Battery manufacturing knowledge infrastructure requirements for multicriteria optimization based decision support in design of simulation

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Abstract

This position paper reports on the requirements analysis within the project Battery Cell Assembly Twin (BatCAT), which develops a digital twin for battery manufacturing. The focus is on the aspects of this work that are at the intersection between semantic web technology and materials science and engineering, specifically, the co-design of the architecture of the semantic interoperability layer and the decision support system (DSS). First, visions and ideas are provided on how the architecture will look, and what technology and previous work it will be based on. Key elements to this include, on the side of the semantic technology, the Meta Object Facility (MOF) with the OntoCommons ecosystem as a meta-metamodel (MOF M3 level), a system of ontologies with OWL EL or RL expressivity as a metamodel (MOF M2 level), and a MOF M1-level model based on OO-LD. On the side of the DSS, answer set programming will be combined with multicriteria optimization (MCO), such that MCO can be applied to model parameterization and design of simulation to make best use of computational resources and data.

Keywords

decision support system, design of simulation, digital twin, multicriteria optimization, requirements analysis

1. Introduction

BatCAT is the project that realizes the Battery2030+ manufacturability programme [1, pp. 70–80] by developing a digital twin platform and data space for manufacturing of vanadium-based redox-flow batteries as well as Li-ion and Na-ion coin cells. BatCAT combines two approaches to decision support: First, logical reasoning by answer set programming [2, 3] (ASP), which can increase the efficiency of neural-network surrogate modelling while also ensuring its interpretability; second, multicriteria optimization [4, 5] (MCO), integrating surrogate models into model parameterization, interoperating with the MolMod database [6]. This line of work can build on *business decision support systems* (BDSS) from previous projects [4, 7]. Model accuracy and reliability will be documented through epistemic

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metadata [8]. Physics-based modelling in BatCAT includes molecular dynamics and Monte Carlo simulation based on classical mechanical pair potentials, using the DL_POLY and ms2 codes; mesoscopic DPD simulations will be carried out using DL_MESO, employing an nDPD potential [9]. The molecular and mesoscopic simulation results will feed into continuum simulations, equivalent-circuit models, and population balance models. Surrogate models, *e.g.*, representing results from continuum simulation [10], will include cellular neural networks (with the potential for exploitation by on-chip deployment [11]). For use in production, it is necessary to make the models XAIR, *i.e.*, explainable-AI-ready [12].

The present work summarizes reflections from the requirements analysis [13] and initial steps of work done within the project, with a focus on the architecture and functional requirements for the data space, semantic artefacts, and multicriteria optimization. For this purpose, we analyse pre-existing lines of work that will be combined within BatCAT in view of insights from the requirements analysis. Specifically, we consider here the conditions and options for deploying MCO in modelling and simulation for *design of simulation* (DoS). This is taken to include both model parameterization and surrogate model development guided by MCO, with the potential of addressing further aspects of simulation workflow design and deployment if the requirements analysis indicates it to be appropriate.

2. Requirements procurement and analysis methodology

An agile requirements analysis was conducted based on interviews with team members and external stakeholders. For this purpose, fifteen 30-minute interviews were conducted. Subsequently, the discussed content was evaluated in combination with the BatCAT project work plan and the relevant policy papers; the latter include the Battery2030+ Roadmap [1] and the Flow Batteries Europe Manifesto [14].

