

# Documentation of Research Software

Dini/nestor-Workshop

Forschungssoftware managen

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Hermann

# Background

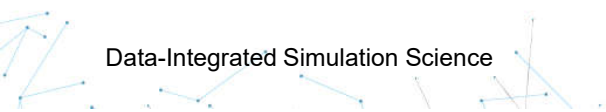
- Institute of Engineering and Computational Mechanics
- No formal education in software engineering
- Research software as a means to an end
- What is required to write good research software?
- No time for documentation



Dilbert.com DilbertCartoonist@gmail.com



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# Evaluation of

## ❖ Recommendations



## ❖ Best Practice examples, which receive funding from the DFG Call e-Research-Technologien “Nachhaltigkeit von Forschungssoftware”\*



\* [https://www.dfg.de/foerderung/info\\_wissenschaft/2016/info\\_wissenschaft\\_16\\_71/index.html](https://www.dfg.de/foerderung/info_wissenschaft/2016/info_wissenschaft_16_71/index.html)

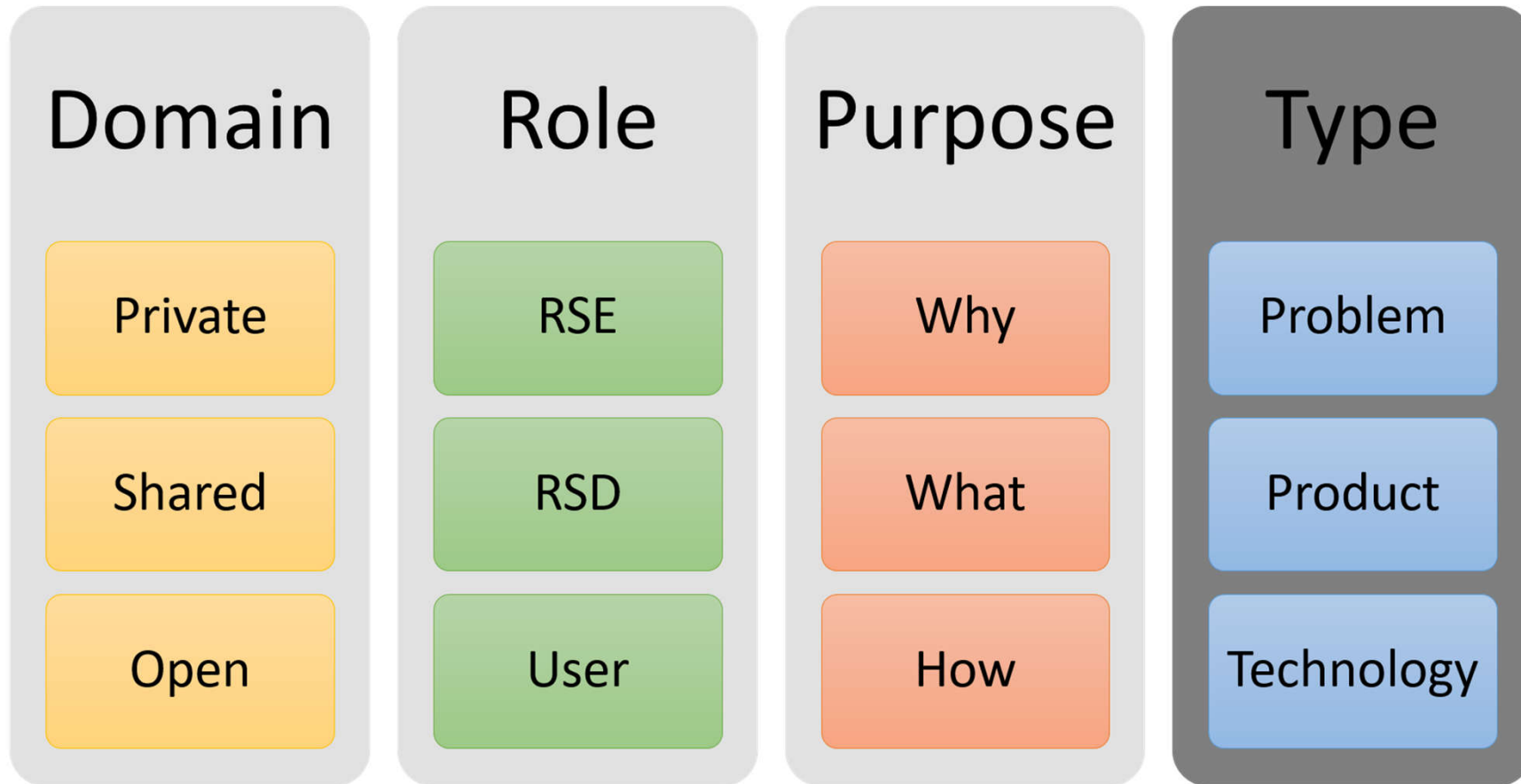
# What I expected

I read some recommendations and see how we can implement the advice in practice.

