GENERIC BI-LAYERED NET MODEL

General Methodology for Process Simulation

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Abstract: The recently developed Generic Bi-layered Net model provides a common framework for the simulation of the hybrid (continuous and discrete, quantitative and qualitative) balance-based and/or rule-based processes. The common features of the process models are represented by a bi-layered net of variable structure also determines the network (ring) structures of the influence routes and flux routes, as well as the Gantt Chart view of the process. The advantage of the new methodology is that the computational model is specified by the very structures and building elements of the process to be modeled. Using this approach, the qualitative complexity of the usual mathematical models can be transformed into the multiplication of the building elements of four types.

Key words: net and network (ring) structures, conservational and informational processes, Direct Computer Mapping, Generic Bi-layered Net, hybrid dynamic simulation, cybernetics

1. INTRODUCTION

The computer simulation of the continuous processes is usually based on the numerical solution of a set of algebraic, differential and/or integro-differential equations (IPDAE). The discrete simulation models are represented by various structures. Many net models, like the pioneering Petri Net [1], as well as, the various State Transition Nets belong to the family of General Nets [2]. Recently Quantitative Petri Nets offer a combined approach for modeling of the various systems [3]. Kalmans' State Space Model [4] established a general framework for the description of formal

models, while this approach does not describe the knowledge about the structure. Artificial Intelligence developed various knowledge representation and search methods, without the explicit consideration of domain specific structures and of fundamental conservation laws. The tools of Computational Intelligence (neural networks, genetic algorithm, fuzzy sets) were derived from the simplified pattern of the biological systems, as well as from the human reasoning. Regardless to the existing combined methods, there is no single unified methodology that covers all aspects of process simulation.

2. THE GENERIC BI-LAYERED NET MODEL

Direct Computer Mapping [5,6] of Generic Bi-layered Net model [7] integrates the structural capabilities of the general net models with the functional abilities of the state space model. The formal description determines a general skeleton for the adequate software implementation of a model-driven and model specific computing architecture.

2.1 Formal Description of the Generic Bi-layered Net

The basic notions and the inherent feedback structure of the process models are shown on Fig. 1 (left), while a simplified example for the structure of a fictitious process is illustrated on the right hand side.

Figure 1. Simplified generic bi-layered structure of process models

The **generic, bi-layered net model** can be defined by the ten-tuplet of

$$\langle P, A, B, G, X, Y, \Phi, \Psi, r, t \rangle \quad (1)$$

The communication channels B and G determine the passive→active

$$B(\tau) \subset P(\tau) \times A(\tau) \quad (2)$$

$${}_j b_i(\tau) = (p_j(\tau), a_i(\tau)) \in B(\tau) \quad (3)$$

$$\exists_j b(\tau) \mid \forall_i (p_j(\tau), a_i(\tau)) \in {}_j b(\tau) \quad (4)$$

$$\exists b_i(\tau) \mid \forall_j (p_j(\tau), a_i(\tau)) \in b_i(\tau) \quad (5)$$

and active→passive data flows

$$G(\tau) \subset A(\tau) \times P(\tau) \quad (6)$$

$${}_i g_j(\tau) = (a_i(\tau), p_j(\tau)) \in G(\tau) \quad (7)$$

$$\exists_i g(\tau) \mid \forall_j (a_i(\tau), p_j(\tau)) \in {}_i g(\tau) \quad (8)$$

$$\exists g_j(\tau) \mid \forall_i (a_i(\tau), p_j(\tau)) \in g_j(\tau) \quad (9)$$

respectively. Index j designates the ordered sets of the existing output (${}_j b$ (4)) and input (${}_j g$ (9)) connections for the j -th passive element. Similarly, index i defines the ordered sets of the existing output (${}_i g$ (8)) and input (${}_i b$ (5)) connections for the i -th active element. Variable τ denotes the optional points or intervals of the continuous or discrete time t , declaring the existence of the respective elements and connections.

The **passive elements** P are associated with state variables X_j and with an operator, describing the change of the state:

$$\forall_j p_j \rightarrow X_j \in X; \quad \psi_j \in \Psi; \quad \psi_j = \left[\begin{array}{c} y_j \\ x_j \end{array} \middle| \begin{array}{c} g_j \\ b_j \end{array} \right] \quad (10)$$

where X_j contains any structured data set, and operator ψ_j describes how y_j changes the state via the channels g_j .

The **active elements** A are characterized by the operators ϕ_i , providing a mapping. This determines how the output changes ${}_i y_j \in {}_i y$, carried by ${}_i g$ are calculated from the coordinated input readings ${}_j x_i \in {}_i x$ that comes from the passive elements through the channels ${}_i b$:

$$\forall_i a_i \rightarrow \phi_i \in \Phi; \quad \phi_i = \left[\begin{array}{c} x_i \\ y_i \end{array} \middle| \begin{array}{c} b_i \\ g_i \end{array} \right] \quad (11)$$

The operators $\psi_i \in \Psi$ and $\phi_i \in \Phi$ *may be anything from a simple input/output mapping to a brief program*, calculating the elementary process or the rule.