Following common practice in agile requirements analysis [16], the requirements obtained from these sources were formulated as (low-level) user stories, grouped into (high-level) epics. More user stories were procured from team members in a dedicated session at a project workshop. Both the user stories and the epics have the format: "As *<role>*, I intend to do *<action>* in order to progress toward *<overarching objective>*." ISO 6515:2018 defines an *epic* as a "major collection of related feature sets broken down into individual *features* or *user stories* and implemented in parts over a longer period of time" [17]. Here, in the case of a user story, the overarching objective is the relevant epic, whereas in the case of an epic, the overarching objective represents a goal at a longer time scale or an even higher degree of abstraction. The *role* label used in the expression above is a *persona*, corresponding to a type of stakeholders. Following ISO 6515:2018, a *persona* is a "model of a user with defined characteristics, based on research", while a *user story* is a "simple narrative illustrating a user requirement from the perspective of a persona" [17]. Accordingly, the personas are not real individuals [16] – they are a means of structuring the requirements [18]. Consequently, multiple people's input can contribute to the same persona, and different requirements formulated by the same individual can be categorized under different personas. The following nine personas were defined for this purpose based on our assessment of key roles related to the BatCAT architecture: (1) AI: Administrator – internal; (2) DI: Digital twin technology user – internal; (3) EI: Experimentalist – internal; (4) MI: Manufacturing use-case owner – internal; (5) SI: Simulation researcher – internal; (6) CE: Customer – external; (7) DE: Developer of a related platform – external; (8) EE: Experimentalist – external; (9) PE: Policy expert – external.

Beside grouping user stories into epics and mapping them to personas, the user stories expressing functional requirements are also attributed to a design target, *i.e.*, a component of the BatCAT architecture. (Epics and non-functional requirements are not assigned a design target.) The twelve design targets are shown as ellipses in Fig. 1. The components most relevant to the topic discussed in the present work are the semantic interoperability layer (SIL) and the decision support system (DSS). In case of the semantic interoperability layer, in addition to the user stories, requirements were also collected in the format of competency questions [19, 20, 21], following standard ontology engineering practices (*e.g.*, the LOT methodology [22]). Moreover, a questionnaire was sent to project participants and external stakeholders in order to identify the most relevant use case scenarios and problems to which MCO (and the DSS in general) should be applied: In this instance, 19 responses were received and evaluated [13].

