Cause-Effect Structures Behaving like Reaction Systems

Ludwik Czaja[1,2]

[1]Vistula University, Warsaw, Poland
[2]Institute of Informatics, The University of Warsaw, Poland

Abstract
Cause-effect (c-e) structures, a net-like algebraic formalism for describing and analysing systems, primarily parallel, may be adapted to work as Reaction Systems. This is acquired by a simple modification of the c-e structures' semantics

Keywords
cause-effect structure, reaction system, quasi semiring

1. Summary of elementary cause-effect structures

Cause-effect structures (c-e) are objects of an algebraic calculus called a *quasi-semiring*[1], for describing and analysing systems built up as nets. Among a number of similarities to Petri nets, the noticeable is graphic presentation of systems' dynamics. The complete presentation of c-e structures is in [Cza 2019].

Definition 1.1 (set $\boldsymbol{F}[\mathbb{X}]$, quasi-semiring of formal polynomials)

Let $\mathbb{X}$ be a non-empty enumerable set. Its elements, called *nodes*, are counterparts of places in Petri nets. $\theta \notin \mathbb{X}$ is a symbol called *neutral*. It plays role of neutral element for operations on terms, called *formal polynomials over* $\mathbb{X}$. The names of nodes, symbol θ, operators +, $\bullet$, called addition and multiplication, and parentheses are symbols out of which formal polynomials are formed. A node's name and θ is a formal polynomial; if K and L are formal polynomials, then $(K + L)$ and $(K \bullet L)$ are too. Their set is denoted by $\boldsymbol{F}[\mathbb{X}]$. Assume stronger binding of $\bullet$ than +, which allows for dropping some parentheses. Addition and multiplication of formal polynomials is defined as follows: $K \oplus L = (K + L)$, $K \odot L = (K \bullet L)$. To simplify notation, let us use + and $\bullet$ instead of $\oplus$ and $\odot$. It is required that the system $\langle \boldsymbol{F}[\mathbb{X}], +, \bullet, \theta \rangle$ obeys the following equality axioms for all $K, L, M \in \boldsymbol{F}[\mathbb{X}]$, $x \in \mathbb{X}$:

(+) $\quad \theta + K = K + \theta = K$ $\qquad$ (•) $\quad \theta \bullet K = K \bullet \theta = K$

29th International Workshop on Concurrency, Specification and Programming (CS&P'21)
lczaja@mimuw.edu.pl (L. Czaja)
0000-0003-4675-816X (L. Czaja)

[1]This calculus differs from the standard semiring by restricted distributivity law: $a \cdot (b + c) = a \cdot b + a \cdot c$ satisfied provided that $b \neq \theta$ if and only if $c \neq \theta$ where θ is a neutral element for both operations (simultaneity and nondeterministic choice). Hence the preposition "quasi". Note that due to the conditional distributivity, the calculus neither reduces to the single element θ, nor makes both operations coincide.

(++) $K + K = K$ (••) $x \bullet x = x$
(+++) $K + L = L + K$ (• • •) $K \bullet L = L \bullet K$
(++++) $K + (L + M) = (K + L) + M$ (• • ••) $K \bullet (L \bullet M) = (K \bullet L) \bullet M$
(+•) If $L \neq \theta \Leftrightarrow M \neq \theta$ then $K \bullet (L + M) = K \bullet L + K \bullet M$

Algebraic system which obeys these axioms will be referred to as a *quasi-semiring of formal polynomials*. □

Definition 1.2 (cause-effect structure, carrier, set ***CE***[$\mathbb{X}$])

A cause-effect structure (c-e structure) over $\mathbb{X}$ is a pair $U = \langle C, E \rangle$ of total functions:

C: $\mathbb{X} \to \boldsymbol{F}[\mathbb{X}]$ (*cause function*; nodes occuring in $C(x)$ are *causes* of x)
E: $\mathbb{X} \to \boldsymbol{F}[\mathbb{X}]$ (*effect function*; nodes occuring in $E(x)$ are *effects* of x)

such that x occurs in the formal polynomial $C(y)$ iff y occurs in $E(x)$. *Carrier* of U is the set $car(U) = \{x \in \mathbb{X} : C(x) \neq \theta \vee E(x) \neq \theta\}$. U is of *finite carrier* iff $|car(U)| < \infty$ ($|...|$ denotes cardinality). The set of all c-e structures over $\mathbb{X}$ is denoted by ***CE***[$\mathbb{X}$]. Since $\mathbb{X}$ is fixed, we write just ***CE***. □

C and E are total, thus each c-e structure comprises all nodes from $\mathbb{X}$, also the isolated ones - those from outside of its carrier. In presenting c-e structures graphically, only their carriers are drawn. A representation of a c-e structure $U = \langle C, E \rangle$ as a set of annotated nodes is $\{x_{E(x)}^{C(x)} : x \in car(U)\}$. U is also presented as a directed graph with $car(U)$ as set of vertices labelled with objects of the form $x_{E(x)}^{C(x)}$ ($x \in car(U)$); there is an edge from x to y iff y occurs in the polynomial $E(x)$. Fig. 1 (a) and (b) depict two graphical presentations of the same c-e structure with carrier $\{a, b, c, d, e, f, g, h\}$; in (a) the encircled nodes comprise groups making products in formal polynomials in (b), where the sums of the products create families of the groups. This c-e structure is the set $\{a_e^\theta, b_e^\theta, c_e^\theta, d_e^\theta, e_{f \cdot g+h}^{a+b \cdot c+c \cdot d}, f_\theta^e, g_\theta^e, h_\theta^e\}$. Sometimes the empty subscript/superscript θ by node names is omitted.

