DIRECT COMPUTER MAPPING OF PROCESS MODELS

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Abstract

The formal description of a novel process model has been introduced, that gives a common framework for the balance based conservational and rule based informational processes. The models are represented by a bi-layered net (di-digraph) that determines also the network structures of influence routes and flux routes. In the direct computer mapping of these process models the balance elements and the signs, as well as the elementary transitions and the rules can be described by two kinds of uniform, brief declarative programs or dynamic databases, executed by the same kernel program. The method supports the parallel execution.

Keywords

Generic modeling and simulation, Dynamic net and network structures, Direct computer mapping of process models, Structure and function, Large scale dynamic models

Introduction

Nowadays there are new challenges of process modeling, especially in understanding of complex biological processes (e.g. Stephanapoulos, Aristi-dou and Nielsen, 1998), and the in simulation based process design and control of large production systems (e.g. Perea, Grossmann, Ydstie and Tah-massebi, 2001). Regardless to the existing excellent modular, equation oriented, object oriented and black box methods, it is worth to develop and to try novel ideas and, non-conventional methods.

Lessons from Simple and Realistic Examples

Let us study first the *natural process* of the gross metabolic reaction $S+I=W$, where say $S=C_4H_4O_4$, $I=H_2O$, $W=C_4H_6O_5$ and E=enzyme (see Fig. 1a). The state of the enzyme controlled reaction is described by the measures (rectangles) $\underline{M}=[S,I,W,E,ES,ESI,EW]$, built from the constant measures $\underline{C}=[C,H,O,E]$. The changes are characte-rized by the rates (triangles) $v=[v_1,v_2,v_3,v_4,v_5,v_6,v_7,v_8,v_9]$ of the reactions $a_1{:}E+S\rightarrow ES$, $a_2{:}\ ES\rightarrow E+S$, $a_3{:}ES+I\rightarrow ESI$, $a_4{:}ESI\rightarrow EW$, $a_5{:}\ EW\rightarrow E+W$, $a_6{:}E+W\rightarrow E$ and of the feeds (a_7,a_8,a_9). The rate expressions can be calculated with the knowledge of the concentrations (dotted lines), while the balance equations are determined by the weighted sum of the process rates (full lines). The edges determine a bi-layered net structure.

It is similar in the other example (see Fig. 1b), where we model the mixing of raw materials S (corn) and I (maize) to produce fodder $W=S_\alpha I_\beta$ in the drum a_3. The conservational process can be modeled by the initial state of measures $\underline{M}=[S,I,W]$, built from the constant measures $\underline{C}=[S,I]$, by the change v_3 determined by the mapping a_3 and by the feeds a_7,a_8,a_9. However, *the rate of the mixing is not determined by the measures themselves, but we need the add-on control*, carried out by the measurement and execution rules (bar nodes) a_1, a_2, a_4, a_5, a_6, manipulating the signs (circles), charac-terizing the storages, the receipt and the drum.

In Fig. 2 the three dimensional illustration of a chicken meal *production system with variable structure* is seen. The process starts (a_1) from dressed poultry (***Ch***) and cuts (a_2) them into characteristic pieces $\underline{C}=[$***Leg,Breast,Back, Wing, Neck***$]$, that are the constant measures of this model.

