Recent Advances in Process Systems Engineering

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Abstract – A crucial success factor in a technology driven market is coupled with the ability to understand and interpret new technologies expeditiously and convert this knowledge into a competitive advantage. In search for procedures to advance corporate know-how faster, mathematical modeling is becoming an indispensable tool. The new challenge for systems research is to create a new breed of computer-based technologies for assistance and/or partial automation of the creative modeling process. Meta-modeling is a modeling paradigm for rapid computer-aided model generation of large multi-scale systems in the industrial practice. It proposes model building by means of phenomena-oriented modeling languages. Using the domain-specific language concepts, users compose process models by specifying the physical and chemical phenomena in a fully declarative fashion. Automatic interpretation of the high-level concepts of the model application leads to an equivalent set of system equations. Computer-aided model generation enables engineering teams to formulate highly structured process models in short amount of time. It also focuses the modeling effort onto the fundamental principles governing a process model without the need for explicit coding of all constitutive and balance equations. This article discusses recent advances and open challenges for computer-aided model generation.

Keywords – modeling and simulation, computer-aided model generation

I. INTRODUCTION

Phenomena-oriented modeling is a research initiative for the computer-aided support and partial automation of the creative task of process modeling. Recent reviews give a comprehensive account of the state-of-the-art and new challenges for computer-aided model building [1,2]. This presentation focuses on recent trends in computer-aided generation of mathematical process models.

This task belongs to the most challenging phases of the life-cycle of a process model [3]. Enabling technologies to support life-cycle considerations are also analyzed in [4]. Computer-aided approaches for improved integration of software components involved in concurrent engineering is discussed in [5].

On-going research effort provide faster algorithms for simulation and optimization [6,8], address dynamic simulation of continuous and discrete processes, i.e. hybrid simulation [9,10], and point towards solution approaches in dynamic optimization [11,12]. Open interfaces and data sharing among commercial and academic flowsheet simulators and physical property packages are the target of initiatives such as Global CAPE-OPEN [13,14].

Several research groups have also developed computer-aided process modeling and simulation tools. The Model.Ia language was a pioneering effort towards model generation [15-19]. Modkit [19-20] also offers tools for supporting the work flow in model development. The MODELLER project [21] proposed a formal framework for declarative model building. Model generation is the focus of systems research in hardware-software co-design. The multi-graph approach supports the design and simulation of architecture and performance of electric circuits and their functionality [22,23].

Despite recent progress, methodologies for the computer-aided support of the modeling activity itself have evolved slowly. There is still a need for further automation to enhance large-scale process modeling in the industrial practice. The following paragraphs reflect a topic list expressing the expectations of practicing process engineers [24].

Fast equation generation. Commercial equation-oriented modeling and simulation is becoming an industrial routine. However, equation-oriented process modeling is still a laborious task requiring the implementation of all constitutive equations by hand. For process models of industrial size and complexity this may amount to encoding several thousands or more equations. This effort is time-consuming and error-prone. Could we generate mathematical artifacts without explicitly editing every single balance equation?

Inclusion of high-level knowledge. Model equations are essential to the mathematical solution of process models. The mathematical relations alone correspond to a high level of abstractions ill-suited for conserving model intention, assumptions and simplifications. Can new model representations incorporate both phenomenological knowledge and rationale alongside the highly abstract mathematical expressions?

Multi-disciplinary approach. Larger and more complex process models require multi-disciplinary developer teams. Which type of information technology will provide an electronic workbench for distributed collaborative development of large projects?
Consistency and Structural Analysis. Consistent formulation of large-scale process models commands meticulous bookkeeping of variables, degrees of freedom and versatility in problem scaling and initialization. Is it possible to design algorithms that can examine consistency, solvability and structural properties of mathematical artifacts?

Few research contributions target at developing solution strategies for the latter more difficult problems. It is a conservative yet common opinion to consider modeling an art not amenable to systematic treatment by information scientific approaches. This work aims at challenging some aspects of this point of view.

Motivation.

Computer-based modeling approaches face a dilemma between two extremes: specificity versus generality. Specialized modeling languages allow the fast model development for expert users [25-26]. They provide a concise vocabulary of high-level language constructs suited for a specific modeling purpose. When applied outside their original scope, modeling becomes cumbersome or impossible for want of desired expressions. Furthermore, rigid modeling languages fail to fully attend to the human factor. Model developers often prefer software environments in which language and functionality can be customized.

On the other hand, the equation-oriented approach permits the description of a wide range of phenomena via abstract mathematical expressions. Clearly, models based on purely mathematical abstractions are generic, but fail to capture valuable features of a process model such as the underlying phenomena, the intention or work progress. In consequence, both monolithic specialized modeling languages as well as generic equation-oriented systems fail to address the needs of new computer-based model generation.

