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Multi-model ecologies for shaping future energy systems: Design patterns and development paths

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ABSTRACT

As energy systems grow more complex, modeling efforts spanning multiple scales, disciplines and perspectives are essential. Improved methods are needed to guide the development of not just individual models, but also *multi-model ecologies* – systems of interacting models. Currently there is a lack of knowledge concerning how multi-model ecologies can and should be designed to facilitate adequate understanding of energy system complexity and its consequences. Via an analysis of twelve multi-model initiatives both within and outside the energy domain, this paper elucidates possible design patterns and development paths for multi-model ecologies.

The results highlight two broad paths to developing energy system multi-model ecologies, one prioritizing interoperability and the other prioritizing diversity. The former path facilitates the efficient development of models spanning multiple scales and (to a degree) disciplines, and can ease systematic testing of assumptions. The latter is suited to bridging traditional disciplines and perspectives and advancing knowledge within the interstices of different knowledge communities. It is furthermore suggested that a combination of diversity, connectivity and hierarchy in multi-model ecology composition is central to enabling the development of complex webs of models capable of addressing the complexity of real-world energy systems.

1. Introduction

Current trends towards less carbon intensive, more decentralized, more interconnected and smarter energy systems are threads in a continuous process of energy systems evolution. The need to understand and steer this evolution with effective policies demands knowledge creation and management processes aligned with the complexity of the energy system itself. Insofar as they enable systematic exploration of the consequences of complex sets of technical and societal interactions, computer models are vital tools in this process.

The implementation of mathematical relations in the form of computer models combined with ongoing advancements in computational capabilities have drastically expanded our ability to grasp complex interactions. However, individual computer models are still undeniably restricted in the scope of system complexity they are able to effectively capture [1–3]. This limits our ability to holistically understand the operation and development of energy systems – across scales, disciplines and perspectives – and thus our capacity to effectively shape their evolution.

As energy systems grow more complex and society's demands on their performance more stringent, we need improved methods to guide the development of not just individual models, but also of *multi-model ecologies* – systems of interacting models [4]. Multi-model ecologies are essential for exploring the interactions amongst energy consumption, production, distribution and transmission; amongst different energy and non-energy infrastructures such as electricity, heat, gas, transportation and communications; and amongst socio-economic, environmental and technical phenomena. By facilitating exploration of complex energy system dynamics on multiple scales and from multiple perspectives and disciplines, multi-model ecologies open up possibilities for addressing problems and questions that were previously beyond reach, and enable systematic testing of assumptions.

Moreover, deliberately viewing systems of models as multi-model ecologies enhances our capacity to strategically steer their combined development. Rather than starting from scratch with each new problem, question or research agenda, existing models can be reused, combined, expanded or adapted to address new questions that arise. Focus shifts from the development of individual models to the

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deliberate *cultivation* of a system of models in a manner which provides ongoing value and effectively adapts to changes in knowledge needs.

The relevance of multi-model ecologies for energy systems is highlighted by a variety of research initiatives seeking to develop and integrate energy system models addressing different scales, scopes and disciplines, and by recent appeals to the need for such research:

- Spataru, et al [5] cite the need for a “holistic, multi-dimensional and multi-scale framework” to address urban energy challenges.
- Grijalva [6] suggests that emerging engineering challenges in the electricity sector require a “holistic, multi-dimensional, multi-scale framework”, and notes specific challenges aggravated by computational limitations, such as dispatch with large penetration of wind generation, demand response in smart grids and multi-level information in transmission and distribution.
- Strachan, et al [7] describe the danger of silos built around specific modeling approaches in energy modeling, and the need for explicit model comparisons for effectively informing policy.
- Ferris [8] calls for layered or hierarchical models to support decision processes in power systems planning, and notes specifically a need for coupled smaller models with well-defined interfaces.
- Brummitt et al [9] point to a lack of scientific analyses of the interactions among human operators, protocols, automatic controls, and physical grids, and state a critical need for “accurately yet insightfully modeling the feedbacks surrounding electrical infrastructure”.

Complementary to this is the challenge of dealing with increasing volumes of diverse *data*, including real-time operational data (e.g. from sensors), market data, infrastructure data and others. Just as with models, the integration of data across scales, disciplines and perspectives is essential. However, effective data integration is hindered by a lack of standard data structures, formats and assumptions, and increasingly also by the sheer quantity of available data.

The challenge of spanning multiple scales, disciplines and perspectives in energy systems research – both in terms of models and data – can be addressed by effectively designed and cultivated multi-model ecologies. However, existing multi-model initiatives adopt vastly different approaches and techniques to representing energy systems and to integrating models and data. These differences may have important implications for the nature of generated knowledge, and thus the ensuing decisions made in shaping future energy systems. Currently lacking is adequate knowledge regarding how multi-model ecologies can be designed and cultivated such that they effectively contribute to holistic understanding of energy systems on the part of policy makers, planners and energy system operators.

The objective of this review is to identify possible *design patterns* and *development paths* for multi-model ecologies – from both a technical (i.e. computational) and social (i.e. organizational/institutional) perspective – and to evaluate the suitability of these for energy systems (multi-) modeling initiatives. We continue in the following section by motivating the need for the use of multi-model ecologies in energy systems research. Building on this, we describe and assess a set of six existing multi-model ecologies dealing with different energy systems topics. We accompany this with an analysis of complementary initiatives in other domains. Finally, we synthesize the insights from these analyses with the aim of extracting design patterns and identifying development paths for multi-model ecologies in the energy systems domain.

2. Multi-model ecologies and the challenge of complexity

Foreseen developments over the coming decades will likely lead to an expansion in the complexity of energy systems, manifested in a greater diversity of technical (and social) elements, an increased degree of interconnection/interdependency between them, and greater vertical differentiation [10]. Though greater energy systems complexity is not a

goal in itself – and indeed brings many challenges – it is a fundamental side-effect of efforts to enhance energy system sustainability, flexibility, efficiency and resilience. This is illustrated by several trends:

- The push towards smarter and more distributed energy systems will entail the instantiation of more and faster communication feedbacks between system elements and levels – from the scale of buildings and neighbourhoods to countries and continents – as well as the integration of a diversity of IT devices into the existing infrastructure.
- The liberalization/deregulation of energy systems has already led to a variety of new roles and markets and, in the future, can be expected to further the involvement of a greater diversity of autonomous actors in the energy system – e.g. power producers, transmission and distribution system operators, retailers, aggregators – interacting with one another within an increasing diversity of markets.
- The integration of different infrastructures – such as electricity, gas, heat, transport and IT – will create new feedbacks and interdependencies, local and global, amongst infrastructures that have historically been developed and operated independently.
- Large-scale integration of renewables will require rapid system adjustment to changes in the availability of wind and solar radiation, and thus rapid and automated feedback between system elements.

