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Data- and simulation-based material behaviour prediction

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Abstract

In research environments and laboratories e.g. for material sciences the in- and output of simulation data is manually managed. Therefore, physical experiments as well as simulations might be carried out several times, learnings are not systematically gathered, and experiments do not systematically build on learnings from data. This paper proposes to engage an ontology in conjunction with a simulation to use data from already carried out experiments and on that basis predict material behaviour under certain condition and plan further physical experiments.

Keywords: ontology, simulation, behavioural design

1. Introduction

Data management in experimental environments or laboratories is often carried out in a manual manner. Material researchers focus on material parameters, a rigorous experimental approach, or consider an appropriate measurement technique. The preparation and pre-processing of experimental data for simulation purposes or in a re-usable manner e.g. for other experiments is considered as a necessary but non-value adding task. The required flexibility for testing, trying, and researching is considered preferential compared to rigid and systematic storage, curation, and knowledge learning principles from a data management perspective. This results in unstructured data in various sources, different formats, occurring at different steps in the process. Moreover, the availability of data is limited due to spread data, or missing rigour when supplying data. In order not to repeat the same virtual or physical experiments, it is necessary to structure the approach and demonstrate benefits.

1.1. Motivation

Simulation is often used as means for subsequent calculations, whereas predictive capabilities remain underachieved. Reasons might be seen in a lack of credibility for simulations (Eichenseer et al. 2023) as well as in valuable input data (Skoog et al. 2012). Input data processing for simulation is proposed in four manners: 1. completely manual input of data, 2. manually prepared e.g. to excel files, 3. automatically populated as information from external sources (e.g. by edge devices in a fabrication) or 4. pushed from other corporate business systems (Skoog et al. 2012). Experimental data as for example accruing in material research labs are often treated in either the first or second manner described before. That means a systematic approach for data storage, (re)using existing data and reducing manual effort is missing.
Simulation Data Management tools (SDM) were primarily developed to manage CAD files and to link CAE tools and thereby the appropriate solver, pre- and postprocessor (Röhm 2021). In that manner SDM provides storing a model, its input parameters, as well as calculated results. The preparation of the input data to an adequate quality is accomplished by the simulation engineer often in a manual approach.

Ontological support with the purpose of ordering and preparing insight in an easy to reuse manner is rarely applied in this context (Wu and Tian 2015).
Keeping an overview of input data resulting from experiments or production processes, as well as already performed calculations is challenging. This applies for a simulation specialist involved in an investigation, but if several persons from different disciplines or roles work together and refer to a common or shared database and simulation a managed overview is required. This paper proposes a data pipeline where ontologies are used to structure and organise experimental and process data so that they are available in a structured and re-useable manner. Furthermore, the ontology will host the simulation models, so that material scientists can use the simulation in the laboratories when planning physical experiments as means for prediction.
The BMBF funded PlattformMaterialDigital[1] (PMD) initiative was launched to tackle these obstacles for the material research community. This paper describes the current state of research in the publicly funded PMD KnowNow project. The remainder of this paper details firstly the current state of simulation data, their usage and thus underpins the need and benefit for improved data preparation. After a short introduction to the research approach in section three the implementation of ontological use as input for is described.

1.2. Application example - multi-layer ceramics research data

Ceramics are electrical insulators and as such engaged as carrier material for electrical devices. Multi-layer ceramics strengthen certain electrical or magnetic behaviour such as shielding, insulating, etc within each of the stapled layers and embed electrical components. The layering technology requires a sophisticated five-step production process, as illustrated in a simplified manner in Figure 1 . For this research, ceramic foils are combined to an inductor, also referred to as component.