Variable $\underline{r}$ designates the geometrical and/or the property coordinates of the distributed systems and/or population balances.

In the network view of the net we can interpret the alternating, connected, ordered set of the communication channels

$$\{j_1 b_{i_1}, i_1 g_{j_2}, j_2 b_{i_2}, i_2 g_{j_3}, \dots, j_n b_{i_n}, i_n g_{j_{n+1}}\}. \quad (12)$$

They are called ***influence routes***, which determine a special network structure. The influence routes carry the influence. E.g. the perturbation of the content X_{j_i} of the element p_{j_i} affects the content $X_{j_{n+1}}$ of the element $p_{j_{n+1}}$, according to the influence:

$$\{j_1 \Delta x_{i_1}(t_1), i_1 \Delta y_{j_2}, j_2 \Delta x(t_2)_{i_2}, \dots, i_n \Delta y_{j_{n+1}}\} \quad (13)$$

where $j \Delta x_i$ and $i \Delta y_j$ refer to the perturbation of the state and the change, respectively. The sensitivity and its special forms, such as observability and controllability can be studied by means of the influence route network. The minimal (generating) influence routes are the basic edges. The maximal influence routes are the transferring routes and the complete loops. The simplified structure of the influence routes is a special ring, where the two algebraic operations are the concatenation and the common part.

2.2 GBN model of problems with increasing complexity

The detailed features of the GBN model are illustrated in Fig. 2 by the example of an isothermic chemical reaction in a perfectly mixed volume. Expanding the model for a continuous vessel, equipped with control devices the homogeneous ODE should be replaced for an inhomogeneous DAE system. However in the GBN model this change can be solved of introducing passive and active elements of informational type, as well as by new connections (see Fig. 3).

When modeling a tubular reactor of distributed parameters (Fig. 4), the mathematical complexity increases for the system of inhomogeneous partial differential equations of second order. In the GBN it means the simple multiplication of the elements and of the (mainly local) connections, along the actual coordinate $\underline{r}$. (accompanied with compensation of the numerical dispersion).

Furthermore, in the case of a, say, fuzzy controlled side flow reactor (Fig. 5) the mathematical construct becomes extremely complex (IPDAE), but in the GBN model we have to add passive and active elements of new functionalities, as well as, the respective new connections simply.

Example 1.
Simple chemical reaction

Mathematical model:
homogeneous ordinary differential equations

$$\frac{dc_A}{dt} = -kc_A c_B \quad \frac{dc_B}{dt} = -kc_A c_B \quad \frac{dc_C}{dt} = +2kc_A c_B$$

$$c_A(0) = c_{A0} \quad c_B(0) = c_{B0} \quad c_C(0) = c_{C0}$$

Figure 2. Mathematical and GBN models of a simple reaction

Example 2. Controlled reactor of concentrated parameters

Mathematical model:
Inhomogeneous differential algebraic equations

$$\frac{dVc_A}{dt} = -kc_A c_B V + F_A c_{A,in} - F_4 c_A; \quad \frac{dVc_B}{dt} = -kc_A c_B V + F_B c_{B,in} - F_4 c_B;$$

$$\frac{dVc_C}{dt} = 2kc_A c_B V - F_4 c_C; \quad F_A = f(c_C, c_{sel})$$

$$F_B = f(c_C, c_{sel})$$

GBN model:
additional elements of informational process:
circle = sign
bar = rule

Figure 3. Effect of controlled flows on the mathematical and GBN models

Figure 4. Effect of distributed parameters on the math and GBN complexity

Figure 5. GBN representation of a hybrid IPDAE model

Example 5. Generic Bi-layered Net representation of a hybrid process with variable structure

Figure 6. Network and Gantt Chart views of a model with variable structure

Finally, the methodology supports also the adequate description of hybrid processes with variable structure. As it can be seen in the Gantt Chart view of the GBN model (Fig. 6), the existence of the respective passive and active elements can be changed in time t .

An important special case of net (1) is the class of **balance processes**, where the basic part of the state X_j is a measure and, the operator ψ_j summarizes the simultaneous rates. Depending on the discrete or continuous time, operator ψ_j generates also the appropriate

$$\psi_j(\underline{y}_j) = \frac{dX_j[p_j]}{dt} \approx \frac{\Delta X_j[p_j]}{\Delta t} = \sum_i i y_j \quad (14)$$

difference or differential equations, called balance equations. In the balance model the descendent of the mappings, ϕ_i can be divided into two disjunct parts, corresponding to the increases (+) and decreases (-) of the characteristic measures:

$${}_i \underline{y}[{}_i \underline{g}] = {}_i \underline{y}^+ [{}_i \underline{g}^+] \cup {}_i \underline{y}^- [{}_i \underline{g}^-] \quad (15)$$

