



BerlinUP
Journals

Electronic Communications of the EASST

Volume 85 Year 2025

**deRSE25 - Selected Contributions of the 5th Conference for
Research Software Engineering in Germany**

*Edited by: René Caspart, Florian Goth, Oliver Karras, Jan Linxweiler, Florian Thiery,
Joachim Wuttke*

**From Start to Finish - A Process of Using
Simulation Software in Energy Research
Projects**

Corinna Seiwerth, Jan Sören Schwarz, Laura Fuentes Grau, Ramiz Qussous, Philipp
Schmurr, Nan Liu, Zhiyu Pan, and Alexandro Steinert

DOI: 10.14279/eceasst.v85.2714

License: © ⓘ This article is licensed under a CC-BY 4.0 License.

Electronic Communications of the EASST (<https://eceasst.org>).

Published by **Berlin Universities Publishing**
(<https://www.berlin-universities-publishing.de/>)

From Start to Finish – A Process of Using Simulation Software in Energy Research Projects

Corinna Seiwerth¹, Jan Sören Schwarz^{2,3}, Laura Fuentes Grau⁴, Ramiz Qussous⁵, Philipp Schmurr⁶, Nan Liu⁶, Zhiyu Pan⁴, and Alexandro Steinert^{2,3}

¹ corinna.seiwerth@fau.de

Chair of Computer Science 7 (Computer Networks and Communication Systems)
Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

² jan.soeren.schwarz@uol.de, alexandro.steinert@uol.de

Department for Computing Science
Carl von Ossietzky Universität Oldenburg, Germany

³ jan.soeren.schwarz@offis.de, alexandro.steinert@offis.de

Energy Division
OFFIS - Institute for Information Technology, Germany

⁴ laura.fuentes-grau@eonerc.rwth-aachen.de, zhiyu.pan@eonerc.rwth-aachen.de

Institute for Automation of Complex Power Systems
RWTH Aachen University, Germany

⁵ ramiz.qussous@inatech.uni-freiburg.de

Institut für Nachhaltige Technische Systeme
University of Freiburg, Germany

⁶ philipp.schmurr@kit.edu, nan.liu@kit.edu

Institute for Automation and Applied Informatics
Karlsruhe Institute of Technology, Germany

Abstract:

Simulation software is crucial in energy research, serving as a key tool for analyzing complex systems and testing innovative solutions. Simulations are used in this context because real-world testing is typically expensive and time-consuming and may jeopardize the stability and safety of critical infrastructure systems. As part of NFDI4Energy, we are developing services to support researchers in effectively integrating simulation into their workflows. To better understand the research community's needs, we developed and analyzed multiple use cases that illustrate the diverse simulation-based processes in energy research. Based on these, we designed a structured process model that guides the use of simulation software, from planning and the initial setup over the execution to sharing results following the FAIR principles. Notably, the process also emphasizes the value of sharing simulation models and software, not just data, via dedicated software registries, thus enabling research data management. Our goal within NFDI4Energy is to create new tools

and services while integrating and connecting existing solutions through a shared service portfolio. This paper presents an overview of the identified requirements and the conceptual design of a Simulation-as-a-Service (SimaaS) approach tailored to the energy research domain, offering early insights into a potential future service landscape.

Keywords: Simulation-as-a-Service, Co-Simulation, Workflow, Use Case

1 Introduction

The use of simulation is of central importance in energy research. A simulation is a model calculation that reproduces the behavior of real-world processes or systems [ESK⁺]. Particularly when analyzing complex systems, such as the integration of renewable energies, simulation enables testing new concepts and solutions under controlled conditions. It provides a solid basis for decision-making for political and regulatory processes. By enabling controlled experimentation without the risks, costs, or constraints of real-world implementation, simulations allow researchers to evaluate the behavior of energy systems under varying conditions and to assess the impact of novel technologies before deployment [PDR]. However, simulation is often associated with a high demand for computing resources. In addition, many research groups face the challenge of only needing performance-intensive IT infrastructure at certain times. At the same time, the acquisition and maintenance of dedicated machines is associated with high costs [GD].

One approach to solve this problem is Simulation-as-a-Service (SimaaS), a concept that enables shared computing nodes. Using cloud computing resources, simulations can be run flexibly and efficiently on heterogeneous infrastructures [WMR⁺]. This reduces investment costs for in-house hardware and improves the utilization of existing resources. SimaaS makes it possible to carry out complex simulations without significant IT investments and thus supports the rapid and flexible scaling of research activities [GD].

Particularly in energy research, easy access to powerful simulation tools accelerates the investigation of key issues and provides important insights for the energy transition [PDR]. Nevertheless, technical challenges remain concerning the standardization and interoperability of the services offered, which restricts broad access to SimaaS offerings.

In the consortium NFDI4Energy¹ (National Research Data Infrastructure for Interdisciplinary Energy System Research), Task Area 5 specifically addresses challenges related to the accessibility and usability of simulation tools. NFDI² as a whole has the mission to implement the FAIR principles for research data and software [WDA⁺]. While not every outcome is legally required to be released as open source, there is a strong commitment across all consortia, including NFDI4Energy, to openly publish tools, services, and data whenever possible, thereby fostering reproducibility, transparency, and long-term accessibility. Within this context, our work contributes to the development of methods and services that lower entry barriers to simulation, with a particular focus on reproducibility and alignment with the FAIR principles for research software. As a first step, we analyzed a set of use cases that highlight typical requirements and

¹ <https://nfdi4energy.uol.de/>

² <https://www.nfdi.de/>

challenges when using simulations in the energy domain. Based on these use cases, we developed a systematic workflow that defines the central steps and functions of a SimaaS for the energy domain. In addition, we examined existing services and assigned them to these use cases to identify potential gaps in the current service landscape. A crucial gap is a missing SimaaS for the energy domain, offering access to established co-simulation frameworks. With this work, we provide an overview of the requirements and design of the SimaaS approach and offer first insights into a possible future service landscape.

