Towards a Research Software Categorization

Wilhelm (Willi) Hasselbring

Software Engineering
http://se.informatik.uni-kiel.de

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Kiel University
Christian-Albrechts-Universität zu Kiel

Research Software

"Research Software includes source code files, algorithms, scripts, computational workflows and executables that were ***created during the research process or for a research purpose****."*

[Gruenpeter et al. 2021]

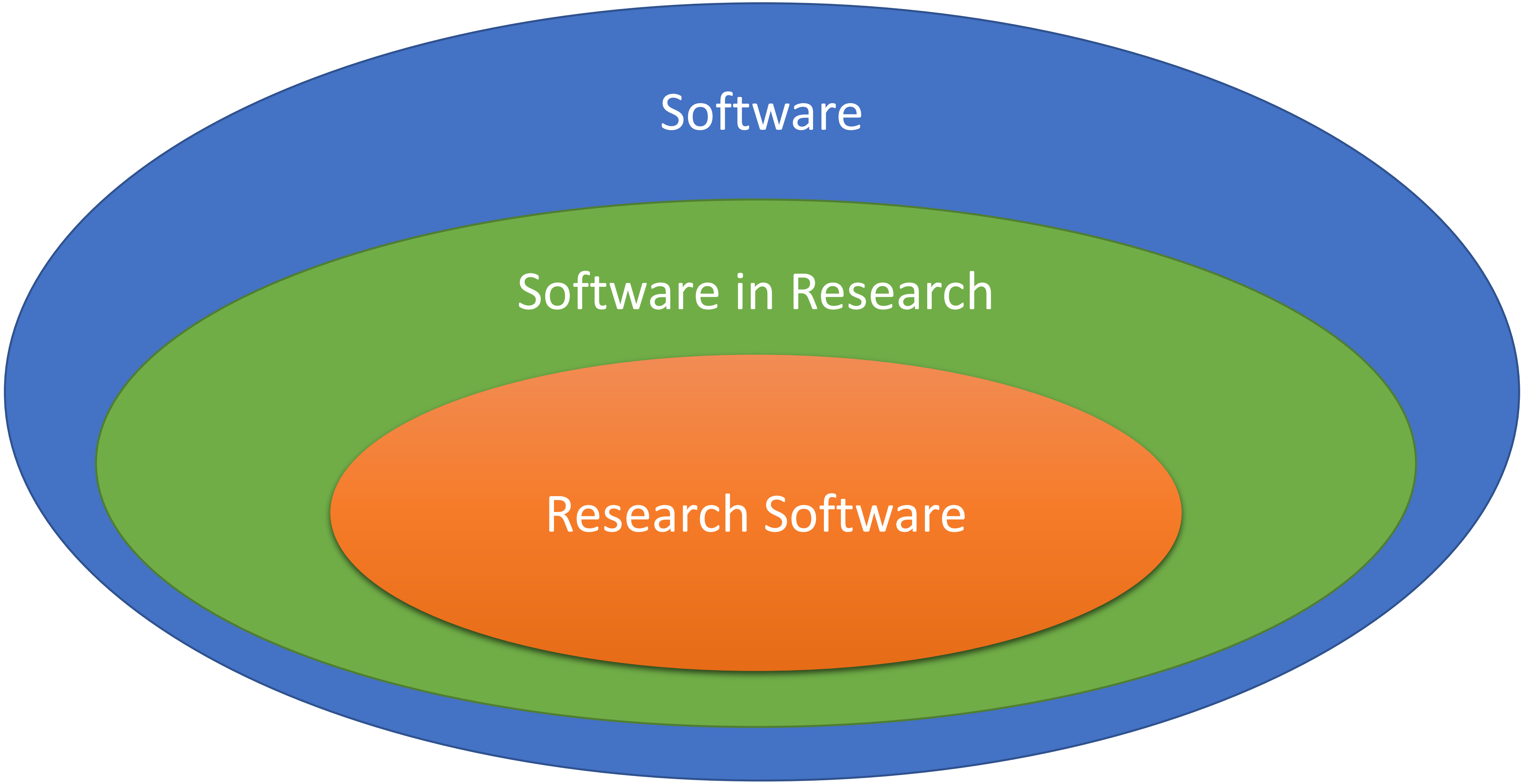
FAIR Research Software

RDA FAIR for Research Software (FAIR4RS) WG [Chue Hong et al. 2022] :

- Research software includes source code files, algorithms, scripts, computational workflows, and executables that are created **during** the research process or **for** a research purpose.
- Software components (e.g., operating systems, programming languages, libraries, etc.) that are used for research but were not created during or with a clear research intent should be considered `**software in research**´ and not `research software´.
- Thus, research software is a separate metaphor of software in research.