One approach to overcome this dilemma in information modeling is entitled meta-modelling [23]. Meta-modelling is a modeling philosophy that supports custom-built modeling languages. Its main conjecture is user adaptability. It encourages users to create their specific modeling language. Each user-defined modeling paradigm constitutes a distinct modeling dialect with domain-specific building blocks, semantic rules, and modeling activities. Each language definition also encodes the mapping between high-level language constructs into equivalent mathematical relations. The challenge for such an open environment is to uphold user innovation, while providing generic consistency control mechanisms.

This article gives an overview of new directions in computer-aided model generation based on meta-modelling. The fundamental design of meta-modelling rooted in four building paradigms will be presented. The discussion will further describe solutions towards (i) data-driven automatic equation generation, (ii) an information model for representing the modeling activity and (iii) implementation of a consistency maintenance mechanism based on agents.

II. META-MODELING ENVIRONMENTS.

A meta-modeling environment is a platform for the ad-hoc definition of formal modeling languages, i.e. modeling dialects. Fig. 1 offers an overview of a meta-modeling methodology rooted in just four formal entities: (i) sme for structuring knowledge, (ii) pme for modeling the behavior of sme (iii) properties objects for automatic equation generation and (iv) Agents for consistency maintenance. The functionality of each element is discussed next.

Modeling Concepts.

Each modeling dialect needs to provide for modeling concepts to structure the modeling world. The proposed system offers two logical entities for structuring process knowledge and defines means for implementing their behavior, i.e. substantial (sme) and phenomenological modeling elements (pme).

Substantial modeling elements (sme):

Sme delineate a separate quantity of matter or information. Thus sme store the data nodes of a process model. The primal purpose of the sme is to introduce the process quantities and their connectivity. Sme can own attributes to improve the inner organization of the embedded knowledge. Attributes are user-defined features belonging to three distinct categories: (i) fundamental properties, (ii) auxiliary properties or (iii) associations. In addition, an actionlist is set of procedures for controlling the communication of each sme instance.
and its environment. The actions in the actionlist define the messages an instance of a sme is able to interpret.

**Phenomenological Modeling Elements (pme):**

Structural dependencies alone are insufficient for complex model building. An orthogonal property governing the behavior of each balance envelope was proposed in the systems literature and its value recognized by Marquardt [27]. The pme ascertain the behavior of their associated sme. More specifically, they provide the knowledge for the specific implementation of balance equations. Thus pme introduce constraints among the attributes of the underlying sme. This active task gives them procedural character when compared to the information structuring and storage function of the sme “data” objects.

**Equation Generation via Fundamental Properties (fp):**

A key objective in meta-modeling aims at consistent generation of balance equations. In order to ensure their consistency, balances can only be synthesized for registered fundamental properties (fp). All fundamental properties are derived from a virtual root class, see Fig. 1. They define basic entities that quantify the state of a modeling object.

Typical fp in chemical engineering systems include moles as a unit for the amount of matter, total enthalpy and fugacity as a measure for thermal and chemical potential. Definition of a fundamental property implies intent to exchange or equilibrate it among different sme objects along their connections. Independent of their domain, the full semantic meaning of the new quantity is completely delineated by (i) the attributes of the sme (ii) the knowledge provided by the union of pme and sme and (iii) the consistency maintenance mechanism.

Based on the fundamental property concept, the generation of balance equation can be implemented as a data-driven search over the network of modeling objects. Equations are generated via selecting a particular type of fp from among the available object property slots. A data-driven search engine scans all sme in the network for the selected concept in order to synthesize the appropriate mathematical expressions. The necessary query information can be deduced from the fundamental properties in the meta-modeling hierarchy as well as the published set of object properties. The actual instantiation of equation objects can thus be automated to a large degree.

The equation generation mechanism is depicted schematically in Fig. 2. The nodes belong to the class of substantial modeling elements, sme, representing data objects. The arcs between the sme nodes indicate associations to other objects within the model hierarchy. Each sme possesses fundamental properties of particular type symbolized by a particular shape of the property tokens, i.e. rectangle, rhomboid, etc. Complex fundamental properties may be linked to auxiliary properties via constraints. Association between a phenomenon, pme, and an sme creates additional relations among fundamental and auxiliary properties of the sme. Pme encode the specific information, the fundamental property contributes to the proper balance equation of that particular type.

Automatic balance equations can only be generated for tokens of type fundamental properties. The actual generation of balance equation entails a search of the object network according to a specific fp type. Each objects supplies the information that it contributes to the balance equation. This information typically entails mathematical expressions that capture physical properties, constitutive equations or other context-specific object properties.

It should be noted that this equation "seeking" approach is entirely generic. Hence, the procedure can effectively synthesize mathematical expressions for any modeling language, which was defined by the concepts outlined above. This procedure also requires no knowledge about the particular semantic meaning of the fundamental properties or their corresponding balance equations.

**Consistency Maintenance by Independent Symbolic Procedures - Agents**

In the proposed methodology, the pme and sme contribute the specific aspects of process knowledge. Consistent association of sme and their subparts is supervised by Agents. They also