2 State of the Art

SimaaS or Modeling and Simulation as a Service (MSaaS) describes an approach in which modeling and simulation capabilities are provided as a cloud-based service. The aim is to make the entire life cycle of simulation, from modeling to execution and evaluation, available via abstracted, user-friendly interfaces [GD]. In this context, we define a simulation model as a representation that reproduces the behavior of a system without necessarily including a target function [ESK⁺]. Building on such models, a simulation scenario specifies a concrete plan that references a given simulation configuration and formulates objectives that motivate and guide the planned analysis. In more complex cases, co-simulation is employed. Co-simulation is a special kind of simulation, where multiple models are executed in individual runtime environments. A central challenge in co-simulation lies in the synchronization and orchestration of these heterogeneous models and their solvers [SRL⁺15]. The SimaaS paradigm addresses these challenges by making complex simulation infrastructures accessible through standardized interfaces, thereby lowering the threshold for interdisciplinary research applications [GD]. To analyze the state of the art, we discuss different aspects that SimaaS can encompass and review existing implementations reported in the literature.

2.1 Aspects of SimaaS

Current SimaaS platforms offer a wide range of functionalities, which can typically be divided into the following categories:

Modeling and configuration: SimaaS enables the web-based definition and adaptation of simulation models. Users can vary parameters and define scenarios via intuitive interfaces [GD]. This is supported by functions for managing input and output data and repositories for model storage and reuse. Some platforms explicitly offer MSaaS to provide executable model components.

Provision and execution of simulations: Simulations can be started on demand, scaled, and executed in a distributed manner. Various types of simulation are supported, such as agent-based models, discrete event simulations, or complex models [HAT⁺]. Technically, this is often done via containerization (e.g., Docker) or virtual machines, combined with load distribution and prioritization of jobs [SBC]. APIs enable cross-system integration [WW].

Experiment and workflow management: SimaaS offers options for orchestrating multiple simulation runs, including scheduling, repetitions, deadline management, and status monitor-

ing [SAW⁺]. Complex experiments and co-simulations can be realized by combining several services [PDR].

Data management: A central function is collecting, aggregating, and providing simulation results. This includes user-defined aggregation logic, data persistence, and interfaces for evaluating or forwarding results [SAW⁺].

Analysis and visualization: Real-time visualizations, 3D representations, and tools for parameter analysis, sensitivity analysis, or live queries support the analysis of simulation results. Presentation services prepare results specifically for different target groups [HAT⁺].

User interaction and access: SimaaS platforms offer interactive web interfaces and APIs for simulation control. Users receive abstracted access to complex processes, can manage simulations, and dynamically adjust parameters [SBC].

Platform services and infrastructure management: In the background, services provide resource management, elastic scaling, security mechanisms, monitoring, and support for multi-tenancy and portability. Virtualization technologies ensure isolated, secure execution of simulations [SBC].

2.2 Implementations of SimaaS

Numerous research and development projects have explored the concept of SimaaS in various domains, demonstrating its practical applicability and adaptability to domain-specific requirements.

One prominent example is the **GEWISS** [PDR] project in the energy domain, which focuses on simulating the interactions between urban development and district heating expansion in Hamburg. The project utilizes a multi-agent-based co-simulation system that combines building-level simulations with urban planning models. The underlying platform leverages loosely coupled REST-based web services and cloud infrastructure to enable scalable execution of simulations involving more than 100,000 agents [PDR].

Another SimaaS from the energy domain is **open-plan-tool**³, developed by researchers at the Reiner Lemoine Institute. It supports the optimized planning of decentralized energy systems for partially covering electricity and heat demand in residential neighborhoods and industrial areas based on oemof [HKK⁺18]. The tool follows an open-science approach, providing all methods, data, and source code under an open-source license. It is designed to be accessible to non-expert users, such as municipal utilities, engineering firms, and engaged citizens, and promote reproducibility and transparency in energy system planning. It provides a scenario editor and simulation server, which allows creating, executing, and analyzing scenarios in a web-based environment.

In the context of electrical power systems, [MVSM] addresses the real-time simulation of fast, nonlinear grid phenomena. The project developed a distributed co-simulation architecture that supports hardware-in-the-loop testing and virtualized simulation laboratories. Its flexible infrastructure allows for high-fidelity simulation and validation of power system automation solutions [MVSM].

³ <https://open-plan-tool.org>

Beyond energy systems, the **MaSS/Galaxy platform** [WMR⁺] targets the biophysical modeling domain. It supports the sharing, reusing, and composing of complex models in a web-based environment, focusing on reproducibility. Users can load and combine models and simulation data from curated databases and collaboratively edit simulation setups [WMR⁺].

Another domain-specific application is **C2SuMo** [CSG⁺], a traffic simulation platform tailored to educational use cases. Built on the SUMO traffic simulator, C2SuMo offers a simplified web-based interface for configuring, executing, and visualizing simulations, making advanced modeling capabilities more accessible to students and non-experts [CSG⁺].

Despite the progress demonstrated by these initiatives, several challenges remain unresolved. Most existing SimaaS approaches are limited in interoperability, typically supporting only specific simulation tools or frameworks. Integrating multiple heterogeneous simulation environments within a unified service architecture is still rare. Furthermore, standardization, interoperability, and long-term maintainability pose significant barriers, particularly in domain-specific contexts such as energy research.

