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MEETING ABSTRACTS

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Introduction

Welcome message from the organizers

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Introduction
Dear readers,
In this supplement of the proceedings of the 11th DACH+ Conference on Energy Informatics 2022, we present the extended poster abstracts, including seven contributions from the co-located Energy Informatics Doctoral Workshop.
Sincerely,
Anke Weidlich (General Chair)
Gunther Gust (Poster Chair)
Mirko Schäfer (Publication Chair)

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Not applicable.

Author's contributions
The authors read and approved the final manuscript.

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S8
GB-Flex: Automated and Distributed Decision-Making in Energy Balancing Groups

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Keywords: energy balancing groups; distributed decision-making; automated energy negotiation

Introduction
Balancing Groups (BGs) are Distribution System Operators (DSO) that balance energy production and consumption — possibly aggregated if small. Larger consumers/producers could be considered separated entities in a BG, although these are mostly DSOs. To generalize the discussion, we refer to them as *sub-balance groups* (SBGs).
Each BG performs day-ahead forecasting and announces it to the Transmission System Operators (TSOs) – who rely on it to adjust energy production and expects BGs to follow the plan as close as possible. If BGs deviate, the TSOs penalize them. Likewise, with intraday (more accurate) markets and local flexibility, SBGs could – but do not do it – react to minimize the penalties [1]. Small SBGs do not have trading departments and cannot foresee deviations nor take necessary actions.
This paper briefly summarizes the possible strategies and shows the feasibility and profits of automatizing the BGs.
To systematically reduce transaction costs, the decision-making for balancing (i.e., contracting) and their implementation (i.e., contract fulfillment) need to be automated. Prompt reactions and correcting measures can lead to more effective balancing. Despite singular deviations/fines are small quantities, they can add up to avoidable expensive costs.

Background and State of the Art
In the electricity market, it is imperative to punctually equilibrate supply and demand. TSOs are provided balanced forecasts of feed-ins and withdrawals. However, SBGs can take a strategic position by participating in a local energy trading market. Local energy balancing follows the real-time balancing in European electricity markets. The dual-price system is applied in Switzerland, where the TSO will set the costs/penalties for positive/negative deviation for each settlement period [2].

We share some methodological approaches (e.g., the distributed nature and automated negotiation approaches) with existing research. For example, Wu et al. [3] validate their pricing strategies via simulations, and Hayes et al. [4] propose a co-simulation including P2P energy platforms and energy distribution networks. Other approaches adopt statistical learning algorithms (e.g., reinforcement learning and Q-learning) and game theory, enabling agents to trade autonomously and derive long-term profit-making policies (e.g., see [5, 6]). Approaches using aggregators often try to bring together smaller entities (e.g., on the household level, and allow them to provide their services to the energy market levels [7]). Similarly, they valorize flexibility. However, they typically ignore the existing and, in practice, established form of balancing groups. Our approach relies on existing structures in the energy balancing and enables them to act more dynamically and integrate more partners.

Decision-making approaches for balancing groups

Centralized decision-making: the BG centralizes all the partners, enabling optimization. It requires data centralization (often impossible), and it is implemented either by the BG itself or by the given SBG(s) following the BG's indications to adjust their schedules. In turn, it distributes the financial efforts/benefits among the partners. The advantages of this approach are possible optimization, risk-sharing, and limited balancing concerns. However, technical and organizational challenges (i.e., implementation/scaling) carry disadvantages, including explicit management of trust, transparency, and privacy, and practical difficulties in data integration.

Decentralized decision-making: Single actors (DSOs) make autonomous decisions and are responsible for their balancing (not viable w.r.t. the current regulative framework). Indeed, the concept of balancing groups has been introduced to avoid such a decentralized solution [2]. The (theoretically) full decentralization entails advantages including actors' autonomy and no need for data integration. Nevertheless, it is discouraged by significant disadvantages such as the absence of risk-sharing (everyone is exposed to the risk), every actor needs to invest in balancing efforts (more effort per partner), possible increase of the costs, and not technologically viable.

Hybrid solution: It combines the previously mentioned approaches and valorizes optimization and risk-sharing, with only a limited amount of actors needing to set up resources for balancing. It would still maintain actors' autonomy, reduce the need for data integration, and reduce the sharing of sensitive information with competitors. Besides the hybrid approach, neither of the extreme approaches can be unconditionally recommended for future balancing solutions.

The GB-Flex Simulator

The GB-Flex simulator enables the definition, simulation, and evaluation of several BGs/SBGs strategies leveraging both synthetic and real-world data[1] to mimic today's SBGs (including independent DSOs). Therefore, leveraging the multi-agent paradigm, autonomous agents can make decisions on their behalf and represent their interests. Hereafter, we refer to agents/actors interchangeably as synonymous with SBGs. Several nuances (i.e., politically-driven decisions and local markets' flexibility) have been not considered, given the lack of characterizing data and the difficulty of clearly quantifying their relevance in simulated environments. Despite this simplification, the study results are not necessarily jeopardized. Nevertheless, we rely only on the available data to ensure plausibility and grounding of the results.

We implemented the following strategies: **Do nothing** — SBGs do nothing to prevent penalties (current real-world scenario and baseline for penalties). **Competitive** — SBGs deal with only the outside market. If the forecasts are short, an SBG can minimize its final share of penalties. If they are long, selling would avoid paying penalties. **Cooperative** — SBGs exchange energy with each other exclusively. If the forecast is long, they try to sell to those short (preventing penalties in the BG). **Opportunistic** — SBGs aim to optimize their profits while preventing penalties for the whole BG. If a surplus cannot be placed

within the BG, it is sold to the outside market (partially or entirely). The simulator comprises a web front-end to configure the scenario, set the inputs, and visualize the results, and a back-end enacting BG, SBGs, and their behaviors. The configurable inputs are load/generate data-sets, scenarios, market prices, energy market prices, penalties, buying/selling strategies, and related boundaries. The simulation clock triggers a check of the intraday forecast every 15 *simulated* minutes. GB-Flex includes 3 types of agents: *BG, SBG* and External market (EM). The main aim of all SBGs is to get their delta (the difference between their day-ahead and their intraday forecast) to zero — thus avoiding penalties — according to the strategy (unless it is *do nothing*).

Results

To enact BGs and SBGs' strategies and dynamics, we used six months of real-world data (Feb 21-Jul 21) from three main actors (*FMV, INERA,* and *OIKEN*) of the BG-Valais. Clearly, six months do not cover the full seasonality of the market. Nevertheless, the selected period suffices for the purpose and avoids strong summer/winter biases. This period tends to genera a surplus in the region, implying over-production. However, conversely to the current exposure to penalties, some strategies proved the benefits of buying/selling energy on the intraday market. We reasonably assume that the intraday energy markets have enough liquidity. In particular, we assume that all bits (buying/selling) an agent places at the market are accepted for the given price. Given the BG's size, this seems a reasonable simplification w.r.t. the traded volume in the energy markets. In theory, all penalties can be avoided if the market price is below the penalty imposed by the TSO. Hence, this assumption always holds because the penalty is related to energy price.

We assumed that the intraday forecasts represent the ground *truth*. This is, in practice, not fully correct and thus also limits the effectiveness of the proposed methods. However, intraday forecasts represent the best information available before execution time — thus, to act on. As mentioned above, current real-world approaches do not employ corrective measures (*do nothing* strategy), the worst possible solution for every entity within the BG. Computing the results for the BG, we speculate on the possible behaviors of some companies.

The potential impact of implementing an active balancing strategy rather than the *doing nothing* approach is confirmed by the several simulations. The SBGs took the initiative to place a surplus or to look for the missing amount of energy. Most of the time, demands and offers among the SBGs have shown to only partially satisfy each other. Nevertheless, seeking the EM has always allowed avoiding penalties (in some cases of 8'326 CHF **in a day**) and possibly generating profits. Our experiments investigate both scenarios with *aligned* strategies (i.e., all actors follow the same strategy) and *mixed* strategies (i.e., the actors have different strategies within the same run). Mixed strategies are particularly interesting to assess situations where single SGBs decide (for whatever reasons) to deviate from a commonly agreed strategy within the entire BG. This allows for each SBG, as well as for the overall BG, to consider strategization and incentivization for desired outcomes. Thus, our hypothesis **"hybrid solutions can be significantly beneficial to the BG, similarly to centralized solutions"** is supported by all empirical evidence we could observe for this balancing group over a period of six months of operational data. Thereby, the need for centralization fades, sparing the actors from its related drawbacks.

Conclusions

This paper investigated the needs, requirements, and constraints of automated decision-making for BG. Hybrid approaches overperformed the unpracticable purely (de)centralized solutions in competitive, cooperative, and opportunistic settings.

Summarizing, the further development of hybrid automated solutions for balancing BGs is a promising direction. They allow for economically efficient and technically feasible implementation, offer a reasonable foundation for further technological and organizational developments, and provide scalability and transferability to other BGs. Moreover, we recommend developing a solution actualizing the GB-Flex simulator in the real world to investigate further the agent-based approach's potential in more realistic settings. Finally, the developed simulator could be refined to ease its usability for non-experts. Such a system is envisioned as an aid for the SBGs in defining and evaluating their strategies ahead of their deployment.

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[1] 96-intervals day-basis data acquired from 02/2021 to 08/2021 by Valais BG.

Availability of data and materials
Detailed material can be found in the project report https://www.ara-mis.admin.ch/Dokument.aspx?DocumentID=68395.

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S14
Explainable AI for power grid frequency stability and control

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Abstract
Balancing power supply and demand is a central task in the operation of power systems. To optimise system control and balancing, we need a solid understanding of emerging power imbalances that manifest in deviations of the grid frequency from its reference. However, understanding grid frequency deviations is challenging as diverse and interacting factors impact the frequency, ranging from volatile renewable generation to deterministic effects of electricity trading. Here, we use explainable machine learning to disentangle different effects on frequency stability. Training gradient boosted trees, we successfully predict frequency stability and frequency control activation from techno-economic features. Interpreting the model with SHapely Additive exPlanations (SHAP), we reveal and compare drivers and risks for frequency stability in major European power grids.
Keywords: machine learning; explainable; grid frequency; stability

Introduction
Balancing power supply and demand is central to power system operation [1]. Large power imbalances threaten the security of supply, which, in extreme cases, can lead to large-scale blackouts [2]. While electricity markets are used to match supply and demand within intervals of typically one hour, additional control schemes are necessary to balance the power system on shorter time scales. The power grid frequency is the central target of these control schemes [3]. It reflects power imbalances through deviations from its reference value of 50 (or 60) Hz, which should remain small to ensure a stable grid operation.

Grid frequency deviations have various different causes, which become more diverse through the transition to renewable energy sources. The market-based dispatch of generators leads to regular deterministic frequency deviations [4], and large social events [5] as well as local legislation [6, 7] can have further effects on the grid frequency. The large-scale integration of wind and solar power generation into modern power grids introduces new challenges, as these energy sources do not provide intrinsic inertia [8] and their fluctuating nature [9, 10] can lead to additional power imbalances and frequency deviations. Due to the importance of power system stability, it is essential to understand and disentangle these different effects on the grid frequency. Furthermore, to stabilise the frequency, control actions are needed [1]. Understanding how these control needs are driven by external factors also remains an active field of research [11].

In this contribution, we demonstrate how eXplainable Artificial Intelligence (XAI) can help to understand the risks and drivers for frequency stability and control. Using operational data from major European power systems, we show applications of our method to frequency stability indicators [12] and deterministic frequency deviations [6] in Europe as well as frequency control activation in Germany [11].

