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Towards a multi-model infrastructure for integrated decision-making in energy transition

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Abstract

Computational simulation models serve as powerful instruments for analysing complex systems, but individually they are often limited in representing systems of an interdisciplinary nature. This paper presents a multi-modelling project that takes the first steps towards an open generic solution of multi-model infrastructure (MMI). It aims to loosely couple individual independent (often already existing) models, facilitate model reuse and meaningful model interoperation in order to support integral decision-making in the Dutch energy transition. The MMI is a minimal viable product collaboratively designed and developed by a diverse group of modellers and energy experts. It includes facilitating services such as software and methods that enable multi-modelling but not the individual independent models themselves. We share the vision, approach and initial outcomes of the project, in particular, give an overview of the multi-model platform architecture design and the three use cases (and multi-models) of marco, meso and micro scales developed to demonstrate the potential of MMI. We also discuss the lessons learnt and future work, with the intension to invite more research, debate and collaboration on topics of multi-modelling, in particular simulation model reuse and interoperation, and to form an even stronger and broader interdisciplinary community of multi-modellers.

Keywords: multi-model; multi-modelling; simulation; model reuse; energy transition

1. Introduction

In this paper, multi-models (MMs) refer to computational simulation models that are formed by coupling individual independent (often already existing) participating models. They can serve as powerful instruments for analysing complex large-scale real-world problems. If well-designed, MMs can join the capabilities of the participating models and save the modellers considerable effort and time by model reuse. The creation of MMs, however, can be highly challenging as well, ranging from technical challenges (such as managing data exchange and coordinating model runs), conceptual complexities (e.g., aligning different model scales and resolutions including the underlying assumptions) to legal, institutional, and ethical issues (such as licensing, intellectual property (IP) rights of data and models, privacy and confidentiality).

The MMviB project (*Naar een Nationale Multi-Model infrastructuur voor integrale Besluitvorming in de energie transitie* in Dutch, multi-model.nl) has the ambition to tackle these challenges in the context of Dutch energy transition, and to develop a minimum viable product (hereinafter called MM infrastructure or MMI), including an open MM communication platform, in order to generate insights from repeatable and verifiable interactions of existing models for decision-making on integrated energy systems. The design and development of the MM infrastructure is supported by a broad community of modellers, energy experts, decision makers and researchers (i.e., communities of practice) from eleven consortium partners where the authors take part in.

This paper aims to share the vision, approach, initial outcomes and lessons learnt of this effort, with the goal to invite more research, debate and collaboration on topics of multi-modelling, e.g., simulation model reuse, interoperation and open-source solutions, and to form an even stronger and broader interdisciplinary community of multi-modellers.

2. Motivation and Background

Energy transition is interdisciplinary (Köhler et al., 2019). It involves the physical infrastructure, supply and demand balance, systemic planning, policy-making, governance, regulations, economics, ecological and environmental issues, etc. To make it more complex, the decisions in energy transition need to be operational, tactical and strategic so that they can bring about hopefully speedy positive changes to our energy systems while maintaining economic, social and environmental sustainability, benefiting our society and living environment as a whole.

Computational models are powerful instruments for systems analysis, but individually they are often limited in representing the interdisciplinary complexity of energy transitions. In energy systems, the diverse scales, scopes and natural characteristic of the interacting parts and factors call for different types of models and modelling methods. Many disciplines and domains that concern energy generation, distribution, asset management, consumption and economics, etc., often have computational models tailored for analysing specific problems. Since these models are developed independently for problems of different nature, they often use heterogeneous modelling solutions. All these point to the new, yet old, approach of multi-modelling (Bollinger et al., 2015). This approach combines individual independent (often already exiting) models to analyse problems that can hardly or not be analysed by individual models separately.