Insofar as complex systems have the potential to generate nonlinear and non-intuitive behavior, however, the growing complexity of energy systems may challenge our ability to effectively control their operation and steer their development with suitable policies and designs. While system feedbacks may help to preserve the stability of a system under certain conditions, they may exacerbate the effects of disruptions under others [11,12]. Likewise, while the introduction of competition into energy systems can enhance efficiency, it may also incite strategic behavior and investment patterns deviating from the social optimum [13].

A side effect of increasing system complexity is a proliferation of perspectives and approaches for understanding and guiding the development of energy systems. Rather than contributing to a more holistic view of energy systems, this tends to feed the formation of silos around different modeling approaches, impeding the ability of policy makers and utility regulators to effectively assess insights from competing models and methodologies [7].

Alleviating the potential risks of energy system complexity requires an ability to holistically explore the consequences of energy system developments and possible technical or policy solutions such as market designs, control algorithms and network investments. This requires tools that enable (1) systemic exploration of multi-scale, multi-disciplinary and multi-infrastructure interactions within energy systems, (2) adequate consideration of the range and types of uncertainties to which these interactions may be subject, and (3) systematic testing of different assumptions and approaches. Such capabilities are beyond the competence of any single model or algorithm. Their realization demands improved approaches to cultivating and deploying interacting sets of models and data, and to effectively synthesizing, comparing and transferring their insights.

Several previous reviews have highlighted the need for and progress towards multi-scale, multi-model initiatives in the energy domain. In a review of energy systems models for energy policy, [14] identifies how different categories of models address growing energy systems complexity, and particularly the links across scales/layers in energy systems. In a review of building energy models at the district and urban scale, [15] notes an outstanding need “for more systemic, multi-scale and transversal approaches able to deal with the intrinsic complexity of urban tissues”. In a review of methodologies for integrating short-term variations of the power system into energy system models, [16] evaluates different methodologies for soft-linking of models representing different time scales versus direct representation of multiple time scales.

Fig. 1. Left pane: Illustration of interactions within a hypothetical multi-model ecology, including models, datasets and actors interacting in different ways. Right pane: Illustration of interactions amongst model and data elements in the HUES platform, including data exchanges (DE) and results comparisons (RC) between modules.

The need for integration of computer models reflecting different perspectives, disciplines, scopes and scales is not specific to the energy systems domain, and is indeed fundamental to addressing problems in a variety of fields [17–19]. Approaches such as integrated modeling [2], model webs [20], multisimulation [21] and cosimulation [22] – as well as modeling frameworks [23–26] and interface standards [27] – have emerged to facilitate model integration and reuse efforts in different fields.

The concept of *multi-model ecologies* [4] offers an overarching perspective on multi-model environments in a manner which emphasizes their socio-technical interactions and evolution. From this perspective, models constitute sets of co-evolving memes, or memplexes [28]. Models in a multi-model ecology may have different scopes, resolutions, and perspectives, and different models may represent different theoretical viewpoints. Just as the interactions of elements in a memplex reinforce one another, the interactions of resources in a multi-model ecology enhance one another's usefulness. The interactions amongst models, datasets and actors in a multi-model ecology may take various forms, including:

- *Model-model interactions*, e.g. data transfer/exchange, branching, structural comparison
- *Model-data interactions*, e.g. model input, model output, model calibration
- *Data-data interactions*, e.g. data transformation, numerical comparison
- *Data-actor interactions*, e.g. data collection, data analysis
- *Actor-model interactions*, e.g. model development, model execution
- *Actor-actor interactions*, e.g. knowledge transfer/exchange, research questions

Fig. 1 (left pane) shows a hypothetical example of how these different forms of interactions might play out in a multi-model ecology. Model A is developed as a branch of Model B (1), and outputs results in the form of a number of datasets (2). These datasets are analyzed by Actor A (3), who exchanges knowledge with Actor B (4). Drawing from this knowledge, Actor B develops Model C based on an alternate set of assumptions (5) which interacts with a suite of existing models (6). The outputs of Model B and Model C are compared with one another (7). The results of Model C are analyzed by Actor C, (8) who transfers the developed knowledge to a group of policy makers (9).

A more concrete example is shown in the right pane of Fig. 1, which illustrates a simplified structure of interactions between models and data in the *Holistic Urban Energy Simulation (HUES)* platform (described in Appendix A), including data exchanges (DE) and results comparisons (RC) between modules in the platform. In the HUES platform, building occupancy models, weather data and building data may serve as inputs to building energy performance models. The outputs of these models, in

turn, may serve as inputs to energy system models, which draw from a technology database, as well as different forms of weather and climate data. The results of these models – which take the form of optimal technology capacities and dispatch patterns in a multi-energy system – may then be compared with detailed simulation models for validation or calibration purposes.

As these examples illustrate, multiple interaction pathways are possible in a multi-model ecology and new pathways may emerge over time. Many different interaction structures are possible, e.g. centralized, decentralized, tightly connected, loosely connected. Independently, each model provides a partial picture of the components and relationships underlying a given problem. Together, they provide a more multi-dimensional, and constantly changing, representation of the system at hand. As this set of resources grows and develops over time, involved actors improve their ability to gain a holistic and multi-dimensional understanding of the problem/system of interest. Viewing systems of interacting models as multi-model ecologies enhances our capacity to strategically develop and effectively deploy the knowledge contained within them.

Many ongoing initiatives have recognized the need for further integration and reuse of energy systems modeling activities, giving rise to a number of multi-model ecologies. Examples include the Energy Modeling Laboratory (EMLab),¹ the Holistic Urban Energy Simulation (HUES) platform,² the Modelica ecosystem of tools,³ the Whole Systems Energy Modeling (wholeSEM) Consortium,⁴ the Integrated Energy Systems Modeling Platform (Nexus),⁵ Enipedia⁶ and the Open Energy Modeling (Openmod) Initiative.⁷ Each of these ecologies takes a different approach to the integration and reuse of models and data in the energy domain, and uses different sets of tools and techniques to accomplish this. Currently, there exists little understanding of how initiatives like these can and should be designed and managed, though this may have important consequences for the types of insights an ecology is suited to deliver and the contributions it may make to shaping the design and operation of future energy systems.