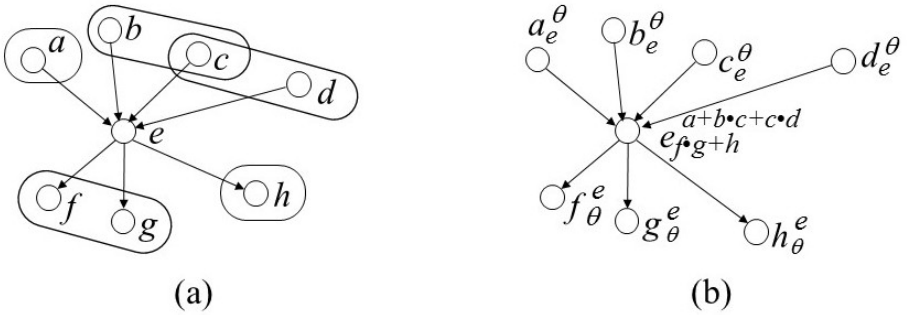

Figure 1: (a) Predecessors and successors of the node e, grouped into families: $\{\{a\}, \{b, c\}, \{c, d\}\}$ and $\{\{f, g\}, \{h\}\}$. (b) Notation by means of polynomials; the arrows are redundant: used only for graphic presentation of c-e structures.

Definition 1.3 (addition and multiplication, monomial c-e structure)

For c-e structures $U = \langle C_U, E_U\rangle,\ V = \langle C_V, E_V\rangle$ define:
$U + V = \langle C_{U+V}, E_{U+V}\rangle = \langle C_U + C_V, E_U + E_V\rangle$ where
$(C_U + C_V)(x) = C_U(x) + C_V(x)$ and similarly for E
$U \bullet V = (C_{U\bullet V}, E_{U\bullet V}) = (C_U \bullet C_V, E_U \bullet E_V)$ where
$(C_U \bullet C_V)(x) = C_U(x) \bullet C_V(x)$ and similarly for E

(The same symbols "+" and "•" are used for operations on c-e structures and formal polynomials). U is a *monomial* c-e structure iff each polynomial $C_U(x)$ and $E_U(x)$ is a monomial, i.e. does not comprise non-reducible (relative to equations in Definition 1.1) operation "+". □

Apart from the representation of c-e structures as a set $\{x_{E(x)}^{C(x)} : x \in car(U)\}$, their linear notation is used as the so-called "*arrow-expressions*": $\{x_y^\theta,\ y_\theta^x\}$ is an arrow, denoted as $x \to y$ and, consequently, $\{x_y^\theta, y_\theta^x\}\bullet\{y_z^\theta, z_\theta^y\}\bullet\{z_u^\theta, u_\theta^z\}..... = \{x_y^\theta, y_z^x, z_u^y, u_{....}^z.....\}$ is a chain, denoted as $x \to y \to z \to u....$. Bidirectional arrow $x \leftrightarrow y$ denotes $x \to y \to x$ (equivalent to $y \to x \to y$), that is, the close cycle $\{x_y^y, y_x^x\}$. Chains and arrows in particular, may be combined into "arrow expressions" representing some c-e structures. For instance c-e structure $\{a_{x+y}^\theta, b_{x\bullet y}^\theta, x_\theta^{a\bullet b}, y_\theta^{a\bullet b}\}$ may be written as $(a \to x + a \to y) \bullet (b \to x) \bullet (b \to y)$.

The set ***CE*** with addition, multiplication and a distinguished element denoted also by θ and understood as the empty c-e structure (θ, θ), where θ is a constant function $\theta(x) = \theta$ for all $x \in \mathbb{X}$, makes an algebraic system similar to that in Definition 1.1, the quasi-semiring of c-e structures. Therefore the Proposition 1.1:

Proposition 1.1 The system $\langle \boldsymbol{CE}[\mathbb{X}], +, \bullet, \theta\rangle$ obeys the following equations for all $U, V, W \in \boldsymbol{CE}[\mathbb{X}],\ x, y \in \mathbb{X}$:

(+) $\theta + U = U + \theta = U$ (•) $\theta \bullet U = U \bullet \theta = U$
(++) $U + U = U$ (••) $(x \to y) \bullet (x \to y) = x \to y$
(+++) $U + V = U + V$ (• • •) $U \bullet V = V \bullet U$
(++++) $U + (V + W) = (U + V) + W$ (• • ••) $U \bullet (V \bullet W) = (U \bullet V) \bullet W$
(+•) If $C_V(x) \neq \theta \Leftrightarrow C_W(x) \neq \theta$ and $E_V(x) \neq \theta \Leftrightarrow E_W(x) \neq \theta$ then
$U \bullet (V + W) = U \bullet V + U \bullet W$ □