Early work on connecting (or coupling) different simulation models started about 30 years ago and went through considerable development (e.g., Dahmann, 1997, 1999; Davis and Anderson, 2003; Turnitsa, 2005; Yilmaz and Tolk, 2006; Tolk et al., 2007, 2013; Tolk, 2023). This body of work in the domain of modelling and simulation (M&S) is often referred to in terms of model *interoperability* or model *composability*. Interoperability is generally defined as the ability of two or more systems or components to exchange information and to use the information that has been exchanged (IEEE, 1990). Model composability is defined by Petty and Weisel (2003) as the capability to select and assemble simulation components in various combinations into valid simulation systems to satisfy specific user requirements.

In M&S theory, the level of conceptual interoperability model (LCIM) distinguishes six levels of low to high capabilities of model interoperation, namely technical, syntactic, semantic, pragmatic, dynamic and conceptual (Tolk, 2010). Broadly speaking, successful interoperation of heterogeneous modelling solutions can have three categories: (1) integratability of infrastructures, (2) interoperability of M&S systems, and (3) composability of models (Tolk, 2010). Integratability (of infrastructures) contends with the physical/technical realms of connections between M&S systems. Interoperability (of M&S systems) contends with the software and implementation details of interoperations, which includes exchange of data elements via interfaces, the use of middleware, mapping to common information exchange models, etc. Composability (of models) contends with the alignment of conceptual issues on the modelling level, i.e., the participating models have consistent representation of interpretations of reality (Page et al., 2004; Page, 2007; Tolk, 2010). Integratability and interoperability can be engineered into a system or service after definition and implementation. By way of contrast, composability cannot be engineered into a system after the fact (see, e.g., Huang et al., 2015, 2016). It requires often significant changes to the simulation to ensure that a research question is either answered consistently and equivalently by participating simulation systems or else the conceptual interoperability among the models fails (Tolk, 2023).

Notably, not all model interoperation projects have the participating models interoperate in all three LCIM categories. Many cases may prefer or require loosely-coupled models due to business interests, data security, proprietary rights, or constrains on modifying the existing models, etc.; see, e.g., Lu and Issa (2005); Goodall et al. (2011); Bollinger et al. (2015); Ferreira et al. (2017). When models are loosely-coupled, the output data from one model is channelled as input data into another model (Antle et al., 2001). The variables in such models are distinct, separate and infrequently interact or overlap across models (Orton and Weick, 1990). These characteristics differ from those that are required by strict conceptual alignment in the LCIM model. Thus the resulting multi-models may achieve integration and interoperation but not necessary neat and tidy composition. The MMviB project focuses on developing such loosely-coupled (multi-) models where reusing existing models is a strong desire. Instead of working in a “greenfield”, the project works in a “greyfield” or “brownfield” of modelling where adapting existing models, and creating generic solutions and methodological supports thereof are the primary goals.

3. Vision, Approach and Outcomes

The MMviB project takes the first steps towards a multi-model infrastructure (MMI) that aims to facilitate model reuse and meaningful model interoperation to support integral decision-making in the Dutch energy transition.

The vision of the project is that, by coupling existing (validated) independent models that describe different (local, municipal, regional and national) energy system levels and system aspects (e.g., spatial, technological, economical, behavioural and social), the resulting multi-models can provide more complete, understandable, and verifiable bases for complex decision-making. This way, we can bring together different expertise to complement one another, and to plan and manage the energy transition more inclusively and effectively.

The MMI refers to facilitating services (including software and methods) that enable multi-modelling. This, however, does not include the individual independent models themselves. The MMI is collaboratively designed and developed by diverse and extensive communities of practice including modellers, energy experts, decision-makers, and researchers. This collective effort involves eleven consortium partners who share a common commitment to advancing the field of integrated energy system decision-making. The approach and main outcomes of the project are summarized as follows.