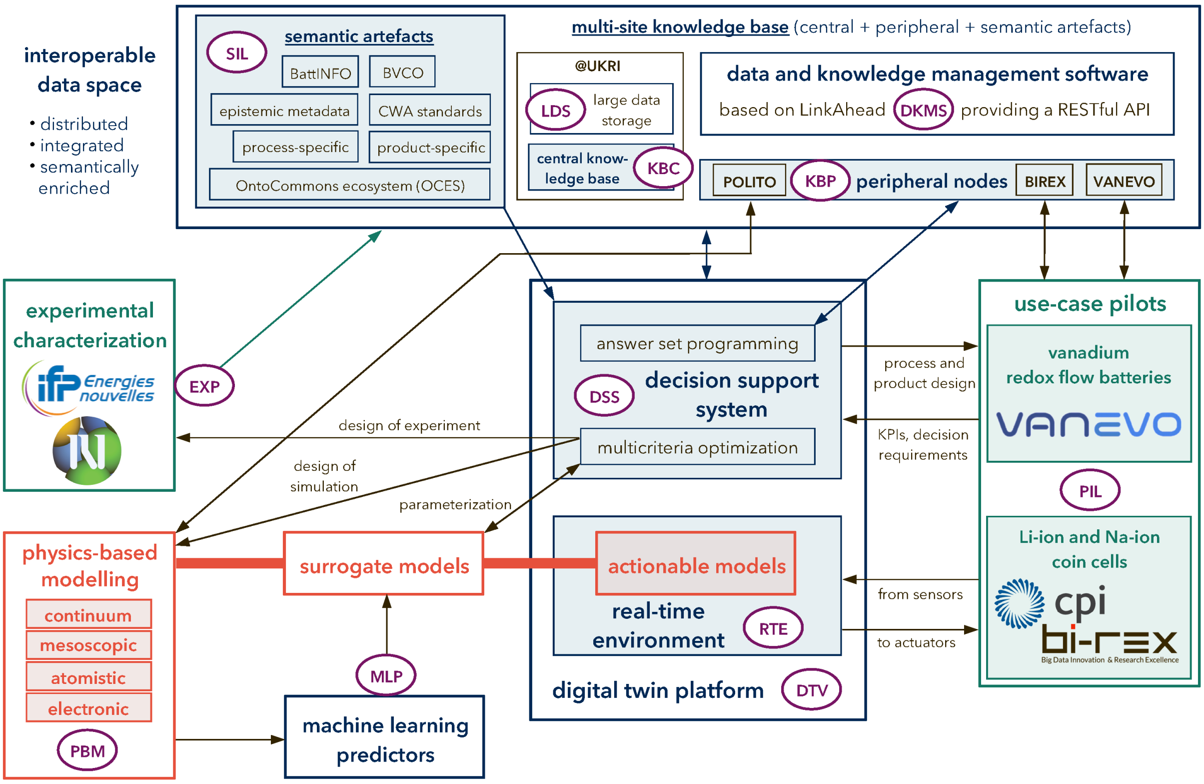

Figure 1: Architecture of the system developed by BatCAT, including a data space and a digital twin platform, applied to two manufacturing use cases. For the present requirements analysis, the following twelve design targets were defined: (1) DSS: Decision support system; (2) KBC: Knowledge base – central; (3) KBP: Knowledge base – peripheral; (4) RTE: Real-time environment; (5) SIL: Semantic interoperability layer; (6) DKMS: Data and knowledge management software (LinkAhead [15]); (7) MLP: Machine learning predictors; (8) PBM: Physics-based modelling; (9) EXP: Experimental characterization and electronic lab notebook; (10) PIL: Pilots; (11) LDS: Large data storage; (12) DTV: Digital twin visualization and front end.

The complete output from the knowledge infrastructure requirements analysis (excluding any sensitive information) will be made openly accessible through CORDIS in due course as part of BatCAT deliverable 4.1, "Data landscape and infrastructure related requirements."

3. Aspects of the requirements analysis

3.1. Multicriteria optimization

From the responses to the questionnaire, the potential MCO problems most frequently selected as relevant were "Slurry Formulation Optimization" and "Design of Simulation (DoS)" both leading at each 45% affirmative answers. Following closely are "Electrode Material Selection", "Coating Thickness and Uniformity", "Electrolyte Composition", and "Design of Experiment (DoE)" each at 40%.

DoS is prioritized by respondents mapped to the following personas: Manufacturing use-case owner (MI), experimentalist (EI), digital twin technology user (DI), simulation researcher (SI), and developer of a related platform (DE). The high priority from diverse personas suggests that simulation is a central component that integrates various aspects of the battery design process. Similarly, the personas highlighting DoE include manufacturing use-case owner (MI), experimentalist (EI), digital twin technology user (DI), simulation researcher (SI), and policy expert (PE). This broad interest reflects the key role of experimental characterization, but also concerns about the resources required to generate all the experimental data that will be needed in order to parameterize and validate models [13].

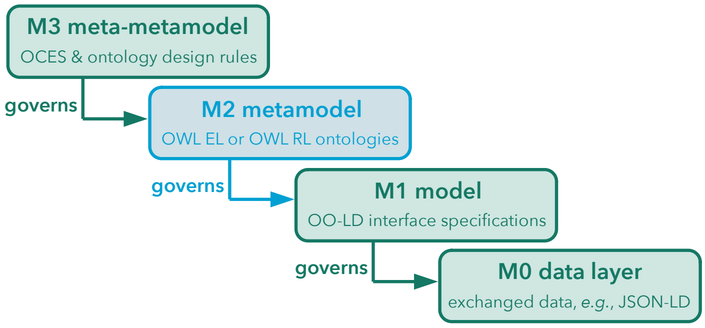

Figure 2: Architecture of the semantic interoperability layer (SIL) in view of the requirements analysis, following the meta object facility (MOF) convention for the four hierarchy levels [28].

3.2. Explainable-AI-readiness

As regards explainable-AI-readiness [12], we follow the definition given by the *XAIR principles* working group of the Knowledge Graph Alliance [23].[1] Accordingly, data and models are XAIR to the degree that their documentation and annotation is both consistent with and conducive to best practices in making use of interpretable learning techniques. Therein, interpretable learning includes both deduction (by logical reasoning) and induction (machine learning), and any combination of them or other kind of acquisition of knowledge from knowledge, insofar as some support through explanation or grounding can be given for it. Epistemic metadata [8] are the annotation through which the explanation, grounding, and knowledge status of data and models can be documented. Currently, the concept of interpretability in machine learning lacks standard metrics and a universally agreed-upon definition, complicating the development and evaluation of models that are expected to be interpretable [24]. Types of interpretability include transparency, which involves a direct understanding of a model's workings, and post-hoc explanations that provide insights after predictions are made, *e.g.*, through techniques like feature importance. Organizations including IEEE have developed standards for ethical AI, emphasizing transparency and explainability, with the IEEE's Ethically Aligned Design guidelines highlighting the importance of designing AI systems that are understandable to users and stakeholders [25]. Widespread misconceptions (criticized, *e.g.*, by Lipton [24]) include an overemphasis on accuracy over interpretability and the notion that linear models are always more interpretable than complex models.

