Bridging granularity gaps to decarbonize large-scale energy systems

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Abstract

The comprehensive evaluation of strategies for decarbonizing large-scale energy systems requires insights from many different perspectives. In energy systems analysis, optimization models are widely used for this purpose. However, they are limited in incorporating all crucial aspects of such a complex system to be sustainably transformed. Hence, they differ in terms of their spatial, temporal, technological and economic perspective and either have a narrow focus with high resolution or a broad scope with little detail. Against this background, we introduce the so-called granularity gaps and discuss two possibilities to address them: increasing the resolutions of the established optimization models, and the different kinds of model coupling. After laying out open challenges, we propose a novel framework to design power systems. Our exemplary concept exploits the capabilities of energy system optimization, transmission network simulation, distribution grid planning and agent-based simulation. This integrated framework can serve to study the energy transition with greater comprehensibility and may be a blueprint for similar multi-model analyses.

1 Analyzing future energy systems

In order to evaluate strategies for decarbonizing energy systems, optimization models are widely used. Since their first application in the 1960's (Hoffman and Wood 1976), these computer tools have permanently been compromising between providing a wide system's perspective and a sufficient level of detail or granularity. For effective decision making, a wide perspective is relevant to comprehensively account for the side-effects or synergies in a system, while the level of detail is associated to the capability of assessing concrete, individual measures.

Due to computational or also institutional limitations (Krey 2014), improvements towards higher detail or broader scope are always accompanied by simplifications on the complementary side. This trade-off leads to deficiencies, which we refer to as granularity gaps in the following.

Established approaches for energy systems planning are highly diverse in terms of their spatial, temporal, technological and economic perspective. Current models span from assessments on the household-level and small districts, e.g. (Kneiske, Braun, and Hidalgo-Rodriguez 2018) up to the modeling of individual or multiple countries (Gils et al. 2017) and even global systems (Teske et al. 2019). The temporal scale plays a crucial role when it comes to planning of infrastructures with lifetimes of several decades on the one hand. On the other hand, verifying the operational feasibility and reliability of such infrastructures as well as fully exploiting power balancing potentials of batteries require short term system analyses (Hedegaard and Meibom 2012). In terms of technology representations, models range from detailed process simulations up to the coupling of energy sectors and interactions with other systems (e.g. energy-economy-climate) (Howells et al. 2013). The spectrum of economic perspectives comprehends simulations from individual decision-makers up to entire economies.

The ranges of the four dimensions introduced (space, time, technology, and economic perspective) are illustrated in Figure 1. There, we outline, from our perspective, a categorization of one popular model type which allows studies on large-scale energy systems: Energy System Optimization Models (ESOMs).