- Multi-model infrastructure (MMI) requirements
- Model description template
- Multi-modelling terminology
- Multi-model (MM) platform
- Energy system multi-modelling use cases

At the beginning of the MMviB project, two requirement workshops were organised with the consortium. The goal was threefold: (1) to generate ideas for the desired features of MMI as a long-term vision; (2) to reach a consensus on the priorities of the features for this project; and (3) to enhance understanding and promote trust among partners through collaborative co-created effort. The resulting requirement features are divided into five categories: (1) infrastructure deployment, (2) model description and alignment, (3) model connection and multi-model setup, (4) model interoperation, and (5) model experimentation and output.

To facilitate model understanding and assessment, we iteratively designed an elaborate *model description template*. It provides a general structure and explanation of how to produce a model description (aimed for a potential user) that can give an overview of the defining characteristics of an energy model. The information includes, among others, the intended purpose of the model, the levels and types of decisions that model developers aim to support, model type, model scope and scale, model assumptions, strengths and limitations, levels and methods of energy system integration, data sources, and the status of verification, validation, and test. Together with the model description template, six *model descriptions* are prepared for the six energy models used in the project. These energy models were all developed and are owned by the consortium members, who are experts and key stakeholders in the Dutch energy system.

During many meetings and discussions, we realized that although we are all within the energy domain and many are also modelling experts, we do not always communicate with one another smoothly. This challenge often started with the terminology we used: sometimes different terms, first appeared to mean differently, turned out to express the same idea, while some other times, the same term might refer to different concepts. To tackle the issue, we compiled a list of modelling *terminology*. Some terms therein are based on simulation modelling literature, and some defined during collaborative design and development processes in the project. We included, e.g., terms of strategic, tactical, operational goals within energy systems, model scope and scale, granularity and resolution, multi-model workflow, among others. In many places, examples are also given for clarification.

A key outcome of the project is the MM communication platform, or simply the MM platform. This includes a software architecture design and the corresponding implementation. They address the prioritized requirements resulted from the requirement workshops mentioned earlier. The design and implementation are again collaborative and iterative by the partners. The MM platform architecture consists of four main components: (1) an orchestrator, (2) model adapters, (3) a model registry, and (4) an intermediate model/data storage. The platform is presented in Section 4.

To demonstrate the use of the MM platform and the potential of multi-models in supporting energy transition, the consortium collaboratively created multi-models in three use cases at three different scales of the Dutch energy transition: (1) Macro scale case – the Dutch national infrastructure, (2) Meso scale case – a provincial business park, and (3) Micro scale case – a local business park. The use cases are presented in Section 6.

4. Multi-Model Platform

To support reusing existing models and maintaining their independence, we choose to couple models in a generic and loose manner. By generic, we mean that the project aims for a generic MM IT architecture and a generic IT infrastructure for multi-modelling that can ease multi-model creation and connection. These needs are translated to the following four principles in the architecture design:

- A participating model does not know and does not need to know that it is part of a multi-model.
- A participating model does not need to be open (source) to become part of a multi-model.
- An external software component (to a participating model) handles the multi-model execution.
- Data exchange among models has standardized format.

Figure 1 provides an overview of the MM platform architecture design. As shown, the *Orchestrator* forms the central part of the MM platform. Its main responsibility is to manage multi-model workflow runs. A multi-model workflow defines a sequence of tasks (and thereby the sequence of individual model runs and the corresponding data flow) through which a multi-model experiment can