NFDI4Energy aims to address these gaps by developing a service-oriented platform that integrates existing and newly developed SimaaS components. A key objective is to align simulation-based research with the FAIR principles to make simulation models, scenarios, and results findable, accessible, interoperable, and reusable across the energy research community [WDA⁺].

3 Overview of Use Cases

A set of representative use cases was compiled within the scope of Task Area 5 to better understand the current application of simulation technologies in the energy domain and identify specific requirements for supporting services. The overarching goal of this task area is to simplify and promote the use of simulation software in energy research by addressing common challenges related to the FAIR principles.

As part of this effort, several supporting components are being developed:

- A research software registry aimed at increasing the visibility and accessibility of simulation models and tools relevant to energy research.
- A scenario ontology that captures and formalizes key concepts and relationships associated with simulation scenarios, enabling semantic annotation, discovery, and reasoning to facilitate the whole process from development to evaluation of co-simulation scenarios [SSF⁺25].
- A SimaaS platform for three co-simulation frameworks widely used in the domain: mosaik [SBE⁺19], VILLASframework [VMRM17], and DaceDS [GD22]. This platform will enable the on-demand, integrated execution of co-simulations using these frameworks.

The identified use cases help guide the development of the aforementioned services by capturing user needs and workflows and assessing the capabilities and limitations of existing solutions. These use cases reflect various practical activities and challenges in simulation-based energy research.

The following use cases exemplify typical tasks researchers face and provide insight into user requirements for simulation support infrastructure:

- UC1: Search for simulation software
- UC2: Compare simulation software and models
- UC3: Find best-suited co-simulation framework
- UC4: Find simulation models and data for co-simulation
- UC5: Find and reuse existing co-simulation scenarios
- UC6: Creation of co-simulation scenarios
- UC7: Guided creation of co-simulation scenario based on research goal
- UC8: Automated execution of a co-simulation scenario
- UC9: Investigate and reproduce the results of a co-simulation
- UC10: Add software to the NFDI4Energy research software registry
- UC11: Add simulation model to the NFDI4Energy research software registry
- UC12: Share the results of a co-simulation FAIRly

Each use case is documented in detail in a publicly accessible repository on GitHub ⁴. The documentation follows a structured format, including:

- Scope and objectives
- Relevant stakeholders
- Assumptions and prerequisites
- Possible execution sequences and workflows

By systematically analyzing these use cases, we gain a deeper understanding of the functional, technical, and organizational requirements for enabling simulation as a FAIR, service-oriented activity in the energy research domain. These insights directly inform the development of tools and services within NFDI4Energy and contribute to the broader goal of supporting reproducible, transparent, and efficient simulation-based research.

4 Workflow for Using Simulation in the Energy Domain

To comprehensively capture the diverse applications of co-simulation in energy systems research, we organized the identified use cases into a structured workflow. This workflow is aligned with the Research and Transfer Cycle described by Ferenz et al. [Fer22]. Additionally, we mapped the use cases with services from the NFDI and energy systems research communities to identify the services that should be integrated and the gaps that need new development.

4.1 Mapping to Research and Transfer Cycle

The Research and Transfer Cycle, shown in Figure 1, outlines five iterative phases of energy systems research [Fer22]:

⁴ https://github.com/NFDI4Energy/simulation-service-requirements/blob/main/use_cases.md

- (I) Identify competences, expertise, and related work,
- (II) Define relevant scenarios based on (existing) models and data,
- (III) Integrate models and data, configure interfaces, and couple tools and laboratories,
- (IV) Extract and ensure the persistence of results, public consultation, and discourse,
- (V) Identify research gaps and challenges for follow-up activities.

The mapping of those phases with the developed use cases is visualized in Figure 2 and described in the following.

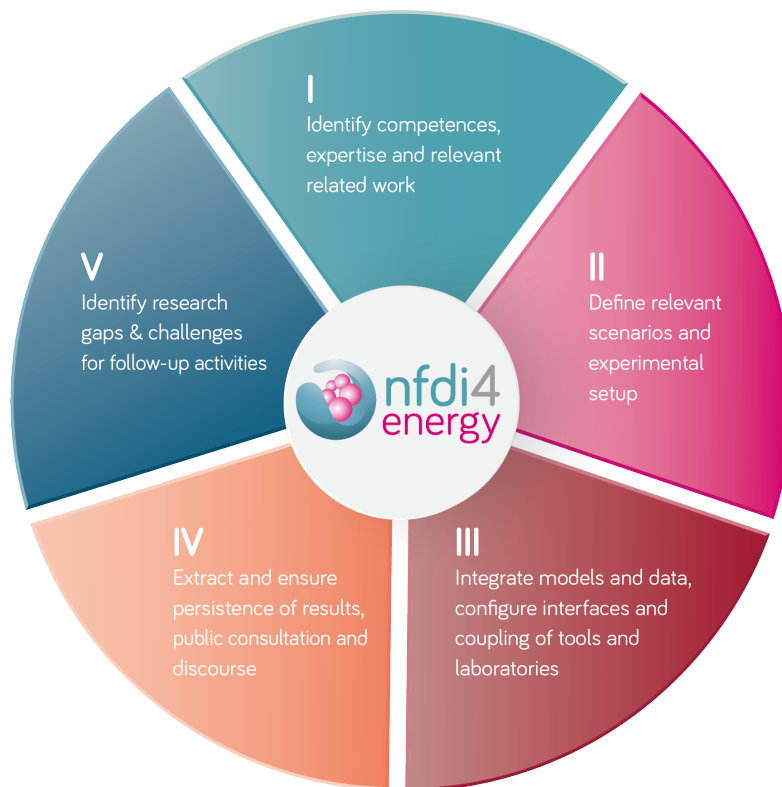


Figure 1: Research and Transfer Cycle [Fer22]

Our workflow begins with the use cases UC1 and UC2, which map to phases I and V of the Research and Transfer Cycle. These use cases enable researchers to explore available tools and identify new research directions by comparing capabilities and identifying gaps.