3. Overview of the analyzed initiatives

This section introduces the initiatives covered by the analysis, including six initiatives from the energy domain and six from a variety of other domains. In both cases, these initiatives have been selected based

¹ <http://emlab.tudelft.nl/>.

² <https://hues.empa.ch/>.

³ <https://www.modelica.org/>.

⁴ <http://www.wholesem.ac.uk/>.

⁵ <http://www.esc.ethz.ch/research/research-projects/Nexus.html>.

⁶ <http://enipedia.tudelft.nl/>.

⁷ <http://wiki.openmod-initiative.org/>.

Table 1
Overview of the analyzed initiatives from the energy domain.

Initiative	Description	References
EMLab	A platform for open source, multi-tool, multi-model, multi-level energy modeling. Modularity of EMLab is built around interchangeable scripts for e.g. market clearing, investment and power plant dispatch. Switching scripts allows for testing assumptions and addressing research questions concerning energy policies and electricity market design issues.	[29–32]
Enipedia	A linked data platform enabling energy system data from different sources to be connected, queried, and visualized from different perspectives.	[33,34]
Modelica	Integrates data on electricity production and storage, natural gas infrastructure and flows, and industrial production chains from various sources.	[35–38]
	An object-oriented modeling language for the dynamic analysis of complex, highly-integrated physical systems using differential, algebraic, and discrete equations. Clustering of component models into libraries together with the ease of nesting components leads to a set of computational modules that can be readily reused and integrated in different ways.	
HUES	A set of models and databases to aid in the design and operation of district and urban energy systems. Modules are implemented using different computer languages and modeling techniques and are accompanied by a semantic wiki-based software infrastructure to support navigation, sharing and understanding of the modules.	[39,40]
Openmod	Initiative focused on enhancing transparency, credibility, efficiency and quality of energy modeling efforts. In addition to collating and disseminating open models and data, Openmod steers modeling work by developing guidelines on practical aspects such as software licensing and data sharing techniques.	[41]
WholeSEM	Multi-institutional initiative with a focus on building and linking energy models to support the UK's national strategic energy modeling activity [42]. Modeling activities span different techniques and scales and include energy system evolution, unit commitment, network planning, social practices and others.	[42,43]

on the qualitatively different nature of their compositions. We have only included initiatives that seek to significantly bridge different scales, disciplines or perspectives, and with clear ambitions for sustained future development. Some energy domain initiatives similar in composition to the analyzed initiatives have been excluded.⁸

In Table 1, each of the six initiatives from the energy domain is described. An extended description of each of these initiatives can be found in Appendix A. One or more of the authors of this paper have been directly involved – to a greater or lesser degree – in four of the six energy domain initiatives.⁹ The details of the remaining energy domain initiatives, and the six initiatives from other domains, have been derived from a systematic search of available literature (using peer-reviewed literature databases), including journal and conference publications, as well as the initiatives' websites. In discussing and analyzing these initiatives, we frame them as multi-model ecologies, emphasizing the interactions and evolution of their social and technical elements.

Table 2 provides an overview of the analyzed initiatives from other domains. These initiatives have been selected to exemplify alternative or complementary approaches to those currently being pursued in the energy domain. They are drawn from a range of fields, including earth sciences, biology, agriculture, health, neuroscience and statistics. Though not all of these initiatives may be strictly defined as multi-model ecologies, their approaches offer insights into how multi-model ecologies may be designed and developed.

4. Analysis

The initiatives introduced above reflect a variety of possible configurations for multi-model ecologies. Building on the ecological metaphor core to the multi-model ecologies concept [4], this section assesses the selected initiatives according to three fundamental ecosystem metrics: diversity, connectivity and hierarchy. These metrics have been selected to provide a comprehensive view of the elements and relationships within each initiative, both technically/computationally and socially/organizationally.

For each of these metrics, we analyze each initiative along two dimensions – the technical dimension and the social dimension. The technical dimension encompasses the (interactions amongst) models and datasets in an ecology, and the social dimension the (interactions amongst) actors in an ecology. For purposes of this analysis, the metrics are defined as follows:

Diversity is the variety and relative abundance of models, datasets and actors representing different disciplines, perspectives and system scales (builds on the definition of [55]). This includes: (1) the diversity of disciplines, perspectives and system scales represented within the initiative's constituent models and datasets, and (2) the diversity of disciplines and perspectives represented by the actors involved in the initiative.

Connectivity is the degree to which an initiative facilitates the flow of data, information and knowledge amongst the involved actors, models and datasets (builds on the definition of [56]). From a technical perspective, connectivity is equated with the degree of interoperability amongst models/datasets in a multi-model ecology which enable data to flow easily amongst elements. For the purposes of this investigation, technical connectivity is evaluated on the basis of the *levels of conceptual interoperability* framework of [57]. From a social perspective, connectivity is defined in terms of the quantity and quality of communication channels within a multi-model ecology, which facilitate the flow of information and knowledge both amongst actors within the ecology and with external actors. This includes in-person communication channels such as meetings or conferences, web-based channels such as wikis, and, perhaps most importantly, adequate documentation.

Hierarchy is characterized by the presence of multiple semi-autonomous levels which communicate data, information or knowledge amongst one another (builds on the definition of [58,59]). In the technical dimension, hierarchy implies the existence of different levels of interacting models and/or datasets in a multi-model ecology. In the social dimension, it implies the existence of different levels of interacting actors.

On the basis of these metrics, we aim to identify patterns in the composition and development of the selected initiatives and thus different pathways to the realization of multi-model ecologies of energy systems. Additionally, we relate this to the purpose of the selected initiatives (as defined by the initiative's architects and/or community). Detailed results of the analysis can be found in Appendix B. Fig. 2 summarizes the results for all twelve of the analyzed initiatives.