Methods
To model frequency stability and control based on operational data, we built a machine learning (ML) model that predicts central indicators of frequency stability from techno-economic features.

As inputs, we used time series data such as load, generation and electricity price time series [13]. The time series contain ex-post (actually measured) data as well as day-ahead available data such as generation forecasts, which can be used in day-ahead predictions of frequency stability. As outputs (targets), we constructed stability indicators from grid frequency measurements [14, 15, 16] in the Continental European, the Nordic and the Great Britain synchronous areas. To model control activation in Germany, we instead used the activated control volumes as output data [17]. The data comes with an hourly or 15 min resolution and all data sources are publicly available.

We mapped inputs to outputs by using a Gradient Boosted Tree (GBT) model to fit the data [18]. We then used a method from XAI, SHapely Additive exPlanations (SHAP), to explain the machine learning model and extract important input features and dependencies [19]. This enables rich ex-post interpretations of historic operational data as well as transparent day-ahead predictions.

Results
Our method revealed risks and drivers for frequency stability in major European power systems [12]. Frequency gradients are mostly affected by fast generation ramps, and we extracted three different classes of generation types that have opposite impacts. The stability indicator that measures the required control effort is mostly related to forecast errors and electricity prices. In the Nordic grid, forecast errors generally play a major role to explain frequency deviations, while the Continental European grid is dominated by fast load and generation ramps, and renewable generation as well as electricity prices are important in Great Britain.

Furthermore, our approach elucidated how deterministic frequency deviations (DFDs) emerge from different load and generation characteristics [6]. DFDs are typically explained by the daily cycle of the load, in particular the load gradients, which already explain a large part of the daily DFD pattern. However, this model fails especially before and around noonday. By using multiple input features, we related this observation to solar power ramps and constructed a model that nearly perfectly reproduces the daily DFD pattern in the data.

Finally, we used our method to analyse the historic activation of control power in Germany as well as its day-ahead predictability [11]. We showed that the control power only exhibits weak daily patterns, but forecast errors and the generation mix strongly affect its activation. Appropriate forecast error estimates also appear as important factors to increase the day-ahead predictability of control. In general, different loss functions and model training schemes have to be used for either ex-post analysis or day-ahead prediction.

Conclusion and Outlook

In this contribution we give an overview over our XAI applications to frequency stability and control. Using techno-economic operational data, we predicted frequency stability indicators and control activation and identified key drivers and risks for frequency stability.

Our ML approach provides a powerful alternative to simulation-based analyses, but also complements physical models. In contrast to physical models, our method is purely data-driven and does not rely on parameter assumptions and approximations. It can therefore identify and quantify unknown effects in historic operational data, which can be used to refine physical models. However, our ML model does only fit associations in the data, which do not necessarily correspond to causal relationships. Therefore, we need domain knowledge, e.g., from physical models, to discuss and validate our data-driven results (cf. ref. [12]).

In contrast to existing data-driven approaches, we go beyond pure linear correlation studies for grid stability analyses. Previous data-driven studies investigated the impact of single features on grid frequency stability based on correlation coefficients and scatter plots [20, 21, 22, 23], which faces different limitations. First, linear correlation analysis can overlook or underestimate important effects that are non-linear. Second, only the impact of a single feature/covariate is examined in most cases. However, this can be misleading if features are correlated, e.g., due to confounding (cf. [12]). Therefore, a multivariate regression can be helpful to adjust for the effect of other variables. We present a multivariate, non-linear regression model, which can contribute as an advanced analysis tool for grid frequency stability and control.

With our case studies, we demonstrate the versatile application of our ML method, which can further be used to optimise power system operation and control. The importance of forecast errors in the Nordic grid and fast generation ramps in Continental Europe revealed risks for frequency stability that can be mitigated by additional optimisation or new system regulations. Day-ahead predictions of frequency deviations can be used for preventive control actions or model predictive control. Finally, SHAP offers further tools such as interaction analysis and monitoring plots, which can be applied both to frequency stability but also to other aspects of the energy system in the future.

Availability of data and materials

All our data sets are available on Zenodo [24, 25]. The code is published on GitHub and archived on Zenodo [26, 27, 28].

Author's contributions

J.K.: Conceptualisation, Investigation, Formal analysis, Visualisation, Writing. B.S.: Supervision, Writing, Conceptualisation. D.W.: Project administration, Funding acquisition, Supervision, Writing, Conceptualisation.

Competing interests

The authors declare that they have no competing interests.

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S19

Towards Verification in Decentralized Energy Systems

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Summary

Distributed Energy Resources play an ever increasing role as the existing centralized energy system is transformed to use more decentralized renewable energy sources. Multi-agent systems are an intuitive paradigm for modeling and control of this type of system. Since the energy system is safety-critical infrastructure it is necessary to ensure its reliability. Formal verification is one way to achieve this. In this poster we motivate possible approaches to the verification problem for MAS as well as their application to energy systems. We outline key challenges that such an approach must address.
Keywords: Multi-agent-systems; Formal Verification; Energy Systems

Introduction and Related Work

The power system is a key piece of safety-critical infrastructure. The transition from fossil-fuel-based energy generation to renewable sources is connected with an ever increasing number of Distributed Energy Resources (DER). This development is an opportunity to create a truly resilient, self-regulating decentralized energy grid without large single points of failure. In Multi-agent systems (MAS)[1] agents act independently towards a common goal. This makes MAS a natural paradigm to model a decentralized energy system as shown in Figure 1, capturing the decentralized and independent nature of different actors. As such, MAS have already been applied to various use-cases within the energy domain [2, 3, 4].
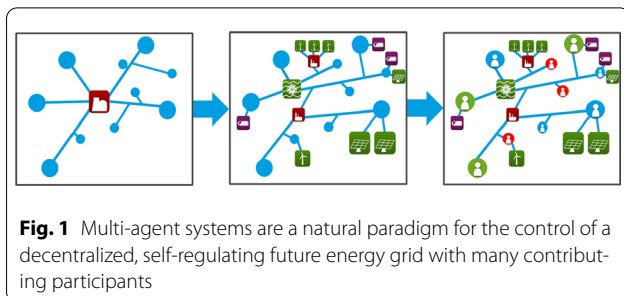

Fig. 1 Multi-agent systems are a natural paradigm for the control of a decentralized, self-regulating future energy grid with many contributing participants

A major problem for a DER-based system is the increased uncertainty of generation due to weather dependence, combined with the inherent complexity of MAS. We want to enable high trust in distributed energy systems by formally verifying desired properties of MAS. These systems are **open** (agents may join or leave the system at run-time), **stochastic** and **heterogeneous**. Prior works in this area usually focus on some, but not all, of these aspects [5, 6, 7]. Verification results may then be used to combine MAS with traditional systems. Contract-Based Design [8] allows MAS to be considered black boxes with a set of assumptions and guarantees. Through this interface, MAS can be included in larger systems.

Example problem: congestion management

We use decentralized distribution grid congestion management [9, 10, 11] as an example problem where generation and storage resources of different participants can dynamically form coalitions to alleviate a congestion. In the simplified model shown in Figure 2 each agent can observe the active power at a target transformer. Each agent knows the bounds of its own power input and output as well as associated costs and the probability of being able to supply a certain amount of flexibility via a prediction function. In case of a congestion, they calculate the flexibility demand and form a coalition to compute a solution as an optimization problem such that:

1. Flexibility is provided to solve the congestion within a maximum time t_{max}.
2. The joint probability of supplying the flexibility exceeds the threshold P_{min}.
3. The total costs for the coalition are (close to) minimal.

The verification problem for this system is to show that, given some environmental boundaries (e.g. a weather forecast for a DER) and the expected size of the congestion, the agent system can calculate and apply a solution within the given time limit and with sufficient certainty. For all investigated and future approaches the desired verification result remains as described here.
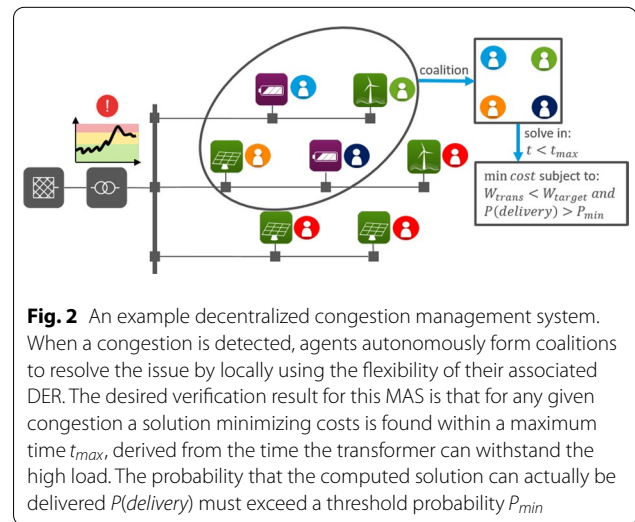

Fig. 2 An example decentralized congestion management system. When a congestion is detected, agents autonomously form coalitions to resolve the issue by locally using the flexibility of their associated DER. The desired verification result for this MAS is that for any given congestion a solution minimizing costs is found within a maximum time t_{max}, derived from the time the transformer can withstand the high load. The probability that the computed solution can actually be delivered $P(delivery)$ must exceed a threshold probability P_{min}

Possible approaches and challenges

In this section we discuss two approaches of formally describing a MAS to achieve verification results. This is not an exhaustive list of approaches. MAS as automata and decentralized algorithms were chosen because they are the areas most familiar to the authors at the time of writing.

MAS as automata

One approach to model verifiable MAS is to describe an agents behavior as a stochastic hybrid automaton [12] and then derive the full system behavior through the parallel composition of all participants. The biggest advantage and disadvantage of such a model is that it captures all possible system states and their probabilities. A property can then be shown to hold over all possible runs of the automaton.

In our example system we could model each agent as a (hybrid) automaton with the active power at the transformer as an input and its contribution to a possible solution as an output as well as inputs and outputs for the communication with other agents. The local cost and prediction functions need to be embedded in the internal states together with the current state of the negotiation. This iterative communication and the dynamic changes in the solution space are not easily captured in classic automata.

Furthermore, it is well known that in general the state space of composite automata grows exponentially, making model checking for the composite automaton infeasible even with relatively small numbers of agents. Under certain conditions the size of the composite automaton can be drastically reduced by using symmetry and similar properties [13, 14]. The design challenge then becomes to make the agents simple enough to have symmetries while being expressive enough to fulfill the task.

Additionally, for **open** MAS it is not viable to create and verify the composite automaton every time the number of agents changes. In these cases an abstraction is needed to reason over automata groups of varying sizes.

MAS as implementations of decentralized algorithms

Modeling the entire physical context of an agent and environment is not always necessary. For many applications it is sufficient to implement a fitting decentralized algorithm using agents. The verification procedure then includes proving the correctness of the algorithm and its implementation, and showing that a solution can be computed in the expected environmental conditions of the agent.

A core part of such algorithms is the exchange and aggregation of information between agents. To allow efficient decentralized aggregation, a function must be decomposable [15], meaning the aggregation operator is both commutative and associative. This ensures that the order in which information is aggregated does not matter and thus not all data must be gathered in one place first.

