Trust for multi-x simulation through documentation from a philosophy of science perspective

Whether technological processes or artifacts can be trusted or relied on is of particular importance in multi-X simulation. This type of simulation involves modeling spatial and temporal scales of various orders, a wide range of coupled physical phenomena, fluids, and materials, and different modeling approaches. Additionally, it deals with heterogeneous data fidelity and faces widely different demands on output dimensionality and response. One challenge of using multi-X simulation is the reuse and verifiability of existing models. Often, researchers need to use models from other domains without having expertise in those domains. On the one hand, one must be able to trust these models without being able to understand them in detail, and on the other hand, the combined model must be understood and trusted as a whole.

One approach to establishing trust is through adequate documentation. However, the question remains: what should be documented and how? Especially in research data management, this question is answered with the FAIR (Findable, Accessible, Interoperable, and Reusable) principles and metadata. In the context of NFDIs (National Research Data Infrastructures), ontology and subject-specific metadata are developed to facilitate data discovery, interoperability, and reuse.

Metadata is helpful in finding relevant models, but more information is needed to effectively reuse them. Other approaches aim to empower non-computer scientists in software development or the use of tools such as version control, but simulation goes beyond software development. But what are we actually doing in the simulation, and what needs to be documented as a result?

To address this question, we looked at approaches from the philosophy of science and how they can be applied to multi-X simulation in a concrete example. We conducted a case study to evaluate the concepts of epistemology, emergence, and validation and verification and their consequences for documentation on a specific example.
Applying these concepts to multi-X modeling, we can develop a more comprehensive and systematic approach to documenting the simulation process. In the case study, we found that underlying decisions were not documented in articles or research data, making it difficult to understand the research. Additionally, the coupling of the model and the model as a whole was not documented. By applying the concepts of epistemology, emergence, validation, and verification to multi-X modeling, we can ensure that the simulation process is properly documented and can be effectively reused in future research.