4. Analysis and consequences for the architecture

4.1. Semantic architecture

It is planned that the digital twin platform will use BPMN 2.0 (business model process and notation [26]) for some of the required deployable workflows; possibly, *e.g.*, for integrating elements such as surrogate models into the Pareto front computation for the MCO module. Such an enterprise architecture would be able to build on the previous work by Kavka *et al.* [27] in the COMPOSELECTOR project (H2020 GA no. 721105). In view of this, the meta object facility [28] (MOF) will be used as a formalism for designing and specifying the architecture of the semantic interoperability layer (*cf.* Fig. 2); both BPMN and MOF are standards devised by the Object Management Group and therefore designed to be technically interoperable. Leveraging MOF, we can establish a unified semantic model [29] that encapsulates diverse aspects of battery design, including materials, processes, and performance metrics. This model can serve as a foundation for interoperable tools and systems, promoting efficient data exchange and collaboration among stakeholders. Additionally, a semantic architecture based on MOF can support advanced query capabilities, allowing users to retrieve and analyse data across domains.

Core elements to the M2-level metamodel are the battery domain ontologies BattINFO and BVCO [7], ontologies for representing content from BPMN [30, 31, 32], and mid-level ontologies for epistemic meta-

[1]See also https://www.kg-alliance.org/kga-wg-xai-24-4/.

data [8], presently undergoing refactoring as *MSO-EM: Ontologies for modelling, simulation, optimization and epistemic metadata* [23].[2] These ontologies will connect to the OntoCommons ecosystem [33] (OCES) and rely on various mechanisms for alignment with other semantic artefacts, including strong alignment (RDFS/OWL), weak alignment using SKOS [34], and bridge concepts [33].

4.2. MCO in model parameterization

Deploying semantics can streamline optimization by providing a common understanding of terms and concepts, *e.g.*, across simulation methods. Promising approaches to be explored for this purpose include CWA ModGra [12, 35, 36] and the ongoing CWA 17815 revision process.[3] MCO-based model parameterization in BatCAT can build on substantial previous work, from which there is a well-established methodology [5, 37, 38, 39, 40]. However, to apply these methods in concrete scenarios, multiple prerequisites must be met: First, the model class must be characterized, *i.e.*, it must be known how the model behaves as a function of the model parameters. Second, the quantities for which the model behaviour is known must be those for which experimental data are available (or other data used instead of experiments, *e.g.*, ab initio calculations). Third, a model (re-)parameterization must be admissible: It does not make sense to optimize one model if there are other models or elements of the simulation workflow that rely on a specific pre-existing model parameterization. This requires a comprehensive understanding of the simulation workflows and their logic. Additionally, characterizing the model class requires systematically exploring the model parameter space and constructing a surrogate model. It is the first of these tasks, sampling model properties as a function of model parameters over the whole relevant parameter space, that can be computationally demanding and that could benefit greatly from design of simulation; the accuracy of the surrogate model can be a metric for the information gained.

4.3. MCO in design of simulation

MCO-based design of simulation (DoS) and experiment (DoE) are foreseen in the BatCAT architecture, and will be applied both to the VRFB and the Li-/Na-ion use cases. The approach to DoS and DoE is in principle the same, except that there usually is more flexibility at varying simulation parameters than experimental parameters; in the case of DoE, there will be additional non-trivial constraints, which might be accounted for through the answer-set (logical) programming component of the decision support system. In design of simulation, MCO consists in selecting simulation parameters to optimize the use of data and computational resources. This includes selecting the most relevant variables, designing simulations that provide the most informative data, and configuring simulations to accurately reflect real-world conditions. The MCO-based DoS can be used when characterizing a model class (*cf.* Section 4.2); however, it is not limited to this. Its potential scope extends at least to all the simulation workflows that explore some parameter space and from which surrogate models are to be developed.