4.1. Design patterns

Fig. 2 highlights several important patterns in the composition of the analyzed initiatives. First, no initiatives were found to feature both high diversity and high connectivity in the technical dimension. This may be partially attributed to the challenge of enabling a high degree of

⁸ This includes Trnsys (<http://www.trnsys.com/>), Matlab Simulink (<https://ch.mathworks.com/products/simulink/>), OpenEI (<http://en.openei.org/>) and Reegle (<http://data.reegle.info/>).

⁹ This includes EMLab, Enipedia, HUES and Openmod.

Table 2
Overview of the analyzed initiatives outside the energy domain.

Initiative & domain	Description	References
GEO Model Web (Earth sciences)	A dynamic and distributed web of models, databases and websites forming consultative infrastructure for researchers, managers, policy makers and the general public; based heavily on principles of the World Wide Web, the Semantic Web and Web 2.0.	[44]
Geppetto & OpenWorm (Biology)	Geppetto is a web-based multi-algorithm, multi-scale platform for the simulation of complex biological systems. It was originally conceived as a resource for the OpenWorm project, an open source initiative to create a virtual <i>C. elegans</i> nematode.	[45–47]
AgMIP (Agriculture)	An international effort linking the climate, crop, and economic modeling communities with the aim of producing improved crop and economic models and next generation climate impact projections for the agricultural sector.	[48,49]
Splash (Health)	A project of IBM Research for combining existing heterogeneous simulation models and datasets to create composite simulation models of complex systems; seeks to enable the integration of models across domains without specifying strict standards for the development of component models.	[50,51]
MUSIC (Neuroscience)	A standard API to facilitate run-time communication between large-scale neuron simulators using different model description languages, enabling plug-and-play interoperability of software components.	[52,53]
R (Statistics)	An open source and widely used computer language and software environment for statistical computing and graphics. A key element is a packaging system which allows for simple extension of R's base language and environment.	[54]

Fig. 2. Summary of the analysis results, comparing the diversity (Div), connectivity (Conn), hierarchy (Hier) and purpose of the selected initiatives. Energy-focused initiatives are indicated in bold.

interoperability amongst conceptually and semantically diverse technical elements. Initiatives that come closest in this regard include Modelica, the GEO Model Web Initiative, Openworm, MUSIC and R. Most of these initiatives also feature a (relatively) high level of technical hierarchy, suggesting that hierarchy plays a role in facilitating simultaneously diverse and connected multi-model ecologies. This may be explained by the role of hierarchy in enabling the realization and communication of ontologically diverse elements. In Modelica, for instance, a DC electrical load in a building may be created as a sub-sub-sub-component of the building itself – a single branch in a tree of highly diverse elements. The intermediate levels in this tree allow these elements to interact by defining shared concepts, which forms a basis for semantic interoperability.

In the social dimension, there exists no clear relationship between diversity, connectivity and hierarchy. However, the lack of strong social hierarchy in the case of any of the analyzed initiatives is remarkable, given the highly structured technical outputs that characterize these initiatives. To a large degree, the emergence of technical hierarchy despite relatively flat social structure may be attributed to tools such as web-based code management systems (e.g. Github), semantic wikis (e.g. Semantic Mediawiki), issue tracking systems and package repositories (e.g. CRAN), all of which facilitate systematic collaboration on software projects. In essence, tools such as these create transient social hierarchies by structuring interactions in a way that enables the sharing of information across levels within a multi-model ecology. The structure of the technical hierarchy lays a structure for these transient social hierarchies. This is illustrated by R, in which popular packages exhibit a mutualistic relationship with the more specialized packages that depend on them (e.g. authors of specialized packages help fix bugs

in the popular packages). The dependencies in packages dictate a web whose connections help to direct people's energy around.

Interestingly, those initiatives with the highest levels of social hierarchy (Modelica, R and AgMIP) are also generally observed to have high levels of technical hierarchy. Both Modelica and R are highly developed initiatives, involving a large number and (relatively) high diversity of models/packages and actors. In these cases, some degree of social hierarchy aids the emergence and evolution of standards (e.g. licenses and modeling languages) underlying the initiative by facilitating communication and coordination amongst involved actors. These standards, in turn, are fundamental to the realization and sustained development of technical hierarchy, connectivity and diversity. In the case of AgMIP, social hierarchy is also elemental to the development of standards which facilitate technical connectivity. Unlike Modelica and R, however, the initiative's primary purpose (model intercomparison) does not require or incentivize high levels of technical hierarchy.

4.2. Relationship between purpose and composition

The purposes of the selected initiatives are found to fall into one of two categories: (1) *enhancing modeling competencies*, e.g. in terms of model interoperability, quality and/or disciplinary scope, and (2) *transparency and dissemination* of modeling work and associated knowledge. Based on the analysis, a clear link between the purpose and technical composition of initiatives can be seen. Namely, initiatives focusing primarily on transparency, dissemination and reuse tend to feature relatively high levels of technical diversity, lower levels of technical connectivity and hierarchy and relatively high levels of social

Fig. 3. Conceptual illustration of the two identified paths for realizing multi-model ecologies, and the approximate locations of the analyzed energy initiatives. Path 1 prioritizes connectivity; path 2 prioritizes diversity.

connectivity. Initiatives focusing more on modeling competencies tend to feature higher technical connectivity and (relatively) lower levels of technical diversity. Both of the initiatives featuring high levels of technical hierarchy entail a purpose mixing the pursuit of transparency, dissemination and reuse with enhancement of modeling competencies.

These relationships may be explained by the fact that initiatives focused strongly on transparency and dissemination do not necessarily require a highly connected technical ecosystem, but do require a highly connected social ecosystem to facilitate dissemination and reuse of models and data. On the other hand, initiatives focused strongly on enhancing modeling competencies benefit from high levels of technical interoperability, which greatly expands the capabilities of the model system. A high degree of community engagement is feasible (and beneficial) in both of these cases, but the need for clear community standards and guidelines (e.g. to enable module interoperability or inter-comparison) in the latter case demands more defined coordination mechanisms. This is particularly true in the case of larger initiatives spanning many organizations, such as Modelica, AgMIP, the GEO Model Web and R.