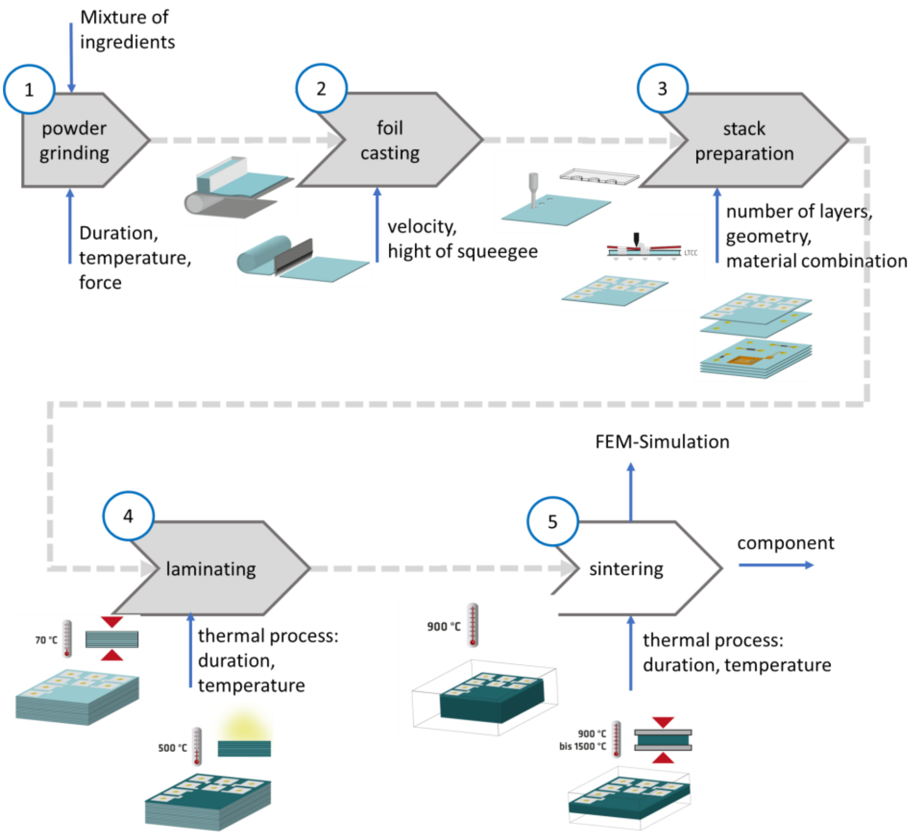

Figure 1. Overview of the five-step production process for ceramic multi-layer [Source: Bundesanstalt für Materialforschung und -prüfung (BAM)]

[1] https://www.materialdigital.de/

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This paper focuses on the sintering process, step 5, where stacks of different ceramic foils carrying an inductor element are laminated. That means the ceramic material itself with its manifold ingredients is processed into foils, step 2, these are punched into required forms, step 3. For research requirements regularly squares with a size from several millimetres to several centimetres are used. During the stack preparation so called vias are pierced into the individual layer allowing to place electrical conductors on or between the layers. When sintering the pre-processed electrical conductor in step 5, the question is if the layers remain in their intended position or if they delaminate. The intend of the FEM-Simulation at this point is to predict if dedicated oven temperatures and exposure times lead to a potential delamination. The figure shows next to the blue arrows process parameters that might influence the sintering process. During the underlying research project all steps are carried out manually, data are mainly stored as excel files as well as some pictures in order to document the experimental setting.

2. State of the art and research goal

This section summarizes the ways in which input and output data for simulations are prepared and processed. SDM tools are shortly introduced as they form the basis for this purpose, in a next section the potential use of ontologies as add-on to conventional simulation data management especially in conjunction with experimental settings is discussed.

2.1. Simulation data management

(Skoog et. al 2008) describe SDM as the identification of relevant input parameters, the collection of all information required to represent the parameters as appropriate simulation input, the conversion of raw data to a quality assured representation, and the documentation of data for future reference and re-use. State of the art SDM systems such as simworx provide capabilities for the storage of different document types such as CAD, PPT, PDF etc. That means the SDMS expects already sorted, structured and relevant data only to be provided by the simulation specialist. Variants of simulation models might be managed, and consecutive activities might be automated in graphical supported workflow editors. In this workflow editors only data that are already stored in the simulation data base might be managed.