For our example system, a reasonable abstraction for the local prediction and cost functions is needed. Agents may contribute flexibility offers of active power supply to the solution. If these offers can be efficiently aggregated, then a solution - in this case a combination of offers to select - can be computed in a given time limit. In practice, heuristic approaches would likely perform better on average than an algorithm that is provably correct in all cases. This results in a conflict between desired hard guarantees and timely solutions that are "good enough".

A totally different approach is chosen in the field of controlled self-organization inspired by organic computing: It includes the embedding of a self-organized system not capable of fulfilling guarantees by itself into an observation and control concept [16]. Control actions limit the state space of the self-organized system, enabling the verification of the full system. From the view of the MAS, these control actions may be treated as environmental boundaries. While transfer of this concept to energy systems has been presented [17], the issue of hard guarantees is not yet solved for **open**, **stochastic** and **heterogeneous** MAS in energy systems.

Conclusion

A recurring point of complexity in both approaches presented here is the need for efficient aggregation of MAS either through symmetry properties or aggregation operators that are both commutative and associative. A point of tension exists between the practical desire for fast heuristic solutions and the need for hard system guarantees. Consequently, these will be the key areas of research going forward to enable a fully decentralized and reliable future energy grid.

Availability of data and materials

Not applicable.

Author's contributions

J.S. created the example system, automata and algorithmic approaches. A.N. provided the organic computing approach and substantial feedback.

Competing interests

The authors declare that they have no competing interests.

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Digital Twin Architecture and Technologies for Hydrogen Electrolyser Applications

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Summary

In this work, a service oriented digital twin (DT) architecture and concept is introduced in the context of hydrogen electrolysers. For this, current literature on DT architectures and concepts was researched and taken into consideration. The approach focuses on a core DT, consisting of a publish subscribe system, a component for integrating sensors and actuators, and a state estimation component. Connected to the core are the services, enhancing the core with additional features, e.g. remaining useful life estimation. The architecture aims to allow creating scalable, extendable, inter-operable and dynamic DTs for electrolysers.

Introduction

Hydrogen is considered to be a key element of the energy transition towards renewable energy [1]. A considerable increase in the demand of hydrogen is expected in the medium to long term in Germany, which will be accompanied with an accelerated roll-out of the hydrogen technology [1]. The production of hydrogen using water electrolysis is the preferred method for producing green hydrogen, utilizing renewable energy [2]. As part of the German National Hydrogen Strategy Action Plan, hydrogen production using electrolysers is supported by providing funding for investments in electrolysers as well as by constructing demonstration plants at industrial scale and scale-up the production plants with the goal of decreasing the hydrogen production costs [1]. The increased scale of the hydrogen production plants

requires efficient, durable, cost effective and scalable electrolysers [3]. In this regard, the emergence of DT technology is of great advantage for the electrolysers' manufacturing and operation processes. DTs can supply a cyber-physical manufacturing system with information on real-world situation and operation status [4]. This can enhance the manufacturing system's intelligence regarding analytical assessment, predictive diagnosis, and performance optimization [4]. DTs extend the use of simulations to all phases of the life cycle of a product, which is the basis of design decisions and validation [5]. The architecture as well as the technologies used to construct the DT differ in literature and industry depending on the application. A definition, that summarizes the characteristics of a DT with a strong focus on real time data and adaptability of the models used in a DT was given by Semararo et al. [5]:

"A set of adaptive models that emulate the behaviour of a physical system in a virtual system getting real time data to update itself along its life cycle. The digital twin replicates the physical system to predict failures and opportunities for changing, to prescribe real time actions for optimizing and/or mitigating unexpected events observing and evaluating the operating profile system."

In this work, a service-oriented architecture of DTs developed for industrial scale hydrogen electrolysers is presented. The design as well as the relations between the DT elements are given in section Architecture Design and Technologies, the technologies are presented in subsections Core Elements and Data Storage & Services, along with the advantages of such architecture.

Architecture Design and Technologies

The architecture is based on the concept of the 5-Dimensional DT by Tao et al.[6]. The architecture consists of core and peripheral elements, with the goal of the core to provide accurate and fast state estimation of the electrolyser. The core design was kept as minimal as possible, with services placed outside of the DT core.

As shown in Figure 1, the architecture's core elements consist of components for sensors and actuators integration, the state estimation as a virtual entity and a communication element. Here a publish-subscribe communication method was selected to provide the communication between the DT entities. This allows for scalable, flexible, high-speed, and high fidelity implementation. Connected to the core are the data storage entity and the services. The services part can include elements for visualization, estimation of remaining useful life, and others. This modular structure of the services allows for easy and fast expansion with additional services. This allows executing computationally demanding processes on external hardware, such as degradation simulations and co-simulations, as well as research and development focused services. To further increase the modularity as well as scalability in combination with continuous integration and continuous deployment, each component of the DT will be running within a Docker container [7]. This allows, in conjunction with the publish-subscribe system, for run-time deployment and updating of services.
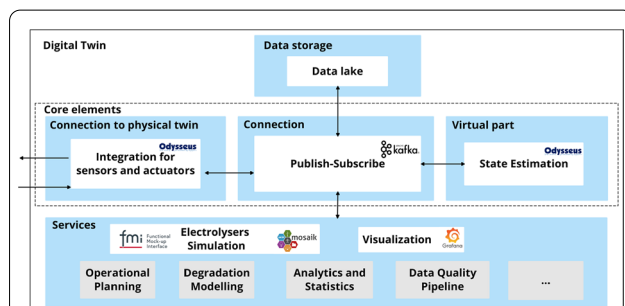

Fig. 1 Electrolysers DT architecture and technologies from the 5D DT concept point of view as in Tao et al. [6]

Core Elements

The overall goal of a DT is to provide an automated bi-directional connection with the physical object in real time or near real time, as well as to be able to deal with high volumes of data [8]. In addition, the data shall also be available on demand, as will be requested by the services. For that, a publish-subscribe system is selected for the connection dimension of the DT. The capabilities for this are met by Apache Kafka (including Kafka Connect), an open-sources distributed event streaming platform [9]. In Kafka, data is captured in form of events or event streams. The data is published in topics by producers and read/processed by consumers. As producers and consumers are working independently, streams can be routed to different services, accessing the same or different topics [9], without a need for producers to wait. Kafka represents a scalable, durable, reliable and highly supported platform [10].

One producer is the electrolyser, which is simulated for the purpose of this work and will be populated with real-time data in the future. Functional mockup units (FMUs) of the functional mock-up interface (FMI) standard are used to encapsulate the models of the electrolysers [11]. The electrolysers FMU is connected, managed and run through the co-simulation framework mosaik [12].

All data regarding the DT is received by the sensors integration component. Such data can be sensor data or if an asset is not yet realized simulation data. The interpretation of the received data will be realized in Odysseus. It enables the stream processing of the data with respect of cleaning and transformation, and extends to different data protocols [13]. This component is crucial, as the DT can therefore work with different data formats and types, which enables easy transformation of data for services into the necessary format.

To mirror the current state of the physical entity as fast and accurate as possible, Odysseus has been selected for running state estimations [13]. Odysseus enables the formulation of queries to process incoming data in the main memory (e.g. manipulation, selection, aggregation, correlation, prediction) and publish the data stream back to a Kafka topic. In addition, Odysseus offers the capabilities to run on clusters (Odysseus NET), as well as in virtual environments including Docker, and can be extended easily with custom or existing plugins. Due to its flexibility, modularity as well as scalability, Odysseus is selected for all tasks regarding data stream processing.

Data Storage & Services

The data storage and services are considered peripheral to the core of the DT, which creates a service based modular DT. Grafana [14] is used as a visualizing service of the DT states, such as trends, errors or anomalies in order to supervise and track the entire system. Grafana is capable to visualize data from different services in dashboards without the need for a specific back-end database [14]. Furthermore, Grafana is well suited for such a dynamic system, as dynamic dashboards can be easily created and customized in combination with alerts and warnings [14].

The utilization of FMU models along with mosaik can also be used for simulation related services of the DT (such as predictive maintenance, operational planning as well as remaining useful lifetime estimation) as shown in Figure 1. The usage of mosaik improves the interoperability of the DT as it allows to connect to simulation models written in different programming languages. Mosaik provides a high level API for Python, Java, C#, and MatLab [12], while the FMUs allows utilizing modelica language models [11].

Conclusion and Future Work

The proposed core of the DT architecture consists of a containerized communication and state estimation. This makes this core not only flexible and extensible, but also enables services to be added, removed or updated without the need to interrupt the core. With technologies such as Docker, Kafka and Odysseus, a fast, reliable and modular DT core will be realized.

With the addition of mosaik into the ecosystem, co-simulation capabilities are enabled for the DT. The simulations can be written in different programming languages or pre-compiled FMUs can be used. This will enable planned future services, such as operational planning, degradation modelling, data quality pipeline, grid integration and remaining useful life calculation. The next planned steps are the

implementation of this architecture with the addition of some services, followed by an evaluation and demonstration of the results.

Availability of data and materials
There are no additional sources of data and materials in this article.

Author's contributions
Conceptualization and architecture design: N.H, S.A, J.C.D, T.B and M.B; writing: N.H, S.A and JCD; review and editing: T.B and M.B.

Competing interests
The authors declare that they have no competing interests.

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Cyber Security in Energy Informatics: A Non-technical Perspective

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Summary
Literature in cyber security including cyber security in energy informatics are overly technocentric focuses that may miss the chances of understanding a bigger picture of cyber security measures. This research thus aims to conduct a literature review focusing on non-technical issues in cyber security in the energy informatics field. The findings show that there are seven non-technical issues have been discussed in literature, including education, awareness, policy, standards, human, and risks, challenges, and solutions. These findings can be valuable for not only researchers, but also managers, policy makers, and educators.
Keywords: energy informatics; cyber security; non-technical; literature review

Introduction
Energy transition is becoming an important trend nowadays. This trend brings cyber threats from information and communications technology (ICT) to the energy sector as ICT is embedded into energy systems. Although scholars have focused on cyber security to improve the cyber security of the energy system, the majority of literature focuses on technical aspects of cyber security. However, literature shows that technology is not enough in preventing cyber threats [1] as technical systems, the humans who operate them, and organizational contexts are all important [2].
Scholars thus call for a more holistic approach for effectiveness of security measures [1]. As a result, we conducted this study by focusing on non-technical issues in cyber security in energy informatics research. We particularly focus on the following research question: What are the main themes related to non-technical issues of cyber security in energy informatics? In this paper, aspects like awareness, policies, and organizational structures can be seen as non-technical aspects, while the specific technologies (e.g., firewalls, cyber-physical systems, algorithms) can be categorized as the technical aspects [3].

Methods
To answer the research question, we conducted a systematic literature review in the field of cyber security in energy informatics. The search was carried out in March, 2022 by using the Scopus database. It is noted that IEEE Xplore and ACM Digital Library, which are largely Scopus-indexed. We focused on journals, conferences and book chapters with the following search string is used: (("smart grid" OR "energy informatics") AND ("cyber security" OR "cybersecurity" OR "cyber-security")) AND (LIMIT-TO ("journals" or "conferences" or "chapters") AND
(LIMIT-TO (LANGUAGE, "English")). The result was 1151 papers with this search string. We then performed checking duplicated or not-relevant papers. Next, we eliminated those survey and literature review papers, as well as omitted pure technical papers. After that, we read the remaining papers in full to eliminate those papers that do not discuss issues related to the review's scope. After this step, 211 papers were selected for review. Moreover, given that Energy Informatics journal is one of the main outlets in the field, we conducted a search on this journal. Two additional papers were found. It means that 213 papers were selected for this study.