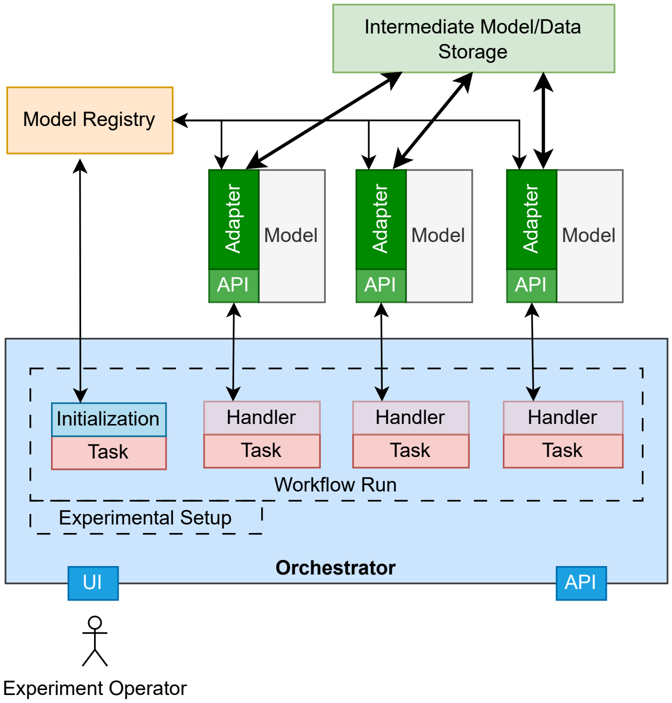

Figure 1. An Overview of the Multi-model (MM) Platform Architecture

be conducted from initialization to completion. Based on MM experimental setups (defined by human modellers), the orchestrator instantiates workflow runs with the corresponding parameters and datasets.

A *Model Adapter* provides a generic interface for the orchestrator to communicate with a model. The adapter is responsible for collecting the input data, instructing the model execution (by translating generic orchestration messages to model-specific instructions) and storing the output data.

The results are passed on from one model to another (by their corresponding adapters) via an *Intermediate Model / Data Storage*. The orchestrator configuration determines how and where in the storage the input data and output data are collected and stored. The data format is defined with *ESDL* (Energy System Description Language), by which the information about an energy system can be formally defined in XML format.

The *Model Registry* is the place where information about models is stored and exchanged. It is used to look up available models and their capabilities, and to (automatically) find the exact URL locations, registered by the adapters, where the models are connected to the MM platform.

The architecture is implemented as follows. For the orchestrator, we chose to use Apache Airflow since it is open source and extensible, and can programmatically author, schedule and monitor workflows, well-suited for our purpose. The open source MinIO, which is a high-performance S3-compatible object storage, is used for the Intermediate Model / Data Storage. We developed the model registry and all model adapters for the participating models in the three MM use cases. The MM platform is open source and can be found at https://github.com/MultiModelling. Note that the individual models belong to their corresponding owners and are not part of the MM platform.

5. Models in Use Cases

Three use cases (and multi-models) are developed collaboratively to demonstrate the use and potential of the MM platform. They are chosen to be at macro, meso, micro scales of the Dutch energy transition. The following six independent models are used by the three use cases: (1) *CTM* – Carbon Transition Model, (2) *ESSIM* – Energy System Simulator, (3) *ETM* – Energy Transition Model, (4) *MOTER* – Modeler of Three Energy Regimes, (5) *OPERA* – Option Portfolio for Emissions Reduction Assessment, and (6) *TEACOS* – Techno-Economic Analysis Of Complex Option Spaces. They are briefly presented as follows; more information can be found on the project website.

CTM is a tool that calculates emissions, costs, energy, feedstock, among others, of present and future Dutch industries that produce synthetic molecules (e.g., steel, refineries, fertilizer plants, large base chemical plants, industrial gases and methanol production). Its goal is to explore pathways to zero emission in industry.

ESSIM is a discrete-time simulation tool and collection of models that calculates energy flows in an interconnected hybrid energy system. Its goal is to assess how the assets in an energy network are dimensioned, detect overloading in any transport asset (e.g., pipes, cables) and analyse the effect of storage in the network.

ETM is a tool for (copper plate) modelling energy systems in a country, region or city. The energy flows are captured in a graph structure which describes the routes for exchanging energy between sectors and processes. The tool calculates yearly energy balances for energy carriers and hourly balances for electricity, heat, and hydrogen.

MOTER is an optimization tool for the dispatch of "multi-commodity" energy systems consisting of interconnected electricity, natural gas, hydrogen and heat networks. Its goal is to find the optimal techno-economic performance of an externally provided multi-commodity energy system.

