

# Bridging granularity gaps to decarbonize large-scale energy systems

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11 flexibility, security of supply

## 12 **Abstract**

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

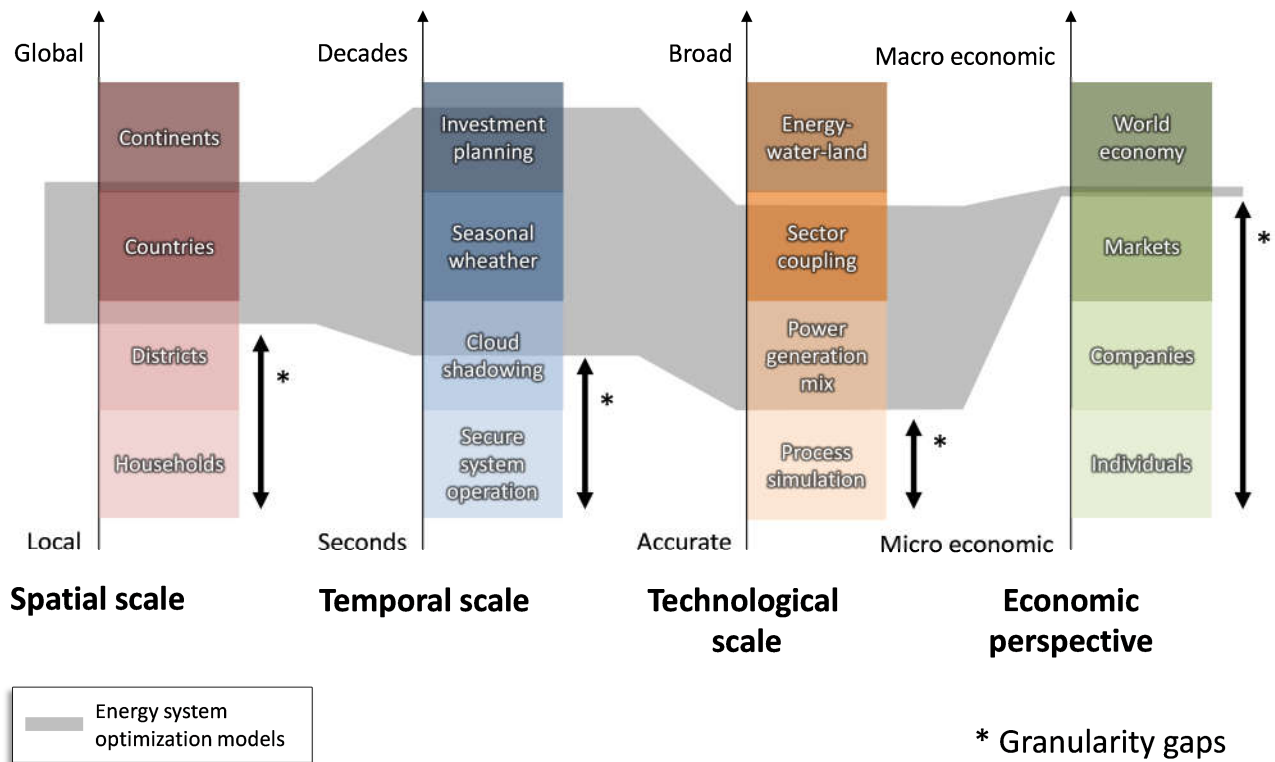
## 25 1 Analyzing future energy systems

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

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

35 Established approaches for energy systems planning are highly diverse in terms of their spatial,  
36 temporal, technological and economic perspective. Current models span from assessments on the  
37 household-level and small districts, e.g. (Kneiske, Braun, and Hidalgo-Rodriguez 2018) up to the  
38 modeling of individual or multiple countries (Gils et al. 2017) and even global systems (Teske et al.  
39 2019). The temporal scale plays a crucial role when it comes to planning of infrastructures with  
40 lifetimes of several decades on the one hand. On the other hand, verifying the operational feasibility  
41 and reliability of such infrastructures as well as fully exploiting power balancing potentials of  
42 batteries require short term system analyses (Hedegaard and Meibom 2012). In terms of technology  
43 representations, models range from detailed process simulations up to the coupling of energy sectors  
44 and interactions with other systems (e.g. energy-economy-climate) (Howells et al. 2013). The  
45 spectrum of economic perspectives comprehends simulations from individual decision-makers up to  
46 entire economies.