Research software should be **FAIR** [Hasselbring et al. 2020b, Lamprecht et al. 2020] and **open** [Hasselbring et al. 2020a].

Software Segmentation



We intend to further categorize the orange ellipse.

Categories of Research Software

Research software mainly falls into one of the following categories (and sometimes combinations):

1. **Modeling, Simulation and Data Analytics** of, e.g., physical, chemical, social, or biological processes in spatio-temporal contexts.
   - Numerical and agent-based modeling and simulation (in silico experiments)
   - Data-driven modeling
   - Data science and data engineering, incl. LLMs
   - Analytics pipelines
   - Data assimilation
2. **(Embedded) Control Software** for complex physical or chemical experiments and instruments, including many forms of sensor-based data collection.
3. **Proof-of-Concept Software Prototypes** in science and engineering research.
4. **Infrastructure** and platform software, such as research data and software management systems.

These categories have varying quality requirements!

[Felderer et al. 2023]

What could we / others do with a Research Software Categorization?

- Assign specific quality requirements to the individual categories
- Recommend appropriate software engineering methods for the individual categories
  - This is, for instance, relevant for institutional software engineering guidelines and checklists.
  - For instance, requirements engineering may be relevant for Category 4, but not for Category 1.
  - For instance, a safety analysis may be relevant for Category 2, but not for Category 1 and 3.
  - Good Practices for High-Quality Scientific Computing [Dubey 2022]
- Design appropriate teaching / education programs for the individual categories
- Explain the relation to stakeholders
- Rationale:
  - We need to understand what kinds of software we have to deal with, and their specific quality requirements

Category 1 in Earth System Sciences

Computational research in the Earth System Sciences

Simulation of Earth system processes by	▪ Earth system models (climate and weather models) and integrated assessment models ▪ sectoral models of, e.g., deep Earth processes, water on the continents, ocean processes, biogeochemical cycles and vegetation
Design, processing and analysis of	▪ Earth observations, e.g., • processing of GRACE satellite signals to derive time series of mass change • geomorphometric analyses of land surface elevations • object identification in satellite images ▪ lab and field observations and experiments, e.g., • luminescence dating • geostatistical analysis
Integrative analysis of	▪ simulation models and Earth observations by, e.g., data assimilation ▪ large databases using statistical analyses or machine learning ("big data" analyses) ▪ stakeholder knowledge by, e.g. multiple-criteria decision analysis or Bayesian networks

[Döll et al. 2023]

Refinement of Category 1

1. **Modeling, Simulation and Data Analytics** of, e.g., physical, chemical, social, or biological processes in spatio-temporal contexts.
    1. Numerical and agent-based modeling and simulation (in silico experiments)
    2. Data-driven modeling
    3. Observation data collection, related to Category 2 & 4
    4. Data science and data engineering, incl. LLMs and data generation
    5. Analytics pipelines for automation and integration, coupling of models, CI/CD
        1. This is related to Category 4 (Infrastructure)
    6. Data assimilation
    7. Scientific visualizations

Defining the roles of research software

[van Nieuwpoort 2022, van Nieuwpoort and Katz 2023]

Research software is a component of our instruments	Category 2
Research software *<u>is</u>* the instrument	Category 1 (& 3 ?)
Research software analyses research data	Category 1.4
Research software presents research results	Category 1.6
Research software assembles or integrates existing components into a working whole	Category 1.5 & 4
Research software is infrastructure or an underlying tool	Category 4
Research software facilitates distinctively research-oriented collaboration	Category 4

Category 3 not included. “proof of concept” is mentioned, but for simulations.

A National Agenda for Research Software
[Australian Research Data Commons 2022]

ANALYSIS CODE	capture research processes and methodology: the steps taken for tasks like data generation, preparation, analysis and visualisation	Category 1
PROTOTYPE TOOLS	demonstrate a new idea, method or model for research	Category 3 (?)
RESEARCH SOFTWARE INFRASTRUCTURE	capture more broadly accepted and used ideas, methods and models for research	Category 4

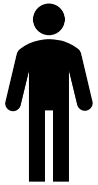
(Category 2 not included)

https://ardc.edu.au/article/research-software-a-first-class-research-output/

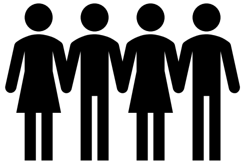
WHAT ARE THE CHALLENGES?