4.3. Development paths

The analyzed initiatives highlight two distinct paths to the realization and development of multi-model ecologies, conceptually illustrated in Fig. 3. Path 1 is exemplified by Modelica, R, EMLab, MUSIC and Openworm. This path prioritizes *connectivity* by basing modeling work on an agreed set of standards, such as a common modeling and/or programming language. This enables emergence over time of diversity and hierarchy amongst the technical elements (models and datasets) of the ecology, as well as the systematic testing of model assumptions. It also lays a basis for addressing problems of increasing specificity. As the ecology grows, more and more computation can be shifted to other resources in the technical hierarchy, reducing the cost of addressing problems of high specificity – a pattern aptly illustrated by the development paths of Modelica and R. In some cases, social hierarchy follows as a way of coordinating the evolution of standards.

Path 2 is exemplified by Openmod, HUES, WholeSEM, the GEO Model Web, Splash and AgMIP.¹⁰ In these cases, priority is given to

¹⁰ While AgMIP is focused primarily on enhancing connectivity (e.g. inter-comparisons, data alignment) between models and datasets, the path followed by the set of technical resources within AgMIP is better characterized by the second path.

diversity – enabling the integration of models representing different spatial/temporal scales, disciplines and perspectives within a common platform. Interoperability, if present at all, emerges over time as models and datasets are gradually adapted to interact with one another. In such cases, social connectivity can play an important role in driving the integration and dissemination of diverse resources in the platform.

Both of these paths can lead to vibrant multi-model ecologies under the condition that they are able to provide sustained usefulness to their social communities. Modelica and R have succeeded because they enhance the modeling and analysis capabilities of their users by enabling them to take advantage of a wealth of computational resources developed within the community. The basis of these ecologies on a foundation of clear standards means that they are able to leverage network effects and autocatalytic dynamics, with the development of one model or package catalyzing the development of others. Openmod also succeeds because it enhances the modeling capabilities of its participants. However, it accomplishes this not by offering a wholly interoperable suite of models, but by facilitating the sharing of diverse resources and by advancing and disseminating best practices, both of which provide value to its social community.

In the case of both of these paths, standards can be an important enabler of interoperability by helping to align the ontological bases and data structures of models and datasets in diverse ecologies. Insofar as standards form a potential barrier to entry by placing additional requirements on developers, however, they must be accompanied by mechanisms to incentivize ongoing contributions, such as long-term project funding. Another option is to allow standards to emerge over time in interaction with an ecology's social community. This creates low barriers to entry in the initial stages of ecology development, encouraging contributions and facilitating the formation of a community. Once a stable community has emerged, it can be engaged to develop standards that enhance the overall usefulness of the ecology. Openmod, a relatively new initiative, has managed to create a relatively stable community and has recently begun, in a limited way at least, to develop community guidelines, e.g. with regard to licensing.

An absence of stringent or obligatory standards, however, need not preclude opportunities for module interoperability within a multi-model ecology. A number of approaches are available to enable interoperability in the absence of standards, including registration processes and metadata files (Splash), ad-hoc linking via scripts (HUES), and reflective middleware approaches [60]. Efforts within AgMIP aptly illustrate possible methods and challenges for enabling interoperability and inter-comparison amongst a highly diverse set of modeling resources.

5. Discussion

Both technical diversity and connectivity (interoperability) are key to realizing the full benefits of multi-model ecologies in terms of enhancing our ability to address the complexity of energy systems. Greater interoperability enables researchers to progressively shift operations below the level of active comprehension by enabling the creation of automated data transformation pipelines. This allows research efforts to focus on domain-relevant questions instead of on computational infrastructure. Next to this, technical diversity ensures that modeling activities sufficiently reflect the variety found in real world (energy) systems. Technical hierarchy furthers the advantages of interoperability and diversity, enabling the development of complex (not just complicated¹¹) webs of models capable of addressing the complexity of real-world (energy) systems.

However, it must be kept in mind that with more complex systems

¹¹ With a sheer increase in the number of parts, complicatedness increases; with an accompanying increase in the depth of interaction structure (hierarchy), complexity increases [10].

of models come increased needs for input data and model parameterization. Systematic approaches for managing model input and output data (e.g. relational or graph databases) can facilitate this. The approaches taken by Enipedia, AgMIP and Openmod are instructive here. Also essential are systematic approaches for dealing with model and parameter uncertainties, such as exploratory modeling [61,62] and internal discrepancy analysis [63].

The most successful of the analyzed initiatives demonstrate the importance of an engaged *social community* to provide the impetus and effort that drive the development of a multi-model ecology. As highlighted by the analyzed initiatives, *openness* is an important element of encouraging community engagement, and can be achieved in different ways that do not necessarily conflict with commercial interests. In this vein, [7] proposes the creation of *expert user groups* around modeling platforms to facilitate ongoing maintenance of complex tools, alleviate issues caused by high turnover rates of technical staff and allow policy makers to draw from a deeper institutional memory. However, in the domain of energy systems where strongly embedded and distinct communities exist based on traditional organizational and disciplinary boundaries, a key issue is how these disparate communities can be effectively bridged.

An important question is which of the aforementioned paths is most suitable for energy systems initiatives. Clearly, energy systems span a number of conventional disciplines – from physics to economics – with very different ontologies and worldviews. The development of ecologies that seek to span a breadth of disciplines, scales and perspectives, may benefit from the latter path. This allows greater flexibility in integrating a diversity of models, and increasing degrees of interoperability over time. Importantly, this approach can also facilitate the sharing of diverse modeling resources, enabling the spread of modeling concepts and hindering the formation of silos based around specific disciplines, scales and perspectives. Ecologies with a narrower focus may benefit from the former path, which allows for greater interoperability – and thus greater capability to build on the work of others – out of the box. This can contribute to greater efficiency and innovation in model development and knowledge generation.

Relevant in this context is also the reality that different multi-model ecologies are not independent of one another (Fig. 4). EMLab-Generation, for instance, is represented on the Openmod wiki; Enipedia feeds data into EMLab; and HUES aims in the near future to incorporate Modelica modules. Such links between ecologies may be social – individuals involved in one ecology may be involved in another – or technical – models may simultaneously participate in multiple ecologies. Just as models may be seen as wholes in themselves as well as elements of a multi-model ecology, multi-model ecologies may be seen as part of a larger *ecology of ecologies*.