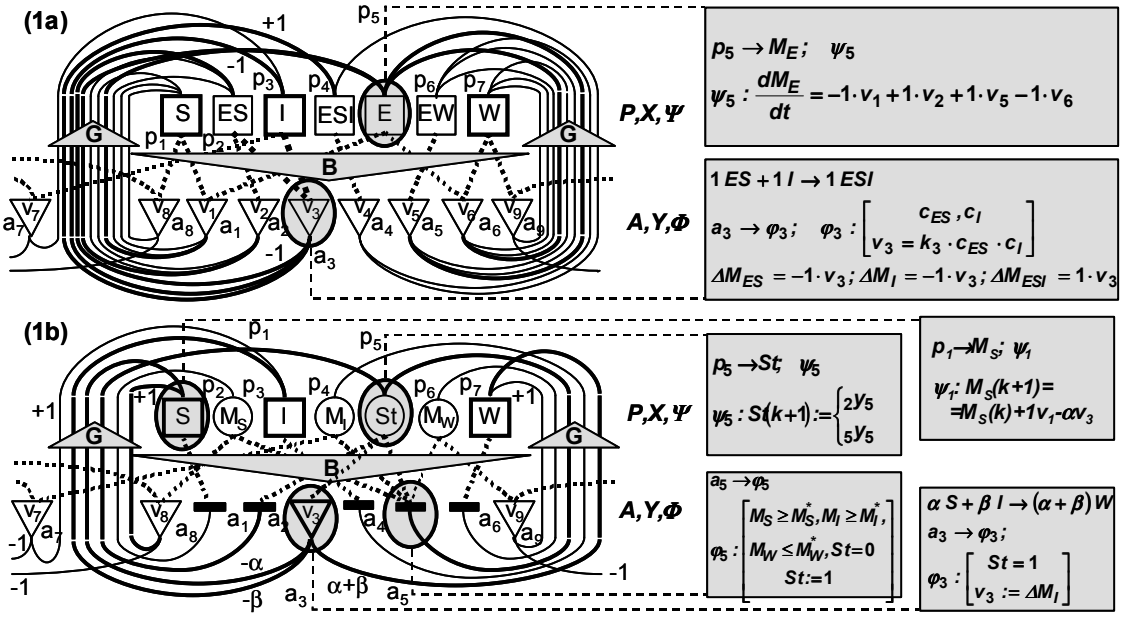

Figure 1. Comparison of a natural (1a) and an artificial (1b) process

Three kinds of **Pa**ckages (*Pa1,Pa2,Pa3*) are manufactured (a_3,a_4,a_5) for sale (a_6,a_7,a_8). The operation of the conservational process depends on the availability of the dressed chicken, and on the demands for the various products. The faint dotted lines designate the necessary, add-on control functionalities. The signed integers refer to the stoichiometric coefficients (e.g. $4Le+2Br= 1Pa_1$).

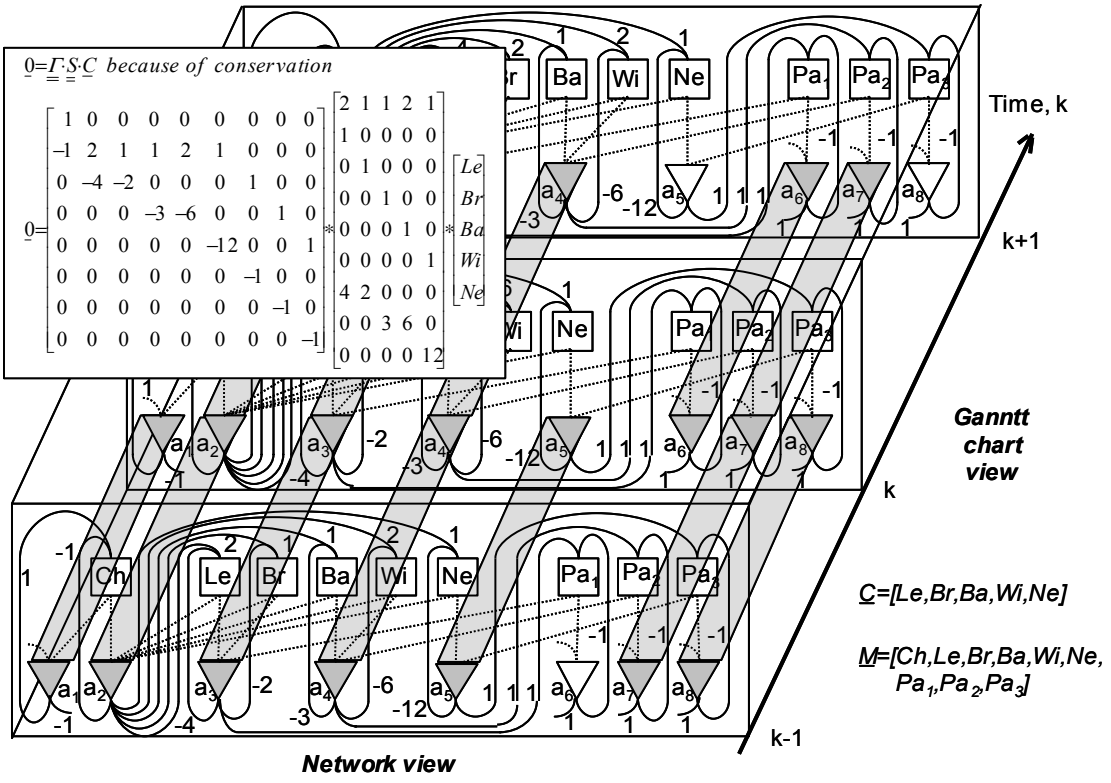

Figure 2. Bi-layered net model of a simplified chicken meal production system

The steadiness of the conservation is determined by the stoichiometries $\underline{S}$ (21) and $\underline{\underline{\Gamma}}$ (18). The gray triangles and shadows are examples for the Gannt chart view, described by variable τ (see later on).

Similar structures have been used in the solution of many practical problems (preparative SMB chromatography, batch co-polymerization, simulation based farm logistics, etc.).