Findings
This section presents non-technical issues that have been discussed in selected papers.
Education. Literature discussed two main program types of educations on cyber security in energy informatics, that are training program for professional [4] (e.g., Skill gaps, workforce, team-taught, living lab), and training program for students [5] (e.g., Curriculum, course for STEM students, courses for undergraduate students). The curriculum for cyber security is discussed in three different levels that are equally important: Cyber security for all, cyber operations, and cyber-informed engineering curriculum [6]. Moreover, pedagogical pillars for energy informatics cyber security education are active learning, project-based learning, Piaget's learn-by-doing posture, and constructivism [7].
Awareness. Cyber security awareness is crucial for the effectiveness of organizational security [8]. Two types of awareness are often discussed in those selected papers, including social awareness and situation awareness. Social awareness helps enhance and improve cyber security in energy informatics. The awareness includes socio-economic consumer data; load disaggregation capability; end-use device database; and smart power hub [9]. Situation awareness indicates that architecture and tools are needed to help operators monitor and be aware of actual threats that exist between the network level and the business level [10].
Policy. There are two categories that have been discussed in those selected papers regarding policy (including legal, and regulatory), that

are policy challenges and policy itself [11]. Policy challenges regarding cyber security in energy informatics is one of the main concerns of scholars. Examples of those concerns include privacy, personal data, data security of sharing information in applications used by the smarter grid devices. Scholars also discuss unclear guidance on mandates and roles of organizations/countries on the topics of cyber security [12].

Geography. Majority selected articles come from the EU [13], North America [14], and Asia [15]. The NIST and the ISO frameworks/standards are widely adopted by the EU Critical Infrastructure (e.g., ISO 27001 for IT security, or ISA 62443 for Operational Technology security). The European Union Agency for Cyber Security (ENISA) and the Department of Homeland Security (DHS) in the USA provides security guidelines to support the implementation of high security standards for critical infrastructures. While the US and the EU's scholars focus on solutions, it seems that Asian researchers are interested in threats, and needs for cyber security solutions (e.g., a need for a domain specific regulatory framework in India [15]).

Standards. Standards (including frameworks and models) have been categorized into two types: Standards in general (e.g., Cyber security assessment [16]) and specific standards for a system (e.g., SCADA system cyber security standards [17]). Scholars discussed security assessment techniques [16], such as reviews passive, vulnerability identification, and vulnerability analysis (e.g., IEC 62351, IEC 62443, IEC 62056-5-3, ISO 15118, ISO/IEC 27019). Literature also discussed particular standards for a specific system, such as SCADA system [17].

Humans. Literature indicates that human behavior is considered one of the important factors in cyber security in energy informatics [18]. Two main issues of human factors have been discussed are roles of human failures in security, and cyber security leadership. For example, the security of smart technologies in the energy systems cannot rely only on technical solutions; humans play a significant role in failure in cyber security, whether it is intentional or unintentional [19]. Human aspects also include management (c.f., [20]).

Solutions. Solutions for cyber security in energy informatic include issues related to risks [21], challenges [22], and solutions [23]. Risk topics include risk assessment of power information control systems [24], energy internet, digital secondary substations, renewable energy, smart grids, physical systems [25], and economic risk [26]. Challenges in smart grid include, for example, hyperphysical challenges in smart grid, information security and privacy challenges, technology challenges (AI, big data, IoT) [27], and communications [28]. Solutions include solution in general, solution in cyber security in smart grid, and solution in cyber security in physical system [29].

Conclusion and Outlook

We have retrieved seven non-technical issues on cyber security in energy informatics, they include education, awareness, policy, geography, standard, human, and solution. From these findings, it can be argued that security awareness is one of the important issues in cyber-defense. Energy system devices are gradually replaced by standard IT protocols and commercial-of-the-shelf hardware and software. Energy systems thus do no longer rely on physical and local measures for their operations. We thus suggest that more study in assessments of maturity cyber security awareness in organizations are needed, such as awareness models or frameworks in cyber security in energy informatics.

Future research will focus on synthesizing these findings to benefit not only researchers, but also managers, policy makers, and educators. For example, identifying socio-technical gaps in the context of digital transformation [30] could help measures on preventing cybercrimes in a holistic way in cyber security in energy informatics.

Author's contributions
D.D. designed, conducted, analyzed, and drafted the manuscript. T.V. discussed and commented on the manuscript. M.M. commented on the final draft of the manuscript. All authors have read and approved the manuscript.

Competing interests
The authors declare that they have no competing interests.

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Towards More Findable Energy Research Software by Introducing a Metadata-based Registry

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Summary
Research software in the energy domain becomes increasingly important to analyze, simulate and optimize energy systems and, therefore, supports the required transition of energy systems as important part to tackle the climate crisis. To make energy research software more findable, it should be described with metadata following the FAIR (findable, accessible, interoperable and reusable) criteria and be registered in a common registry. Within the doctoral research project, a metadata schema to describe energy research software and an according registry will be developed. With these artifacts, the software gets easier to find and, thus, its reuse is supported.

Introduction
In energy research, self-designed software is a basic tool for multiple purposes like the visualization of processes and values, e.g., power quality, the (co-)simulation of smart grids or the analysis of transition pathways. Within a typically exemplary research cycle, this self-designed software is often a starting point and, therefore, fundamental for producing new research results while it also presents a research result by itself (see Figure 1).

Energy research software (ERS) can be defined as software that is employed in the scientific discovery process to understand, analyze, improve and/or design energy systems. Software-wise, ERS ranges from simple scripts over libraries (e.g. for python) up to full software solutions. Content-wise, it can for example visualize, analyze and/or generate (artificial) data from energy (sub-)components or grids in laboratories or the real world. Alternatively, it can also represent particular energy (sub-)components, energy (distribution) systems and transition paths of energy use, distribution, conversion, and/or generation to analyze the design and/or control in simulations and optimizations. The increased need for ERS led to the development of multiple models and frameworks partly with overlapping scope coming from different subdomains. Often new tools are developed without reusing the already existing ones while ERS becomes even more complex in the upcoming years [1]. Therefore, a lot of time is spent on (re)developing software instead of doing research slowing down the progress in research.
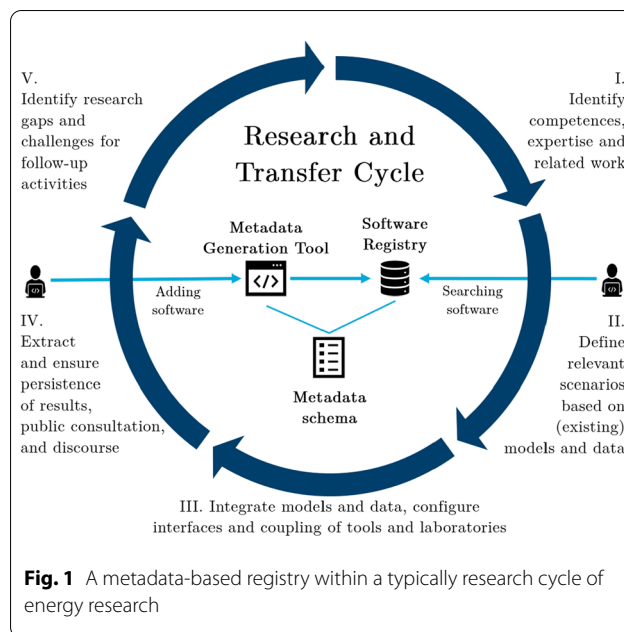

Fig. 1 A metadata-based registry within a typically research cycle of energy research

Different approaches to formulate the FAIR criteria for research software show that metadata and repositories for these metadata, software registries, are key elements for FAIR research software [2, 3, 4]. Especially the findability of ERS can be increased by describing it with useful metadata and registering it into a registry. This is a first step for increasing the reuse of ERS and improving the research process.

Therefore, three different artifacts (see Figure 1) with separate requirements are proposed. A metadata schema for ERS should be usable for all different types of ERS to increase their findability and is the foundation for the other two artifacts. A metadata generation tool should support researchers to create high-quality metadata for their ERS. It should lower the entrance barrier for creating metadata for all researchers in the energy domain without the need for a deeper understanding of the underlying technologies. A registry for ERS should help researchers to find the right software based on multiple search criteria.

The requirements for the three artifacts lead to multiple relevant research questions (RQs). Within this doctoral project, the following RQs will be focused:

- RQ1: Which metadata elements are required to enable a useful classification and description of ERS to make it more FAIR and which elements from existing metadata schemas are suitable to be reused to describe ERS?
- RQ2: Which domain-specific ontologies can be used as a value vocabulary for describing ERS?
- RQ3: How can additional input information like keywords or already used software be used to improve the search results when looking for ERS?

Approach

A four-step approach for the doctoral project is formulated to address the research questions. The first two steps focus on creating an application profile as metadata schema and follow the method of Curado Malta and Baptista [5].

The goal of the first step is to develop a domain model. Therefore, first, requirements will be defined following the approach of Curado Malta and Baptista [5]. Semi-structural interviews will be performed to analyze which metadata elements are required for users of the search service. From the interview results, use cases will be formulated. In parallel, an environmental scan [6] will be started to analyze existing

approaches, like general work on metadata for research software, e.g., CodeMeta[2], and domain-specific developments like the metadata schemas of the Open Energy Platform[3]. The domain model will be developed based on these requirements and the first results of the environmental scan. It will contain desired elements with short descriptions, examples and their relations. These elements and their description will be formulated in English to be available to the international research community. The domain model will address RQ1. It will be tested with different developers of ERS who will also be asked for requirements for the metadata generation tool.

In the second step, a description set profile will be developed. Therefore, the environmental scan will be extended to determine if elements (described in RDF) can be reused addressing RQ1 as part of a state of the art report [5]. For each element, it will be specified if it is mandatory or optional and if constrains exist, e.g., if the use of a controlled value vocabulary is required or not. Especially for the domain specific elements, value vocabularies will be used. It will be carefully analyzed if one or multiple ontologies, like OEO [7], can be integrated as value vocabulary to address RQ2. The description set profile will be formalized and encoded to be used by the registry and the metadata generation in the following steps.

In the third step, a registry for ERS will be implemented. This development will start from existing frameworks, like the one of bio.tools[4] [8]. The registry will be based on the new developed metadata schema for ERS and will support an extensive search functionality based on semantic web technologies, e.g., based on already used software. This feature will be analyzed in depth to address RQ3 by primary testing with manually created metadata.

In the fourth and last step, a tool to assist researchers with creating metadata will be developed. It will support the use of controlled value vocabularies as defined in the specification of the metadata schema and will allow to integrate additional ontologies to include many links to other semantic web sources like DBpedia[5]. Additionally, the tool will be able to automatically extract many metadata from existing software repositories like GitLab. With this tool, many entries in registry will be created allowing it to evaluate the registry and the metadata schema. Tools like the one for Geoscience by Garijo et al. [9] and the one for EngMeta [10] will be used as starting point.

Conclusion and Outlook

ERS needs to be described with more metadata stored in a common repository to improve the FAIRness and the overall findability of research software in the energy domain. This doctoral proposal focuses on the development of a **metadata-based registry for ERS** to enable this process.

By learning from other domains and analyzing the special requirements from the energy domain, a metadata schema, a registry, and a metadata generation tool should be constructed. Therefore, four steps are planned: determination of a domain model based on a requirement analysis, definition of a formalized metadata schema including domain ontologies as controlled value vocabularies, development of a metadata registry based on the formalized schema including advanced search functionality and creation of a metadata generation tool to support researchers in creating useful metadata based on the formalized schema.