In phase II, which focuses on scenario development based on existing data and models, we assigned the use cases UC3, UC4, and UC5. The latter use case is conditionally reached in the workflow through a decision point asking whether a new scenario needs to be created. If the answer is no, the researcher is directed to reuse existing scenarios. If yes, the workflow proceeds to the use case UC6. This branching reflects typical decision paths in research: depending on prior experience, one may prefer to reuse existing scenarios or develop a new one from scratch.

The subsequent use cases — UC6, UC7, and UC8— correspond to phase III of the cycle, which centers on the integration and configuration of simulation environments. All paths con-

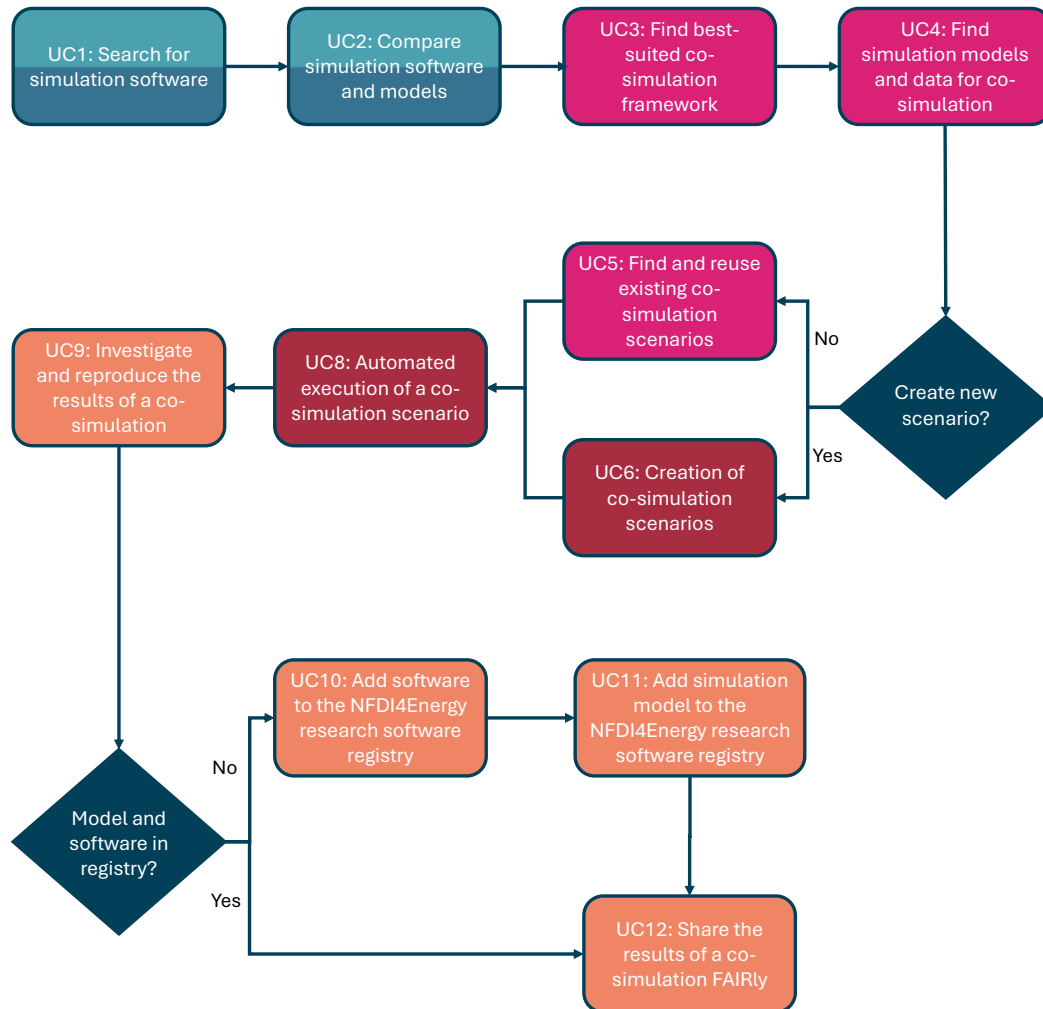


Figure 2: Workflow for using simulation in the energy domain

verge at the automated execution step, emphasizing its central role in simulation-based research workflows.

The use case UC9 addresses Phase IV, following directly after the execution phase. A subsequent branching decision determines whether the models and software used have already been published in a registry. If not, users are guided through the steps UC10 and UC11. If the components are already registered, the workflow proceeds directly to UC12, promoting adherence to the FAIR principles (Findable, Accessible, Interoperable, Reusable).

UC7 is excluded from the core sequence of the workflow, as it serves as an overarching use case that integrates multiple other use cases rather than representing a discrete step.

It is important to note that the workflow is not designed as a strictly sequential process. Instead, it allows for flexible entry and exit points, enabling researchers to adapt the process to their specific project requirements and prior knowledge. This flexibility supports targeted and efficient planning of simulation activities and simultaneously informs the development of the SimaaS platform by highlighting functional and interoperability requirements across use cases.

Further, the described workflow systematically supports implementing the FAIR principles for research software in energy research. By explicitly considering use cases such as UC1, UC10, and UC5, central aspects such as the findability, accessibility, and reusability of software, models, and scenarios are addressed. The structured documentation and registration of software and simulation models increase visibility and facilitate reusability in research projects. The selection of suitable co-simulation frameworks and the configuration of interoperable models promote the use of standard interfaces and data formats. In addition, the workflow strengthens the sustainability of research results through the targeted support of reproducibility and reuse, for example, through the FAIR-compliant publication of simulation results.