2.2. Ontologies as data mean for simulation data organisation

(Benjamin et. al 1995) defines ontologies as a list of the types of entities that exist in a domain, their essential properties, and the essential relationships that may exist between them. An ontology means a certain representation of data or a set of objects and the relationships between them (Guarino 2009, Jepsen 2009). Ontologies refer toa certain field of work. The domain knowledge is essential to create ontologies of work processes and correctly describe all relations (Elnagar 2020). Therefore, before using it in practical tasks, data is organized, transformed, and brought into a form that is effective for storage and use. The conventional way to store and use data through relational databases refer to matrices. These relational databases are restricted by their capacity to manipulate the tabular framework once there are filled with data. In their place, engineers can use ontologies that have flexibility in organizing and representing data. The ontology serves as the basis for organizing knowledge and is used to discover new facts, identify hidden or non-obvious relationships between elements and parameters of an experiment. By connecting larger amounts of data, it will be possible to connect different process parameters and experimental results in a logical chain. Such a chain will reflect both certain parameters and the connection between objects and actions. Thus, enabling reasoning on the process-object relations (Alam, Birkholz. et al 2021). (Benjamin et. al 2006) Ontologies are useful in simulation modelling and especially in problem analysis during the conceptual model development phase.

Engineers from different disciplines can use ontologies as a common framework to facilitate communication, collaboration, and integration of knowledge and data from different engineering disciplines. Using ontologies, engineers bring all definitions and names of objects and phenomena to one level. Ontologies provide definitions that help to limit misunderstanding. Ontologies also help to combine engineering knowledge from different domains. Engineers can map their data to concepts already in the ontology, allowing them to aggregate and analyse data from different sources and domains. This is especially valuable in projects that involve data from multiple engineering disciplines.

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In addition, engineers can share their knowledge and experience through ontologies. Each discipline can contribute to the ontology, expanding the common knowledge base for all participants. This collaborative approach can lead to more comprehensive ontologies.
Data storage in ontologies is carried out in triples in a structured manner. To store data, it is required to map data to the according position in the ontology and wrap them to an appropriate format. Thereby accruing experimental data such as protocols or photographs in different data formats or mixes are accessible and comparable. For example, one may measure the hight of a multi-layer stack and note that in his or her protocol under the term "hight" and a unit of "µm", whereas the second measurement is a photograph with a measurement device next to the component. Both measurements are "understood in context" by the ontology and might be given as answer to the user request "stack hight of multi-layer xyz?".

2.3. Research goal

This paper targets to structure experimental and process data as input for simulations. Thereby the manual workload for simulation experts is expected to be reduced. The ontological data structuring approach is proposed in a manner that non-IT experts as laboratory assistants can propose their data to the ontology. The embedding of the simulation model in the ontology and the connection of both simulation and data intends to engage the simulation as means to predict the material behaviour during the sintering process (see section 3). This question obviously strongly depends on the quality and manner the simulation model is build, the current understanding of the influence of process parameters from a material research perspective, the used solver and simulation tools etc. However, this contribution focusses on the data preparation and the application of the simulation in an appropriate tool frame including an ontology so that different user may benefit from it.
Next to there here intended and further detailed approach ontologies provide the opportunity of sharing knowledge between different engineers and thereby provide equal access and understanding to a larger group. Simulation specialist need data that are relevant in the context, trustful and pre-processed e.g. with respect to dimensions or data formats for an easy input as parameters into their models. Material engineers currently rely on experimental data only and do not benefit from simulation insight. Therefore, the prediction capabilities of simulations remain unutilized e.g. when planning experiments. This research is based on the assumption, that both groups benefit from an integrated environment, connecting divers' experimental data including their context, a data pipeline including the preparation work in an automated manner and accessible results of virtual as well as physical experiments for both user groups. Furthermore, the longer-term organized data acquisition and curation may serve as source for reusing both real and simulated experiments.