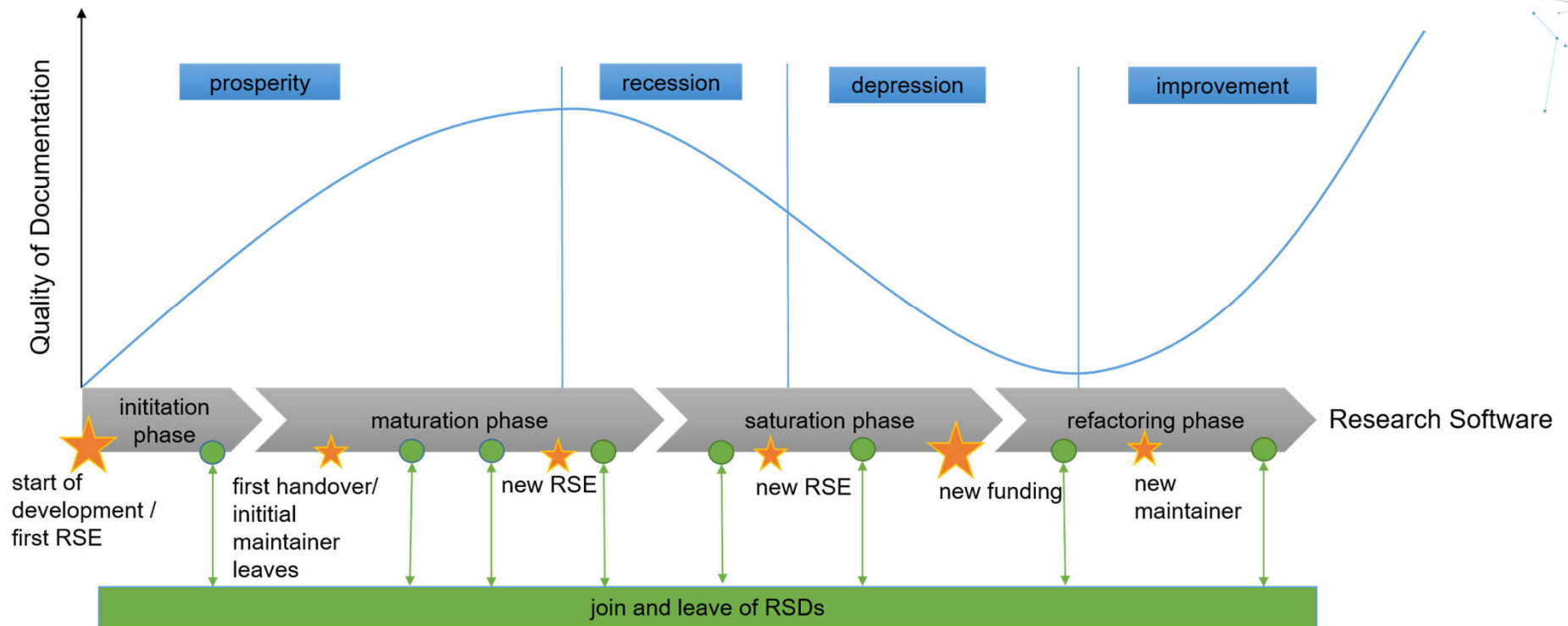
## What I found ...

- ... it is a bit more complex.
- ... explanations why documentation is not good, but not how to document.
- ... focus on tools not on content

