DigitalEnergyTwin

Definition of requirements for modelling, simulation, optimization, interfaces and standards

Work package 2

D2.2

DIGITAL ENERGY TWIN – OPTIMISED OPERATION AND DESIGN OF INDUSTRIAL ENERGY SYSTEMS

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Inhalt

1 Executive summary

Co-simulation is very promising in the context of the project. Literature shows that the Functional Mock-Up interface is the most promising standard for continuous time, discrete event and hybrid co-simulation. The support of the Functional Mock-Up interface standard was a central criterion in the selection of suitable tools for modelling, simulation and optimization.

The following requirements have been defined for selecting suitable tools and methods for physical modelling, data-driven modelling and optimization: (i) availability of models, frameworks and libraries, (ii) availability of knowledge in the consortium, (iii) scalability of the models, (iv) community (academic and practical), and (v) support for FMI (to enable co-simulation). After evaluating these requirements, the consortium concluded to use Modelica for physical modelling and Python for data-driven modelling.

The requirements to set up an operational optimization have been worked out. The operational optimization includes all manufacturing processes, the energy supply and distribution as well as the interconnection to external supply grids. The target of the operational optimization is to find the best energy supply considering energetic, exegetic, economic, ecologic and technical aspects. As restriction it has been found, that the production program cannot be changed, so the order of the products is fixed. The 4 pillars of optimization (i) technical on process and component level, (ii) system (demand and supply) level, (iii) integration of renewable and efficient supply technologies including (conventional, renewable and volatile) energy sector coupling (based on exegetic and time-dependent considerations) and (iv) energy exchange over company boundaries (grid) are integrated in the operation optimization concept.

2 Modelling, Simulation and Optimization

The following general requirements have been defined for modelling, simulation and optimization: (i) availability of models, (ii) availability of knowledge in the consortium, (iii) scalability of the models, and (iv) community (academic and practical).

Due to the increasing complexity of systems, evaluating the overall behaviour of industrial energy systems including its processes for different applications (control, design, what-if, etc.) and at different stages of their development is becoming steadily more difficult. In order to keep benefiting from the results of simulation-based analyses, new techniques are required to efficiently simulate the interactions between different subsystems. There are two ways to achieve this goal: (i) the entire system can be modelled and simulated with a single tool which is referred to as monolithic simulation; or (ii) established tools for the respective subsystems can be coupled in a so-called co-simulation[1]. As our knowledge of each subsystem matures, simulation tools become more specialized, accumulating years of research and practical experience in their respective domains. As such, the use of the co-simulation approach allows existing simulation tools to be leveraged. Thus, co-simulation is very promising in the context of the project.

2.1 Co-Simulation

In co-simulation, the subsystem models are interconnected at their behavioural levels, through the traces computed by the corresponding simulation tools. To run a co-simulation, one needs a co-simulation scenario and an orchestrator algorithm. The co-simulation scenario points to one or more simulation units, describing how the inputs and outputs of their models are related. Each simulation unit is seen as a black box, capable of producing outputs and consuming inputs, according to the model it represents. To produce behavior, the simulation unit needs to have a notion of:

- model, which is created by the modeller based on his knowledge of the system under study;
- solver, which is part of the modeling tool used by the modeller that approximates the behavior of the model; and
- an input approximation, which approximates the inputs of the model over time, to be used by the solver; as well as
- input reactivity and output reactivity, which determine which inputs the simulation unit receives from the orchestrator.

A recent study on promising standards and tools for co-simulation shows that the Functional Mock-up Interface (FMI) is the most promising standard for co-simulation [2]. The Functional Mock-up Interface is a tool independent standard for co-simulation and the exchange of

[1] Gomes, Cláudio, et al. "Co-simulation: a survey." *ACM Computing Surveys (CSUR)* 51.3 (2018): 1-33.

[2] Schweiger, Gerald, et al. "An empirical survey on co-simulation: Promising standards, challenges and research needs." Simulation modelling practice and theory 95 (2019): 148-163

dynamic models which is currently supported by more than 140 tools [3]. A discussion on research challenges and current barriers of the FMI standard can be found here [4].

Requirement for DigitalEnergyTwin: Tools for modelling, simulation and optimization must support FMI for co-simulation.

2.2 Physical Modelling

A fundamental distinction in physical modelling can be made between acausal and causal modelling approaches. In causal modelling, the modelled system is, directly or indirectly, described by a system of ordinary differential equations in explicit form. In acausal modelling, the modelled system is expressed as a system of differential algebraic equations in implicit form. Literature shows that acausal modelling techniques are well suited for modelling large-scale multi-domain systems[5]. A literature review shows that Modelica is a promising language since there is an active development community and there is a wealth of (open source) libraries for energy related applications such as energy supply and distribution, HVAC systems or storage technologies[6]. Various Modelica tools support FMI for co-simulation (e.g. Dymola and Open Modelica) and Modelica was previously used by TUG7, AEE, MUL and FHV. In the context of DigitalEnergyTwin acausal modelling approaches have the following advantages:

- It is simple to read and write physical models [8].
- The model development time in acausal languages is expected to be five to ten timers shorter compared that for causal languages [9].
- They are well suited for dynamic optimization problems [10].

In addition, in some engineering disciplines MATLAB/Simulink are a preferred tool for modelling, especially for robotic or controller components. They are also capable of exporting FMUs. Since their availability in industrial settings is limited due to a high price tag, Modelica is the preferred choice for DET.