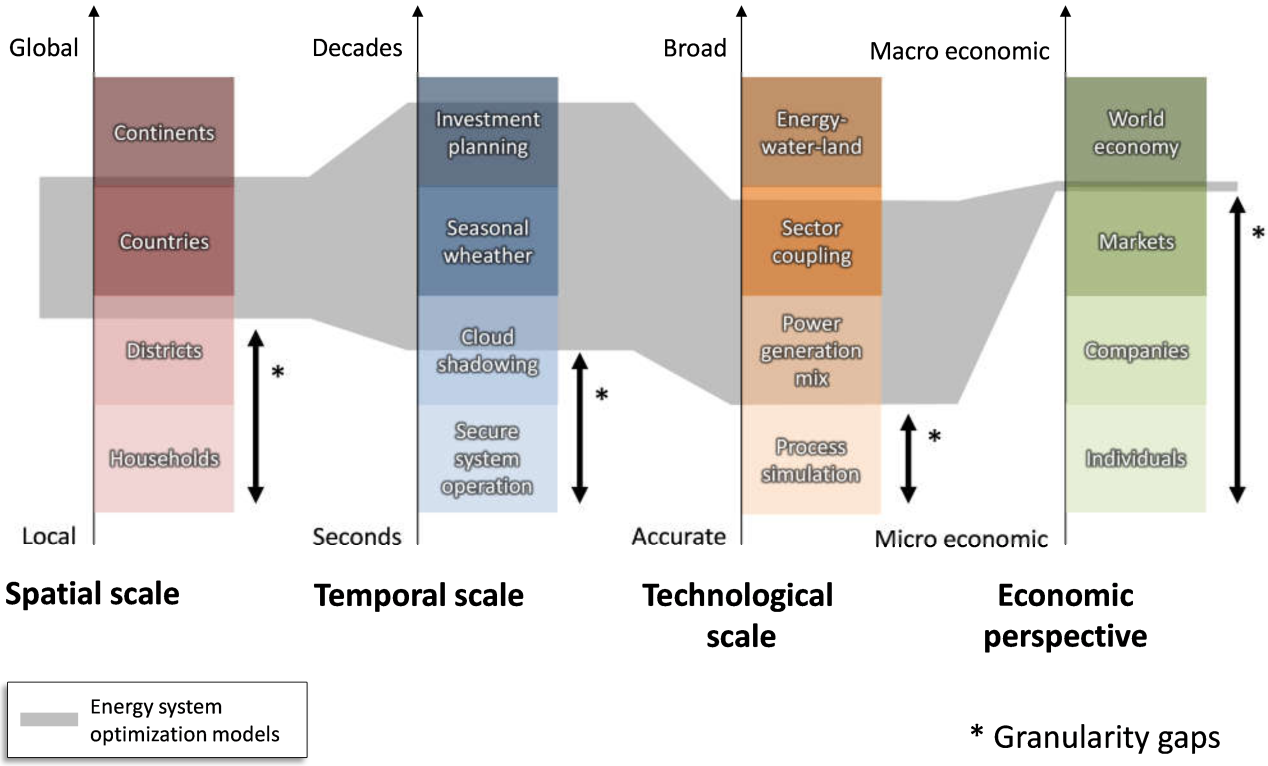

Figure 1: Illustration of different spatial, temporal and technological scales, and economic perspectives of energy system models with a categorization of ESOMs.

1.1 Characteristics of large-scale energy system optimization models

ESOMs are often applied to study the possible development of entire energy systems. For example, Haller et al. do this for Europe including Middle East and North Africa (Haller, Ludig, and Bauer 2012). Their large geographic scope allows for investigating the benefits from international cooperation, but their low spatial resolution limits the findings of, for example, concrete measures of grid expansion needed for the integration of renewable energy sources (RES). Compared to Haller et al., more recent studies such as (Sgobbi et al. 2016), (Child et al. 2019), (Bernath, Deac, and Sensfuß 2019) are more comprehensive in terms of the technologies considered. This development is fostered by the trend of analyzing multi-technology interactions, especially in energy systems with high shares of RES (Markard 2018). Resulting extensions of the energy models include other energy sectors (e.g. the electrification of the heating sector as presented by Bernath et al.) or the introduction of new technologies (e.g. hydrogen as fuel and long-term storage option as presented by Sgobbi et al.). However, the spatial resolution usually remains rather coarse and the results are limited to the perspective of a central system planner.

1.2 The granularity gaps

Successful energy policies rely on the implementation of concrete strategies. Finding such strategies with the corresponding level of detail, for example on a local municipality level, often remains elusive, especially in those studies that rely on broad scope models. At first glance, a direct straight-forward approach would be deriving local strategies by breaking down the actions identified from the global and national level. Although such top-down approaches exist (Müller et al. 2019), they ignore two crucial aspects.

First, in markets (such as within the European Union), decisions cannot simply be instructed top-down. They are rather made by the interaction of various stakeholders with heterogeneous interests. This self-interested stakeholder behavior leads to investment decisions and operation strategies that may strongly deviate from the desired optimal system states. This aggregation bias (also caused by market imperfections) is well-known in economic modeling theory (Fagiolo and Roventini 2017), and sometimes called "behavioral complexity of actors" (Li 2017) in the context of energy system modeling. Hereafter, we refer to it as "economic granularity gap", in line with the wording of the other granularity gaps treated.