As future work, a detailed requirement analysis will be performed as basis for the domain model.

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Author's contributions
The literature review as well as the formulation of the approach were performed by the author during his doctoral project.

Competing interests
The author declares that he has no competing interests.

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S50

Grid- and market-oriented integration of flexible prosumer households into the energy system

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Summary
Energy management systems (EMS) in households can contribute to the efficiency and stability of the energy system if they receive information from the relevant actors. This includes the volatile supply of renewable energy and the distribution grid load. In addition, household

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residents have to get incentives to provide flexibility from devices like battery electric vehicles, heat pumps, or stationary batteries, as providing flexibility can result in different levels of comfort loss. In order to convey both information and incentives to EMS, price signals are suitable. To incentivize the balancing of renewable energy fluctuations, time-varying energy prices are an obvious instrument. Avoiding distribution grid congestion requires a reliable limitation of power at the grid connection point. To implement this power limitation in the form of a price signal, energy prices are only suitable to a limited extent. For this purpose, a grid fee can be defined that is both power- and time-dependent, making it very unattractive to exceed a power limit at the grid connection point at certain times of potential grid overloading, but avoiding the need for external control of household devices. The goal of the doctoral project is to concretize and evaluate these time- and load-dependent price signals as a way to better integrate residential EMS into the energy system. Therefore, those price signals, generated by electricity suppliers and distribution system operators, should reflect both electricity grid and market situations. In addition to the regulatory framework conditions, meaning the unbundling of the energy market and grid operation, it must be taken into account that the aforementioned goals can be contradictory.

Motivation

Households with photovoltaic (PV) power plants and flexible devices like electric vehicle (EV) charging equipment, heat pumps and/or stationary batteries can be called flexible prosumer households. Often, they are equipped with energy management systems (EMS) that control devices in order to maximize self-consumption of their solar generation. However, this optimization objective does not exploit the full potential of flexibility that those households could provide to the electrical energy system. In the context of the energy transition, two purposes of flexibility gain significance: The first one is the balancing of the residual load, meaning the electricity demand minus the generation from volatile renewable energy sources (VRE), namely wind and solar power power plants. One of the most important mechanisms to balance the residual load is the trading on spot markets. Therefore, passing spot market results to customers, which some suppliers are already doing, is a market-oriented integration of households into the energy system.

Independent of that, as the heating and transportation sectors are being electrified and an increasing number of PV power plants feed into the low-voltage grids, it becomes increasingly important to limit the power drawn from or fed into the grid reliably. This is called grid-oriented flexibility. Grid- and market-oriented flexibility can also be contradictory, due to different system boundaries and - due to an unbundled energy market - also different actors. Furthermore, market signals can put additional strain on the distribution grids due to herding effects, meaning the simultaneous load increase at the price minimum [1]. While more flexible devices and PV systems are being installed, a potential conflict of interest is emerging: Distribution system operators (DSOs) probably need a way to reliably limit the power of households so that grid expansion requirements do not become too high. Suppliers, on the other hand, would like to take advantage of their customers' flexibility to use cheap electricity from renewable sources when it is available on the market and lower the energy demand during a high residual load. Both can result in lower electricity costs for households, but only if EMS get the necessary information in the form of price signals. These signals must adequately address both grid and market views. The contribution of this doctoral project is the concretization of overlapping grid and market signals for decentralized EMS in households.

Related Work

Possible regulatory concepts to solve the described potential conflict are compared in an own publication [2]. Direct control by the DSO, dynamic grid fees, quotas, and flexibility markets are compared with respect to their reliability, complexity, acceptance, and macroeconomic effects. The existing literature provides studies on further development of the regulatory system. The authors of [3] model the effects of a reformed regulation on the power demand of grid users, but declare concrete implementation possibilities of grid- and market-oriented incentives to be subject of further research. Gottwalt states in his thesis

[1] that a power-based surcharge can counteract herding effects, which is a basis for the concept presented here. The authors of [4] discuss load-oriented grid fees and point out the need for research especially in the interaction with the electricity price signal. The effects of grid- and market-oriented EV charging as a major provider of flexibility in households is investigated by Uhlig [5] who assumes a central charging management system instead of incentive signals. Fattler [6] examines optimized charging for different purposes, meaning either grid- or market-oriented optimization and states that its combination to be subject of further research. It can be seen that often either market- or grid signals are considered or a central controlling instance is assumed.

Concept

The concept for overlapping grid- and market signals is visualized in Figure 1 and can be described as follows: Electricity suppliers send a dynamic energy price to their customers that is based on stock market results (1). Some suppliers are already doing this today. Based on stock market results, weather forecasts as well as information about flexibility options of its grid users, the DSO sends time- and load-variable grid fees to all grid users (2). Those define a considerable price for exceeding a certain power limit at a certain time. Accordingly, the grid fees here do not represent a further energy price that is simply added to the supplier's energy price. Rather, they define a grid restriction in the form of a maximum power profile at the grid connection point that can be exceeded at the cost of higher charges. The goal is to parameterize those grid fees in a way that grid users only exceed the power limit if adhering to the limit would mean considerable losses in comfort. Those market- and grid-signals would define framework conditions for the prosumer on a daily basis with an hourly or quarter-hourly resolution. It also has to be investigated if those signals have to be updated during the day. The focus here is a low-voltage grid segment, starting with an equal grid signal for all grid users. Grid signals have to be parameterized in terms of an adequate power limit, the price for exceeding the limit, and time spans of the limitation.
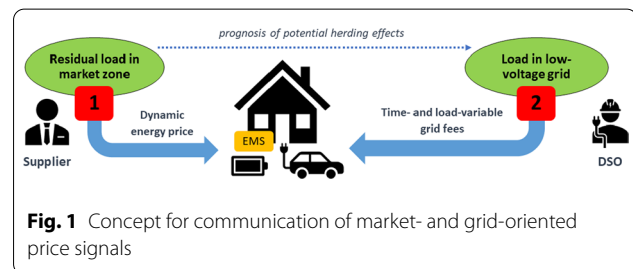

Fig. 1 Concept for communication of market- and grid-oriented price signals

Research questions

the investigation of the described concept is guided by the following research questions:

- RQ1: To what extent are spot market prices suitable for incentivizing flexible prosumer households to minimize the residual load and what is their contribution to do so?
- RQ2: How would time- and load-variable grid fees have to be designed and parameterized to satisfy the potentially opposed requirements of grid users and actors in the energy system?
- RQ3: How can grid operators define and communicate load-variable grid fees that satisfy the criteria of the previous question?
- RQ4: Given the elaborated market- and grid-oriented signals, what is the potential contribution of flexible prosumer households to the security of supply?

Methodology

The data sources to answer the given research questions are electricity system and market data provided by ENTSO-E and EPEX as well as collected data from a field test in the research project *SynergieQuartier* [7]. In the given field test, data of charging stations, PV plants, heat

pumps, batteries as well as the inflexible power demand of 30 prosumer households is being recorded. The participants get a dynamic tariff based on EPEX market prices, according to which they are actually billed during the field test duration if there are savings for them compared to their previous constant tariff. Therefore, user behavior can be observed, while the effects of an EMS that reacts on grid- and market-oriented signals are simulated as part of the doctoral project. The optimized power at the grid connection point of each household is being used as input for a low-voltage grid model that is implemented by using the framework *pandapower* [8]. By modeling relevant actors in the energy system - households, suppliers, and grid operators - the design and parameterization of the described concept can be evaluated based on their requirements and costs.

First Results and Outlook

First simulations of charging processes show that optimization towards exchange prices is suitable to not only lower the charging costs but also increase the share of VRE of the energy charged. However, by using the residual load itself instead of exchange prices, the share of VRE becomes higher. Related to RQ1, this indicates that passing on EPEX day-ahead prices to households has similar effects as passing on the predicted residual load itself. However, the effects are not the same, since exchange prices are also influenced by other factors. The simulation also shows that variable energy prices are not sufficient to avoid charging with high power during the highest residual load, as the residual load can remain close to its maximum for many hours. The next steps are modeling and optimization of more flexible devices in households, collecting more field test data, and modeling the relevant actors in the energy system to parameterize the described concept.

Availability of data and materials

Not applicable.

Competing interests

The author declares that he has no competing interests.

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Summary

The increasing digitization in power distribution grids leads to a more complex overall system, but increases the monitoring and control capabilities for active grid operational management. In the future, malfunctions of Information and Communications Technology in the process network can have a direct impact on grid operation and thus on the reliability of the power supply. In this paper, a methodological approach to evaluate resilience for cyber-physical distribution grids in case of disruptions in the process network is presented. The basis of this is a co-simulation environment for power grids and process networks which can be used to evaluate existing process networks and their expansion possibilities.

Keywords: Co-Simulation; Cyber-Physical Power System; Resilience

Introduction

Current developments in power supply make an increasingly active operational management at the distribution grid level essential [1]. This leads to a growing need for communication, which is being met by the increased digitization and thus integration of Information and Communications Technology (ICT) in the distribution grid to achieve a sufficient level of grid transparency and the ability to control the relevant assets [2]. The domains of Energy Technology (ET), Operational Technology (OT) and Information Technology (IT) become equally significant for reliable operation and data aggregation in all domains and data exchange between these domains is required. This is accompanied by cross-domain interactions that must be considered when analyzing the reliability of such a system [3].

Operational management is becoming increasingly dependent on the ICT used and malfunctions of IT (e. g., switches, firewalls) and OT (e. g. Remote Terminal Units (RTUs), Intelligent Electronic Devices (IEDs)) can have a direct impact on the security of supply. This makes it necessary to introduce preventive measures against ICT failures and cyberattacks, which include, for instance the expansion of monitoring capabilities and intrusion detection systems [4, 5]. Nevertheless, malfunctions of ICT can never be completely prevented and potential impacts should be assessed on the one hand and mitigated as far as possible on the other hand to achieve resilient operation of the overall system. This requires a structured definition of possible malfunctions in the process network and their potential effects as well as realistic test environments that enable the cross-domain interdependencies to be analyzed in the sense of a cyber-physical system.

Problem Statement

The scope of this work is to provide a methodology to make the resilience in the event of disruptions in the process network of cyber-physical power distribution grids evaluable and comparable. This work can be utilized to evaluate resilience of existing process networks when operational management is increasingly dependent on ICT, and it can serve to compare different options for process network expansion or adaption using qualitative metrics. Consequently, the following research questions will be addressed in the context of this work:

- RQ 1: What models and modeling depth are required to map the interactions during ICT disruptions between the aforementioned domains ET/IT/OT?
- RQ 2: How can process networks be compared in terms of their resilience and which metrics are suitable for such a comparison?
- RQ 3: How can measures for process network expansion or adaption be identified that effectively increase the resilience of cyber-physical power distribution grids?

Related Work

In the field of mutual simulation of power grids and ICT, various approaches exist that usually pursue a specific investigation objective in terms of impact of cyberattacks, malfunctions, or infrastructure design for monitoring and control applications [3]. Happ (2020) [6] presents a scalable, agent-based simulation environment for cyber-physical power systems with control logics. In Veith et al. (2020) [7], a software/in/the/loop approach for co-simulation is proposed to enable prior testing of software rollouts for smart power systems. Wermann et al. (2016) [8] use a co-simulation framework to enable the mapping of cyberattacks for vulnerability analysis in smart grids.