CREATORS OF	Analysis Code	**STRUGGLE WITH**	making their research practices more transparent
AUTHORS OF	Prototype Tools		enabling broad impact through quality software
MAINTAINERS OF	Research Software Infrastructure		lack of support for research software infrastructure

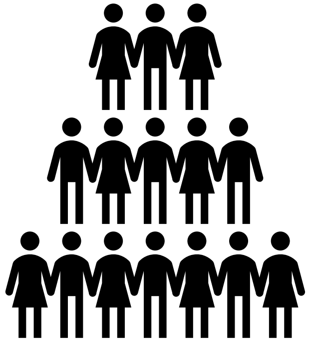
Another Categorization:
Stages of Research Software,
both for Developers and Users



Individual Researcher



Local Research Group



Community (incl. Non-Researchers)

Infrastructures for Quality Research Software Task Force

User stories for the software and research lifecycle:

1. Individual creating research software for own use (e.g. a PhD student)
2. A research team creating an application or workflow for use within the team
3. A team / community developing (possibly broadly applicable) open source research software
4. A team or community creating a research service

Source:

- [Courbebaisse et al. 2023]
- https://eosc.eu/advisory-groups/infrastructures-quality-research-software

Application classes (https://elib.dlr.de/148645/)

Application Class 0	Small scope, personal use	• Scripts to process data for a publication. • Simple administrative scripts to automate specific tasks • Software that demonstrates or tests certain functions
Application Class 1	Narrow scope, beyond personal use	• Software from Bachelor/Master/PhD theses • Software from smaller/shorter research projects
Application Class 2	Extended scope, wider use	• Software from longer-term research projects • Software libraries, frameworks
Application Class 3	Critical software, software products	• Mission-critical software • Software that is sold as a produt (with warranties) • Software that serves as research infrastructure

[Schlauch et al. 2018]
[Fritzsch 2023]