Definition 1.4 (partial order $\leq$; substructure, set ***SUB***$[V]$, firing component, set ***FC***, pre-set and post-set)

For $U, V \in \boldsymbol{CE}$ let $U \leq V \Leftrightarrow V = U + V;\ \leq$ is a partial order in ***CE***. If $U \leq V$ then U is a *substructure* of V; ***SUB***$[V]$= $\{U : U \leq V\}$ is the set of all substructures of V. For $A \subseteq$***CE***: $V \in A$ is *minimal* (wrt $\leq$) in A iff $\forall W \in A$: $(W \leq V \Rightarrow W = V)$.
A minimal in ***CE***$\backslash\{\theta\}$ c-e structure $Q = \langle C_Q, E_Q\rangle$ is a *firing component* iff Q is a monomial c-e structure and $C_Q(x) = \theta \Leftrightarrow E_Q(x) \neq \theta$ for any $x \in car(Q)$. The set of all firing components

is denoted by ***FC***, thus the set of all firing components of $U \in$***CE*** is ***FC***$[U] =$ ***SUB***$[U] \cap$ ***FC***. Let for $Q \in$ ***FC*** and $G \subseteq$ ***FC***:

$^\bullet Q = \{x \in car(Q) : C_Q(x) = \theta\}$ (*pre-set* or causes of Q)
$Q^\bullet = \{x \in car(Q) : E_Q(x) = \theta\}$ (*post-set* or effects of Q)
$^\bullet Q^\bullet = {}^\bullet Q \cup Q^\bullet$
$^\bullet G = \bigcup_{Q \in G} {}^\bullet Q$ (*pre-set* or causes of G)
$G^\bullet = \bigcup_{Q \in G} Q^\bullet$ (*post-set* or effects of G)
$^\bullet G^\bullet = {}^\bullet G \cup G^\bullet$ □

Thus, the firing component is a connected graph, due to the required minimality. Elements of the pre-set are its *causes* and elements of the post-set are its *effects*.

Definition 1.5 (**salvo** - pairwise detached firing components; family ***FCS***)

Firing components Q and P are *detached* if and only if $^\bullet Q^\bullet \cap {}^\bullet P^\bullet = \varnothing$. Any set $G \subseteq$***FC*** of pairwise detached firing components is called their ***salvo***. The family of salvos is denoted by ***FCS***. So, if $G \subseteq$***FC***$[U]$ then ***FCS***$[U] \subseteq 2^{\mathbf{FC}[U]}$ for a c-e structure U, denotes a collection of salvos in U. The intention is that firing components in a salvo are capable of acting ("firing") simultaneously. This notion will be used in definition of parallel semantics of c-e structures.□

Definition 1.6 (state of elementary c-e structures)

A *state* is a subset of the set of nodes: $s \subseteq \mathbb{X}$. The set of all states: $\mathbb{S} = 2^{\mathbb{X}}$. A node x is *active* in the state s iff $x \in s$ and *passive* otherwise. As in case of Petri nets, we say "x holds a token" when x is active. Obviously, the state might be defined equivalently as a two-valued function s: $\mathbb{X} \to \{0, 1\}$. □

Definition 1.7 (sequential and parallel semantics of elementary c-e structures)

Sequential. For $Q \in$***FC***$[U]$, $s \in \mathbb{S}$, let $[[Q]] \subseteq \mathbb{S} \times \mathbb{S}$ be a binary relation defined as:
$(s,t) \in [[Q]]$ iff $^\bullet Q \subseteq s \wedge Q^\bullet \cap s = \varnothing \wedge t = (s \backslash {}^\bullet Q) \cup Q^\bullet$ (Q transforms state s into t).
Semantics $[[U]]$ of $U \in$***CE*** is: $[[U]] = \bigcup_{Q \in FC[U]} [[Q]]$. $[[U]]^*$ is its reflexive and transitive closure, that is $(s,t) \in [[U]]^*$ if and only if $s = t$ or there exists a sequence of states $s_0, s_1, ..., s_n$ with $s = s_0$, $t = s_n$ and $(s_j, s_{j+1}) \in [[U]]$ for $j = 0, 1, ..., n-1$. State t is *reachable* from s in semantics $[[\ ]]$ and the sequence $s_0, s_1, ..., s_n$ is a *computation* performed by U.
Parallel. For a salvo $G \in$***FCS***$[U], G \neq \varnothing$, relations $[[G]]$ and $[[U]]_{par}$ are defined in the same way as $[[Q]]$ and $[[U]]$ in the sequential case but with Q replaced with G and ***FC***$[U]$ replaced with ***FCS***$[U]$. Closure $[[U]]^*_{par}$, reachability and computation are defined as in the sequential case. □

Note that $[[U]] = \varnothing$ iff ***FC***$[U] = \varnothing$. Behaviour of elementary c-e structures may be thought of as a token game: if each node in a firing component's pre-set holds a token and none in

its post-set does, then remove tokens from the pre-set and put them in the post-set. This is illustrated in Fig. 2. Properties inferred from above definitions are proved in [Cza 2019].