Concerning the development of metrics for resilience assessment and the design of resilient infrastructures, mainly conceptual approaches are available in the research landscape, but there has been a lack of standardized metrics to describe resilient operation [9, 2]. Drayer (2018) [10] conceptually investigates to what extent distributed/hierarchical architectures can contribute to resilience in an automated operation of distribution grids. Hammad (2018) [11] proposes resilient/by/design approaches for microgrids, focusing on impacts on transient stability in the event of cyberattacks. Das et al. (2020) [2] survey available qualitative and quantitative metrics that could potentially be used to assess smart grid resilience.

However, there is no comprehensive approach that practically implements the resilience assessment for process networks and applies it to specific cyber-physical distribution system topologies in the context of a cross-domain simulation.

Methodology

Consequently, within this work an environment for the simulation of disruptive events in the process network of active distribution grids is developed. An overview of the methodological approach combining the generation of scenarios, a co-simulation environment for power grids and process networks as well as the resulting assessment of the resilience of the simulated infrastructure in a novel manner is shown in Figure 1.
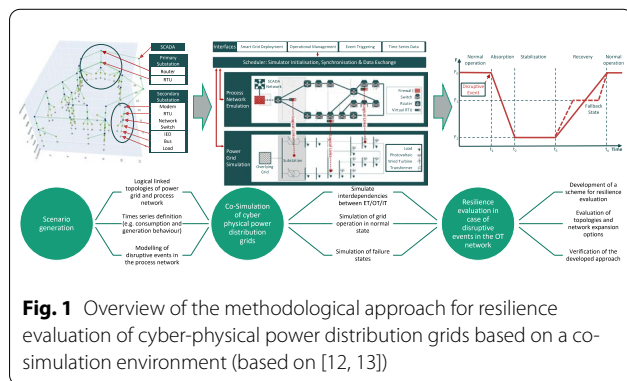

Fig. 1 Overview of the methodological approach for resilience evaluation of cyber-physical power distribution grids based on a co-simulation environment (based on [12, 13])

Scenario Generation. To be able to simulate realistic topology sizes, one goal has been the widely automated execution of large-scale scenarios. Open-source benchmark data sets of high and medium voltage topologies are to be used on the power grid side. While this data is publicly available for power grids in large numbers, this is not the case for the associated process network topologies. Therefore, we use a graph-based approach to generate the process network corresponding to a power grid [12]. Based on a previously defined rule set and the ET components of the given power grid, the process network topology (e.g., including RTUs and information about the OT protocols used) is gradually created. An exemplary output graph based on a medium voltage topology is shown in Figure 1 on the left.

Co-Simulation. These topologies are part of the input data for the co-simulation, of which the structural design is shown in the middle of Figure 1. The functional requirements, analyzed in detail in [13], account for the fact that both the power grid and the process network and their interdependencies must be simulated. Also, there must be the ability to map component-specific failures that can occur due to malfunctions as well as cyberattacks. We use a static power flow simulation representing the power grid, while we can deploy the emulated components of the process network using a container-based network emulation method. Both simulators are connected through a scheduler using step-based synchronisation. We use a self-developed virtual remote terminal unit (vRTU) that allows the use of typically used OT communication protocols (IEC 60870-5-104, Modbus) and the mapping of an internal logic, which can be used, for example, to logically link several internal data points.

Resilience Evaluation. The simulation results enable the application and the comparison of different methods to evaluate the resilience against disruptions in the process network. Resilience in general is defined as the capability to absorb, adapt to, or recover rapidly from a disruptive event and maintain ongoing operation (cf. right side of Figure 1) [9]. In this work, disruptive events are considered exclusively on the ICT side in the process network of cyber-physical power systems, which can be failures or limitations in the functionality of specific components. Targeted disruption through cyberattacks is another form that is taken into account. Suitable frameworks in terms of threat modeling are available for structuring these type of events, and they are mapped as single- or multi-stage events within the co-simulation (see [5]).

With regard to maintaining ongoing operation, the primary criterion is the continued supply of all participants on the grid or – in case of outages – the recovery time from supply failures. In addition, other criteria such as compliance with voltage and current limits can be considered on the ET domain. The consequences of disruptive events can also be assessed directly in the IT and OT domain. Thus, the maintaining of the grid operator's monitoring and control abilities must be ensured. In the future, a suitable method for resilience assessment can also be used to make different options for adaptions in the process network comparable.

Conclusion and Outlook

In this paper, a methodological approach based on a co/simulation environment is presented to enable investigation of process network resilience for cyber/physical power distribution systems. For this purpose, a simulation of the power grid, an emulation of the process network and the interdependencies between both systems are mapped within the co-simulation environment. Furthermore, the focus is on the appropriate modeling of the necessary input data for the simulation, which includes in particular information about the process network topologies and the structured mapping of ICT malfunctions and cyberattacks. The next steps are to utilize the simulation environment to apply and compare existing concepts and metrics for resilience assessment in the research landscape to identify a suitable assessment scheme.

Competing interests
The authors declare that they have no competing interests.

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ISoLATE: Integrated distributed SCADA security through local approximations of power flow equations

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Abstract

To ensure a safe and secure operation of electricity grids now and in the future new security measures have to be developed. Many existing security solutions are either only centrally applied at the SCADA server or do not focus on the underlying physical process. This project investigates distributed, process-aware intrusion detection for electricity grids. We research how knowledge about the physical process can be integrated into a decentralised intrusion detection system (IDS). Further, we present an implementation of the IDS using secure, separated communication channels, and a corresponding testbed including an attack tool.

Keywords: Intrusion Detection; SCADA network; process awareness

Introduction

The ongoing energy transition does not only affect the way the electricity grid is produced and operated, but also requires full integration of information and communication technology (ICT) within Supervisory Control and Data Acquisition (SCADA) networks. In Figure 1 an overview over an electricity grid and its SCADA network is given. Until the 2000s *"security through obscurity"* has been the major security paradigm in this context [1]. Now that interconnectivity between (field) devices, remote access and commonly used protocols play a larger role, additional vulnerabilities are introduced to the grid. In that sense, it is now more lucrative to e.g. develop hacking tools with the energy sector in mind. Because of the underlying physical layer and its hard boundaries regarding space- and time complexity as well as real time requirements, solutions from normal ICT security cannot be directly applied here. Approaches of Intrusion Detection Systems (IDS) for electrical grids include a) specification based (e.g. [2]), b) behaviour based (e.g. [3]) and c) anomaly based (e.g. [4]) approaches. Even though machine learning has been successfully applied to network intrusion detection in general [5], in case of electricity grids this is not yet that common (exceptions are e.g. [6] and [7]). Another widely applied measure, to identify whether a manipulation was conducted within the grid, is *state estimation* (SE). In SE, available measurements are used

to calculate the system state [8]. The calculated state is then used to cross-check if the measurements received from the system are consistent all together. One short coming is that this method relies directly the assumption that the data has not been manipulated beforehand. Since the communication protocols used within the SCADA network are not necessarily secure, this assumption is not correct. It has been shown that the overall state can be manipulated in a way that it remains consistent without being detected by these approaches [9]. A possible mitigation to this problem was proposed in a recent line of work done by Chromik et al. ([10, 11, 12, 13]). The work follows a process-aware approach and evaluates local data directly against various physical and safety requirements. By doing this, the IDS is able to detect manipulations before the normal SCADA communication happens. In this project, the approach from Chromik et al. is lifted from a pure local view to a broader, distributed view of the electricity grid and its topology. The prototype implementation of distributed IDS presented in [14] is improved to use separate, secure communication channels and the testbed is advanced with a designated attack tool.
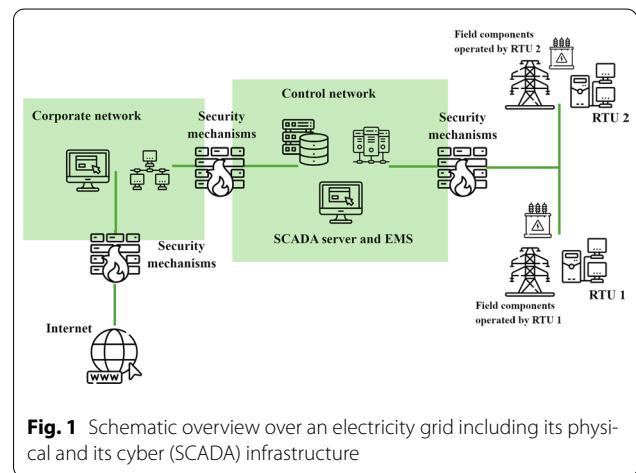

Fig. 1 Schematic overview over an electricity grid including its physical and its cyber (SCADA) infrastructure

Methodology

The proposed IDS supervises the current state of the electricity grid, based on a electricity grid model proposed by Chromik et al. in [12]. Along with the model, Chromik et al. defined a set of physical and safety requirements, which cover basic physical laws (e.g. like Kirchhoff's Law) and desired properties of the grid (e.g. a reference voltage). Those requirements are checked for a given state of a specific electricity grid. Violations of requirements are considered a fault and a potential attack. This model was adapted in [14] to cover a distributed setting: Instead of supervising a complete electricity grid, the grid is split into smaller parts, so called *subgrids*, which are connected through *border regions*. Along with the grid model, the physical and safety requirements are also adapted to the distributed setting. Concretely, three *scopes* of requirement evaluation are formed: *local* evaluation within a *subgrid*, *neighbourhood* evaluation within the *border region* between to subgrids and *global* evaluation, which requires knowledge about the complete grid. The distributed IDS works with so called monitors, which evaluate the requirements according to their matching *scope*. As the local monitors (LM), i.e. the monitors evaluating the *local* scope, are directly deployed at each subgrid (e.g. a field station), local communication of the sensor data is possible directly, without the need to use the normal, potentially insecure, communication infrastructure of the SCADA network. The LMs communicate the data received from their subgrid to the neighbourhood and global monitors via an additional secure communication channel, that is independent of the normal SCADA traffic.

Results

Testing the IDS on a real SCADA network of an electricity grid is in general not possible. Chromik et al. developed a testbed using the co-simulation framework MOSAIK [15], therefore this testbed was adapted to

fit the requirements of the new, distributed setting. Through the test-bed we can ensure that the capabilities and limitations of the proposed IDS are well understood before adapting it for real world experiments. The communication implemented within the distributed IDS should not only be encrypted, e.g. via Transport Layer Security (TLS), but also have an authentication system to prevent malicious parties from falsely identifying as one of the monitors or executing Man-in-the-Middle (MITM) attacks. To directly communicate information as soon as it is available instead of pulling for new data a push-based data flow should be used to ensure real-time capability. In consideration of these requirements, we selected the OPC Unified Architecture (OPC-UA) [16] and adapted the IDS implementation presented in [14] to use OPC-UA. Further, we developed an attack tool to start predefined (distributed) attack routines against the testbed. The attack tool directly connects to the Modbus server of the field stations within the testbed, simulating the attacker's ability to get into the internal communication channels at the field stations. The user can inspect the sensor data to generate comprised and yet plausible data sets and execute attacks against the testbed. An exemplary screenshot of the current IDS implementation and the attack tool is given in 2.
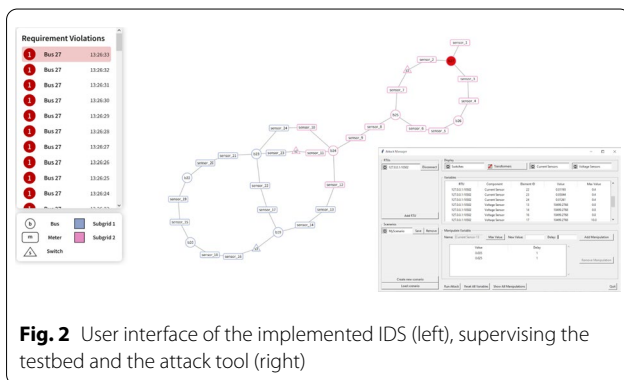

Fig. 2 User interface of the implemented IDS (left), supervising the testbed and the attack tool (right)

Conclusion and Future Work

Electricity grids need to be better protected against cyber attacks as new challenges and attack vectors recently have arisen. In this work, an IDS is proposed to detect stealthy sensor attacks and command manipulations within the SCADA network operating electricity grids. Therefore, the local, process-aware approach presented by Chromik et al. was lifted to supervise *neighbourhoods* of field stations using a secure and distributed infrastructure. Further, an attack tool was developed to deploy more elaborate and repeatable attacks against the testbed infrastructure, which remain a coherent state locally. Future work aims to, (1) include power flow equations to enhance the plausibility checks within the IDS and, (2) conduct field tests both on the smaller scale of the living laboratory parking lot at the University of Twente as well as on the larger scale with our industry partners.