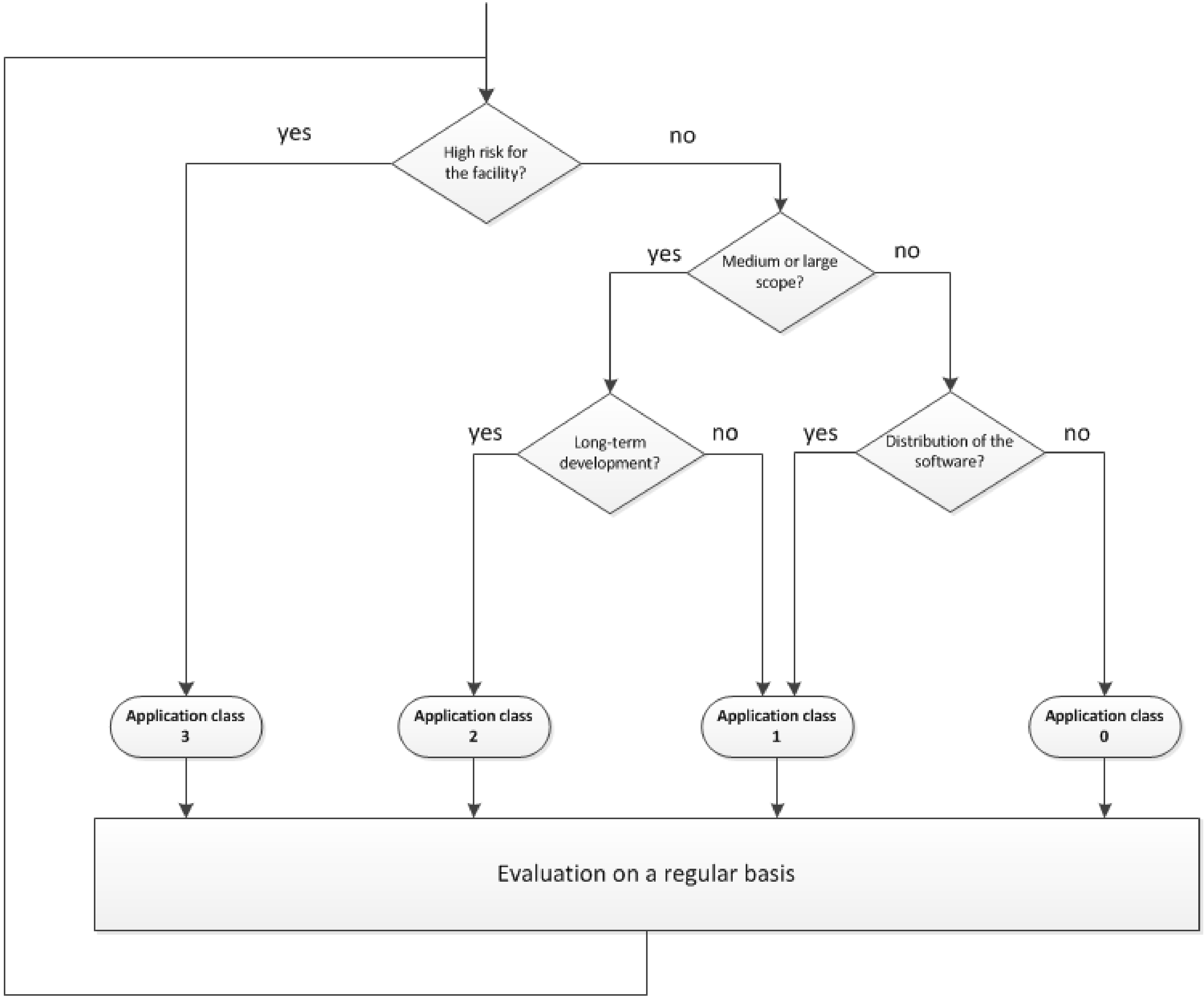
Categorization based on Criticality

- Safety-critical software
  - Failure results in loss of life, injury or damage to the environment;
  - Example: Railway interlocking system
- Mission-critical software
  - Failure results in failure of some goal-directed activity and/or loss of critical infrastructure;
  - Example: Spacecraft navigation system
- Business-critical software
  - Failure results in high economic losses or damage to reputation;
  - Example: Customer accounting system in a bank

⇒ Dependability

- Policy-critical software (?)

Potential risks, expected scope and lifetime determine the application class



[Schlauch et al. 2018]