The presented workflow describes an idealized process for using co-simulations in the energy domain. The workflow is intentionally high-level, making it generally applicable for co-simulation use across different domains. However, the frameworks we plan to integrate into the SimaaS hub are specifically designed for co-simulations in the energy domain. Therefore, our focus in the following discussion is on this particular domain.

4.2 Mapping to Services

After developing the workflow, we analyzed existing services, primarily from the NFDI community, that aim to support various phases of the research process. The analysis included generic base services provided by Base4NFDI, such as IAM4NFDI, Jupyter4NFDI, PID4NFDI, and nfdi.software, as well as domain-specific tools and registries. The Base Services of the Base4NFDI initiative provide basic infrastructure components to enable efficient and cross-consortia use of digital resources within the NFDI. IAM4NFDI⁵ offers an integrated solution for Identity and Access Management and enables researchers from different disciplines and institutions to easily and securely access digital resources within the NFDI [GHH⁺24]. Jupyter4NFDI⁶ supports the cross-consortia provision and use of Jupyter notebooks through a central service for the execution, versioning, and reproducibility of scientific analyses [HBF⁺24]. PID4NFDI⁷ aims to improve the integration of persistent identifiers in the NFDI consortia, taking into account different levels of maturity of service providers and community adoption [BBB⁺24]. nfdi.software⁸ aims to establish a central marketplace for research software within the NFDI in order to promote cross-disciplinary access as well as the sustainable use and further development of scientific software [HHG⁺24].

⁵ <https://base4nfdi.de/projects/iam4nfdi>

⁶ <https://base4nfdi.de/projects/jupyter4nfdi>

⁷ <https://base4nfdi.de/projects/pid4nfdi>

⁸ <https://base4nfdi.de/projects/nfdi-software>

Among the registries considered were Open Energy Factsheets, which include the Open Energy Model Factsheets⁹ and Framework Factsheets¹⁰, Helmholtz.Software¹¹, Software Heritage¹², re3data.org¹³, and the Open Energy Database¹⁴.

In addition, we examined a variety of research data management and supplementary services. The Open Energy Databus¹⁵ is a transformative platform for agile data integration, collaboration, and automation, built upon a structured metadata knowledge graph to support open energy data management. The Leibnitz Data Manager¹⁶ is a data management system for federated search. Ontology Mapping by NFDI4Ing¹⁷ uses the Metadata4Ing ontology to semantically describe research data, particularly in engineering and related disciplines. The Open Energy Knowledge Graph (OEKG)¹⁸ represents a semantic network of entities, types, properties, and relationships relevant to energy system analysis. It follows the RDF standard and uses the Turtle format. The Open Energy Academy¹⁹ provides a collection of training materials, tutorials, and FAQs to support users in interacting with the Open Energy Platform. The NFDI4Ing Terminology Service²⁰ is a web-based application designed to reveal and connect terminologies across different research communities, supporting interoperability within the Semantic Web framework. DBpedia Lookup²¹ is a web service that allows users to retrieve DBpedia URIs based on relevant keywords, facilitating semantic annotation. SMECS²² is a web application for extracting and curating research software metadata following the CodeMeta standard. Finally, the EOSC Exchange and Validation Node (EOSC EV Node)²³ provides infrastructure for validating, exchanging, and integrating research services within the European Open Science Cloud ecosystem.

These services were systematically mapped to the previously developed use cases to identify coverage gaps and derive implications for service development and integration. Table 1 presents the results of this mapping, showing which services support which use cases.

Use cases UC1 and UC3 focus on the search for suitable simulation software. This should take place via a registry provided on the NFDI4Energy platform. In particular, the Open Energy Factsheets and the nfdi.software registry are taken into account for this purpose. The Open Energy Databus can be used to support the management and structuring of the registry data to make this registry searchable.

⁹ <https://openenergyplatform.org/factsheets/models/>

¹⁰ <https://openenergyplatform.org/factsheets/frameworks/>

¹¹ <https://helmholtz.software/>

¹² <https://www.softwareheritage.org/>

¹³ <https://www.re3data.org/>

¹⁴ <https://openenergyplatform.org/dataedit/schemas>

¹⁵ <https://databus.openenergyplatform.org/>

¹⁶ <https://projects.tib.eu/datamanager/>

¹⁷ <https://nfdi4ing.pages.rwth-aachen.de/metadata4ing/metadata4ing/>

¹⁸ https://openenergyplatform.github.io/organisation/family_members/knowledge-representation/oekg/

¹⁹ <https://openenergyplatform.github.io/academy/>

²⁰ <https://nfdi4ing.de/5-3/>

²¹ <https://lookup.hu.dbpedia.org/lookup-application/>

²² <https://github.com/NFDI4Energy/SMECS>

²³ <https://open-science-cloud.ec.europa.eu/>

Table 1: Services related to the use cases

Use Case	Related Services
UC1: Search for simulation software	Open Energy Factsheets Open Energy Databus nfdi.software
UC2: Compare simulation software and models	Open Energy Factsheets Ontology Mapping by NFDI4Ing OEKG
UC3: Find best-suited co-simulation framework	Open Energy Factsheets Open Energy Databus nfdi.software
UC4: Find simulation models and data for co-simulation	Open Energy Factsheets Open Energy Databus Open Energy Database
UC5: Find and reuse existing co-simulation scenarios	Open Energy Factsheets
UC6: Creation of co-simulation scenarios	Open Energy Academy IAM4NFDI
UC7: Guided creation of simulation scenario based on research goal	Open Energy Database
UC8: Automated execution of a co-simulation scenario	Leibnitz Data Manager Open Energy Database EOSC EV Node IAM4NFDI
UC9: Investigate and reproduce the results of a co-simulation	Jupyter4NFDI
UC10: Add software to the NFDI4Energy research software registry	Helmholz.Software Software Heritage Open Energy Factsheets re3data.org IAM4NFDI PID4NFDI SMECS
UC11: Add simulation model to the NFDI4Energy research software registry	re3data.org Open Energy Factsheets IAM4NFDI PID4NFDI
UC12: Share the results of a co-simulation FAIRly	Jupyter4NFDI Terminology Service DBpedia Lookup PID4NFDI