Author's contributions
The literature research, the adaption of the electricity grid model, the adaption of the IDS beyond the local approach and for the distributed setting as well as the adaption of the testbed and the new IDS implementation were all performed by the author during her doctorate. The author supervised, instructed and contributed to the implementation of the separate communication channels within the IDS and the attack tool as part of a Bachelor and Master course in Computer Science at the Westfälische Wilhelms-Universität, Germany.

Competing interests
The author declares that she has no competing interests.

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Taxonomy of Local Flexibility Markets

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Abstract

Flexibility has risen as a potential solution and complement for system operators' current and future problems (e.g., congestion, voltage) caused by integrating distributed renewable resources (e.g., wind, solar) and electric vehicles. In parallel, local flexibility markets (LFM) emerge as a possible smart grid solution to bridge between flexibility-seeking customers and flexibility-offering customers in localized areas. Nevertheless, there is no unique, standard, or simple solution to tackle all the problems system operators and other energy actors face. Therefore, many local flexibility market concepts, initiatives (projects), and companies have developed various solutions over the last few years. At the same time, they increased the complexity of the topic. Thus, this research paper aims to describe several local flexibility market concepts, initiatives (projects), and companies in Europe. To do so, we propose a taxonomy derived from LFMs descriptions. We use the taxonomy-building research method proposed by [1] to develop our taxonomy. Moreover, we use the smart grid architecture model (SGAM) as a structural and foundation guideline. Given the numerous and diverse LFM solutions, we delimit the taxonomy by considering solutions focused on congestion management on medium and low voltage (meta-characteristic).

Keywords: Local Flexibility Markets; SGAM; Taxonomy; Congestion Management

Introduction

Smart grids in power systems are growing, driven by decentralization, decarbonization, and digitalization trends [2]. Examples of these trends are the integration of distributed energy resource (DER) and electric vehicle (EV) or the massive data created by metering devices (i.e., smart meters). Flexibility is becoming an essential part of current and future energy systems in modern power systems. Notably, they complement traditional solutions to tackle typical power system problems (e.g., congestion, balancing, voltage, grid expansion) caused, for example, by the integration of DERs and EVs. For the most part, DER, particularly renewable sources, located on medium voltage (MV) and low voltage (LV) voltage networks, will provide flexibility. Consequently, the focus shifts to local distribution areas, where the Distribution System Operator (DSO) operates and challenges their planning and operation.

Thus, a rising concept considering the trends and their challenges; and local flexibility as a partial solution over the last years, and even pushed by adaption of the Clean Energy Package (CEP) (i.e., Regulation (EU) 2019/943, Directive (EU) 2019/944), are local flexibility market (LFM). LFM capitalize on asset data extraction and control to provide services at the local area level. The services offered by LFMs can go beyond typical DSO and transmission system operator (TSO) services. An example beyond service is, enabling and managing local energy trading among peers (Peer-to-peer). Consequently, numerous LFM concepts arose within the last five years. For example, Nodes deployed their LFM in several countries (e.g., Norway, Germany, Portugal, Canada, Finland, and the United Kingdom), adapting to their needs [3]. Another example is the Gopacs platform [4] launched as an initiative by Dutch grid operators. However, the associated literature body is also growing considerably [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]. Nevertheless, to date, literature on LFM focuses mainly on clearing algorithms, services development, payments, and trading. Still, one crucial point, the system architecture used to implement these concepts, is not yet fully explored.

Thus, as solutions and literature grow, a description gap can help developers, regulators, and system operators understand the different solutions the market and research offer. Furthermore, as solutions grow, it is inevitable to ask from a research perspective: what are the local flexibility markets archetypes?

The associated benefits of understanding LFM architectures can bring many benefits to developers but especially to both system operators, the TSO and DSO. These benefits are, for instance, to enable the clear identification of LFM scope, what are the main smart functions these LFM bring, clarify which components are necessary for operation, and who owns them and their location or how these components might communicate. There is a mix of what LFM functions currently provide. These solutions involve several stakeholders, not always present in all LFM concepts. Moreover, different LFM solutions implement divergent logic (i.e., coordination of DSO-DSO; DSO-TSO; DSO provision, TSO provision, Peer-2-Peer, etc.). Overall, the topic of LFM is growing fast and encompasses many subtopics challenging its comprehension.

To bridge the description gap and contribute to the research question from a holistic system perspective, we develop a LFM taxonomy. To develop the taxonomy, we use the iterative taxonomy building method proposed by [1]. Moreover, we use the Smart Grid Architecture Model (SGAM) as a structural and foundation guideline since LFM are smart grid solutions.

Research approach

Arguably, a complete taxonomy of all LFM depends on the level of abstraction. Consequently, we establish the level of abstraction and narrow down the scope by focusing on (1) European developments, (2) congestion management, and (3) medium and low voltage solutions.

Taxonomy building method

We follow the taxonomy building method proposed by [1]. The authors proposed an iterative method for creating a taxonomy, where the meta-characteristic selection sets the taxonomy's scope. The taxonomy's end product (i.e., artifact's structure) contains a set of dimensions (variable), containing each dimension a set of characteristics (possible values of a variable) such that when considering an object (a LFM) has only one characteristic for each dimension. Additionally, we consider the suggestions provided by [16] to develop taxonomies. Concerning the iterative part of the method, the authors include two types of iterations. On the one hand, the empirical-to-conceptual iteration describes how the researcher should first identify the set of objects to classify and then identify common characteristics among these objects. To identify the objects, the authors in [1] recommend a review of the literature using sampling techniques such as random, a systematic, a convenience, or some other type of sample. On the other hand, in the conceptual-to-empirical approach, the research does not examine actual objects but conceptualizes the dimensions. Therefore, this approach is deductive and complicated since it requires experience.

To develop the taxonomy we propose, we aim to use both iteration approaches, empirical-to-conceptual and conceptual-to-empirical. For the empirical-to-conceptual approach, we use scientific, and grey literature available online as previously exposed [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]. Furthermore, in the empirical-to-conceptual approach, we might consider a set of interviews with several power system experts; company experts already providing LFMs solutions [17,18,3] and other energy experts (subjective). These interviews might assist us to (1) refine and include aspects to the taxonomy that literature or project's description might not include and (2) hit the ending conditions when multiple interviewees add no further details. For the conceptual-to-empirical we initially aim to use previous experience from internal European Union (EU) projects (e.g., InteGrid [19], InterFlex [20], SynErgie [21]), grey literature (e.g., public deliverable) and scientific literature (e.g., [22]) to conceive the taxonomy and identify the first characteristics and domains.

Smart Grid foundations

Energy systems and pointedly smart grids are complex since they encapsulate many aspects. For instance, the smart grid application of LFMs deals with business, regulatory and technical aspects (components, communications, information, and functions). Therefore, to guide the taxonomy in the complex world of smart grids, we would like to use the SGAM [23] as a foundation for developing the taxonomy. The SGAM provides a standard structure for describing smart grid projects and applications, including almost all aspects. The SGAM could endow the taxonomy with a helpful structure already used in smart grids and thus, increase its usefulness. The SGAM interoperability layers (component, communication, information, function, and business) could assist in identifying better characteristics and dimensions within a specific interoperability layer.

Conclusion

This paper project is in its early stage, and thus, we might not be able to assess the conclusions fully. Nevertheless, the taxonomy might enable energy actors to identify their LFM "archetype" in a clear and structured manner. Additionally, it might bring associated business and development advantages to several actors in the energy and, specifically, in the smart grid industry, such as system operators, regulators and policymakers, and even service providers (developers). System operators might benefit from having a taxonomy to understand the LFM potential impact on their current and future systems. Likewise, regulators and policymakers might benefit from the taxonomy to identify archetypes of LFM that might require different regulations for their possible implementation, for example, distributed ledger technologiess (DLTs) such as Blockchain. Finally, service providers (developers) might also benefit from such a taxonomy as they could use it for clear business development and differentiation between solutions. Additionally, the taxonomy could be material for follow-up research, such as evaluating the taxonomy's usefulness by classifying a couple of LFMs currently available in literature or commercially available.

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Availability of data and materials

Not applicable

Author's contributions

SPM contributed to the design of the work. SPM drafted the first version of the paper.

Competing interests

The authors declare that they have no competing interests.

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Framework To Provide A Simulative Comparison Of Different Energy Market Designs

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Abstract

Useful market simulations are key to the evaluation of different market designs existing of multiple market mechanisms or rules. Yet a simulation framework which has a comparison of different market mechanisms in mind was not found. The need to create an objective view on different sets of market rules while investigating meaningful agent strategies concludes that such a simulation framework is needed to advance the research on this subject.

An overview of different existing market simulation models is given which also shows the research gap and the missing capabilities of those systems. Finally, a methodology is outlined how a novel market simulation which can answer the research questions can be developed.

Motivation and Background

In addition to the necessary expansion of the transmission grid [1] and the increasing relevance of Renewable Energy Sources (RES) and battery storage options, the question arises whether the current market model will meet the requirements of the future. Existing research on Local Energy Market (LEM) and Peer-To-Peer (P2P)-based market concepts show the potential of different alternative market designs [2], but often lacks a comparative analysis through simulation.

A market design in this context can be defined as a set of market rules which clarifies the price clearing, special roles and the flow of money, information and energy as well as the admission and access rules. The operation of the power grid represents a natural monopoly, as the provision of parallel infrastructure is not economically feasible. As a consequence, participants with varying consumption and generation capabilities are connected to the power grid in every possible market. This includes consumers, producers and prosumers. The rules governing the interaction between all market participants are part of the market design which is subject of the comparative simulation.
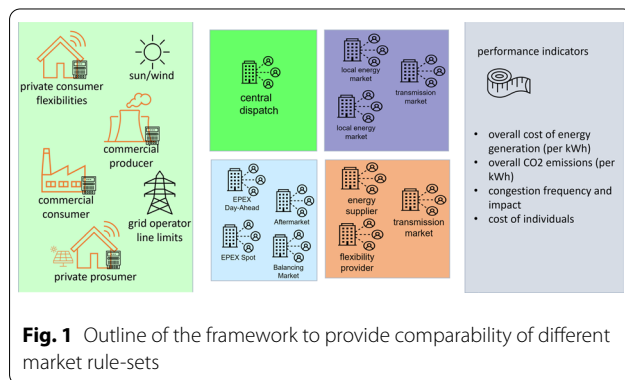

Fig. 1 Outline of the framework to provide comparability of different market rule-sets

The general targets of such a market design, anchored for example in the German EnWG §1, are generally known as:

- security of electricity supply
- economic efficiency
- environmental compatibility

It is of interest, whether a simulation can be done based on a generalized market approach to allow for bench-marking different market rules. This would allow to compare a market with different types of grid fees to Locational marginal pricing (LMP), P2P markets or the current European market design. Agent-based simulations can show the interactive behavior of actual market participants instead of solving for the general market equilibrium.