Software Layers

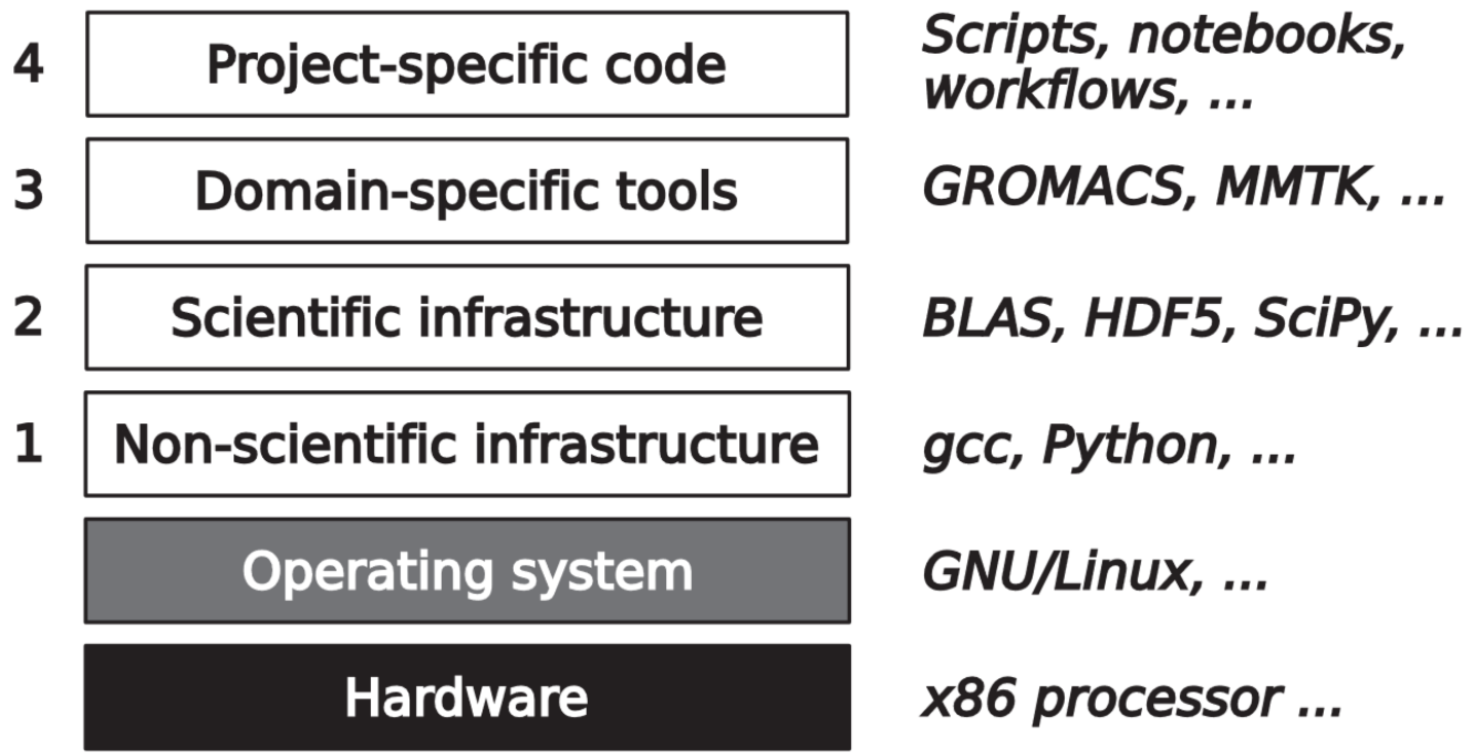


Figure 1. Typical scientific software stack.

Category 1

Category 1

Category 4

(Category 2 & 3 not included)

[Hinsen 2019]

The Research Software Encyclopedia´s Taxonomy

- Software to directly conduct research
  - Domain specific software
    * Domain-specific hardware (e.g., software for physics to control lab equipment, or embedded hardware)
    * Domain-specific optimized software (e.g., neuroscience software optimized for GPU)
    * Domain-specific analysis software (e.g., SPM, fsl, afni for neuroscience)
  - General software
    * Numerical libraries (includes optimization, statistics, simulation, e.g., numpy)
    * Data collection (e.g., web-based experiments or portals)
    * Visualization (interfaces to interact with, understand, and see data, plotting tools)
- Software to support research
  - Explicitly for research
    * Interactive development environments for research (e.g., Matlab, Jupyter)
    * Workflow managers
    * Provenance and metadata collection tools
  - Used for research, but not explicitly for it
    * Databases
    * Application programming interfaces
    * Frameworks (to generate documentation, content management systems, etc.)
  - Incidentally used for research
    * Operating Systems
    * Package Managers
    * Virtualization technologies
    * Formatting, indexing, or other small helper libraries
    * Scheduling and task management (for people)
    * Version Control
    * Text Editors and Integrated Development Environments (IDEs)
    * Communication tools or platforms (e.g., email, video-conferencing, etc.)
    * Infrastructure (e.g., on-prem or cloud servers used for services or research needs)
    * Testing or software libraries

[Sochat et al. 2022], https://rseng.github.io/rseng/

https://rseng.github.io/software/repository/github/containers/podman/annotate-taxonomy/index.html

Software to directly conduct research	Domain-specific software	☐ Domain-specific analysis software
Software to directly conduct research	Domain-specific software	☐ Domain-specific hardware
Software to directly conduct research	Domain-specific software	☐ Domain-specific optimized software
Software to directly conduct research	General software	☐ Data collection
Software to directly conduct research	General software	☐ Numerical libraries
Software to directly conduct research	General software	☐ Visualization
Software to support research	Explicitly for research	☐ Interactive development environments for research
Software to support research	Explicitly for research	☐ Provenance and metadata collection tools
Software to support research	Explicitly for research	☐ Workflow managers
Software to support research	Incidentally used for research	☐ Communication tools or platforms
Software to support research	Incidentally used for research	☐ Formatting, indexing, or other small helper libraries
Software to support research	Incidentally used for research	☐ Infrastructure
Software to support research	Incidentally used for research	☐ Operating systems
Software to support research	Incidentally used for research	☐ Package Management
Software to support research	Incidentally used for research	☐ Personal scheduling and task management
Software to support research	Incidentally used for research	☐ Testing
Software to support research	Incidentally used for research	☐ Text editors and integrated development environments
Software to support research	Incidentally used for research	☐ Version control
Software to support research	Incidentally used for research	☐ Virtualization technologies
Software to support research	Used for research but not explicitly for it	☐ Application Programming Interfaces
Software to support research	Used for research but not explicitly for it	☐ Databases
Software to support research	Used for research but not explicitly for it	☐ Frameworks