# Categories



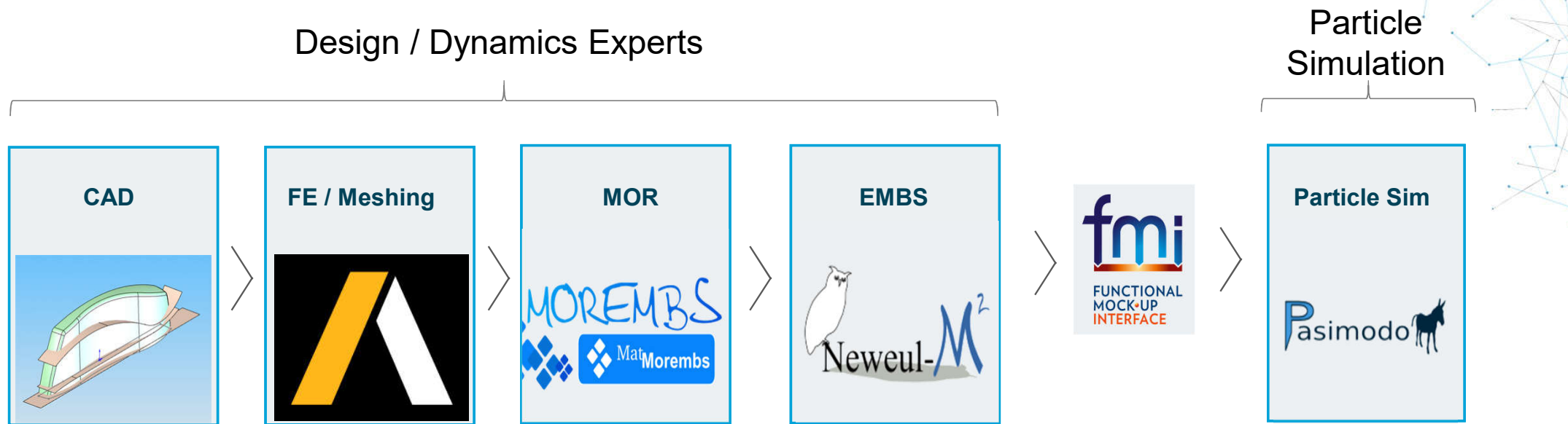
# Research software has a history



Quality of documentation over the development phases of research software

Hermann, S., Fehr, J. Documenting research software in engineering science. *Sci Rep* **12**, 6567 (2022).  
<https://doi.org/10.1038/s41598-0>

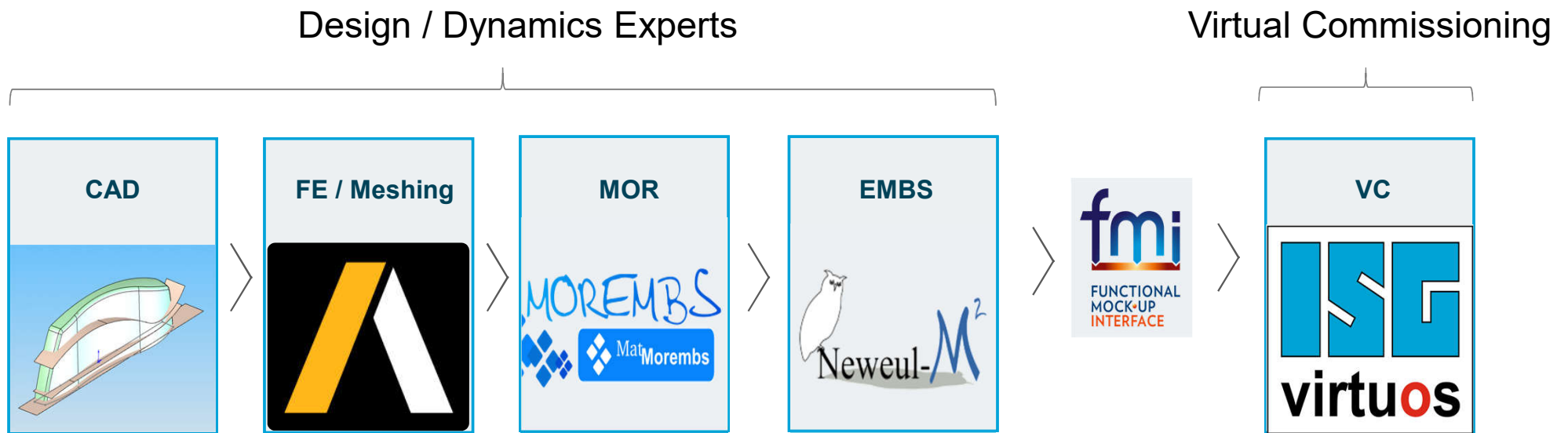
# Toolchain institute



Toolchain to analysis of the cutting fluid behavior with a modified micro single-lip deep hole drilling tool [1]