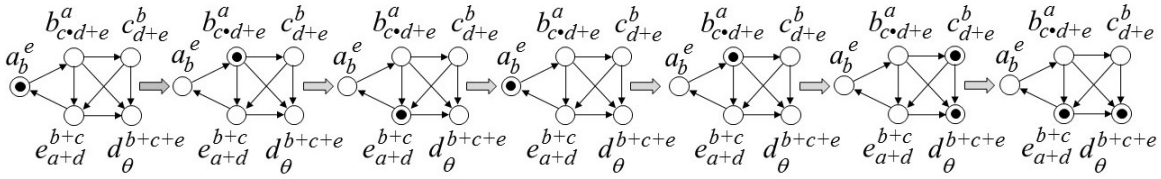

Figure 2: Example of activity (successive transformations) of elementary c-e structure. Its linear notation as an "arrow expression" is the following:
$(a \to b) + (b \to c) \bullet (b \to d) + (b \to e) + (c \to e) + (c \to d) + (e \to d) + (e \to a)$.

2. Summary of extended cause-effect structures

The structure of extended c-e structures, their firing component in particular, is the same as in Definitions 1.1 - 1.4. The extensions consist in redefining the state, treating the pre and post sets of firing components as multisets, and redefining semantics. It is assumed that with a given c-e structure $U \in \boldsymbol{CE}[\mathbb{X}]$ (i.e. already constructed by operations introduced in Definition 1.3) and the set of its firing components $\boldsymbol{FC}[U] = \boldsymbol{SUB}[U] \cap \boldsymbol{FC}$, some additional information is associated. The following extensions of elementary c-e structures with this information will be obtained: multi-valued nodes, capacity of nodes and coefficients of monomials in polynomials annotating nodes (counterparts of weight of arrows in Petri nets), in particular a coefficient ω which represents inhibiting. To this end, a notation for multisets is convenient: let $\mathbb{N}$ be the set of natural numbers including 0 and $\mathbb{N}_\omega = \mathbb{N} \cup \{\omega\}$, where the value ω means infinity, that is $\omega > n$ for each $n \in \mathbb{N}$. A *multiset* over a base set X is a (total) function $f\colon X \to \mathbb{N}_\omega$. If the set $\{x\colon f(x) \neq 0\}$ is finite then the linear-form notation is adopted for multisets , e.g.

X	a	b	c	d	e
$f(X)$	2	0	3	1	ω

is denoted by $2 \otimes a + 3 \otimes c + d + \omega \otimes e$. A multiset is *zero* $\mathbb{O}$, when $\mathbb{O}(x) = 0$ for all x. Addition, subtraction and multiplication on multisets is defined: $(f+g)(x) = f(x)+g(x)$, $(f-g)(x) = f(x)-g(x)$ for $f(x) \geq g(x)$, $(f \cdot g)(x) = f(x) \cdot g(x)$, comparison of multisets: $f \leq g$ iff $f(x) \leq g(x)$ for all x. Assume the customary arithmetic of ω: $\omega + n = \omega, \omega - n = \omega$, $\omega + \omega = \omega$ and additionally $0 - \omega = 0$.

Definition 2.1 (state of extended c-e structures)

A state of extended c-e structure U is a total function $s : car(U) \to \mathbb{N}$, thus a multiset over $car(U)$. The set of all states of U is denoted by $\mathbb{S}$. □

Definition 2.2. (weights of monomials and capacity of nodes)

For a c-e structure $U = \langle C, E \rangle$ and its firing component $Q \in \boldsymbol{FC}[U]$, let with the pre-set ${}^\bullet Q$ and post-set $Q^\bullet$ of Q, some multisets $\overline{{}^\bullet Q}\colon {}^\bullet Q \to \mathbb{N}_\omega$ and $\overline{Q^\bullet}\colon Q^\bullet \to \mathbb{N}_\omega$ be given as additional information. The value $\overline{{}^\bullet Q}(x)$ is a *weight* (or *multiplicity*) of monomial $E_Q(x)$ and the value

$\overline{Q^\bullet}(x)$ - a *weight* (or *multiplicity*) of monomial $C_Q(x)$. For $E_Q(x) = \theta$ or $C_Q(x) = \theta$ assume respectively ${}^\bullet\overline{Q}(x) = 0$ or $\overline{Q^\bullet}(x) = 0$ and additionally let ${}^\bullet\overline{Q}(x) = 0$ for $x \notin {}^\bullet Q$ and $\overline{Q^\bullet}(x) = 0$ for $x \notin Q^\bullet$. Let $cap(U)$ be a total function $cap(U) : car(U) \to \mathbb{N}_\omega \backslash \{0\}$, assigning a *capacity* to nodes in the set $car(U)$. A c-e structure endowed with such information is a *c-e structure-with-weighted monomials and capacity of nodes*. Note that this definition extends directly from the firing components onto their salvos. Indeed, For any non-empty salvo $G \in \boldsymbol{FCS}[U]$ and any $x \in {}^\bullet G^\bullet$ there exists exactly one firing component $Q \in G$, with $x \in {}^\bullet Q^\bullet$ (because firing components in G are pairwise detached). Thus one may define ${}^\bullet\overline{G} = {}^\bullet\overline{Q}$ and $\overline{G^\bullet} = \overline{Q^\bullet}$. It should also be noticed that weights of cause or effect monomials in identical firing components appearing in different c-e structures, may be different. □