3 https://fmi-standard.org

4 Schweiger, Gerald, et al. "Functional Mock-up Interface: An empirical survey identifies research challenges and current barriers." Proceedings of The American Modelica Conference 2018, October 9-10, Somberg Conference Center, Cambridge MA, USA. No. 154. Linköping University Electronic Press, 2019.

5 Schweiger, Gerald, et al. "Modeling and simulation of large-scale systems: A systematic comparison of modeling paradigms." Applied Mathematics and Computation 365 (2020): 124713.

6 Schweiger, Gerald, et al. "District energy systems: Modelling paradigms and general-purpose tools." Energy 164 (2018): 1326-1340.

7 Schweiger, Gerald, et al. "District heating and cooling systems–Framework for Modelica-based simulation and dynamic optimization." Energy 137 (2017): 566-578.

8 F. E. Cellier, et al. “Modeling from Physical Principles,” in The control Handbook (W.S.Leveine, ed.), 1995.

9 Wetter Michael et al. “Modelica Versus TRNSYS - A Comparison Between an Equation-Based and a Procedural Modeling Language for Building Energy Simulation,” in SimBuild, 2006.

10 Wetter Michael et al., “Equation-based languages – A new paradigm for building energy modeling , simulation and optimization,” Energy Build., vol. 117, pp. 290–300, 2016.

Requirement for DigitalEnergyTwin: Modelica is used for physical modelling. Developments should build up on existing (well validated) libraries such as Buildings[11], AixLib[12] or IDEAS[13].

2.3 Data-driven modelling

Python is widely used for various applications in data science. It supports state-of-the-art frameworks for data science such as Tensorflow, Keras and Scikit-learn. Furthermore, Python supports FMI for co-simulation and Python was previously used by TUG[14] and FHV for various machine learning applications. For quick prototyping, MATLAB provides useful functionality for machine learning and neural networks and also supports FMI standards. As mentioned above, it is a highly priced development tool. Therefore, Python is the preferred choice of implementing data driven models in industrial setups.

Requirement for DigitalEnergyTwin: Python is used for data-driven modelling. Tensorflow is used for various neural networks (CNN, RNN, etc.); Scikit-learn is used for other regression (Decision Tree, Support Vector Regression, etc.) and classification (Nearest Neighbors, Decision Tree, etc.) applications.

2.4 Optimization

For the operational optimization historical, future/predicted and live (near-real) data. Due to the fact that input parameters for the optimization like energy demand and energy prices are changing, the optimization must be adapted to these changes. Therefore, a fast calculation of the optimization is needed. A use case which includes all specific components for the operational optimization has been developed. On this use case different optimization approaches will be implemented and evaluated.

Requirement for DigitalEnergyTwin: Most of the requirements for the operational optimization are already defined in SG01. The global optimum needs to be detected. The energy demand on process level and energy supply must be considered. And energetic, exegetic, economic, technical and multi-benefit/non-energy-benefit aspects as well as the four pillars in optimization (process, system, integration of renewables, energy exchange over industry boundaries) need to be included. Additionally to the SG01 requirements it turned out that also the fast calculation of the optimum is essential.

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11 https://simulationresearch.lbl.gov/modelica/

12 https://github.com/RWTH-EBC/AixLib

13 https://github.com/open-ideas/IDEAS

14 Schweiger, Gerald, et al. "The potential of power-to-heat in Swedish district heating systems." Energy 137 (2017): 661-669.

2.5 Accuracy

To reach a high accuracy for a complex system such as the energy systems of industrial processes is a difficult task. There exists a multitude of exogenous inputs and design parameters that affect the dynamic behaviour of such a system, that cannot easily be acquired from data. Examples are detailed information about components or control strategies. An important question raised in Harty 2001 [15] is whether a higher accuracy results in a more useful simulator. In some cases the higher accuracy also comes with a loss of computational performance, or with additional parameters that require calibration, making the simulator less useful from an engineering perspective. While it might be more or less intuitive what a good enough accuracy is within the scope of the project, this can be difficult to quantify.

The accuracy of a simulation is often quantified by metrics such as Root Mean Squared Error (RMSE) and Mean Absolute Percentage Error (MAPE), measuring the deviation of the simulated value compared to the measured value at fixed time instances. Shortcomings of these methods are that they don't take dynamic behaviour into account, so that moderately delayed fast dynamics might be considered by the metric as a large deviation. Approaches exist to mitigate these shortcomings such as dynamic time warping, although not widely adopted by the scientific community. Other cases not being considered are, discrete events like "when A happens, B should happen within a specified time frame".

In the field of data-modelling, the coefficient of determination (R2), the RMSE and mean absolute error (MAE) are typical error metrics for regression problems [16].

Another method that is important in this context are sensitivity analyses. These methods investigate the influence of certain parameters on the overall simulation results.

Requirement for DigitalEnergyTwin: The accuracy of models will be evaluated using a transparent metric consisting of: RMSE, MAE, R2. Furthermore, methods such as Dynamic time warping will be taken into account when event-based accuracy is relevant.

[15] Harty, D. The myth of accuracy. Journal of the Engineering Integrity Society (EIS) 2001, 9, 22–28.

[16] Rätz, Martin, et al. "Automated data-driven modeling of building energy systems via machine learning algorithms." *Energy and Buildings* 202 (2019): 109384.