Second, ensuring an efficient power supply with renewable resources requires adequately dimensioned power transmission infrastructure and – given the increasing penetration of decentral power generators and consumers (Cossent, Gómez, and Frías 2009) – distribution infrastructure. However, even on the coarsest level, the transmission grid, the accordingly required network simulation studies exceed the spatial resolution of ESOMs. Therefore, transferring their findings to concrete implementation strategies for the real grid (including integration measures in the distribution grid) turns out to be much costlier than anticipated or even technically infeasible. Cost underestimations have been observed, for example, for the integration of decentral technologies such as prosumers (Schill, Zerrahn, and Kunz 2019). In order to overcome infeasible system states, bottom-up approaches (such as cellular approaches in (Lehmann, Huber, and Kießling 2019)) are helpful, but they do not guarantee yielding the intended system designs, especially with regard to affordability, reliability or sustainability. These are issues arising from the "spatial granularity gap".

Closely linked to the spatial granularity gap is the trade-off between long-term investment planning and operation of the energy system's components. Validating or optimizing the latter is only possible if both the spatial and the temporal scale are sufficiently detailed. Although especially ESOMs provide extensive temporal scales to sufficiently capture the fluctuating availability of RES while also enabling investment planning (Poncelet et al. 2016), "temporal granularity gaps" still exist. For example, this is triggered by the idea of introducing real-time pricing tariffs (Allcott 2011) in the power market or if effects of local short-term fluctuations of RES on the operational feasibility and affordability of decentral power generators are to be investigated (Schreck et al. 2020).

Now, the crucial question is *how to address these granularity gaps without compromising the desired broad scope*. As mentioned above and detailed below (section 2.1), increasing the granularity of a particular scale automatically results in the need for more accuracy on another.

2 How to bridge the granularity gaps?

Strategies for bridging granularity gaps, based on the aforementioned unidirectional top-down or bottom-up approaches, exhibit strong limitations. In response, iterative approaches are becoming more promising. These can be realized endogenously by increasing model resolutions or exogenously by model coupling.

2.1 Increasing resolutions in energy systems analysis

Increasing model resolutions can be realized by yielding, for example, sufficient spatial resolutions to simulate effects in real transmission grid infrastructures. Cranking-up the resolution only makes sense if, at the same time, the underlying phenomena or technologies are modeled appropriately, for instance extending power flow modeling by voltage constraints (Salam 2020). And still, breaking-down high-level decisions to the local level remains challenging. This would always call for even better resolutions to capture distribution grids. In this case, differentiation between individual system components becomes more important (as opposed to coarse technology-aggregations) and thus, decisions of heterogeneous actors gain in relevance and should be incorporated, too.

In other words, increasing the spatial granularity automatically leads to the need of higher technological resolutions which then also calls for a more detailed economic perspective.

Achieving such resolutions is extremely challenging, not only from a modeling perspective (e.g. required inputs, inter-disciplinarily) but also from a computational perspective (e.g. runtimes and data handling). The authors of several recent publications focus on this issue and strive for a more efficient treatment of the temporal scale, often using clustering algorithms, e.g. (Buchholz, Gamst, and Pisinger 2019). Although there are further attempts to tackle computational limitations, including the application of high performance computing (Breuer et al. 2018), fully integrated tools are not available yet (Mehigan et al. 2018).

2.2 Model coupling in energy systems analysis

An alternative to increasing resolutions of a particular ESOM is model coupling. It allows incorporating detailed findings from diverse domain-specific tools. Top-level system planning can be succeeded by more detailed models allowing for effectively addressing granularity gaps.

In the following, we introduce three modeling approaches to extend the capabilities of techno-economic (top-level) energy system planning: transmission network simulation, distribution grid planning, and agent-based simulation of microeconomic actor decisions.

2.2.1 Transmission network simulation

The main objective for coupling network simulation studies (as performed, e.g., in (ENTSO-E 2019)) to ESOMs is to incorporate information on feasibility constraints for transmission system operation and planning. This is usually done in an iterative manner: Network simulation studies provide power flow constraints for top-level unit commitment and/or extension planning. Based on top-level results, the constraints then are updated by further network simulation studies.