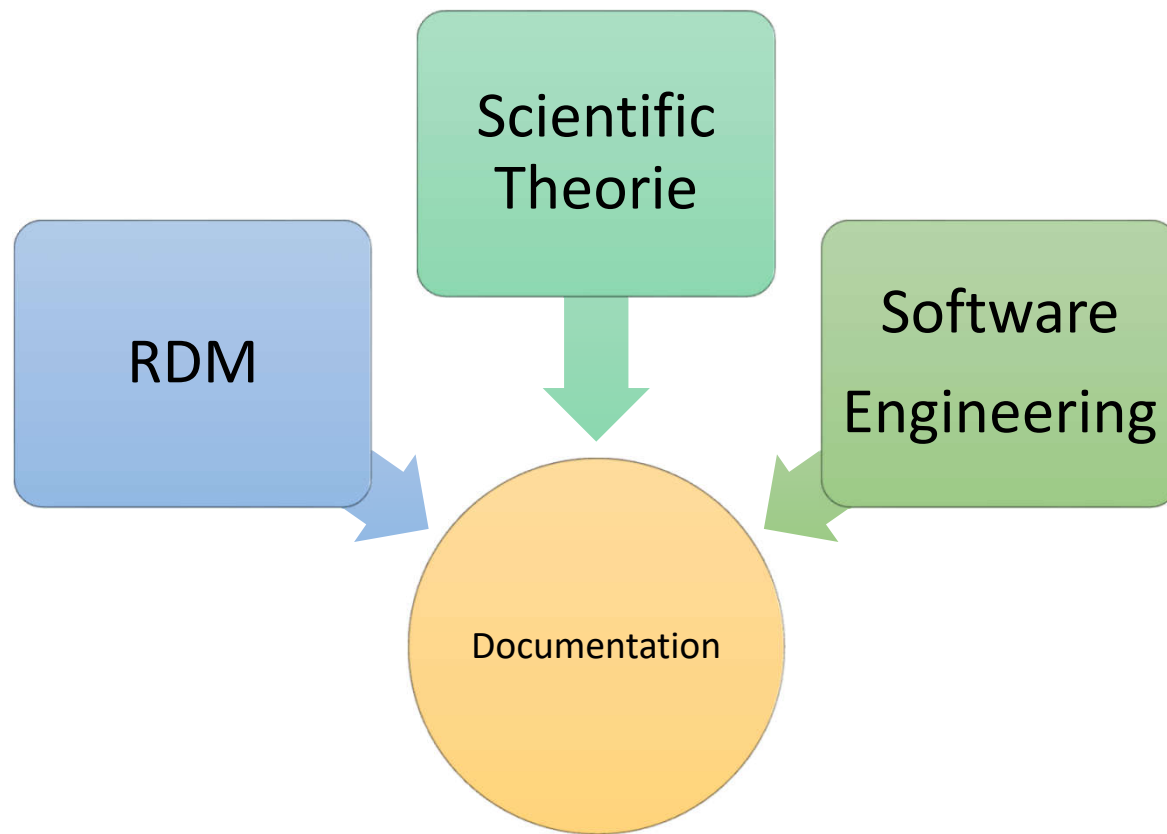


# Toolchain industry



Toolchain for simulation of digital twins within a virtual commissioning approach

# But, how?



# Research Data Management

- Description with metadata
- Describing the finished product
- When, from whom, to which purpose, with which methods
- Focus on publishing
- FAIR Principles – Findability!



# Software Engineering: Docs as code

- Google: change perspective → tie into existing workflow
- Audience: other people with
  - Different background (experience level, domain knowledge, purpose)
  - Different encounter (seekers, stumblers)
- Must not be perfect
- Document should have a single purpose
- Documentation review
  - Technical → expert
  - Audience → newbie
  - Writing → ?

WINTERS, TITUS; MANSHRECK, TOM; HYRUM, WRIGHT. Software engineering at Google: lessons learned from programming over time. Beijing: O'Reilly, 2020.

# Scientific Theorie -- Simulations

Models reduce the reality through decisions

- *First decision (D1):*
  - Model (e.g. Multibodysystems)
- *Second decision (D2):*
  - Research Software (e.g. Neweul-M2)
- *Third decision (D3):* Research Question
  - D1 and D2 decisions are often implicit given

# Scientific Theorie -- Simulations

Verification and Validation through **transparency** and **skill**

- **Transparency**: documentation
- **Skill**: how to document

POMPE-ALAMA, ULRIKE SUSANNE. The Changing Face of Scientific Practice – Seeing Things Virtually. In: *Advanced Optical Technologies* (2019). doi:10.1515/aot-2018-0066.

# Conclusion

- The model determines the documentation
  - Multi-X-Simulation (multi-scale, multi-physics, ...)
- Micro and macro documentation is needed
  - Software documentation and Metadata just parts of documentation
- Focus must be on the method not on tools, they can change