OPERA is an optimization model (van Stralen et al., 2021) that represents the entire Dutch energy system including bunker fuels, feedstocks, and all domestic greenhouse gas (GHG) emissions. The driver of the model is the energy demand, e.g., the steel in tons that need to be produced, and kilometres needed to by passenger cars. The model determines what technologies are used to fulfil these demands.

TEACOS is a optimization tool for the analysis of mid to long-term strategic investment. It models the supply chain as a network. The model selects the best combination of investments and calculates the corresponding product flow such that either the Net Present Value is as high as possible, or the costs are minimized. It aims to answer questions such as which (decarbonization) opportunities to invest in and how much; what is the optimal investment timing.

6. Use Cases and Multi-Models

Each of the three simple use cases (i.e., multi-models) contains three of the six models (Sect. 5) to demonstrate the use and added-value of multi-modelling. The case cases are implemented The cases and their purposes are briefly explained in this Section.

The macro scale case focuses on the Dutch national infrastructure. Typically, the models from Dutch grid operators (TSOs and DSOs) in combination with ETM are used to assess the impact of energy transition scenarios on the energy infrastructure. This approach has limitations in incorporating the changing economic conditions and the optimization of existing assets for the future. By connecting ETM to OPERA and MOTER, future scenarios regarding economic and technological consistency as well as the asset use can be optimized. A methodological focus and challenge of this case is to couple different model granularity (i.e., detail levels) and scope. For that, a regionalization model was developed to bridge the gaps so that the projected national demand and capacity could be "regionalized" to smaller units and be connected to specific locations.

The meso scale case focuses on the industrial area in the South-Western province of Zeeland, which contains major Dutch industries. The case assumes that the major business challenge in Zeeland is the production of hydrogen (H2), which can be made by either electrolysis or the SMR (Methane Steam Reforming) process. Compared to SMR, electrolysis can be considered greener with no (or limited, depending on the generation of electricity) CO2 emissions. The main decision factors between these two are the gas cost, electricity cost, CO2 emissions, and CapEx (Capital Expenditures) for installing the production units. These factors, together with the hydrogen demand and other necessary conditions and processes, are being modelled by coupling CTM, ETM and TEACOS. An interesting methodological aspect is that the models form an iterative loop where TEACOS optimizes processing configuration based on the electricity price, provided by CTM and ETM that calculate the electricity price based on the impact of the new process configuration. The condition for convergence is the occurrence of two same processing configurations in two successive iterations.

The micro scale case concerns a local business park in the municipality of Tholen in the Netherlands. The Regional Energy Community (REC) Tholen aims to collectively invest in renewable energy measures towards a business park that is CO2 neutral or even energy positive. This use case aims to find pathways to an energy transition with PV installations. To that end, three existing models from the consortium are being coupled: ETM, TEACOS and ESSIM. In there, ETM and ESSIM use historical hourly profiles for solar and wind, energy prices and demand to gain insights to the expected balancing in the energy system over an entire year. TEACOS determines the optimal investment in (and capacity of) PV panels by the REC (hence from a perspective of the business park as a whole). ESSIM calculates how much of the given electricity capacity in PV panels can actually be self-consumed by local businesses. To add individual investment behaviour of local businesses – which in real life can be different from "collective decisions" – an agent-based model (ABM) (Prisse, 2023) is developed for this case such that each business takes its own PV investment decisions that are most beneficial for its own situations. The ABM results are compared to TEACOS results to show the difference between what is optimum for the community and what is beneficial hence a more likely decision for an individual business.

7. Lessons Learnt and Future Work

Understanding and harmonising different models, their (input and output) messages, the modelling languages and tools, etc., take time. All these aspects are vital for different models to exchange information in a meaningful and coherent manner. As mentioned, the ESDL provides a semantic for energy system description. It helped information exchange within the use cases. However, a common semantic is necessary but not sufficient for meaningful information exchange. Take the Units of Measurement (UoM) as a simple example, 100 as investment cost may mean 100 Euros, kilo or million Euros, or Euros per MW, etc. Since the models were not designed to work with one another, they inherently have different levels of details, diverse ways of abstraction, units, categorizations, etc. Meaningful information exchange and correct interpretation requires agreements on conceptual alignment, thus often the corresponding model and data transformations from one model to another during multi-model design.