In simple terms, power flow problems for existing or candidate grid infrastructures are solved (Salam 2020) in order to obtain constraints related to transmission adequacy and power system security. The ESOM then trades-off grid expansion measures against other, competing flexibility-providing technologies.

Established modeling tools developed for simulation and planning of power networks are available (FGH GmbH 2020, DIgSILENT GmbH 2020). However, appropriate solving routines can also be conducted with more general software packages such as MATLAB (Zimmerman, Murillo-Sanchez, and Thomas 2011) or Python frameworks (Brown, Hörsch, and Schlachtberger 2018).

While the above mainly refers to electricity grids, similar comments apply to modeling of gas networks (ENTSO-G 2019), which are of increasing importance (Clegg and Mancarella 2016).

2.2.2 Distribution grid planning

Many high-level energy decisions, for example shares of rooftop PV, heat pumps, or mobility occur on the distribution grid level to which ESOMs are blind. Here, the objective of a model coupling is to capture the impact of ESOM decisions on the distribution level and thus its rebound effect caused by the corresponding adaptation costs.

For the analysis of distribution grids, detached from the ESOM, domain-specific tools become essential. This is different to the transmission level, where by justifiable simplifications concerning modeling of power flows (e.g., by using DC-power flow (Stott, Jardim, and Alsac 2009)) an integration to an ESOM is still possible, as computational constraints are not exceeded and the model complexity remains manageable. Relevant tools automatically analyze, optimize and find solutions for imbalanced distribution grids. Examples are EDisGo (Müller et al. 2019), SNOP (Cibis et al. 2019) or pandapower Pro (Scheidler, Thurner, and Braun 2018). The latter, for instance, identifies voltage, transformer and line problems and solves them by the use of heuristic approaches. This includes not only conventional solutions such as line and transformer replacements, but also innovative measures such as regulated distribution transformers or autonomous network re-configuration.

2.2.3 Agent-based simulation of microeconomic actor decisions

Energy system planning often assumes that all actors are motivated by minimizing the total system costs, while in reality they follow their own principles. Incorporating such microeconomic actor behavior is the objective of model coupling using agent-based models (ABMs). In an ABM, actors are modeled as autonomous agents with individual attributes, behaviors and relationships to other agents as well as to their environment (Macal and North 2005). By simulating the behaviors and interactions of individual agents at the micro-level, the system behavior emerges at macro-level (Bonabeau 2002, Bale, Varga, and Foxon 2015). This – more realistic – system behavior can then be transferred to ESOMs in order to, e.g., evaluate discrepancies from a hypothetic cost-minimized system.

In the context of modeling energy markets, this approach is implemented, e.g., in the EMLab model (Chappin et al. 2017). EMLab models power companies as agents which sell their power on the energy markets and perform investment decisions regarding new power plants. The objective of the model is to analyze the aggregate effects of these investment decisions, e.g. on CO_2 mitigation targets, while evaluating different policy scenarios and designs of the European electricity markets. Another example is AMIRIS (Deissenroth et al. 2017), an ABM of the German power market focusing on the market integration of RES. Thereby, special consideration is given to the influence of political framework conditions on the operation and profitability of energy technologies.

2.3 Model coupling via automated workflows: an exemplary coupling concept

Domain-specific models can be coupled with ESOMs by either soft or hard-coupling. Soft-coupling means that independent models interact by exchanging input and output data. Hard-coupling denotes the integration of the domain-specific models, resulting in an extended ESOM. Existing literature on model coupling approaches (Fichtner et al. 2013) reports several challenges concerning soft-coupling of established models. These are, for example, inferior performance due to communication overhead or difficulties in documentation and reproducibility of the integral model execution. However, as access and domain-specific knowledge for the application of modeling tools usually are distributed across institutions, soft-coupling is rather established than hard-coupling. Nevertheless, hybrid models that typically combine bottom-up and top-down energy modeling approaches are representatives for hard-coupling (Herbst et al. 2012).