3. Implementation

Following the global target of an integrated and easy to handle environment for material scientists and simulation specialists, this research is organized in four main steps, see figure 2. Firstly, it focusses on the requirements from a user perspective understanding the needs in detail, step 1. Then it details the required IT-environment based on the material scientist's input in step 2. Ceramic multi-layer test data are created in step 3 as prerequisite to validate the user storis. Finally, in step 4 the IT-framework is used with these data and conclusions are drawn on the effort and insight. This section details each step with a focus on the steps 1 and 2, step 3 has been carried out by another research group, the sections results and conclusions of this paper describe the findings with respect to the research goal.

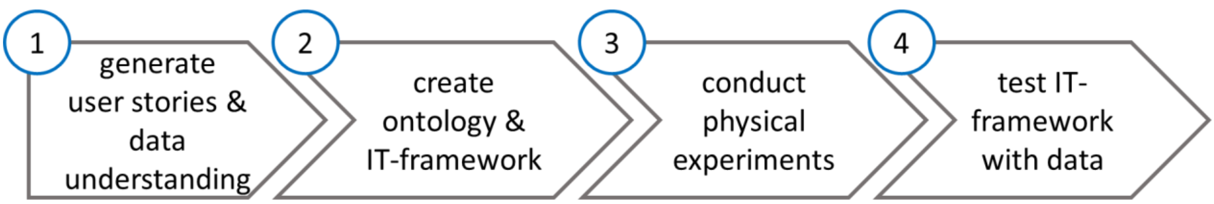

Figure 2. Sequential illustration of the research approach

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3.1. Formulating user stories scenario and analysing data

The first step conducts the requirements and needs from a user perspective. The goal of using simulation as means for material behaviour prediction is relevant to material scientists carrying physical experiments in laboratories. Two user stories were formulated based on the approach described by (Lucassen et. al. 2016). The working group was based in Germany; the user stories are translated for this paper.

1. As material scientist, I want to use the sintering simulation with a dedicated component design, sintering process characteristic, and physical parameters of the material system to predict the bending after the sintering process.
2. As a material scientist, I want to use the sintering simulation to optimize the component design with respect to multi-layer material and sintering process parameter.

From the user stories a rough understanding of input data became clear, a deeper analysis was conducted collecting a data landscape in an MS Visio template. For this purpose, one stakeholder from each main process step, as described in Figure 1, plus one material scientist with a general overview was interviewed. All data, including the format, that are relevant as input for the simulation are noted in a flow format. Through this step all input parameters for the simulation including potential pre-processing is visualized.

3.2. Establishing a corresponding IT-framework including simulation and ontology

Material scientists are specialists on the inner composition, parameters, and behaviour of ceramic or other materials. Laboratory assistants conducting the experiments focus on the operational work in the laboratory, their core knowhow is on programming the machines, handling the probes etc. Using a simulation or an ontology does not belong to the day-to-day business of both user groups, therefore a user interface is required for two cases: a) feeding the ontology with experimental data and b) running simulation-based experiments with stored process and material parameters.