For UC2, in which a comparison of simulation software and models is planned, additional functionalities are required in addition to the registry data, such as those provided by the ontology mapping of NFDI4Ing and the OEKG.

UC4 is about finding suitable models and data for co-simulations. The Open Energy Factsheets and the Open Energy Database are suitable sources for this, ideally managed via the Open Energy Databus.

To reuse co-simulation scenarios in UC5, these should be stored in a registry such as the Open Energy Factsheets. No entirely suitable services are available for UC6, which addresses creating new scenarios. However, the Open Energy Academy can serve as a tool to provide didactic

support for the creation steps. IAM4NFDI could also facilitate saving created scenarios in the personal user profile.

UC7, which provides for guided scenario creation based on research objectives, can be partially supported by the Open Energy Database. However, specialized services for full implementation are still missing.

For UC8, which relates to the automated execution of simulation scenarios, services such as the Leibniz Data Manager, the Open Energy Database, the EOSC EV Node, and the IAM4NFDI basic service can implement the infrastructure. However, additional implementations are necessary to cover the entire use case functionally.

Jupyter notebooks can be used in UC9, which deals with the analysis and reproducibility of simulation results. The basic service Jupyter4NFDI provides a suitable environment for this.

The implementation of UC10, which describes adding software to a registry, can, in principle, be carried out with any suitable software registry. However, IAM4NFDI and PID4NFDI are also required to ensure that entries can be identified, found, and changed in the long term. SMECS can also be used to extract relevant registration information automatically.

The Open Energy Factsheets are also suitable for UC11, where simulation models must be stored in a registry. Integration of IAM4NFDI and PID4NFDI is also essential here. To increase the registry's visibility and referenceability, it should also be listed in re3data.org.

Finally, UC12 deals with the FAIR-compliant publication of simulation results. Existing Jupyter notebooks from UC9 can be reused here. Additionally, results should be published in suitable repositories or registers. The results should be provided with metadata that can be standardized and enriched by the Terminology Service and DBpedia Lookup to improve findability and interoperability. The use of persistent identifiers is also crucial for sustainable findability and accessibility.

The analysis reveals that individual use cases are typically not supported by a single service alone. Instead, several services contribute to different aspects of a use case, and their combined use is often necessary to achieve comprehensive support. In particular, infrastructure-level services such as IAM4NFDI and PID4NFDI function as foundational components that enable essential capabilities like identity management and persistent identification, rather than directly supporting end-user tasks. Their value is facilitating interoperability and FAIR compliance across the broader research software and data landscape. The mapping thus highlights existing strengths within the NFDI service ecosystem and important gaps and opportunities for further development, especially regarding integration and usability.

In this context, it becomes evident that a central, user-oriented SimaaS hub is needed to orchestrate and integrate distributed services. While individual tools already exist to support simulation workflows in research, identifying, combining, and applying them remains a fragmented and time-consuming process. The hub therefore serves as a single entry point where frameworks and services are jointly presented, enabling researchers to access, compare, and employ them in a coherent manner. For newcomers to the field, the hub offers a low-threshold opportunity to explore simulations and gain orientation, while experienced researchers can use it to set up and execute both simple and complex co-simulations.

Beyond this integrative function, the hub is designed to advance reproducibility, transparency, and the implementation of FAIR4RS principles [BCK⁺] in simulation workflows. Simulation scenarios are stored in a dedicated registry to make them findable, and the development of a

scenario ontology provides a shared interface across frameworks, ensuring accessibility and interoperability. The ontology also supports the general description and semantic annotation of scenarios, thus enhancing their reusability. The SimaaS service itself is implemented according to FAIR4RS guidelines: it will be registered in the NFDI4Energy service portfolio, enriched with metadata, and exposed via standardized APIs whose endpoints are aligned with the scenario ontology. Moreover, to foster reuse and community-driven development, the implementation of the SimaaS will be openly published on GitHub.

Within NFDI4Energy, we are developing and implementing this SimaaS hub as an openly available service for the energy research community, aiming to foster broad adoption and collaborative advancement. To ensure long-term sustainability, the hub's development and maintenance are embedded in the organizational structures of NFDI4Energy and supported by institutional partners and dedicated teams, thereby securing both technical continuity and community-driven evolution.

5 Conclusion

In this work, we presented a structured analysis of the application of SimaaS in energy systems research. Based on a comprehensive collection of use cases within the NFDI4Energy consortium, we defined a workflow that reflects typical research processes and the associated simulation activities. This workflow enables a systematic understanding of how co-simulation services can support research, from identifying suitable tools and models to sharing results in a FAIR manner.

We mapped these use cases to existing services from the NFDI community and beyond, revealing both synergies and significant gaps. While various infrastructure-level and domain-specific services already exist and partially support the identified use cases, no single service fully covers the needs of researchers across the entire simulation lifecycle. Moreover, the fragmentation of the service landscape and the lack of integration limit the accessibility and effectiveness of simulation-based research workflows.