No single model or even multi-model ecology is capable of capturing all relevant aspects of the energy system. For this reason, links

within this ecology of ecologies are essential to enabling the cross-fertilization of technologies and ideas and to adequately addressing the complexity of energy systems. Developing a multi-model ecology is thus not about realizing an all-encompassing suite of modeling resources, but about effectively linking with and filling a (perhaps very specific) need or gap within this ecology of ecologies. Policy makers may play an active role in cultivating this ecology of ecologies to encourage the development of modeling initiatives reflecting the full range of relevant scales, perspectives and disciplines, and facilitating connectivity between them.

6. Conclusions

Effectively dealing with increasing energy system complexity demands holistic exploration of the consequences of energy system developments and technical or policy solutions, potentially spanning multiple scales, disciplines and perspectives. Such capabilities are beyond the competence of any single model, thus requiring the development of interacting systems of models, or *multi-model ecologies*. Implementing multi-model ecologies in practice, however, necessitates adequate understanding of available options and best practices for their development – knowledge which is currently lacking. To address this gap, the objective of this review has been to identify design patterns and development paths for multi-model ecologies – from both a technical and social perspective – and to evaluate the suitability of these for energy systems (multi-)modeling initiatives.

With regard to design patterns, the analysis found no initiatives with both high diversity and connectivity in the technical dimension, which may be attributed to the challenge of enabling a high degree of interoperability amongst conceptually/semantically diverse elements. The analysis also identified a lack of strong social hierarchy in the case of any of the analyzed initiatives, but found that those initiatives with the highest levels of social hierarchy are generally characterized also by high levels of technical hierarchy.

With regard to development paths, the analysis suggests that there exists no single route or design template for the realization of energy systems multi-model ecologies. Which path is most suitable depends on the specific goals of an initiative. Initiatives with the goal of enhancing modeling competencies within a (relatively) narrow band of disciplines may best pursue a path prioritizing technical connectivity (interoperability) amongst elements. This requires clear standards which, if a vibrant ecology is to be maintained, should be developed in coordination with other actors in the initiative's community. This, in turn, requires active cultivation of a strong community, and the development of social structures (hierarchy) to facilitate the evolution of standards over time.

Initiatives with the primary goal of model dissemination and transparency may best be served by a path that prioritizes technical diversity. By initially maintaining low barriers to entry and minimizing the stringency of standards, it becomes possible to incorporate models and datasets representing a wide range of scales, disciplines and perspectives. In addition to facilitating knowledge dissemination, this can help to bridge traditional disciplinary silos and advance knowledge within the interstices of different knowledge communities. Technical connectivity may gradually be increased over time by phasing in modeling and data specification standards. Open standards and software, comprehensive documentation and permissive licensing are essential to preserving transparency and enabling broad dissemination.

For energy systems researchers – as well as researchers in other domains – in the process of developing multi-model ecologies, the design patterns and development paths identified in this paper may be instructive in terms of finding an appropriate path forward. Additionally, we hope that our analysis may facilitate and inspire a shift in focus from the development of isolated models to the cultivation of evolving systems of interacting models, in turn enabling researchers to better address the complexity of energy systems.

Fig. 4. As illustrated by the relationships between analyzed initiatives, the social and technical elements of different multi-model ecologies link with one another, forming a larger “ecology of ecologies”.

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Appendix A. Description of the analyzed initiatives

EMLab: The Energy Modeling Laboratory (EMLab)¹² is a platform for open source, multi-tool, multi-model, multi-level energy modeling. The platform has grown out of modeling efforts within an energy and industry research group at Delft University of Technology over the past decade, which have sought to understand and shape the evolution of model systems and ontologies [64–66,34]. EMLab originally encompassed a set of agent-based models dealing with policy questions on the long-term evolution of the electricity sector, but has since grown encompass a diversity of approaches, tools and results. EMLab-Generation, the most comprehensive of the model environments in EMLab, is developed in AgentSpring, a modular agent-based modeling platform based on the concepts of reusable scripts and data storage using graph databases. The modularity of AgentSpring is built around *scripts* – descriptions of actions which together define complex agent behavior. Scripts in EMLab-Generation include market algorithms, investment algorithms, power plant dispatch algorithms, algorithms related to various policies and many others [30–32]. Different versions of many of these scripts exist, some representing previous versions of the same script and others representing distinctly different conceptualizations of the relevant process. Switching out of scripts allows for the testing of different assumptions and addressing of research questions on variety of energy policies and electricity market design issues.

Enipedia: Enipedia¹³ is a linked data platform enabling energy system data from different sources to be connected, queried, and visualized from different perspectives. It includes data on electricity production and storage, natural gas infrastructure and flows, and industrial production chains. Enipedia was developed at Delft University of Technology, and is related to but distinct from EMLab. The majority of data in the platform has been compiled from various open datasets from organizations such as the US EPA, the IAEA and the EU ETS. A pipeline of custom scripts automates the process of aligning these diverse datasets and uploading them to a common graph database, which serves as Enipedia's back-end. Enipedia is accessible via the Web and is implemented as a wiki, with the intent of allowing a diversity of users to contribute and edit data. The use of graph databases and semantic wiki technology enables the linkage of datapoints across wiki pages, and the tailored querying and visualization of datasets for different purposes. The use of machine-readable formats and semantic web protocols enables the integration of data distributed across the Web and interoperability with other semantic web resources.

Modelica: Modelica is an object-oriented modeling language for the dynamic analysis of complex, highly-integrated physical systems using differential, algebraic, and discrete equations. Modelica components are organized as a growing set of free and commercial software libraries e.g. for control, thermal, electrical, hydraulic, pneumatic, mechanical and other types of systems. The clustering of Modelica's component models into libraries together with the ease of nesting components

leads to a set of computational modules that can be readily reused and integrated in different ways. A number of Modelica libraries specifically deal with energy system components. These include libraries for electrical and electronic components, power systems, thermal power plants, HVAC systems, energy storage systems, building energy and control systems, district energy systems and others. Through the integration of these components, Modelica enables the development and testing of multi-scale energy system models based on a detailed representation of physical processes. Development of the Modelica language is overseen by the non-profit *Modelica Association*, which maintains a list of free and commercial Modelica component libraries, as well as a list of Modelica simulation environments. The Modelica Association releases new versions of the Modelica language [67] and the Modelica standard library as well as the Modelica license. Also active in the Modelica “ecology” are the providers of Modelica simulation environments (e.g. Dymola, OpenModelica), Modelica users’ groups in various disciplines, and developers who contribute free and commercial component libraries. The Modelica language is actively used by researchers and commercial actors in different engineering domains, and significant investment in development has left it well-positioned to become the standard for modeling complex multi-engineering systems.