Formal Description of the Generic, Bi-layered Net Model

Abstracted from the above mentioned and other examples the ***generic, bi-layered net model***

$$\langle P, A, B, G, X, Y, \Phi, \Psi, \underline{r}, t \rangle \tag{1}$$

can be defined. Communication channels B deter-mine the passive→active relations (dotted lines):

$$B(\tau) \subset P(\tau) \times A(\tau) \tag{2}$$

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

$$\exists_j \underline{b}(\tau) \mid \forall_i \left(p_j(\tau), a_i(\tau)\right) \in {}_j\underline{b}(\tau) \tag{4}$$

$$\exists \underline{b}_i(\tau) \mid \forall_j \left(p_j(\tau), a_i(\tau)\right) \in \underline{b}_i(\tau). \tag{5}$$

It is similar for channels *G* (full lines):

$$G(\tau) \subset A(\tau) \times P(\tau) \tag{6}$$

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

$$\exists_i \underline{g}(\tau) \mid \forall_j \left(a_i(\tau), p_j(\tau)\right) \in {}_i\underline{g}(\tau) \tag{8}$$

$$\exists \underline{g}_j(\tau) \mid \forall_i \left(a_i(\tau), p_j(\tau)\right) \in \underline{g}_j(\tau) \tag{9}$$

Index *j* designates the ordered sets of the existing output (${}_j\underline{b}$ (4)) and input ($\underline{g}_j$ (9)) connections for the *j*-th passive element. Similarly, index *i* defines the ordered sets of the existing output (${}_i\underline{g}$ (8)) and input ($\underline{b}_i$ (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 relations (see Gannt chart view in Fig. 2).

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

$$\forall_j p_j \rightarrow X_j \in X; \quad \psi_j \in \Psi \tag{10}$$

$$X'_j = \psi_j\left(X_j, \underline{y}_j\left(\underline{g}_j\right)\right) \tag{11}$$

where X_j is any structured data set, while operators ψ_j describe how the changes $\underline{y}_j$, arriving via the channels $\underline{g}_j$, modify the state.

The ***active elements*** *A* (triangles or bars) are characterized by an operator φ_i, resulting a mapping. This determines how the output changes ${}_i y_j \in \underline{y}_j$, carried on ${}_i\underline{g}$ can be calculated from the coordinated input readings ${}_j x_i \in \underline{x}_i$ coming from the passive elements through the channels $\underline{b}_i$:

$$\forall_i a_i \rightarrow \varphi_i \in \Phi; \quad \varphi_i = \begin{bmatrix} \underline{x}_i \left[\underline{b}_i\right] \\ {}_i\underline{y}\left[{}_i\underline{g}\right] \end{bmatrix} \tag{12}$$

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

The alternating, connected, ordered set

$$\left\{{}_{j_1} b_{i_1},\ {}_{i_1} g_{j_2},\ {}_{j_2} b_{i_2},\ {}_{i_2} g_{j_3},\ \ldots\ {}_{j_n} b_{i_n},\ {}_{i_n} g_{j_{n+1}}\right\} \tag{13}$$

of the communication channels is called ***influence route***, which determine a special ring (network) structure. The influence routes carry the influence, e.g. having perturbed the content X_{j_1} of the element p_{j_1}, this change effects on the content $X_{j_{n+1}}$ of the element $p_{j_{n+1}}$ as follows:

$$\left\{{}_{j_1}\Delta x_{i_1}(t_1),\ {}_{i_1}\Delta y_{j_2},\ {}_{j_2}\Delta x(t_2)_{i_2}, \ldots, {}_{i_n}\Delta y_{j_{n+1}}\right\} \tag{14}$$

where ${}_j\Delta x_i$ and ${}_i\Delta y_j$ refer to the perturbation of the state and the change. Obviously, sensitivity and its special forms, such as observability and controllability can be studied by means of the influence route network.

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

$$\psi_j\left(\underline{y}_j\right) = \frac{\Delta X_j\left\lfloor p_j \right\rfloor}{\Delta t} = \sum_i {}_i y_j \tag{15}$$

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:

$${}_i\underline{y}\left\lfloor {}_i\underline{g} \right\rfloor = {}_i\underline{y}^+\left\lfloor {}_i\underline{g}^+ \right\rfloor \cup {}_i\underline{y}^-\left\lfloor {}_i\underline{g}^- \right\rfloor \tag{16}$$

The active elements of the balance process models describe the various transportations and transformations. The operator φ_i can often be determined by the respective rate v_i, i.e.:

$$\varphi_i: \quad {}_i\underline{y} = {}_i\underline{\gamma} \cdot v_i\left(\underline{x}_i\right) \tag{17}$$

while the whole process

$$\underline{Y} = \underline{v} \cdot \underline{\underline{\Gamma}} \tag{18}$$

can be written for, and stoichiometric vectors ${}_i\underline{\gamma}$ are the rows of ***process stoichiometry matrix*** $\underline{\underline{\Gamma}}$.