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



51

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

54 **1.1 Characteristics of large-scale energy system optimization models**

55 ESOMs are often applied to study the possible development of entire energy systems. For example,  
 56 Haller et al. do this for Europe including Middle East and North Africa (Haller, Ludig, and Bauer  
 57 2012). Their large geographic scope allows for investigating the benefits from international  
 58 cooperation, but their low spatial resolution limits the findings of, for example, concrete measures of  
 59 grid expansion needed for the integration of renewable energy sources (RES). Compared to Haller et  
 60 al., more recent studies such as (Sgobbi et al. 2016), (Child et al. 2019), (Bernath, Deac, and Sensfuß  
 61 2019) are more comprehensive in terms of the technologies considered. This development is fostered  
 62 by the trend of analyzing multi-technology interactions, especially in energy systems with high  
 63 shares of RES (Markard 2018). Resulting extensions of the energy models include other energy  
 64 sectors (e.g. the electrification of the heating sector as presented by Bernath et al.) or the introduction  
 65 of new technologies (e.g. hydrogen as fuel and long-term storage option as presented by Sgobbi et  
 66 al.). However, the spatial resolution usually remains rather coarse and the results are limited to the  
 67 perspective of a central system planner.

68 **1.2 The granularity gaps**

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

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

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

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

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

## 106 **2 How to bridge the granularity gaps?**

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

### 111 **2.1 Increasing resolutions in energy systems analysis**

112 Increasing model resolutions can be realized by yielding, for example, sufficient spatial resolutions to  
113 simulate effects in real transmission grid infrastructures. Cranking-up the resolution only makes  
114 sense if, at the same time, the underlying phenomena or technologies are modeled appropriately, for  
115 instance extending power flow modeling by voltage constraints (Salam 2020). And still, breaking-  
116 down high-level decisions to the local level remains challenging. This would always call for even  
117 better resolutions to capture distribution grids. In this case, differentiation between individual system

118 components becomes more important (as opposed to coarse technology-aggregations) and thus,  
119 decisions of heterogeneous actors gain in relevance and should be incorporated, too.

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

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

## 129 **2.2 Model coupling in energy systems analysis**

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

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

### 136 **2.2.1 Transmission network simulation**

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

142 In simple terms, power flow problems for existing or candidate grid infrastructures are solved (Salam  
143 2020) in order to obtain constraints related to transmission adequacy and power system security. The  
144 ESOM then trades-off grid expansion measures against other, competing flexibility-providing  
145 technologies.

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

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

### 152 **2.2.2 Distribution grid planning**

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

157 For the analysis of distribution grids, detached from the ESOM, domain-specific tools become  
158 essential. This is different to the transmission level, where by justifiable simplifications concerning  
159 modeling of power flows (e.g., by using DC-power flow (Stott, Jardim, and Alsac 2009)) an  
160 integration to an ESOM is still possible, as computational constraints are not exceeded and the model  
161 complexity remains manageable. Relevant tools automatically analyze, optimize and find solutions  
162 for imbalanced distribution grids. Examples are EDisGo (Müller et al. 2019), SNOP (Cibis et al.  
163 2019) or pandapower Pro (Scheidler, Thurner, and Braun 2018). The latter, for instance, identifies  
164 voltage, transformer and line problems and solves them by the use of heuristic approaches. This  
165 includes not only conventional solutions such as line and transformer replacements, but also  
166 innovative measures such as regulated distribution transformers or autonomous network re-  
167 configuration.