HUES Platform: The Holistic Urban Energy Simulation (HUES) platform¹⁴ comprises a set of models and datasets to aid in the design and operation of district and urban energy systems. The platform has been developed over several years by researchers at Swiss research institutes and universities including Empa, ETH Zurich, HSLU, EPFL and the University of Geneva. Modules in the platform currently include building occupancy models, building energy models, energy system models, an optimization suite, a technology database, solar radiation and climate data, an electricity network model and others. A set of centrally defined module development guidelines and a nascent ontology encourage a degree of conformity amongst modules. However, development of the platform is highly decentralized – contributions are generally based on independent research, and mostly take the form of independently developed modules with limited interoperability towards one another. The computational modules of the platform – implemented using different computer languages and modeling techniques – are accompanied by a software infrastructure to support the navigation, sharing and understanding of modules. This infrastructure has two main elements – a semantic wiki and a code repository. The wiki enables distributed management of model metadata, allowing platform contributors to directly create and update content associated with their modules. The code repository enables the sharing of module code and data across diverse platform users. Future development of the HUES platform aims to enhance module interoperability through further development of the HUES ontology and the integration of a multi-module workflow development system, while preserving possibilities for including a diversity of new and legacy models into the platform.

Openmod: Openmod¹⁵ is an initiative of energy system modelers from various universities and research institutes (mostly from Europe), aiming to “exchange ideas and source code, lobby for policy support for open projects, and actively share data, code and knowhow” [41]. The central focus of Openmod is

¹² <http://emlab.tudelft.nl/>.

¹³ <http://enipedia.tudelft.nl>.

¹⁴ <https://hues.empa.ch>.

¹⁵ <http://www.openmod-initiative.org/>.

on supporting and promoting openness in energy modeling, with the purpose of enhancing transparency, credibility, efficiency and quality of energy modeling efforts. One specific motivation for this effort is the closed-source nature of models currently used to inform energy policy decisions. The disciplinary scope of Openmod spans energy system models and data. Models covered by the initiative currently primarily include optimization and simulation models for electricity system investment and dispatch from the local to the European scale [68]. Data covered by the initiative includes transmission network data, power plant data, renewables data (e.g. wind and solar), weather data and a limited amount of consumption data [69]. More than the previously described initiatives, Openmod is a *social community* of energy system modelers, and may best be described as a “community of practice” [70]. The initiative has held workshops one or more times per year since 2014, at which various models are presented and relevant topics discussed. The last workshop (Stockholm, 2016) included approximately 50 participants, with the Openmod mailing list extending to several hundred participants. In addition to collating and disseminating open models and data, Openmod plays an important role in steering the modeling work of this emerging community by developing guidelines on practical aspects such as software licensing and data sharing techniques, and disseminating information about best practices in software development.

WholeSEM: The Whole Systems Energy Modeling Consortium¹⁶ (wholeSEM) is “a multi-institutional initiative to develop, integrate and apply state-of-the-art energy models”, the purpose of which is to build and link energy models to support the UK’s national strategic energy modeling activity [42]. The initiative is based on a recognition of the role of models in bridging different scales and time periods, and facilitating decision making under conditions of “pervasive uncertainty” [42]. It is composed of a consortium of four UK universities with complementary research competencies in different aspects of energy systems modeling. Modeling activities of the initiative span different techniques and scales and include energy system evolution, unit commitment, network planning, social practices (related to household energy demand) and others. Several schemes for piecemeal model integration within the consortium have been defined, some of which have already been realized [43]. The independent and linked modeling activities of the consortium are complemented by annual conferences and periodic workshops, as well as a fellowship program to facilitate knowledge exchange internally and externally.

Appendix B. Detailed results of the analysis

B.1. Diversity

With regard to the technical dimension, Openmod, WholeSEM, HUES, AgMIP and the GEO Model Web Initiative include, or foresee that they will include, models and datasets covering a range of disciplines and developed using different software tools and programming languages. Most of the energy-related initiatives focus on a limited range of spatial scales, e.g. the national–regional level or the building–district level. WholeSEM, for instance, includes models covering energy system evolution, unit commitment, network planning and social practices, but focuses most strongly on national level energy systems. HUES also incorporates a significant diversity of models and

datasets – including building occupancy and building energy models, energy system models, an energy conversion and storage technology database, solar radiation and climate data, an electricity network model and others – but focuses most strongly on the level of buildings and urban districts. Many of the initiatives include elements spanning multiple temporal scales – most commonly from hours to years – though none covers the full range of relevant temporal scales (i.e. from milliseconds to decades).

All of the energy-related initiatives span multiple disciplines and perspectives. Where EMLab,¹⁷ WholeSEM, HUES and Openmod focus on a combined technical and social perspective, Modelica is largely limited to the perspective of physical engineered systems. Reflecting the importance of certain environmental variables to renewable energy generation and building energy demand, some of the initiatives also integrate environmental models and/or data. HUES, for instance, includes solar insolation time series and a microclimate emulator. Additionally, some of the initiatives, WholeSEM in particular, also explicitly address non-economic social and behavioral aspects.

To a large degree, the diversity of the initiatives’ social dimensions aligns with that of their technical dimensions. Though it is difficult to precisely qualify the actor diversity of the selected initiatives, it is clear that all of the energy domain initiatives explicitly include individuals and teams representing different disciplines and perspectives. Openmod and Modelica are unique in that they engage individuals from many institutions spanning different areas of expertise. Whereas Openmod is driven largely by the academic research community, Modelica engages both academic and commercial actors. HUES and WholeSEM have also been specifically developed to integrate knowledge from a diversity of actors, but are currently mainly driven by a handful of (academic) institutions with complementary expertise. A notable non-energy initiative in this respect is AgMIP, which includes six distinct teams with expertise in regional and global economics, crop modeling, climate, stakeholders and information technology [48].