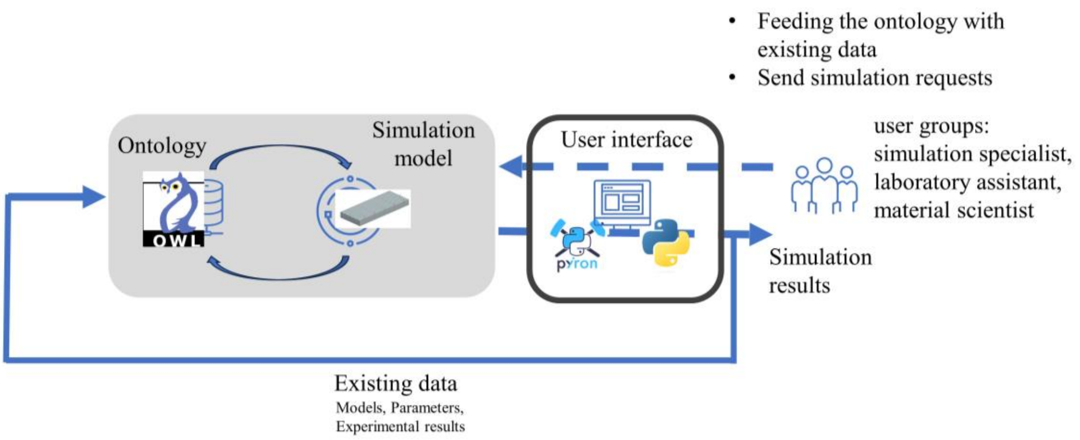

Figure 3. User interaction with the IT-framework

Within the IT-Framework the main purpose of the ontology is to store both the virtual and physical experimental data and to feed the simulation according to a user request. The MS Visio scheme as generated in step 1 is transferred into an OWL-scheme via a script (Stark et al. 2021). This approach enables quickly executed potential manipulations and extensions of the ontology.

Essentially, the process of exploring existing data in an ontology involves a systematic and comprehensive exploration that combines data mining, relationship analysis, and contextual understanding. By drawing information from the ontology's rich repository, users can make informed decisions about the operating parameters of their new experiments, ultimately increasing the credibility and efficiency of their scientific efforts.

The following figure 4 provides an overview of the IT infrastructure functions answering a simulation request from a material scientist. Users may approach the system either through an interface, step1, this

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applies to persons or roles that are less familiar with programming interfaces. The workflow area as well may serve as interface to use the stored data.

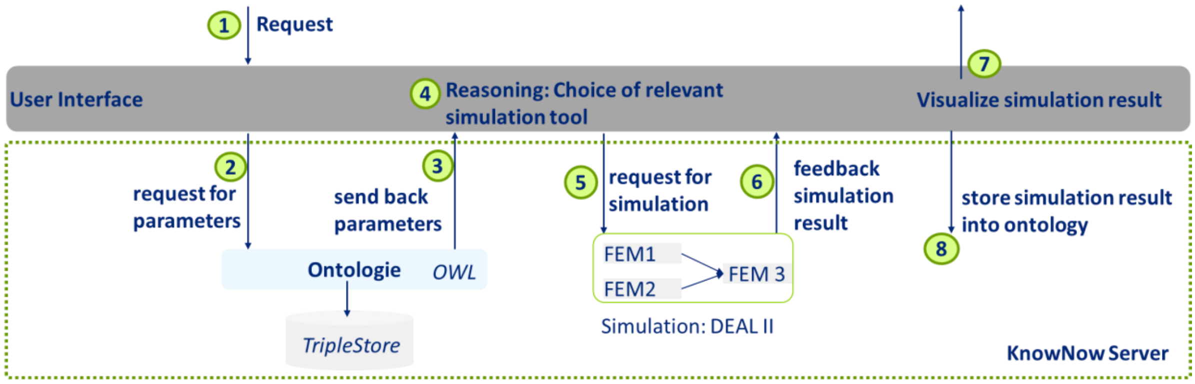

Figure 4. Functional actions between the user interface, the ontology and the simulation