In our opinion, a more favorable compromise between soft and hard-coupling is the integration and interlinkage of existing models in reproducible work-flows that can be distributed across institutional boarders. Dedicated workflow tools developed for design processes in aerospace and shipyard industry enable the automated execution of highly iterative or data-intensive multi-model simulations and thus allow quasi hard-coupling of the corresponding tools (Seider et al. 2012).

In reaction to the challenges related to i) addressing the granularity gaps by ii) a performant and reproducible model coupling approach, we propose a multi-model concept to comprehend the analysis of large-scale energy systems with ESOMs by transmission network simulation, distribution grid planning and agent-based simulation of the power market.

Figure 2 shows how each of the particular models can be characterized in terms of spatial, economic and technological focus.

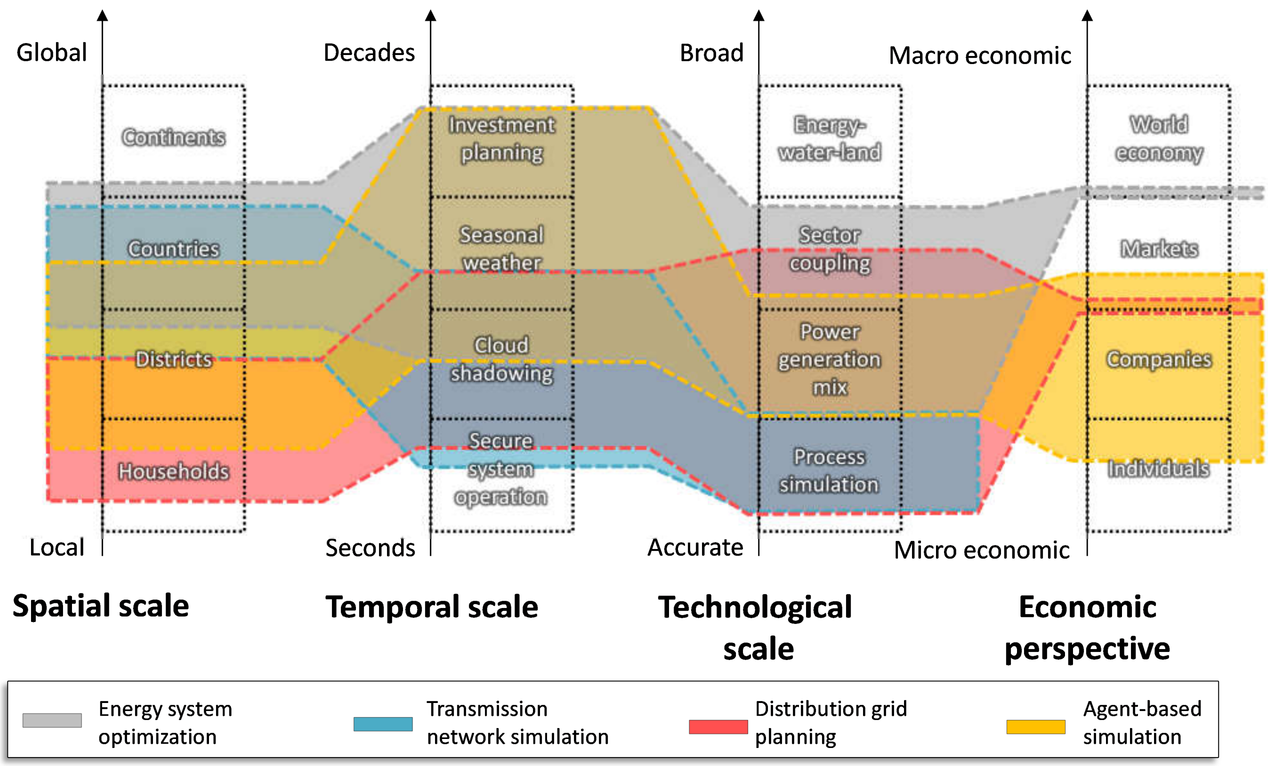

Figure 2: Characterization of the proposed multi-model approach for analyzing decarbonization strategies of energy systems

Besides convergence issues, the major challenge, especially of bi-directional model coupling, is data management and compatibility (i.e. allowing the outputs of a particular model to be inputs for another). In the following, we further discuss these challenges of providing insights from domain specific models to the top-level ESOM.

