State-of-the-Art (SotA) analysis

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Modelling standards and software for digital twins

OpenSCALING will improve simulation-based processes and scalable digital twins. One essential part are extensions of the following existing modelling standards that are in wide-spread use for the development of digital twins and are utilized to describe and to exchange dynamic multi-domain models, in particular from the mechanical, electrical, thermal, fluid, control, energy, building, automotive, aerospace domains. The underlying mathematical description are differential, algebraic and discrete equations:

- The Modelica language standard defines an open object-oriented language with 2-dim. object diagrams to model complex, dynamic systems on a high level supporting acausal connections of components defined by first principle equations. This standard is developed since 1997, is supported by > 10 tools, and is in widespread industrial use. Modelica tools support export of causal Modelica models as FMI components (see next item). A large class of advanced Modelica libraries has been developed in the ITEA EUROSYSLIB project. Developments towards decarbonized energy systems for buildings, district energy systems and factories are often performed with the large, open source Modelica Buildings library.

- FMI (Functional Mock-up Interface) is the leading, open standard to exchange dynamic models on a low level using a combination of (a) an XML-File to define the interface of a parameterized input/output block, (b) a dynamic link library to define the executable code that is accessed via a C-API, and (c) other resources all packed together in a zip-file. This standard was developed in the ITEA MODELISAR project and was afterwards further improved[1] [2]. It is supported by > 180 tools and plays a key role in many industries for collaborative workflows and comprehensive cross-domain system level analysis, optimization and virtual tests.

- The SSP (System Structure & Parametrization) open standard is used to define complete systems consisting of one or more connected FMI components including their parameterizations. It is supported by nearly 10 tools. Developments performed in the SetLevel project extend SSP with

[1] Blochwitz, Otter, Akesson, Arnold, Clauß, Elmqvist, Friedrich, Junghanns, Mauss, Neumerkel, Olsson, Viel (2012): Functional Mock-up Interface 2.0: The Standard for Tool independent Exchange of Simulation Models. DOI 10.3384/ecp12076173.

[2] Junghanns, Blochwitz, Bertsch, Sommer, Wernersson, Pillekeit, Zacharias, Blesken, Mai, Schuch, Schulze, Gomes, Najahfi (2021): The Functional Mock-up Interface 3.0 - New Features Enabling New Applications. DOI 10.3384/ecp2118117.

quality assessment information to support a Credible Simulation Process Framework.

- eFMI (Functional Mock-up Interface for embedded systems) is a recent open standard intended as exchange format for workflows and tool chains from physical models to embedded production code. An eFMI component is FMI compliant and can therefore be simulated by FMI tools to perform Software-in-the-Loop testing. Utilizing an eFMI component on an embedded device requires however dedicated tool support for eFMI. This standard was developed in the ITEA EMPHYSIS project [3]. The first tools with eFMI support are currently coming to the market.
- The ISO 10303-243:2021 MoSSEC (modelling and simulation information in a collaborative system engineering context) standard is an industrial effort to make progress in the representation of the elements "that together comprise a set of "results" for a study including the audit-trail of what is to be done, and what has been done, and evolution", enabling "the representation of the definitions of models and key values that are part of the modelling" among others to allow the proper reuse of simulation models in a collaborative system engineering environment. Currently, some initial reference implementations can be found in the standard. LOTAR (LOng Term Archiving and Retrieval) is an international consortium with the prime objective to create and deploy the EN/NAS 9300 series of standards for long-term archiving and retrieval of digital data in the aerospace domain. The LOTAR MBSE workgroup suggests the usage of Modelica, FMI and SSP as a basis [4].

Other important tools for simulation-based processes and digital twins:

- MATLAB and Simulink to design, simulate and deploy input/output blocks and especially controllers.
- Simscape to model and simulate multi-domain physical systems.
- Open source packages from the Julia ecosystem such as ModelingToolkit.jl or Modia.jl provide high-level descriptions of multi-domain models. The available model libraries are currently very limited when compared with Modelica or Simulink/Simscape. Advantage is the easy combination with many open-source Julia packages, e.g., for error propagation or machine learning.

Multi Physics Simulation

OpenSCALING addresses the field of system simulation which is characterized by the interaction of sub-models from different physical domains. Current industrial

[3] Lenord, Otter, Bürger, Hussmann, Le Bihan, Niere, Pfeiffer, Reicherdt, Werther (2021): eFMI: An open standard for physical models in embedded software. DOI 10.3384/ecp2118157

[4] Coïc, Murton, Mendo, Williams, Tummescheit, Woodham (2021): Modelica, FMI and SSP for LOTAR of Analytical mBSE models: First Implementation and Feedback. DOI 10.3384/ecp2118149.

trends result in new challenges for multi-physics simulations:

- Automotive: HVAC-systems of electric vehicles do not provide a comfort function for the passengers only. Keeping the battery system at the right temperature level is essential for a correct function and a long battery lifetime. In contrast to combustion engines which produce enough waste heat, electrical vehicles must generate extra heat which directly reduces the range. Heat pumps and very efficient HVAC-systems are countermeasures. This leads to more complex and larger multi-physics system models, which are challenges for simulation tools, and to higher requirements to the accuracy of models, which increases the modelling effort and requires expert knowledge.

- Buildings and Energy: Also, in these fields a trend to larger simulation models with more subsystems coming from different physical domains can be observed. The energy field has to consider the interactions between different kinds of energy production like fossil, wind and solar energy. State of the art buildings have multivalent sources for electrical energy, heating, and cooling which are coordinated by energy management systems. To assess the efficiency of such systems, simulations over the whole year are necessary to consider the seasonal weather effects. Simulation tools are confronted with large-scale models which have to be computed extremely fast.