Upper Level Categorization

- Commercial Software
- Research Software
- System Software
- …

Application domains:

- Finance and Banking
- Healthcare
- Education
- Transportation and Logistics
- Retail and E-Commerce
- Manufacturing and Industrial
- Government and Public Sector
- Entertainment and Media

Research Software Examples

Example for Category 1 (Modeling and simulation): Modularization of Earth-system simulation software as basis for domain-specific languages

Software Modularization

How to

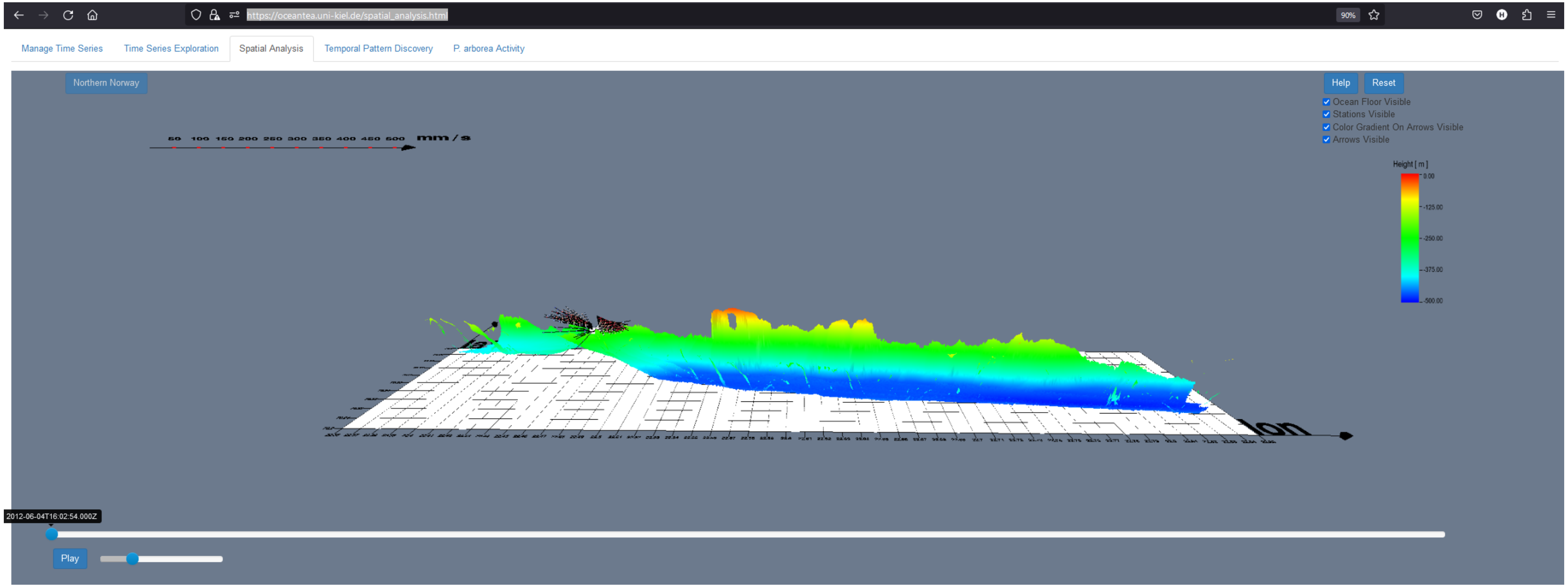
- improve maintainability, stability, reusability, reproducibility, … ?
- enable scalable execution in the Cloud?
- parallelize for high performance computing?
- test for higher quality?
- achieve higher flexibility?