Next, the query is sent to the ontology, step 2 in the figure 4, and results are fed back to the workflow and the user interface according to the origin of the request, step 3. Data handed over at step three might be the certain parameters or the result of an entire experiment. The user decides on further actions: start the simulation, find the necessary parameters in the ontology, or exit the program. When running the simulation, a simulation specialist either enters the desired operating parameters of the simulation or selects the parameters from the ontology that he or she intends to test. After successfully running the simulation, step 6, the user will be given the option to look at the results or download the results and study them afterwards. Simulation results will be stored to the ontology pending on the file format in a post processed manner ensuring a potential reuse of already calculated results, step 6.
A workflow serves as automation tool for the steps 2-8 from Figure 4. The workflow is implemented in Python based on the PMD provided PYIRON templates. The workflow is launched by, sending a SPRQL request to the ontology comprising the necessary samples, parameters, and objects (step 1 in Figure 5). The results will provide a list of operating parameters for the experiment. The user then decides which parameters should be passed into the simulation; if necessary, they can be changed (figure 5, step 2). Next, the user selects a sample plate for which the experiment needs to be carried out (step 3, figure 5).
Finally, the simulation engineer runs the simulation and expects the results (steps 4 and 5, figure 5). The results are automatically saved in the ontology to prevent data loss and to allow the file to be downloaded and studied. All other steps occur in the background and are performed automatically without user intervention.

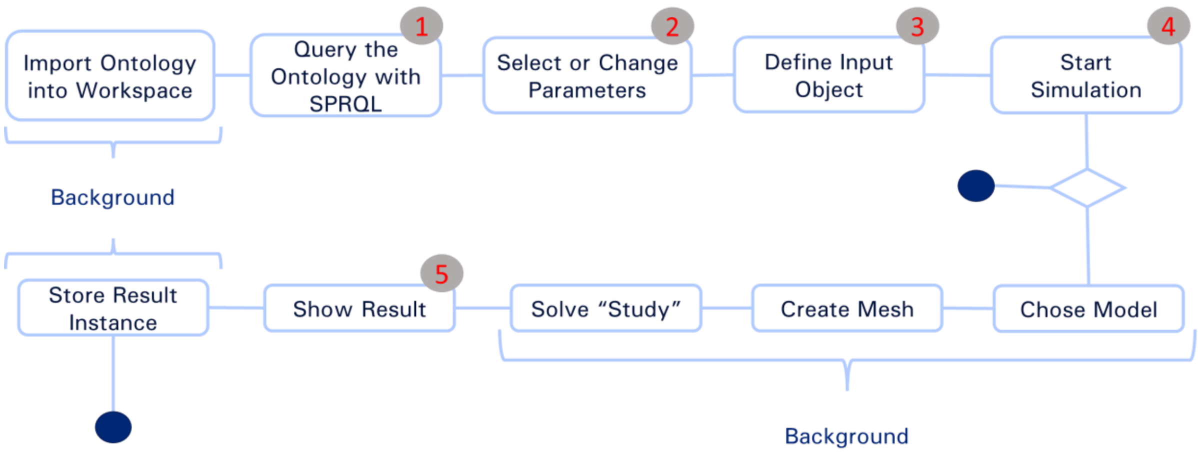

Figure 5. Pyiron-based Workflow linking ontology and simulation

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3.3. Conducting physical experiments and establishing the simulation

Physical experiments are executed by project partners and comprise a choice of different input materials during the ceramic powder process generation (step 1 in figure 1). Furthermore, different ceramic foil production processes are executed resulting in different ceramic foil densities. The hight of the multi-layer stack is varied. The laminating and sintering oven temperature and time of exposure are varied. All data are saved in structured excel files, provided by partners via the user interface and saved to the ontology. These data except for the sintering process serve as input data for the FEM simulation. Deal II is used as simulation environment.

The FEM simulation is calculating the warpage or even potential delamination under sintering temperature influence consists of several blocks which are consecutively executed, see figure 6. Each block, one on the left, one on the right, is performed individually. The left block prepares for the simulation and collects data into clusters. The right block prepares the mesh of the CAD file being examined. The results are then sent to the main simulation script, which calculates the complete sintering process of the ceramic plate in a given period of time.