- All industries: The necessity to include sub-models from different domains leads to an increased exchange of simulation models via FMI. The concept of Terminals, introduced with FMI 3.0 in 2022, simplifies the error-proof interconnection of FMUs due to bus and physical connectors for the modeller. But the FMI 3.0 Terminals concept is based on causal connectors. The selection, which signal becomes an input or an output still needs to be negotiated between the involved parties. Inappropriate constellations lead to algebraic loops over large parts of the combined models which often leads to numerical problems and/or a reduction of the computational performance. The OpenSCALING innovation regarding acausal FMU-interconnections will significantly improve this situation.

Artificial intelligence for modelling and simulation

Following the rapid progress in the field of machine learning in computer vision, classification and further in the last decade, industrialization of these approaches and methodologies already happened or is ongoing. However, the use of machine learning in modelling and simulation for the generation of hybrid models, a combination of physical equations and neural networks, started with the approach of NeuralODEs in 2018 [5] and physics-informed neural networks (PINNs) in 2019

[5] Chen, Ricky TQ, et al. (2018): "Neural ordinary differential equations." Advances in neural information processing systems. https://doi.org/10.48550/arXiv.1806.07366

[6]: .

A NeuralODE is an ordinary differential equation, where a neural network defines the right-hand-side. If the right-hand-side is a combination of neural networks and physical equations no term has become established yet. Within OpenSCALING the term PeN-ODEs (Physics enhanced NeuralODEs) is used since these models can be trained with the same methods as NeuralODEs, however contain explicit physical formulations. In this way, for example, previously constant parameters can be replaced by NNs that can in principle depend on arbitrary other quantities. Another way to utilize NNs is to improve the state derivatives computed using physical equations to match measurement data before passing them to the ODE solver. The gradients with respect to the NN parameters, required for training, can either be computed using AD (Automatic Differentiation) through the solver or sensitivity analysis methods for ODEs. In contrary, for PINNs the physical equations are used as a regularization term in the loss and the model itself is a neural network without any physical equations. This difference can be in turn used to classify different approaches to integrate physical knowledge into hybrid models. Typically, using physical equations inside the model leads to a better extrapolation capability, especially in presence of time-dependent inputs. However, if low computational effort is favoured often models without physical equations are employed. In the recent years many approaches for generating such fast surrogates have been developed. However, testing and validation is in most of the cases done using academic examples. Within project PHyMoS selected approaches, e.g., Proper Orthogonal Decomposition and MeshGraphNets, are investigated in industrial use cases. While great potential has been proven, upscaling to LSS results in unacceptable training times if no application specific measures are taken. After showing the potential of hybrid modelling in academia in the recent years this approach was evaluated in first use cases among different domains from climate modelling, simulation of the human cardiovascular system, modelling of fluid flows to driving simulation. Within the ITEA project UPSIM accuracy boosts up to 40% on validation data were shown for the hybrid modelling of a brake system as PeN-ODEs in form of a NeuralFMU and comparable results for PeN-ODEs of a vehicle's vertical dynamics. Current restrictions of FMI hinder to develop and train more sophisticated architectures for NeuralFMUs that would enable upscaling hybrid modelling with FMUs to more complex systems. Vice versa for the integration of NNs into Modelica models there is no standard allowing a seamless integration in the according system simulation standards. Currently, open standards like NNEF (Neural Network Exchange Format) or ONNX (Open Neural Network Exchange) lack either tool support, sufficient big community, required feature set or suitability for usage in embedded systems. This is in turn also a challenge for the integration of fast surrogates generated with AI methods, e.g., using the aforementioned methods from PHyMoS, into a larger system context.

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[6]Raissi, Maziar, Paris Perdikaris, and George E. Karniadakis. "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations". https://doi.org/10.1016/j.jcp.2018.10.045.

Moreover, recently, the question of uncertainty quantification (UQ) was also raised for hybrid modelling [7], however, an according methodology or toolset available for industry is missing.

To conclude, it is shown that using AI in modelling has the potential to become the standard approach for complex systems. What is still missing for a quicker and wider adoption is on the one hand better support by tools and standards, e.g., extending FMI to represent PeN-ODEs instead of ODEs. On the other hand, adoption of UQ methods for according models respectively training methods that can handle large-scale systems are required to apply the available technology for credible models of complex systems.

Credible digital twins

In the ITEA UPSIM project several elements for credible digital twins are developed, such as the Credibility Development Kit. Partially, the Credible Simulation Process Framework from the SetLevel project is utilized that integrates simulation with SSP models into the development and quality assessment of automated driving functions. In both projects emphasis is on the management process to develop credible digital twins. There is a huge literature on other aspects of credible models, such as calibration, verification, validation, uncertainty analysis, sensitivity analysis, Monte Carlo Simulation, Design of Experiments etc... [8] [9] [10]. All these methods are typically not integrated in a modelling software. For example, the uncertainty information is usually defined in the tools that perform uncertainty analysis, and not in the models where the information naturally belongs to.

[7] Psaros, Apostolos F., et al. "Uncertainty quantification in scientific machine learning: Methods, metrics, and comparisons." arXiv preprint arXiv:2201.07766 (2022). https://doi.org/10.48550/arXiv.2201.07766

[8] Law (2019): How to build valid and credible simulation models. DOI: WSC40007.2019.9004789.

[9] NASA 2019: NASA Handbook for Models and Simulations.

[10] Riedmaier, Danquah, Schick, Diermeyer (2021): Unified Framework and Survey for Model Verification, Validation and Uncertainty Quantification. DOI 10.1007/s11831-020-09473-7.