An effect monomial $E_Q(a)$ of a node $a \in {}^\bullet Q$, with weight ${}^\bullet\overline{Q}(a)$, is denoted by ${}^\bullet\overline{Q}(a) \otimes E_Q(a)$. Similarly for a cause monomial $C_Q(x)$ of a node $x \in Q^\bullet$ with weight $\overline{Q^\bullet}(x)$: $\overline{Q^\bullet}(x) \otimes C_Q(x)$. The coefficient representing weights will be abandoned if they are 1.

Definition 2.3 (inhibitors)

For a firing component $Q \in \boldsymbol{FC}[U]$, let $inh[Q] = \{x \in {}^\bullet Q : {}^\bullet\overline{Q}(x) = \omega\}$, thus a set of nodes in the pre-set of Q, whose effect monomials $E_Q(x)$ are of weight ω. The nodes in $inh[Q]$ will play role of *inhibiting nodes* of firing component Q. In accordance with the note in Definition 1.5 (pairwise detached firing components in salvos), the concept of inhibiting nodes extends directly onto the salvos: $inh[G] = \{x \in {}^\bullet G : {}^\bullet\overline{G}(x) = \omega\}$ where $G \in \boldsymbol{FCS}[U]$. The inhibiting nodes will be called *inhibitors*. □

Definition 2.4. (enabled firing components and enabled salvos)

For a firing component $Q \in \boldsymbol{FC}[U]$ and state s let us define the formula: $enabled[Q](s)$ if and only if:

$$\begin{array}{l} \forall x \in inh[Q] : \ s(x) = 0 \wedge \\ \forall x \in {}^\bullet Q \backslash inh[Q] : \ s(x) > 0 \wedge {}^\bullet\overline{Q}(x) \leq s(x) \leq cap(U)(x) \wedge \\ \forall x \in Q^\bullet : \overline{Q^\bullet}(x) + s(x) \leq cap(U)(x) \end{array}$$

So, Q is enabled in the state s iff none of inhibiting nodes $x \in {}^\bullet Q$ contains a token and each remaining node in ${}^\bullet Q$ contains, with no fewer tokens than is the weight of its effect monomial $E_Q(x)$ and no more than capacity of each $x \in {}^\bullet Q$. Moreover, none of $x \in Q^\bullet$ holds more tokens than their number when increased by the weight of the cause monomial $C_Q(x)$, exceeds capacity of x. Evidently, for a salvo $G \in \boldsymbol{FCS}[U]$, the formula $enabled[G](s)$ is defined as above by replacing Q with G and $\boldsymbol{FC}[U]$ with $\boldsymbol{FCS}[U]$. □

Definition 2.5. (Sequential and parallel semantics of extended c-e structures)

Sequential. For $Q \in \boldsymbol{FC}[U]$, let $[[Q]] \subseteq \mathbb{S} \times \mathbb{S}$ be a binary relation defined as:

$(s,t) \in [[Q]]$ iff $enabled[Q](s) \wedge t = (s - \overline{{}^\bullet Q}) + \overline{Q^\bullet} \leq cap(U)$ (Q transforms state s into t). *Semantics* $[[U]]$ of $U \in$ ***CE*** is $[[U]] = \bigcup_{Q \in \boldsymbol{FC}[U]} [[Q]]$. Closure $[[U]]^*$ and reachability and computation are defined as in Definition 1.7.

Parallel. For a salvo $G \in \boldsymbol{FCS}[U], G \neq \varnothing$, the relations $[[G]]$ and $[[U]]_{par}$ are defined in the same way as $[[Q]]$ and $[[U]]$ in the sequential case, but with Q replaced with G and $\boldsymbol{FC}[U]$ replaced with $\boldsymbol{FCS}[U]$. Closure $[[U]]^*_{par}$, reachability and computation are defined as in the sequential case. □

An example of using inhibitor is in Fig. 3. The weight of one effect (i.e. subscript) monomial $\omega \otimes z$ of the node T is ω, thus traversing arrow from T to z would require infinite number of tokens at T, which is impossible. Thus, T is the inhibiting node in firing component Q_0 and ordinary - in firing component Q_1. In accordance with aforesaid notation of multisets, the weighted monomials are denoted by $w \otimes M$, where w is the weight of M - an unweighted monomial. The weight is skipped if $w = 1$. The corresponding arrows are dashed in the figures if $w = \omega$. In all graphic presentations of c-e structures, nodes of unbounded capacity ω, for storing data (sets of tokens), will be drawn as bigger circles with double edge. Remaining nodes, the "control", are of capacity 1 and drawn as smaller circles.