Research Questions

To investigate different market models and possible behaviors comparably the central research question which will be answered is stated as:

"How can different energy market designs be evaluated in a simulative comparative manner?"

The general input data of a scenario to investigate should be convenient to enter into the model. Further on, generic Key Performance Indicators should be definable in the framework and calculated as a simulation result. A high-level outline of the comparative market simulation framework is shown in Figure 1.

This leads to a refinement of the listed overall research question, which can also be seen as milestones of the project:

1 By which abstract description can market designs be characterized to implement them in software?

2 Can the different market mechanisms successfully be represented in the simulation framework?

3 How can key performance indicators of market mechanisms be applied to evaluate specific market designs through simulation?

The focus lays in the abstraction of different market designs and how those can be simulated with the same framework. The best possible trading strategy of market agents, the most realistic input scenario, as well as finding the best possible key performance indicators will not be the key element of the project, but the integration of those will be made possible based on existing software. Furthermore, trading strategies can be further investigated once a comparative simulation framework is available.

The following section presents which simulation libraries and research already exists in this area.

Related Work

Existing agent-based models of energy systems were analysed and compared with regard to selected characteristics such as

- availability of the sourcecode
- interoperability to other tools
- possibility of distributed computation
- consideration of grid limits and congestion
- comparability of different market designs possible

The consideration of actual grid congestion is often poorly supported, i.e. only based on external timeseries data, or not possible at all. Needed data to calculate the grid congestion is often missing as a simulation input, which is probably a reason why the grid behavior is often not respected in the simulation. Most frameworks have been developed to cover exactly one use case like the ERCOT system [3], Day-Ahead-Market [4, 5, 6] or LEM [7] and can not model different market mechanisms. Other frameworks lack the integration of power flow calculation and can not model dynamic grid fees. The key property of being able to evaluate different market designs is not covered in existing available market simulation software like [8, 9]. This leaves room for a new framework which can be inspired by the existing ones.

Concluding, the majority of existing available models lack a few key features which makes it hard to use them for market comparability. The existing models were developed to study a single market scenario. A generic market modeling approach is therefore not directly possible.

Methodology

To account for the individual risk aversion of traders in a market, an agent-based simulation approach is used. This allows to investigate different game theoretic agent strategies and is therefore more flexible to model real energy market dynamics.

Being able to run the simulation in a distributed manner allows simulating larger scenarios through scalability. On the other hand, a solution with a simple setup routine and low resource requirements is needed to lower the barrier to entry for using the framework. This is also supported by providing a standardized and open-source framework.

A high-level concept is needed to implement an abstraction of different possible markets and provide a framework which covers a wiring between all market participants. Furthermore, the behavior of additional market participants, which only exist in particular cases, must be generically describable in the framework. Such a framework is implemented in the project and furthermore evaluated with regard to the research questions in a design science approach.

Conclusion and Outlook

In this report, an outline of the PhD research topic and a summary of the related work is given. A framework to evaluate different market properties aims to bring a better understanding of the key features of market designs. It can be used to compare different market designs through simulation and reflect changes in agent behavior or strategies.

The next steps include the conception of a generic market description and its implementation to showcase the comparative evaluation of selected market designs by using a set of pre-defined key performance indicators. The framework will then be validated using different scenarios to demonstrate the answering of the research questions.

Availability of data and materials
Not applicable.

Competing interests
The authors declare that they have no competing interests.

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The role of flexibility throughout the decarbonization of the European energy system

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Summary
The successful decarbonization of the European energy system requires a detailed knowledge of the energy systems flexibility and its provision. Since the individual flexibility resources interact with each other in multiple ways, investigating them separately is not feasible. Possible interactions are, among other things, the competitive impact on the market value of one flexibility option by integrating another, as well as synergistic effects for grid stabilization between different sectors or locations. This project aims to analyze these mutual dependencies among different flexibility options throughout the decarbonization of the European energy system. First, the resource allocation of the flexibility resources under explicit consideration of demand-side flexibility will be studied using the open-source energy system model PyPSA-Eur-Sec. Then the resulting PyPSA system models are analyzed in terms of their stability and detailed flexibility provision in presence of emerging flexibility requirements using an envelope-based flexibility model.

Introduction
The change from a conventional to a more sustainable power supply using Renewable Energy Sources (RES) drastically increases the systems variability [1]. Balancing this variability in generation while maintaining system stability is the fundamental challenge of the future sector-coupled European energy system and requires increased system flexibility [2]. Energy system flexibility and its provision become therefore cornerstones of the future energy system. Traditionally provided by conventional power plants in the form of ancillary services, alternative balancing technologies such as dispatchable generation with synthetic fuels, energy storage systems (ESS) or demand-side management (DSM) are increasingly used [3].

Generally, these resources can be characterized based on their technical properties into three main classes, namely, (1) distributed generation, (2) storage units and (3) flexible loads. The new flexibility options open up untapped potentials [4] to balance demand and supply mismatches that are hard to avoid, but their consideration [5] in recent energy system models is still limited. In particular, assessing the interactions of the flexibility resources across different energy sectors along a transformation path is still an open research question [6], as is studying their influence on system stability.

In general, the different flexibility options do not only operate on different time scales (diurnal, synoptic, and seasonal) [7], but are also particularly dependent on the location in the grid. Potential interactions can therefore occur at both temporal and spatial scales and can be either cooperative or competitive in nature. For example, the integration of DSM, as well as increased cross-sectoral electrification, have a competitive influence on the market value of energy storage units and therefore their allocation probability, as both cases lead to a lowered volatility in the residual load [8]. In contrast, the application of power-to-X as long-term energy storage together with the fast dynamics of short-term storage technologies shows synergistic effects in increasing the systems stability against disturbances, such as strong power fluctuations [9].

Within this context, this project aims to study the mutual interaction of different flexibility resources in allocation and flexibility provision throughout the decarbonization of the European energy system.

Related work
Investigating the role of flexibility resources in future energy systems has become subject to many recent research projects in the field of energy system modeling. Victoria et al. [2] analyzed the role of storage technologies throughout the decarbonization of the sector-coupled European energy system. Nebel et al. [10] compared the effects of multiple different flexibility options on the German energy system disregarding the spatial distribution. Heitkoetter et al. [11] determined the flexibility potential of demand response for Germany. And Ruhnau et al. [4] estimated the storage requirements in a fully renewable German electricity system in the presence of extreme events. In general, the current publications have in common that they either use low spatial resolution [10, 11] or solely focus on the role of single flexibility resources as the flexibility providers in a fully decarbonized future energy systems [2, 4], due to which cross-system interactions and interactions with other flexibility resources, particularly DSM, are not sufficiently studied.

In a detailed overview about how different flexibility options are represented in open energy modeling tools Heider et al. [5] shows that the simulation and optimization toolbox Python for Power System Analysis (PyPSA) appears suitable for studying the provision of flexibility over different energy sectors. First investigations by Brown et al. [7] on the synergies of sector coupling in a highly renewable European energy system, stressed their potential to significantly influence total system costs and flexibility provision.
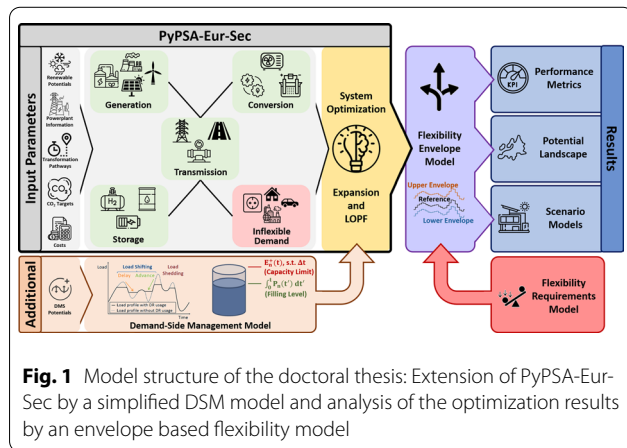
In the literature, several generic models for assessing flexibility are presented, with the best known using envelopes in form of time series [12] or polytopic sets [13] for bounding certain flexibility measures. Nevertheless the use of such a generic envelope-based flexibility

model to assess the flexibility in a large-scale energy system model with respect to spatial constrains is still subject to research [14].

Research questions

This doctoral project aims to address the aforementioned research gap by modeling different scenarios of the European energy system along a given transformation pathway using the open-source energy system model PyPSA-Eur-Sec. The resulting systems are compared based on their resource allocation, their operational flexibility deployment and their stability against emerging flexibility requirements with help of an envelope-based flexibility model. The key questions of interest in this work are the following:

- **Research Question 1:** How do the concepts of flexibility, flexibility requirements, flexibility potentials and flexibility resources relate to each other in terms of flexibility models?
- **Research Question 2:** What is the impact of demand-side flexibility on the storage requirements and resource allocation along the decarbonization of the European energy system?
- **Research Question 3:** What are the resource-specific flexibility potentials and how are they used to ensure balancing of emerging flexibility needs in a future energy system?

Fig. 1 Model structure of the doctoral thesis: Extension of PyPSA-Eur-Sec by a simplified DSM model and analysis of the optimization results by an envelope based flexibility model

Methodology

In order to answer the research questions defined above, the doctoral project will be divided in three consecutive stages. In the first stage, the underlying concepts of flexibility, flexibility requirements, flexibility potentials will be defined from a theoretic perspective, whereas in the second phase, demand-side flexibility will be integrated in the sector-coupled open-source energy system model PyPSA-Eur-Sec [15] as temporal restricted storage units based on results published by Kleinhans et al. [16] and Gils et al. [17]. The resulting model will then be used to study the influence of the impact of demand-side flexibility on the storage requirements and resource allocation along a given decarbonization pathways, similar to the work done in [2]. In the third and final stage, a detailed assessment of the resource-specific flexibility potentials and their deployment will be carried out using an envelope-based flexibility model. The envelopes for this assessment will be generated by comparing the dispatch of a baseline system (undisturbed system) with the dispatch of a system under emerging flexibility requirements (disturbed system). The detailed provision of these flexibility potentials for different categories of flexibility requirements will then be analyzed using flow tracing methods.

Conclusion and outlook

This doctoral project presents an approach to investigate the interactions of different flexibility resources and their flexibility provision in presence of flexibility requirements throughout the decarbonization of the European energy system. In contrast to the recent literature, the focus is placed on the spatial distribution of the flexibility provision and the cross-sectorial interactions between different flexibility resources using a generic flexibility envelope model.

Availability of data and materials

Data sharing is not applicable to this article as no datasets were generated or analysed during the current study.

Competing interests

The author declares that there are no competing interests.

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