B.2. Connectivity

With regard to the technical dimension, Modelica and EMLab are highly interoperable, featuring aspects of technical, syntactic and semantic interoperability. Component models operate in a plug-and-play manner, and are able to run in parallel and interact during runtime. EMLab enables interoperability by way of a common programming language (Java) and ontology, and a core simulation engine (AgentSpring) which coordinates inputs from different modules. A critical distinction of Modelica is that the equations are *acausal*, allowing the separation of the modeling (defining equations) and the simulation (efficient computation of a solution). This means appropriate solvers are used for different problem parts, allowing very different systems to be easily coupled, for example across widely different time resolutions. This setup aims to overcome the limitations of conventional approaches in modeling integrated engineered systems, and encourages a high degree of model reuse since models can be connected in arbitrary ways. The use of standardized interfaces enables compatibility between components without the necessity for translators to convert interface data between components [37]. The exchange of models with other simulation platforms is increasingly possible, particularly using Functional Mockup Units, which entail the packaging of Modelica models as self-contained executables for use with other models via the Functional Mockup Interface.

At the other end of the spectrum is Openmod, in which included models and datasets exist completely independent of one another. Between these extremes are initiatives such as HUES, WholeSEM and Splash in which interoperability largely takes the form of loose coupling

¹⁶ <http://www.wholesem.ac.uk/>.

¹⁷ Throughout this analysis, EMLab refers specifically to EMLab-Generation, the main modeling environment of EMLab.

between modules, with modules running in series and exchanging data via file I/O. In Splash, interoperability between models is enabled via a registration process, in which a description of the relevant model or dataset is specified in the form of a specially formatted metadata file [50]. During this process, “mapping actors” are also defined to automate data transformations between models. The construction and simulation of customized model/data workflows is facilitated via a graphical design environment, in which registered datasets, models and mapping actors are dragged and dropped into a design workspace.

With regard to data, Enipedia and AgMIP exemplify a high degree of interoperability. Enipedia focuses specifically on enabling flexible exploration of linked datasets from different sources, and has a highly developed infrastructure for aligning ontologies and data formats. AgMIP includes a comprehensive central repository featuring model input and output data in harmonized formats [71]. This is complemented by a repository of data translation applications and extensive metadata files to facilitate replication of analyses.

With regard to the social dimension, all of the energy-related initiatives feature a high level of openness, expressed in different ways. Nearly all of these initiatives make their model code and data available via the Web – either through a dedicated website or via code repositories such as Github and Bitbucket – and most of the initiatives invite external developers and scientists to contribute. In many cases, models and data are made available with permissive licenses, such as the GNU General Public License, the MIT License and Creative Commons licenses. Some initiatives go beyond this. Openmod promotes openness by providing explicit guidance to developers in terms of open source licensing and open source software tools. OpenWorm maximizes transparency by providing a video archive of team meetings. In the case of nearly all the initiatives, the internet plays an important role in mediating social organization. The GEO Model Web initiative envisions coordination mechanisms based almost entirely on concepts of the web, and interactions in Openmod are mediated largely via a community wiki and mailing list. On the other hand, it is clear that social connectivity based entirely on internet-mediated communication is limiting. For this reason, nearly all of the larger initiatives (Modelica, Openmod, WholeSEM, OpenWorm, R) complement web-based coordination with regular conferences or workshops that enable participants to interact in person.

B.3. Hierarchy

From a technical perspective, the existence of hierarchy in a multi-model ecology is dependent on a high level of connectivity between components. Hierarchy is particularly evident in Modelica, in which component models (physical representations of engineered systems) may consist of other component models, which in turn may consist of other component models, and so on. This recursive composition is reflected in the structure of Modelica's libraries, many of which contain recursive sets of encapsulated subpackages for representing lower-level components. An example is the Modelica Buildings Library,¹⁸ which amongst others contains an electrical subpackage, which contains a DC subpackage, which contains a loads subpackage. In this manner, a building is represented as a hierarchy of engineered components, sub-components and subsubcomponents.

Similar patterns of hierarchy may be found in R, which includes complex networks of interdependent packages for data manipulation and visualization, with more specialized packages depending on more general-purpose packages, which in turn depend on the R base package. An example is the so-called “Hadleyverse”,¹⁹ a cluster of recursively dependent R packages which themselves are depended upon by myriad more specialized packages within the R ecosystem. Hierarchy is also

evident in the object-oriented composition of some of the smaller initiatives such as EMLab, which is composed of recursively dependent sets of Java classes representing e.g. different energy system actors, markets and technologies.

The existence of clear hierarchy within the social dimension of the analyzed initiatives is less apparent than in the technical dimension. Most of the analyzed initiatives consist of a relatively flat social structure. Exemplary here is Openmod, which is driven by a loose network of researchers spread across different organizations. In a handful of the analyzed initiatives, elements of social hierarchy have emerged over time as the ecology has matured. This is apparent in Modelica, which has seen the emergence of regional users' groups in North America, Europe and Asia, and is overseen by the Modelica Association, which consists of board members from around the world and manages the release of new versions of the Modelica language, the Modelica standard library and the Modelica license. A similar form of hierarchy may be seen in R. In EMLab, social hierarchy merges with academic structures – the initiative is steered by a set of professors, who develop and supervise projects by PhD and MSc students that build on a common technical core.

B.4. Purpose

The purposes of the selected initiatives fall into one of two categories: (1) *enhancing modeling competencies*, e.g. in terms of model interoperability, quality and/or disciplinary scope, and (2) *transparency and dissemination* of modeling work and associated knowledge. Initiatives falling clearly into the first category include EMLab, WholeSEM, AgMIP, Splash, MUSIC and OpenWorm. The precise modeling competencies to which these initiatives seek to contribute differ. EMLab aims to facilitate model reuse and enable new ways of addressing energy policy and design questions; MUSIC focuses on enhancing runtime interoperability amongst models; AgMIP focuses, amongst others, on improving model quality through systematic model inter-comparisons.

Initiatives falling more into the second category include Openmod and HUES. Openmod is focused on advancing the development of open models and data in the energy domain, and HUES on enabling the reuse and dissemination of models and data for building and district energy systems. Some initiatives – such as the GEO Model Web, Modelica and R – strike a balance between these purposes, disseminating modeling resources widely (e.g. through highly developed module libraries/repositories) but maintaining stringent standards to enable module interoperability.

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¹⁸ <https://github.com/lbl-srg/modelica-buildings>.

¹⁹ <http://adolfoalvarez.cl/the-hitchhikers-guide-to-the-hadleyverse/>.

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