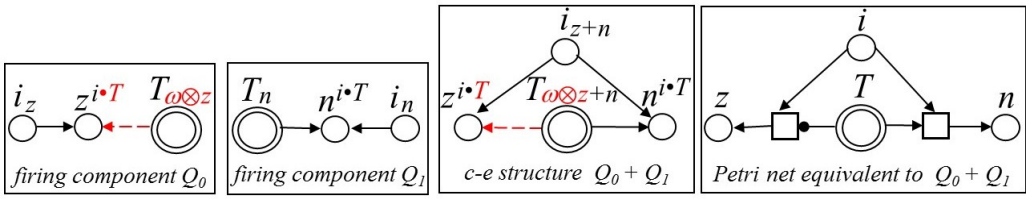

Figure 3: Construction of c-e structure $Q_0 + Q_1$ implementing "test zero". A token at the node i starts testing contents of T; on termination, the token appears at z (zero) if T is empty and at n (not zero) otherwise. The tested node T plays two roles: inhibiting in Q_0 and ordinary in Q_1. Capacity of T is infinite, whereas of remaining nodes is 1. The empty subscript/superscript θ is skipped. In the Petri net counterpart, the inhibiting arrow enters the left transition.

3. Basic notions of reaction systems

This outline of reaction systems [Ehr 2007], [Ehr 2017] is limited to the primary definitions, not their extensions, generalizations and properties established in this theory. The outline serves only as a reference base for the next section concerned with a translation of reaction systems into a version of cause-effect structures. That is why the original (in the literature) denotation of certain constituents of reaction systems, has been somewhat changed, in order to avoid naming collision with the cause-effect structures. But the new presentation is completely equivalent to original and only tailored to the purpose of the next section. The reaction systems will be referred to as ***RE***. The reaction systems as well as cause-effect structures, though devised to describe interactions or cooperation in a network of active objects, both are certain models

of computing - in the broadest meaning of this word. Reaction systems are very inspiring new model of computing, if "computing" is to encompass interaction, not only "number crunching". That is why a certain attempt to translate the reaction systems into c-e structures is undertaken, though for a price of modifying semantics of the latter, but retaining their structure. There have been also other endeavours to relate reaction systems with some formal models, for instance [Kle 2011], [Dut 2018], [Bar 2018], [Gor 2018].

Definition 3.1 (reaction system)

A reaction system A is created of two sets: $A = (\mathbb{B}, \mathbb{R})$ where $\mathbb{B}$ is a set called a **background** (intended to comprise the so-called **entities)**, $\mathbb{R}$ is a set of **reactions**, each reaction $r \in \mathbb{R}$ created of three sets $r = (R_r, I_r, P_r)$ where $R_r \subseteq \mathbb{B}$ is a set of **reactants**, $I_r \subseteq \mathbb{B}$ is a set of **inhibitors** with $R_r \cap I_r = \varnothing$ and $P_r \subseteq \mathbb{B}$ is a set of **products**. The **initial state** of the system A is a set $\mathbb{S}_0 \subseteq \mathbb{B}$. □

In the literature, all the sets in Definition 3.1 are required to be finite. Though the concept of "entity" has not been formally adopted in the definitions, for the purpose of this section it will be understood as an object associated in a given state with an element of the background, likewise a "token", an abstract object, of intuitive, informal status in the c-e structures or Petri nets. Hence, the set phrase "entity present in..." in writings on the reaction systems. Since the notion of "state" of reaction systems is analogous to that in elementary Petri nets (and elementary c-e structures), meaning of the word "entity" may be thought of as an element of state.

Definition 3.2 (state and enabled reactions)

A state $\mathbb{S}$ of reaction system A is a subset of its background: $\mathbb{S} \subseteq \mathbb{B}$. The intention is that $\mathbb{S}$ be the set of those background's members, which comprise entities. A reaction $r = (R_r, I_r, P_r)$ is **enabled** in a state $\mathbb{S}$ iff $R_r \subseteq \mathbb{S}$ and $I_r \cap \mathbb{S} = \varnothing$. □

Definition 3.3 (semantics of reaction systems - change of state)

The **result** of a reaction r in a state $\mathbb{S}$ is the set P_r if r is enabled at $\mathbb{S}$ and the empty set $\varnothing$ otherwise. This result is denoted by $res_r(\mathbb{S})$. The result of the reaction system A in a state $\mathbb{S}$ is the union of all its reactions in this state:

$$res_A(\mathbb{S}) = \bigcup_{r \in \mathbb{R}} res_r(\mathbb{S})$$

□

Note that on completion (if it exists) of reaction system work, the entities in the difference of sets $\mathbb{S} \backslash res_A(\mathbb{S})$ disappear. Note also two features differing the reaction systems from cause-effect structures (or Petri nets): the lack of conflicts and possible absorption of reactants by products.

These features will be taken into account in definition of semantics of reaction c-e structures in the next section.