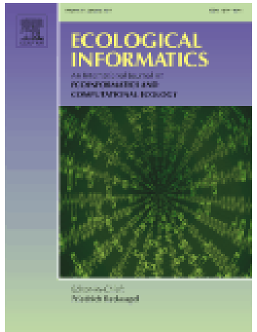
[Johanson & Hasselbring 2017, Claus et al. 2022, Jung et al. 2021, 2022a, 2022b]

OceanDSL

Funded by
DFG Deutsche Forschungsgemeinschaft
German Research Foundation

Example for Category 1 (Data analytics): OceanTEA





Paper on the analysis results: [Johanson et al. 2017]
Paper on the software architecture: [Johanson et al. 2016]
Code: https://github.com/cau-se/oceantea

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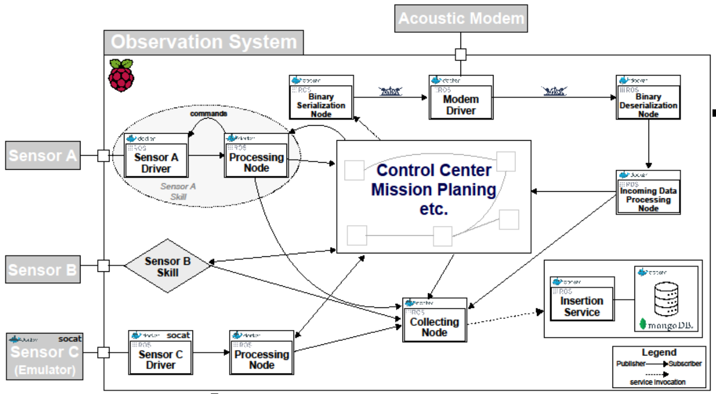
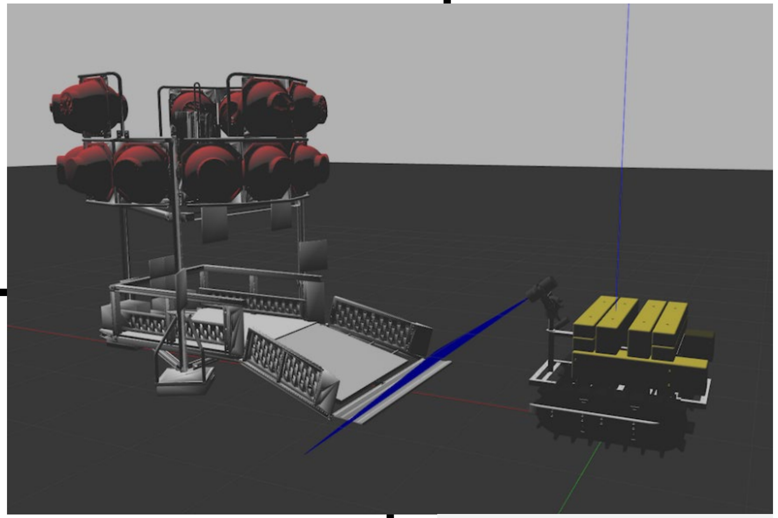
DIE KIELER MEERESWISSENSCHAFTEN

Example for Category 2 (Embedded control software): Entwicklung von Software für Unterwasser-Roboter

Digital Twin Prototype





Digital Twin

Physical Twin

[Barbie et al. 2021]

GEOMAR

Examples for Category 3 (Proof-of-Concept Software Prototypes): Software Impacts

Kieker

https://github.com/kieker-monitoring

Kieker: A monitoring framework for software engineering research
[Hasselbring and van Hoorn 2020]

ExplorViz

https://github.com/ExplorViz

ExplorViz: Research on software visualization, comprehension and collaboration
[Hasselbring et al. 2020c]

titan

https://github.com/cau-se/titan-ccp

The Titan Control Center for Industrial DevOps analytics research
[Henning and Hasselbring 2021]

Examples for Category 3 (Proof-of-Concept Software Prototypes):

Example from Pure Mathematics

- Arbitrary precision math in computer algebra systems
  - Goals for developing research software:
    - Proof of concepts
    - Find counter examples
    - Optimization
  - General purpose software
    - Example: Oscar.jl: https://github.com/oscar-system/Oscar.jl
    - Commercial Example: Mathematica: https://www.wolfram.com/mathematica/
  - Special purpose software
    - Example: polymake: https://polymake.org

(Contributed by Lars Kastner, TU Berlin)

Examples for Category 3 (Proof-of-Concept Software Prototypes):

Automated Theorem Proving

- Lean: https://leanprover.github.io
- KeY: https://www.key-project.org

(Contributed by Lars Kastner, TU Berlin)

Examples for Category 4 (Infrastructure):

D-GRID

nfdi

Nationale
Forschungsdaten
Infrastruktur

Outlook: RSE Research

Research Software Engineering

Software Engineering Research

Research Software Engineering Research
aims at understanding and improving how software is developed for research.

RSE Research, in short.

See also: https://github.com/NLeSC/RSE-research [Lamprecht et al. 2022]

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