Documentation of Research Software

Dini/nestor-Workshop
Forschungssoftware managen

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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
VICTOR DIDN'T LEAVE US MUCH DOCUMENTATION ON HIS PROJECT.

FZEEET!

I GUESS THAT'S WHAT HE MEANT BY "STILL WORKING ON THE GOAT HEAD ISSUE."
Evaluation of

- Recommendations

- **Neweul-M²**

- Best Practice examples, which receive funding from the DFG Call e-Research-Technologien “Nachhaltigkeit von Forschungssoftware”*
  - DuMu²
  - preCICE

* 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
<table>
<thead>
<tr>
<th>Domain</th>
<th>Role</th>
<th>Purpose</th>
<th>Type</th>
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<tbody>
<tr>
<td>Private</td>
<td>RSE</td>
<td>Why</td>
<td>Problem</td>
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<tr>
<td>Shared</td>
<td>RSD</td>
<td>What</td>
<td>Product</td>
</tr>
<tr>
<td>Open</td>
<td>User</td>
<td>How</td>
<td>Technology</td>
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</table>
Research software has a history

Quality of documentation over the development phases of research software

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

Design / Dynamics Experts

Virtual Commissioning

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 $\rightarrow$ 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 $\rightarrow$ expert
  • Audience $\rightarrow$ newbie
  • Writing $\rightarrow$ ?

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

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