These findings underline the necessity of developing a central SimaaS hub that integrates and orchestrates existing services. Such a hub would serve as a unifying interface for researchers, facilitating the reuse of models and software, enhancing interoperability, and lowering the barrier to entry for complex co-simulation tasks. Ultimately, this supports the technical implementation of FAIR principles and the broader goals of transparency, reproducibility, and collaboration in energy systems research.

Future work will focus on the iterative development of this hub in close collaboration with stakeholders, the expansion of the use case catalog, and the refinement of ontology-driven approaches to scenario modeling and service discovery.

Acknowledgements: The authors would like to thank the German Federal Government, the German State Governments, and the Joint Science Conference (GWK) for their funding and support as part of the [NFDI4Energy](#) consortium. The work was funded by the German Research Foundation (DFG, German Research Foundation) under the National Research Data Infrastructure ([NFDI](#)) – NFDI4Energy – 501865131.

Bibliography

- [BBB⁺24] S. Bingert, J. Böhm, M. Buys, S. El-Gebali, S. Genderjahn, S. Hagemann-Wilholt, T. Kahlert, M. Lange, M. Meistring, I. Sens, M. Stocker. Persistent Identifier Services for the German National Research Data Infrastructure: Proposal for the Integration Phase of Base4NFDI. Dec. 2024.
[doi:10.5281/zenodo.14281255](https://doi.org/10.5281/zenodo.14281255)
- [BCK⁺] M. Barker, N. P. Chue Hong, D. S. Katz, A.-L. Lamprecht, C. Martinez-Ortiz, F. Psomopoulos, J. Harrow, L. J. Castro, M. Gruenpeter, P. A. Martinez, T. Honeyman. Introducing the FAIR Principles for research software. 9(1):622. Publisher: Nature Publishing Group.
[doi:10.1038/s41597-022-01710-x](https://doi.org/10.1038/s41597-022-01710-x)
- [CSG⁺] F. Caglar, S. Shekhar, A. Gokhale, S. Basu, T. Rafi, J. Kinnebrew, G. Biswas. Cloud-hosted simulation-as-a-service for high school STEM education. 58:255–273.
[doi:10.1016/j.simpat.2015.06.006](https://doi.org/10.1016/j.simpat.2015.06.006)
- [ESK⁺] L. Emele, M. Stappel, A. Kleinau, J. Hastings, V. Sehn, H. Förster, P. Kuckertz, C. Hoyer-Klick, C. Hofmann, K. Knosala, L. Hülk, I. Killicarslan, F. Drathschmidt, F. Simon, F. Ulrich, C. Muschner, C. Winger, F. Neuhaus, L. Christmann, M. Glauer, P.-F. Duc, S. Cordes, M. Pehl, K. Schnepf, T. Mossakowski, A. Stage, H. Gardian, E. S. Arellano Ruiz, M. Rothkötter, L. Rülcke, A. Seibicke, L. Mittermeier, U. Müller, N. Köhler, H. Spinde, V. Wichern, N. Zielke, U. Stucky, M. Breitkreutz, L. Gerlach, C. Heidfeld, J. S. Schwarz. Open Energy Ontology (OEO). original-date: 2018-06-06T12:04:47Z.
- [Fer22] S. Ferenz. Towards More Findable Energy Research Software by Introducing a Metadata-based Registry. In *Abstracts of the 11th DACH+ Conference on Energy Informatics*. Energy Inform. Springer, 2022.
[doi:10.1186/s42162-022-00215-6](https://doi.org/10.1186/s42162-022-00215-6)
- [GD] M. Gütlein, A. Djanatliev. Modeling and Simulation as a Service using Apache Kafka:. In *Proceedings of the 10th International Conference on Simulation and Modeling Methodologies, Technologies and Applications*. Pp. 171–180. SCITEPRESS - Science and Technology Publications.
[doi:10.5220/0009780501710180](https://doi.org/10.5220/0009780501710180)
- [GD22] M. Gütlein, A. Djanatliev. On-Demand Simulation of Future Mobility Based on Apache Kafka. *Lecture Notes in Networks and Systems* 306(ViM):18–41, 2022.
[doi:10.1007/978-3-030-84811-8_2](https://doi.org/10.1007/978-3-030-84811-8_2)
- [GHH⁺24] P. Gietz, M. Hardt, D. Hübner, W. Pempe, C. Pohl, M. Bonn, S. Apweiler. IAM4NFDI Service description, operating concept and TOMs. July 2024.
[doi:10.5281/zenodo.13149756](https://doi.org/10.5281/zenodo.13149756)