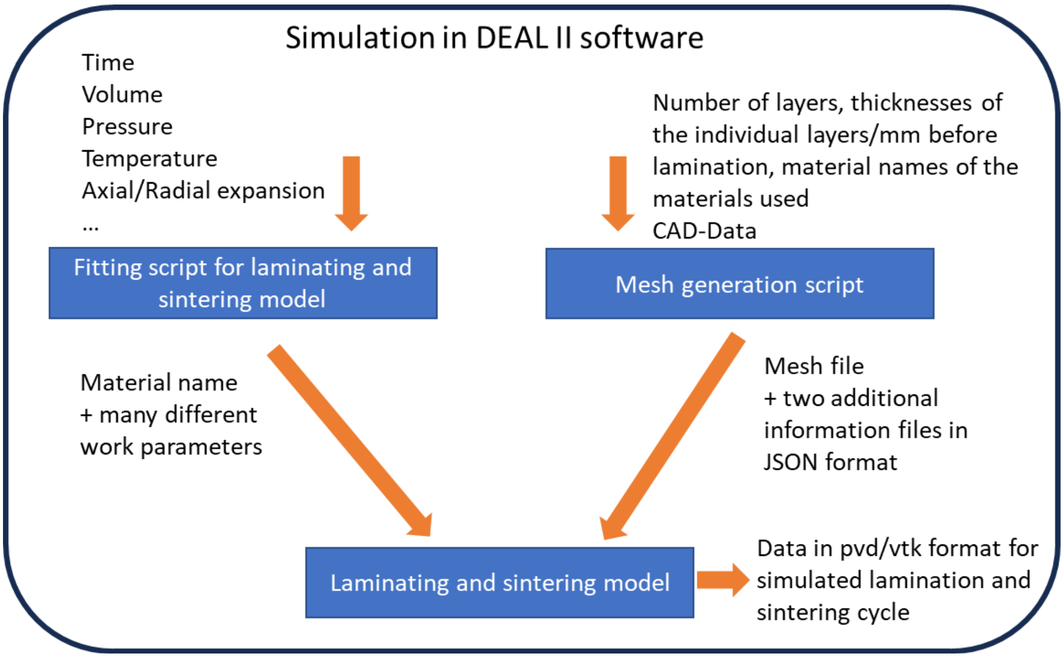

Figure 6. Overview for Deal II FEM based de-lamination simulation

3.4. Testing the simulation in conjunction with the ontology

The user interface serves as working area for material scientist or laboratory assistants as bridge between the complex structure of ontological knowledge representation and the need of certain required data. The user interface is implemented using Python with the connection of various data processing libraries, a library for working with web design and a data transfer server, as well as additional libraries for connecting to the ontology and changing it. The main advantage of this solution is that all the code is located inside one project. This increases the stability and speed of operation, without data loss and transfer delays between different software.

Working models of sintering ceramic plates are presented in the form of three executable files in different programs. Each simulation is independent of the others and refers to a specific operating mode. For example, inputs such as simulation time, process pressure, temperature for ceramic plate can be manipulated depending on the work piece being examined. All parameters of each simulation and work pieces are documented in the ontology and can always be studied before creating a new experiment (Figure 7, right).