### 168 **2.2.3 Agent-based simulation of microeconomic actor decisions**

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

178 In the context of modeling energy markets, this approach is implemented, e.g., in the EMLab model  
179 (Chappin et al. 2017). EMLab models power companies as agents which sell their power on the  
180 energy markets and perform investment decisions regarding new power plants. The objective of the  
181 model is to analyze the aggregate effects of these investment decisions, e.g. on CO<sub>2</sub> mitigation  
182 targets, while evaluating different policy scenarios and designs of the European electricity markets.  
183 Another example is AMIRIS (Deissenroth et al. 2017), an ABM of the German power market  
184 focusing on the market integration of RES. Thereby, special consideration is given to the influence of  
185 political framework conditions on the operation and profitability of energy technologies.

## 186 **2.3 Model coupling via automated workflows: an exemplary coupling concept**

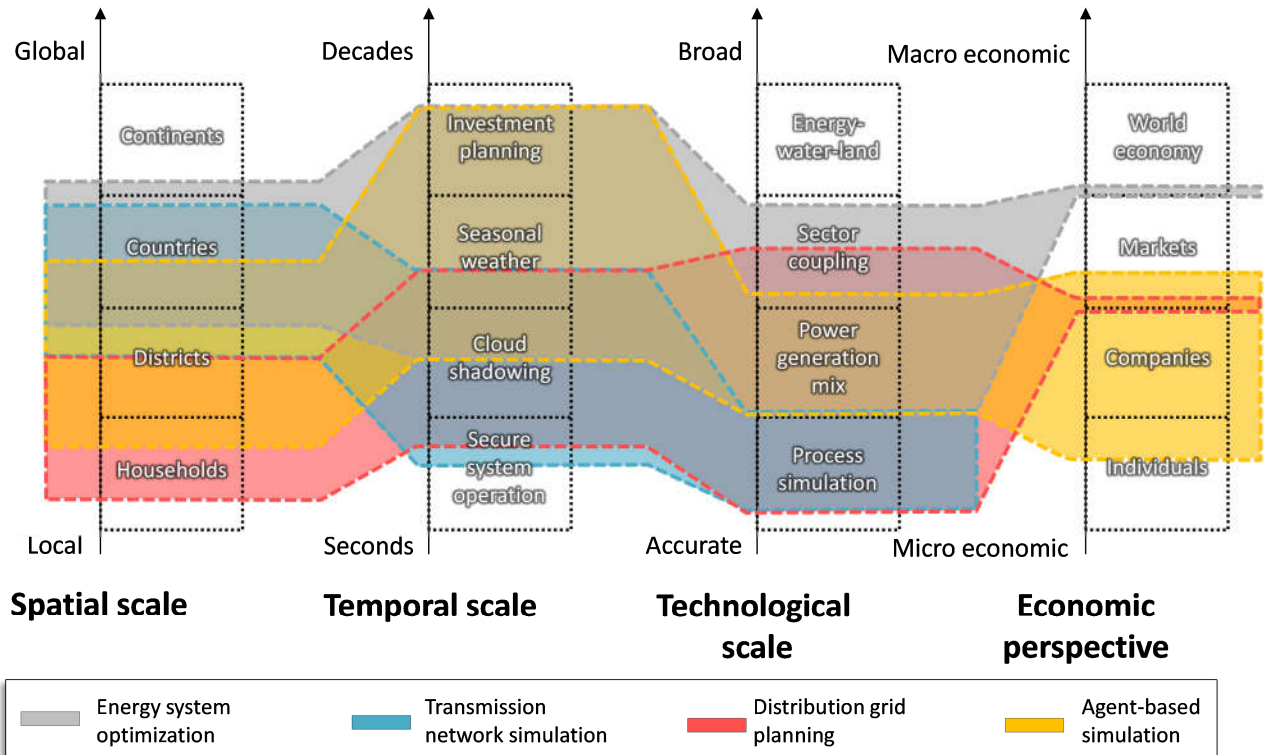
187 Domain-specific models can be coupled with ESOMs by either soft or hard-coupling. Soft-coupling  
188 means that independent models interact by exchanging input and output data. Hard-coupling denotes  
189 the integration of the domain-specific models, resulting in an extended ESOM. Existing literature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