MCO requires well-characterized parameter and objective spaces, and a multicriteria cost function that maps parameters to objectives. To apply MCO to DoS, one must have a clear picture of the parameter space that must be explored. Unimportant technical parameters of the solver are naturally excluded, but depending on the scenario, model and solver parameters *can* be included. In general, therefore, the explored simulation parameters $\mathbf{x} = (x_1, \dots, x_k)$ from some $X \subseteq \mathbb{R}^k$ can include: (1) Physical properties of the simulated system, such as thermodynamic or mechanical boundary conditions; (2) model parameters; (3) solver parameters. However, it is not necessary to include all three types of parameters. The immediate purpose of each simulation is to compute $g_{\mathrm{sim}}(\mathbf{x}) = \mathbf{z} = (z_1, \dots, z_\ell) \in Z \subseteq \mathbb{R}^\ell$, *i.e.*, the quantities that are obtained from the simulation. These are physically/technically meaningful quantities. DoS does not target optimizing a single simulation, but the overall knowledge gained from a simulation series or programme; in our framework, the goal is to

[2]The system of ontologies can be accessed through the persistent URL https://www.purl.org/mso-em. The development is done on a public github repository, for the time being: https://github.com/martinhorsch/mso-em. This will soon be moved to a new BatCAT organization site on github. There will then be a pointer to the new repository at the URL of the present one.
[3]https://www.cencenelec.eu/news-and-events/news/2024/workshop/2024-04-22-nano/

create a surrogate model $g_{\text{corr}} : X \to Z$ that correlates the simulation data, $g_{\text{corr}}(\mathbf{x}) \approx g_{\text{sim}}(\mathbf{x})$, can stand in for the physics-based model, while being much more tractable numerically.

To achieve this goal, we wish to obtain maximum knowledge on how g_{sim} behaves over X by making efficient use of a given amount of computational resources. The objective space for the DoS problem, by convention and without loss of generality defined over minimization objectives, can therefore be expressed in terms of metrics for remaining uncertainty or lack of knowledge (or negative information on g_{sim}, negative success at sampling X, or negative performance of g_{corr}). We can here simplify this by assuming that the number m of simulations to be arranged upon invoking the DoS is predetermined, and that the choice of simulation parameters is restricted (as a boundary condition) such that the expected computational resource requirements are constant. The parameter space for the MCO problem is therefore X^m, *i.e.*, the mk-dimensional space from which simulation parameters for m simulations would be selected. The objective space $Y \subseteq \mathbb{R}^n$ is defined over n uncertainty metrics. Solving the MCO-problem for this kind of DoS requires a cost function $f : X^m \to Y$, expressing the expectation of how well the simulation parameter space X will be sampled upon conducting m additional simulations while choosing the respective parameter values; for this, another surrogate model f_{corr} is needed, which approximates f. On this basis, the Pareto front is computed over the mk-dimensional parameter space X^m and the n-dimensional objective space Y, using the multicriteria cost function $f_{\text{corr}} : X^m \to Y$.

5. Conclusion

For the multicriteria optimization and its use for design of simulation to play together with the whole architecture of a data-driven and knowledge-based digital twin project, it is necessary, but not enough to rely on ontology-based semantic interoperability: Different levels of representation and actionable workflows need to interoperate technically. In the case of the BatCAT project, it appears that the Object Management Group's standards provide a suitable framework, comprising four hierarchy levels of semantics from MOF together with workflow orchestration based on BPMN. It remains a major challenge to formulate the simulation problems, including the interaction between physics-based simulation and data-driven surrogate models, such that multicriteria optimization really can be used to optimize the selection of simulation parameters. Realizing this in practice is beyond what we can report through this position paper. However, there is substantial previous work as a basis for it, to which the requirements analysis in BatCAT, as summarized here, adds one more building block that was needed.

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