaluation of the process