197 In our opinion, a more favorable compromise between soft and hard-coupling is the integration and  
198 interlinkage of existing models in reproducible work-flows that can be distributed across institutional  
199 borders. Dedicated workflow tools developed for design processes in aerospace and shipyard

200 industry enable the automated execution of highly iterative or data-intensive multi-model simulations  
 201 and thus allow quasi hard-coupling of the corresponding tools (Seider et al. 2012).

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

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



208  
 209 **Figure 2: Characterization of the proposed multi-model approach for analyzing decarbonization strategies of**  
 210 **energy systems**

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

### 215 2.3.1 Incorporating aspects of transmission adequacy and security

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

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

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

### 238 **2.3.2 Incorporating costs for decentral technology planning in the distribution grid**

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

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

249 An approach to meet the upscaling challenge is to reduce the highly location-dependent solution  
250 space and determining analogies in terms of decentral technology capacities. In (Meinecke et al.  
251 2020), the authors present a methodology to derive representative benchmark grids which take this  
252 aspect into regard. These grid models are used instead of real networks' datasets to obtain relations  
253 between grid reinforcement costs and the share of new producers and consumers for different urban,  
254 sub-urban or rural areas. To scale-up from benchmark grid specific expansion cost to nationwide  
255 quantities, a mapping is required to match geographical regions, such as municipalities, to the  
256 corresponding benchmark grid. Criteria for appropriate clustering approaches are the ratio between  
257 supplied and total area of a municipality or the population density (Kittl, Sarajlić, and Rehtanz 2018).

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

### 262 **2.3.3 Incorporating aspects of microeconomic actor decisions**

263 Concerning coupling ABM to ESOMs, challenges arise from dealing with different system  
264 boundaries while having significant overlaps when modeling similar phenomena or mechanisms (e.g.  
265 power plant dispatch). In particular, this is related to selecting those outputs of an ESOM that only



266 affect the agents' simulation framework (e.g. the power market) and to ensure that deviations  
267 between model outputs describing congruent phenomena are due to the differences in economic  
268 granularity (rather than the different system boundaries).

269 A way to tackle the challenge of different system boundaries is a model harmonization. This requires  
270 the ABM to be executed in a mode where actor-specific features (e.g. incomplete information) are  
271 disabled. Hence, if equally parameterized (e.g. by using the same techno-economic parameters), both  
272 models should show a congruent system operation and, thus, (sub-)system costs (Schimeczek et al.  
273 2019).

274 From this starting point, the influence of actors' behavior can be investigated by agent-based  
275 simulation. Due to the increasing market penetration, trending examples are prosumers trying to  
276 maximize the self-consumption of photovoltaic-battery systems (Klein, Ziade, and De Vries 2019)  
277 and future heat pump owners who react on real time-pricing signals (Schibuola, Scarpa, and Tambani  
278 2015). If the operation of such technologies is accordingly fixed in an ESOM, increasing system  
279 costs (compared to the macroeconomic optimum) are expectable. This cost difference (also  
280 interpretable as measure for the economic granularity gap) is subject to the regulatory framework  
281 conditions of the ABM and thus, allows for investigations on adapting the regulation regime, e.g. to  
282 incentivize system alignment of decentral actors.

### 283 **3 Discussion**

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

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

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

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

305

## 306 4 Conclusion

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

## 317 **5 Conflict of Interest**

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

## 320 **6 Author Contributions**

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