- [HAT⁺] C. Hüning, M. Adebahr, T. Thiel-Clemen, J. Dalski, U. Lenfers, L. Grundmann. Modeling & simulation as a service with the massive multi-agent system MARS. In *Proceedings of the Agent-Directed Simulation Symposium*. ADS '16, pp. 1–8. Society for Computer Simulation International.
[doi:10.22360/SpringSim.2016.ADS.001](https://doi.org/10.22360/SpringSim.2016.ADS.001)
- [HBF⁺24] B. Hagemeyer, A. Bleier, B. Flemisch, M. Lieber, K. Reuter, G. Dogaru. Jupyter4NFDI. July 2024.
[doi:10.5281/zenodo.12699382](https://doi.org/10.5281/zenodo.12699382)
- [HHG⁺24] M. Hammitzsch, B. Hetenyi, B. Grüning, A. Marcic, M. Löbe, L.-J. Castro, F. Engel, K. Höfner, M. Zacharias, O. Werth, V. Seibert, A. Rausch. nfdi.software - Initialisation Phase. Dec. 2024.
[doi:10.5281/zenodo.14507302](https://doi.org/10.5281/zenodo.14507302)
- [HKK⁺18] S. Hilpert, C. Kaldemeyer, U. Krien, S. Günther, C. Wingenbach, G. Plessmann. The Open Energy Modelling Framework (Oemof) - A New Approach to Facilitate Open Science in Energy System Modelling. *Energy Strategy Reviews* 22(0):16–25, 2018.
[doi:10.1016/j.esr.2018.07.001](https://doi.org/10.1016/j.esr.2018.07.001)
- [MVSM] M. Mirz, S. Vogel, B. Schafer, A. Monti. Distributed real-time co-simulation as a service. In *2018 IEEE International Conference on Industrial Electronics for Sustainable Energy Systems (IESES)*. Pp. 534–539. IEEE.
[doi:10.1109/IESES.2018.8349934](https://doi.org/10.1109/IESES.2018.8349934)
- [PDR] T. Preisler, T. Dethlefs, W. Renz. Simulation as a service: A design approach for large-scale energy network simulations. 5:1765–1772. ISBN: 9788360810651.
[doi:10.15439/2015F116](https://doi.org/10.15439/2015F116)
- [SAW⁺] S. Shekhar, H. Abdel-Aziz, M. Walker, F. Caglar, A. Gokhale, X. Koutsoukos. A simulation as a service cloud middleware. 71(3):93–108.
[doi:10.1007/s12243-015-0475-6](https://doi.org/10.1007/s12243-015-0475-6)
- [SBC] M. Shahin, M. A. Babar, M. A. Chauhan. Architectural Design Space for Modelling and Simulation as a Service: A Review. 170:110752.
[doi:10.1016/j.jss.2020.110752](https://doi.org/10.1016/j.jss.2020.110752)
- [SBE⁺19] C. Steinbrink, M. Blank-Babazadeh, A. El-Ama, S. Holly, B. Lüers, M. Nebel-Wenner, R. Ramírez Acosta, T. Raub, J. S. Schwarz, S. Stark, A. Nieße, S. Lehnhoff. CPES Testing with Mosaik: Co-Simulation Planning, Execution and Analysis. *Applied Sciences* 9(5):923, 2019.
[doi:10.3390/app9050923](https://doi.org/10.3390/app9050923)
- [SRL⁺15] F. Schloegl, S. Rohjans, S. Lehnhoff, J. Velasquez, C. Steinbrink, P. Palensky. Towards a classification scheme for co-simulation approaches in energy systems. In

2015 International Symposium on Smart Electric Distribution Systems and Technologies (EDST). Pp. 516–521. 2015.
[doi:10.1109/SEDST.2015.7315262](https://doi.org/10.1109/SEDST.2015.7315262)

- [SSF⁺25] J. S. Schwarz, A. Steinert, L. Fuentes Grau, Z. Pan, P. Schmurr, N. Liu, C. Seiwert, R. Qussous, R. German, V. Hagenmeyer, S. Lehnhoff, A. Monti, A. Nieße, A. Weidlich, L. Hülk. Developing an ontology for co-simulation scenarios of energy systems. Aug. 2025.
[doi:10.5281/zenodo.16736210](https://doi.org/10.5281/zenodo.16736210)
- [VMRM17] S. Vogel, M. Mirz, L. Razik, A. Monti. An open solution for next-generation real-time power system simulation. In *2017 IEEE Conference on Energy Internet and Energy System Integration (EI2)*. Pp. 1–6. 2017.
[doi:10.1109/EI2.2017.8245739](https://doi.org/10.1109/EI2.2017.8245739)
- [WDA⁺] M. D. Wilkinson, M. Dumontier, I. J. Aalbersberg, G. Appleton, M. Axton, A. Baak, N. Blomberg, J.-W. Boiten, L. B. da Silva Santos, P. E. Bourne, J. Bouwman, A. J. Brookes, T. Clark, M. Crosas, I. Dillo, O. Dumon, S. Edmunds, C. T. Evelo, R. Finkers, A. Gonzalez-Beltran, A. J. G. Gray, P. Groth, C. Goble, J. S. Grethe, J. Heringa, P. A. C. 't Hoen, R. Hooft, T. Kuhn, R. Kok, J. Kok, S. J. Lusher, M. E. Martone, A. Mons, A. L. Packer, B. Persson, P. Rocca-Serra, M. Roos, R. van Schaik, S.-A. Sansone, E. Schultes, T. Sengstag, T. Slater, G. Strawn, M. A. Swertz, M. Thompson, J. van der Lei, E. van Mulligen, J. Velterop, A. Waagmeester, P. Wittenburg, K. Wolstencroft, J. Zhao, B. Mons. The FAIR Guiding Principles for scientific data management and stewardship. 3(1):160018. Publisher: Nature Publishing Group.
[doi:10.1038/sdata.2016.18](https://doi.org/10.1038/sdata.2016.18)
- [WMR⁺] M. A. Walker, R. Madduri, A. Rodriguez, J. L. Greenstein, R. L. Winslow. Models and Simulations as a Service: Exploring the Use of Galaxy for Delivering Computational Models. 110(5):1038–1043.
[doi:10.1016/j.bpj.2015.12.041](https://doi.org/10.1016/j.bpj.2015.12.041)
- [WW] S. Wang, G. Wainer. Semantic Mashups for Simulation As a Service with Tag Mining and Ontology Learning. In *Proceedings of the Symposium on Theory of Modeling & Simulation - DEVS Integrative*. Pp. 25:1–25:8. Society for Computer Simulation International. Series Title: DEVS '14 ISSN: 07359276.
<https://dl.acm.org/doi/10.5555/2665008.2665033>