In the balance process models the alternating, connected, ordered set

$$\left\{{}_{j_1} g^-_{i_1},\ {}_{i_1} g^+_{j_2},\ {}_{j_2} g^-_{i_2},\ {}_{i_2} g^+_{j_3}, \ldots, {}_{j_n} g^-_{i_n},\ {}_{i_n} g^+_{j_{n+1}}\right\} \tag{19}$$

of the communication channels is called ***flux route***. Flux routes determine another special ring structure, which carry the constant and conservational measures and, e.g. having

modified, measure X_{j_1} in element p_{j_1}, this change effects
on measure $X_{j_{n+1}}$ of the element $p_{j_{n+1}}$, i.e.:

$$\left\{{}_{j_1}\Delta y^{-}_{i_1}(t_1),{}_{i_1}\Delta y^{+}_{j_2}(t_2),{}_{j_2}y^{-}_{i_2}(t_1),\ldots,{}_{i_{n-1}}\Delta y^{+}_{j_n}(t_n)\right\} \quad (20)$$

The $\Delta y^{+/-}_{j_i}$ values refer to the dispersion of the changes in the rate of subsequent processes, (multi-plied by the stoichiometric coefficients, see Fig. 2).

Conservational process is special case of the balance process, iff

(i) There are constant measures $\underline{C}$ determined by the model specific conservation laws, and all of the measures $\underline{M}$ contained in the state X of the passive elements P are combined from these constant measures according to the respective stoichiometry $\underline{\underline{S}}$, accordingly (see Fig. 2):

$$\exists\, \underline{C} \quad \exists\, \underline{\underline{S}} \quad | \quad \underline{M} = \underline{\underline{S}} \cdot \underline{C} \quad (21)$$

(ii) The conservation expression

$$\underline{0} = \underline{\underline{\Gamma}} \cdot \underline{M} = \underline{\underline{\Gamma}} \cdot \underline{\underline{S}} \cdot \underline{C} \quad (22)$$

fulfils.

Software Representation of the Direct Computer Mapping

In direct computer mapping of the process models the passive *P* and active *A* elements are described by the

p(Identifiers, Kind, Time, Location, Content, Call_for_Operators, Others)

passive, and

a(Identifiers, Kind, Time, Location, Inputlist, Call_for_Operators, Outputlist, Others)

active dynamic database or program partitions.

These dynamic partitions are executed by a ***general and optionally extendable kernel***. The active elements read the Content (*X*) from the associated passive elements of Inputlist (*B*), and then, according to operators Φ calculate changes (*Y*), finally the passive elements on Outputlist (*G*) are modified according to the operators Ψ.

The method offers robust solution for the hard, multidimensional and non-linear problems, as well as supports parallel programming.

Conclusion

The generic, bi-layered net model has been proved to describe the common and specific features of the various dynamic process models. The suggested novel approach determines the inherent relations between the structure and the functionalities and gives a theoretical basis for the direct computer mapping of the process models.

Outlook

The ongoing work focuses on the *problem solving by direct computer mapping of process models*. Some exciting actual questions are:

- the *analogy between the metabolic networks and the supply* chains (or rather *supply cycles),*
- the *analysis of the influence routes* for the conscious synthesis (planning & sceduling) of the appropriate balance routes; and
- the supplement of the net with a distributed cost function that *generates local economic potential for local decisions* made by operators Φ.

To improve the effectiveness of the method, the ***hardware representation has been initiated***. In the direct hardware mapping, the alternating communication (*x, y*) between the „active" (*A*) and „passive" (*P*) processors can be organized via the programmable (and possibly wireless frequency) channels (*B, G*), while the operators Ψ and Φ are realized by brief, in parallel executable programs.

Nomenclature

$a_i \in A$ = active elements,
${}_jb_i \in B$ = passive →active connections,
$\underline{C}$ = constant conservational measures,
${}_ig_j \in G$ = active →passive connections,
$\underline{M}$ = derived balance measures,
$p_j \in P$ = passive elements,
$\underline{r}$ = geometrical and property coordinates,
$\underline{\underline{S}}$ = stoichiometry between the conser-vational and constant measures,
t = time,
v_i = rate of conservational process of φ_i,
$X_j, {}_jx_i$ = state variables and their readings,
$Y, {}_i\underline{y}, {}_iy_j$ = changes of the state variables,
$\underline{\underline{\Gamma}}$ = process stoichiometry matrix,
$\varphi_i \in \Phi$ = operator (or a brief program) that describes the function of the active elements,
$\psi_j \in \Psi$ = operator (or a brief program) that determines the state of the passive elements,
τ = time interval(s) or time points, when the given item exists.

References

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