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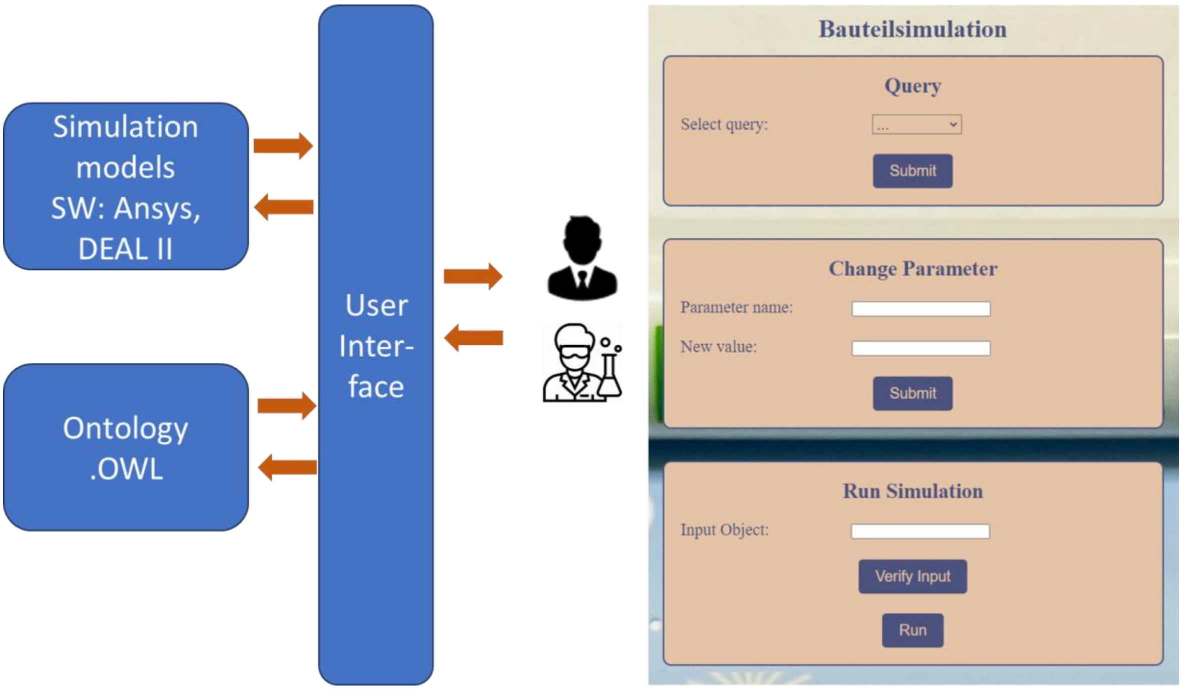

Figure 7. Schematic diagram simulations and ontology access of via the user interface (left); Visual impression of the user interface and manipulation opportunities (right)

The simulation in conjunction with the ontology connected via the workflow serves as working area for the simulation specialist. He or she may research in the ontological database for what objects, parameters, elements are available and what has been simulated already. The second field enables the material scientist to modify the parameters as requested in the user stories. In the third step the simulation experiment is executed and thereby a predictive simulation is conducted. The result of the simulation, as well as the result of each simulation script, can be studied and downloaded by the user for further research.

4. Results

Material scientist, laboratory workers or if relevant simulation experts may query the ontology and search for desired samples, parameters, and process execution details. This support the study the history of experiments and gain insight into the sintering process. Simulation experiments proved that the use of various experimental process data serve well as basis for running simulation experiments and prediction of material behaviour is thereby possible. The user interface eases access to ontologically stored and structured data. This ease of interaction is especially valuable for domain experts and non-technical users who need to work with data conducted in different laboratories. In addition, users often need to create, edit, and maintain ontologies. The user interface simplifies these tasks by allowing users to define objects, their parameters, and required properties without having to delve into the ontology and examine all the relationships between objects. Thus, the user interface in combination with the ontology serves as tool for searching, storing, and using experimental results. It is also a tool for training and predicting the results of the studied sintering processes of work pieces.

5. Conclusion and next steps

By answering the research questions posed at the outset, it can be concluded that material scientist can use ontology-structured data to predict material behaviour of multi-layer ceramic components during the sintering process. Obviously, the larger the knowledge base, the more accurate are predictions within the framework of one operating parameter using similar studies and experiments.
Ontologies offer a structured and standardized way to represent knowledge and data. They provide a basis for defining terms, parameters, and their relationships within a particular experiment or project.

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This structured presentation facilitates clear and unambiguous understanding of complex data. The querying feature proved out successfully.

During the implementation of the workflow an automatic check of already conducted simulation experiments was discussed but not implemented. However, for future installations this deems to be useful preventing from double simulation work. The current setting does not allow to choose from different simulation models. Based on the workshare only one simulation model has been established. An inclusion is considered useful. The used DEAL.II simulation causes that simulation output data format does not allow data to be automatically entered into the ontology. This problem requires additional study and development of data transfer interfaces.

Acknowledgement

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