2.3.1 Incorporating aspects of transmission adequacy and security

In order to include power transmission aspects such as transmission adequacy and system security in energy system planning, the preparation of data for power flow analyses poses a challenging prerequisite. This applies to the compilation of complete and consistent transmission grid datasets, including electrical network parameters. A spatial disaggregation of ESOM output data requires geo-coordinates of substations. Coupling in the opposite direction is less cumbersome as it mostly comes down to spatial aggregation of costs or technical parameters, such as power transfer distribution factors (Cao et al. 2020).

Available transmission grid data models can be categorized in open models (Medjroubi et al. 2017) and proprietary models provided by transmission system operators (TSOs), e.g. (ENTSO-E 2018). The former are mainly based on OpenStreetMap (OpenStreetMap Contributors 2017), or have been applied to maps provided by TSOs (Wiegmans 2016) and therefore need to make assumptions on electrical parameters. Opposed to this, proprietary models contain real electrical parameters and information about power generators, but they usually lack geo-locations. A complete grid dataset can be obtained by first matching proprietary and open grid data models with geo-information from open power plant databases (Gotzens et al. 2019) and then estimating transmission line lengths from electrical parameters. Missing geo-coordinates then can be estimated by triangulation.

For the spatial disaggregation of ESOM output data on generation, appropriate distribution factors are needed. Such factors could be derived using actual power plant contributions to the power balance of a country. However, their validity is limited as they are subject to the actual state of the (transforming) energy system. Disaggregation may also be performed by means of an optimization algorithm. To this end, country-specific ESOM instances are required that fully capture the spatial resolution of the transmission grid.

2.3.2 Incorporating costs for decentral technology planning in the distribution grid

Challenges related to the coupling of the distribution grid planning with the top-level system are twofold. The first is the generalization and spatial upscaling of grid expansion measures (which are usually examined for representative, particularly selected distribution grids) to a nationwide cost indicator, which can then be considered in an ESOM.

The second challenge is the corresponding downscaling. Decentral technologies (renewable energy sources, heat pumps and charging stations) can be assigned to low, medium and high voltage distribution grids. Missing nation-wide distribution grid data, the lack of uniform standards and region-specific geographical conditions imply a high degree of freedom in assumptions regarding the spatial distribution and dimensioning of devices (e.g. many roof-top photovoltaics vs. one free-field photovoltaic plant).

An approach to meet the upscaling challenge is to reduce the highly location-dependent solution space and determining analogies in terms of decentral technology capacities. In (Meinecke et al. 2020), the authors present a methodology to derive representative benchmark grids which take this aspect into regard. These grid models are used instead of real networks' datasets to obtain relations between grid reinforcement costs and the share of new producers and consumers for different urban, sub-urban or rural areas. To scale-up from benchmark grid specific expansion cost to nationwide quantities, a mapping is required to match geographical regions, such as municipalities, to the corresponding benchmark grid. Criteria for appropriate clustering approaches are the ratio between supplied and total area of a municipality or the population density (Kittl, Sarajlić, and Rehtanz 2018).

In order to solve the downscaling problem, probabilistic approaches in terms of grid planning provide a way to deal with unknown future penetrations of decentral technologies. The idea is to distribute those randomly within the previously mentioned representative benchmark grids and examine the required grid expansion multiple times to obtain average and robust costs (Drauz et al. 2019).

2.3.3 Incorporating aspects of microeconomic actor decisions

Concerning coupling ABM to ESOMs, challenges arise from dealing with different system boundaries while having significant overlaps when modeling similar phenomena or mechanisms (e.g. power plant dispatch). In particular, this is related to selecting those outputs of an ESOM that only affect the agents' simulation framework (e.g. the power market) and to ensure that deviations between model outputs describing congruent phenomena are due to the differences in economic granularity (rather than the different system boundaries).