Example 3.1 (test zero)

The "test zero" task (Fig. 3) may be realized in the reaction system $A = (\mathbb{B}, \mathbb{R})$ with $\mathbb{B} = \{i, z, n, T\}$, $\mathbb{R} = \{r1, r2\}$ where $r1 = (\{i\}, \{T\}, \{z\})$, $r2 = (\{i, T\}, \varnothing, \{n\})$. Result of this system's work depends on the initial state $\mathbb{S}_0$ (i.e. what the environment supplies): if $\mathbb{S}_0 = \{i, T\}$ then the result is $\{n\}$ ("not zero" - presence of entity at T), if $\mathbb{S}_0 = \{i\}$ then the result is $\{z\}$ ("zero" - absence of entity at T). Reactant i initiates work of the system, while T is tested for presence/absence of entity. Evolution of the system $A = (\{i, z, n, T\}, \{r1, r2\})$ with initial state $\{i, T\}$ is the following:

$res_{r1}(\{i, T\}) = \varnothing$ (because $\{i\} \subseteq \{i, T\}$ and $\{T\} \cap \{i, T\} \neq \varnothing$)
$res_{r2}(\{i, T\}) = \{n\}$ (because $\{i, T\} \subseteq \{i, T\}$ and $\varnothing \cap \{i, T\} = \varnothing$) thus
$res_A(\{i, T\}) = res_{r1}(\{i, T\}) \cup res_{r2}(\{i, T\}) = \{n\}$ ("not zero")

Evolution of the system A with initial state $\{i\}$ is the following:

$res_{r1}(\{i\}) = \{z\}$ (because $\{i\} \subseteq \{i\}$ and $\{T\} \cap \{i\} = \varnothing$)
$res_{r2}(\{i\}) = \varnothing$ (because $\{i, T\} \nsubseteq \{i\}$ and $\varnothing \cap \{i\} = \varnothing$) thus
$res_A(\{i\}) = res_{r1}(\{i\}) \cup res_{r2}(\{i\}) = \{z\}$ ("zero")

More complex example of evolution of a reaction system, that is its consecutive state changes, is in section 4.

4. Cause-effect structures working similarly to reaction systems

The objective is to build a system structurally identical with c-e structures but working like reaction systems. Let us call them "reaction c-e structures" and denote by ***RECE***. The evident counterparts of some objects in reaction c-e structures and reaction systems are the following:

nodes$\longleftrightarrow$*elements of background*,
firing components$\longleftrightarrow$*reactions*,
causes in a firing component$\longleftrightarrow$*reactants in a reaction*,
effects in a firing component$\longleftrightarrow$*products in a reaction*,
inhibitors in a firing component$\longleftrightarrow$*inhibitors in a reaction*,
tokens$\longleftrightarrow$*entities*.

The state of reaction c-e structures is a restriction of the state introduced in Definition 2.1 with added "ω" to the range (codomain).

Definition 4.1 (state)

A state of reaction c-e structure U is a total function $s : car(U) \to \{0,1,\omega\}$. The set of all states of U is denoted by $\mathbb{S}$. In the following, symbols 0 and 1 will be treated as logical values

of *false* and *true* respectively and operations of propositional calculus on them will be applied. Moreover, operations $\vee$, $\wedge$ on ω, are defined as: $0 \vee \omega = \omega \vee 0 = \omega$, $0 \wedge \omega = \omega \wedge 0 = 0$, $1 \vee \omega = \omega \vee 1 = \omega$, $1 \wedge \omega = \omega \wedge 1 = 1$, $\omega \vee \omega = \omega \wedge \omega = \omega$, $\neg\omega = 0$. As formerly, ω will be used for inhibiting actions. Interpretation of 0 and 1 as *false* and *true* is justified by absorption property of entities in reaction systems and will be made formal in Definition 4.6. □

The lack of conflicts requires introducing for reaction c-e structures concept called here "volley", to differ it from "salvo" for c-e structures introduced in Definition 1.5.

Definition 4.2 (weights of monomials and inconsistent firing components)

Given a c-e structure $U = \langle C, E\rangle$ and its firing component $Q \in \boldsymbol{FC}[U]$, let along with the pre-set ${}^\bullet Q$ and post-set $Q^\bullet$ of Q, some functions
$\overline{{}^\bullet Q}$: ${}^\bullet Q \to \{0,1,\omega\}$ and $\overline{Q^\bullet}$: $Q^\bullet \to \{0,1,\omega\}$ be given as additional information. The value $\overline{{}^\bullet Q}(x)$ is called a *weight* of monomial $E_Q(x)$ and the value $\overline{Q^\bullet}(x)$ - a *weight* of monomial $C_Q(x)$. For $E_Q(x) = \theta$ or $C_Q(x) = \theta$ assume respectively $\overline{{}^\bullet Q}(x) = 0$ or $\overline{Q^\bullet}(x) = 0$. Additionally, $\overline{{}^\bullet Q}(x) = 0$ for $x \notin {}^\bullet Q$ and $\overline{Q^\bullet}(x) = 0$ for $x \notin Q^\bullet$. As formerly, ω is interpreted as a "disable signal" and used for defining inhibiting nodes. Firing components Q and P are *inconsistent* if for a certain $x \in {}^\bullet Q^\bullet \cap {}^\bullet P^\bullet$, weights $\overline{{}^\bullet Q}(x)$ and $\overline{{}^\bullet P}(x)$ or $\overline{Q^\bullet}(x)$ and $\overline{P^\bullet}(x)$ are different: $\overline{{}^\bullet Q}(x) \neq \overline{{}^\bullet P}(x)$ or $\overline{Q^\bullet}(x) \neq \overline{P^\bullet}(x)$. Note that detached Q and P (Definition 1.5) are not inconsistent. □