The active elements of the balance process models describe the various transportations and transformations. In the balance process models the alternating, connected, ordered set of the communication channels

$$\left\{ j_1 g_{i_1}^-, i_1 g_{j_2}^+, j_2 g_{i_2}^-, i_2 g_{j_3}^+, \dots, j_n g_{i_n}^-, i_n g_{j_{n+1}}^+ \right\} \quad (16)$$

is called flux route. Flux routes determine another network structure, which carry the conservational measures. For example, if we modify the value of measure X_{j_1} in element p_{j_1} , then this change effects on measure $X_{j_{n+1}}$ of the element $p_{j_{n+1}}$, i.e.:

$$\left\{ j_1 \Delta y_{i_1}^-(t_1), i_1 \Delta y_{j_2}^+(t_2), j_2 \Delta y_{i_2}^-(t_1), \dots, i_n \Delta y_{j_n}^+(t_n) \right\} \quad (17)$$

The $\Delta y_{j_i}^{+/-}$ values refer to the dispersion of the changes in the rate of subsequent processes (multiplied by the stoichiometric coefficients). The minimal (generating) flux routes are the basic edges. The maximal flux routes are transferring routes and the complete loops. Similarly to influence routes, the simplified structure of the flux routes the is a special ring, where the two algebraic operations are the concatenation and the common part.

Conservational measure is a special case of the balance measure, where there are constant measures $\underline{C}$ determined by the model specific conservation laws. All of the conservational measures $\underline{M}$ can be combined from constant measures, according to the respective stoichiometry $\underline{S}$, i.e.:

$$\exists \underline{C} \quad \exists \underline{S} \quad | \quad \underline{M} = \underline{S} \cdot \underline{C} \quad (18)$$

For the conservational processes

$$0 = \underline{\Gamma} \cdot \underline{M} = \underline{\Gamma} \cdot \underline{S} \cdot \underline{C} \quad (19)$$

is fulfilled, where $\underline{\Gamma}$ is the process rate matrix [8].

2.3 Properties of the GBN Model

GBN architecture offers a general tool to develop robust case specific simulators for any conservational and/or informational process rapidly. When building a simulator for a completely new class of problems, only the respective new dynamic partitions have to be added. The most important useful features of the GBN based generic tools are the following:

Complexity is rather quantitative than qualitative. To move from a lumped balance model to another one of distributed parameters and further to the population balance, usually means the change of complexity from ordinary differential equations to partial differential equations and furthermore to integro-differential equations. In GBN models the above changes can be replaced for declaring the respective new dimensions, while the model generator prepares more elements that will be executed by the same kernel during a longer time.

Easy supplement of new add-on modeling capabilities. In a conventional simulator expert has to write new module with the respective interface. In GBN, the problem specific knowledge can be contained in the expert defined

new program partitions, communicating with the generalized dynamic database.

Full runtime modification. When running the user can pause the simulation and all of the programs and parameters can be modified easily. Afterwards the execution can be continued with the modified structure and parameters.

Macrogranular parallelism: combining generic simulation with genetic algorithm in evolutionary problem solving [7]. First the user must define the so-called possibility space of the given problem of synthesis type. The possibilities can be declared either directly by the full set of the possible active and passive generic elements, or indirectly by the alternative “surface” features and variables. Next the objective(s) have to be declared that can be formulated by an aggregated goal function or by a number of evaluations. The genetic algorithm prepares an initial population. Next the model synthesizing program generates and simulates the variants one after the other, followed by the evaluation of the prescribed objectives. With the knowledge of these evaluations the genetic algorithm proposes a new population to be studied while the new variants will be tendentiously better. The principle is that similarly to the engineering way of thinking, modeling is based on the *a priori* knowledge of the essential features, while the final evaluation is made with the most versatile consideration of the best detailed experiences. Because of the very limited communication between the genetic algorithm and the simulations, the method can be executed by macrogranular parallel architectures (cluster, GRID) effectively.

Microgranular parallelism: possible model-based hardware architectures. The direct mapping of process models onto adequate software architecture gives an idea also for a corresponding hardware implementation. In this hypothetical machine, programming means the configuration of the processors and the communication network, as well as the distribution of data and of brief programs amongst the processors.

3. CONCLUSIONS ABOUT THE “NATURAL INTELLIGENCE” OF PROCESS MODELS

Having studied various process models, coming both from the nature and from the engineer-made artifacts, the following general conclusions can be derived:

a) The natural processes are conservational processes. This means that the state of the natural processes is determined by additive quantities, called measures, while the majority of these measures can be derived from the model specific constant measures (that cannot be formed or decomposed

further within the modeled system). In the feasible formulation of the programs the rate of the processes is controlled by the specific measures, therefore the driving force of the processes converges to zero, if the input measures are exhausted.

b) The analysis of the complex conservational GBN models leads to a new interpretation of the informational process, as a simplified and idealized part of conservational processes. A given subsystem behaves as an informational process with respect to its complement if it consumes and produces significantly less conservational measures than the complementary process, while the informational subprocess affects more influence on the complement than the completing part on it.

ACKNOWLEDGEMENTS

The work was supported by Hungarian Scientific Research Fund T 037-297 and by the Grant of Hungarian Ministry of Economy and Transport GVOP-3.3.1 200404-0091/3.0.

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