A way to tackle the challenge of different system boundaries is a model harmonization. This requires the ABM to be executed in a mode where actor-specific features (e.g. incomplete information) are disabled. Hence, if equally parameterized (e.g. by using the same techno-economic parameters), both models should show a congruent system operation and, thus, (sub-)system costs (Schimeczek et al. 2019).

From this starting point, the influence of actors' behavior can be investigated by agent-based simulation. Due to the increasing market penetration, trending examples are prosumers trying to maximize the self-consumption of photovoltaic-battery systems (Klein, Ziade, and De Vries 2019) and future heat pump owners who react on real time-pricing signals (Schibuola, Scarpa, and Tambani 2015). If the operation of such technologies is accordingly fixed in an ESOM, increasing system costs (compared to the macroeconomic optimum) are expectable. This cost difference (also interpretable as measure for the economic granularity gap) is subject to the regulatory framework conditions of the ABM and thus, allows for investigations on adapting the regulation regime, e.g. to incentivize system alignment of decentral actors.

3 Discussion

Previous studies show that both the increase of the resolutions in ESOMs and the model coupling represent options with partly high methodological and resource challenges.

Our concept of multi-model coupling allows combining top-level investment decisions in the energy system with costs and constraints associated to the spatial granularity such as arising with technology integration in the transmission and distribution grids. Integrating the behavior of decentral actors also enables the identification of appropriate regulatory regimes in order to reduce the economic granularity gap.

Automated workflows based on pre-configured peer-to-peer networks are the core of our concept, coordinating model-calls and data exchange. In this way, the individual models are still executed on their established IT-infrastructure but there are integral work flows that can be started from each point of the peer-to-peer network. This contributes to overcome recurring cross-institutional communication barriers, as well as to keep interdisciplinary expertise that is needed to maintain complex models which have been developed over years. Transparency and traceability of such multi-modeling approaches improve, because the overall data-processing is centrally stored and documented in defined workflows which also allow an easier reproducibility of the scientific outcome.

Downsides of establishing cross-institutional workflows are additional efforts for the setup of the peer-to-peer network (e.g. adapting IT infrastructures such as firewall rules). The proposed concept is therefore best used for extensive model coupling rather than simple unidirectional couplings. Furthermore, the convergence of multi-model coupling can prove challenging and, still, bridging granularity gaps is clearly only possible within the scope of the chosen models.

4 Conclusion

Modeling approaches for energy system planning are subject to the trade-off between claiming holistic perspectives and providing sufficient granularity for decision making. Especially for policy strategies, granularity gaps between what needs to be considered (and, thus, modeled) and the transferability into real actions or policies become evident. We described these gaps and discussed recent research approaches to overcome them. We presented a novel concept based on automated and cross-institutional workflows for bridging these gaps, as a promising perspective for future research. We illustrated this approach with selected model types that are relevant for merging different perspectives on energy system transformation. In this way, we addressed two major challenges in modeling the decarbonization of large-scale energy systems: render granularity gaps comprehensible and make necessary multi-modeling approaches executable in a traceable and efficient way.

5 Conflict of Interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

6 Author Contributions

TP, HL, TK and KKC were responsible for funding acquisition and conceived the concept of model coupling with automatized work-flows. KKC took the lead for the first version of the manuscript and the visualization of granularity gaps. KKC, OA, SD, ES and SFS performed the literature research. SD, TK and KKC contributed the manuscript sections on distribution grid planning. OA, KKC and HL wrote the sections on transmission network simulation, and ES, SFS and KKC did the same for the sub-chapters on agent-based simulation. The remaining text sections were mainly finalized by JH and KKC. TP, JH, SFS, TK, HL and SSS reviewed the full manuscript, provided critical feedback and helped to shape and improve the line of argumentation in different phases of manuscript preparation.

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