Coupling different models together may succeed to provide a more complete picture of the real system but this does not mean that there is no information gap between different models. The gaps may be temporal, spatio, or regarding model resolution or subject classification, etc. For example, some energy models need extensive details on production and consumption profiles and increase (and decrease) merit orders. When such information is not readily available from other participating models, it is necessary to create (new) bridging models or sometimes manually define the data gap based on domain expertise.

The MMviB approach is in principle service-oriented. The ICT complexity of the project is very high in that regard – much more than what the project expected upfront. The consortium members are energy system modelling experts but not necessarily ICT experts or software engineers. Their expertise in the energy domain are exclusive for energy modelling challenges but falls short in bringing the energy models to a web-based service-oriented setting. Since the models (including data) in this setup are at the back-end, server security issues also get into part of the considerations, which require another type of ICT expertise.

A notable benefit of multi-modelling is that it enables the parties (and model owners) to work together in an unprecedented way. All models from the project partners have a long development history. They are highly complex and can only be worked out by their own developers. An attempt to integrate two mature models would require the developers to spend significant time, which they often lack, to understand how their own model and the other model work, before even considering an approach to add functionality to the models without breaking them. A conventional form of model integration would be very challenging under current real-world commercial conditions. But with the loose-coupling approach in the MMviB project, the model owners can develop adapters for their own models, apply ESDL, and resolve ESDL issues (including conceptual issues) for data exchange via the orchestrator. This greatly facilitates creative processes and open communications, and gives all parties involved a way forward in taking their models to the next level. The willingness of project members towards such an approach, collaborative spirit, learning by doing, and the iterative process of trial and error, all contributed positively to the outcome.

That said, while working on a multi-model, interactions between different parties (who are owners of individual models) are significantly more difficult than working on a typical simulation modelling project, because different parties have their own priorities and availabilities. Creating work sessions where people are physically together helps, but the time that was spent waiting on other parties was enormous even with the best intentions from all parties involved. As a result, there are often long hold-ups over the total scope of work. This is understandable and acceptable given the exploratory nature of this project. In a real-life project, however, this would put pressure on the timeline and possibly unacceptable consequences if priorities of different parties are not aligned and formalised upfront.

This proof-of-concept project aims to demonstrate the feasibility and potential of multi-modelling. Three use cases are developed based on real situations but they are not yet meant for real-life decision-making. To that end, future work needs to address numerous conceptual, methodological and organizational issues. For example, regarding the energy domain, after working with ESDL for three cases, all model owners agreed that there is a need for a standardized way of working and communicating with ESDL. The latter provides a semantic, but semantic alone is not sufficient to communicate the information about an energy system in a rigorous and coherent way. A higher or deeper level of conceptual alignment is needed in many aspects of the models for both static and dynamic information. Coupling models and validating multi-models do require in-depth knowledge of each separate model and their dynamics. If such knowledge is not well-documented, it also hinders the multi-modelling process and the understanding of the entire multi-model. The authors believe that the modelling community in the industry and academia is in a strong need for formal ways and methods for model description and documentation. This includes model conceptualization, assumptions, validity conditions, and experimental conditions. As interdisciplinary works are becoming a must dealing with real-world complex challenges, computational models are getting increasingly more complex as well. Curating and reusing our models, at least some of them, is an efficient way – probably the only manageable way – of combining our knowledge facing large-scale highly complex and dynamic challenges in the future. This makes the multi-modelling approach a promising way forward accompanying and empowering interdisciplinary endeavours.

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- https://multi-model.nl
- https://multimodelling.readthedocs.io
- https://github.com/MultiModelling
- ESDL https://energytransition.gitbook.io/esdl

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