Remark. Inconsistency of firing components must be avoided so that to obtain free of conflicts behaviour of the reaction c-e structures. The inconsistency is exemplified by the following c-e structure: $U = \{x_{0\otimes y+z},\ y^x,\ z^x\}$ containing two firing components: $Q = \{x_{0\otimes y},\ y^x\}$, $P = \{x_z\ z^x\}$, thus $\overline{{}^\bullet Q}(x) = 0$, $\overline{{}^\bullet P}(x) = 1$. In the initial state s with $s(x) = 1$, $s(y) = s(z) = 0$ the parallel execution of the set of firing components $G = \{Q, P\}$ yields undetermined state of node x: it might be either 1 or 0. U is a direct translation of the reaction system $(\{x, y, z\}, \{Q, P\}, \{x\})$ with $Q = (\{x\}, \varnothing, \{x, y\})$, $P = (\{x\}, \varnothing, \{z\})$, which performs state transformation $\{x\} \to \{x, y, z\}$. The same transformation of state is performed by the reaction c-e structure $V = \{x_{0\otimes y+0\otimes z},\ y^x,\ z^x\}$, leading to $t(x) = t(y) = t(z) = 1$.

Definition 4.3 (**volley** - simultaneous firing, family ***FCV***, extension of weight functions)

Any set $G \subseteq \boldsymbol{FC}$ without inconsistent firing components is called their *volley*. The family of volleys is denoted by ***FCV***. So, if $G \subseteq \boldsymbol{FC}[U]$ then $\boldsymbol{FCV}[U] \subseteq 2^{\mathbf{FC}[U]}$ for a c-e structure U, denotes a collection of volleys in U. The pre-set ${}^\bullet G$ and post-set $G^\bullet$ of a volley G are defined as in Definition 1.4. Extension of the weight functions $\overline{{}^\bullet Q}$ and $\overline{Q^\bullet}$ onto the volley G are defined as follows:

$$\overline{{}^\bullet G}(x) = \begin{cases} \overline{{}^\bullet Q}(x) & \text{for arbitrary } Q \text{ if it belongs to } G \\ 0 & \text{else} \end{cases}$$

$$\overline{G^\bullet}(x) = \begin{cases} \overline{Q^\bullet}(x) & \text{for arbitrary } Q \text{ if it belongs to } G \\ 0 & \text{else} \end{cases}$$

This is a correct definition, since for any firing components Q and P in G: $\overline{{}^\bullet Q}(x) = \overline{{}^\bullet P}(x)$ if $x \in {}^\bullet G$ and $\overline{Q^\bullet}(x) = \overline{P^\bullet}(x)$ if $x \in G^\bullet$. Functions $\overline{{}^\bullet G}$ and $\overline{G^\bullet}$ will be used in definition of reaction c-e structures semantics. □

Definition 4.4 (inhibitors)

As in Definition 2.3, for a firing component $Q \in \boldsymbol{FC}[U]$, the set $inh[Q] = \{x \in {}^\bullet Q : \overline{{}^\bullet Q}(x) = \omega\}$ comprises all nodes in the pre-set of Q, whose effect monomials $E_Q(x)$ are of weight ω. This also extends onto the volleys: $inh[G] = \{x \in {}^\bullet G : \overline{{}^\bullet G}(x) = \omega\}$ where $G \in \boldsymbol{FCV}[U]$. □

Definition 4.5 (enabled firing components and enabled volleys)

For a firing component $Q \in \mathbf{FC}[U]$ and state s let the formula $enabled[Q](\mathbf{s})$ be defined as:

$\forall x \in inh[Q] : \ s(x) = 0 \wedge \forall x \in {}^\bullet Q \backslash inh[Q] : s(x) = 1$

For a volley $G \in \boldsymbol{FCV}[U]$, the formula $enabled[G](s)$ is defined as above by replacing Q with G and $\boldsymbol{FC}[U]$ with $\boldsymbol{FCV}[U]$.

In the "token game" metaphor, Q (or G) is enabled in the state s iff none of inhibiting nodes $x \in {}^\bullet Q$ (or $x \in {}^\bullet G$) contains a token and each remaining node contains. As formerly, the inhibiting nodes will be called *inhibitors*. □

Definition 4.6 (semantics [[ ]] of reaction c-e structures)

For a volley $G \in \boldsymbol{FCV}[U], G \neq \varnothing$ let $[[G]] \subseteq \mathbb{S} \times \mathbb{S}$ be a binary relation defined as:
$(s,t) \in [[G]]$ iff $enabled[G](s) \wedge \forall x \in car(U) : t(x) = (s(x) \wedge \neg\overline{{}^\bullet G}(x)) \vee \overline{G^\bullet}(x)$
(say: G transforms state s into t). *Semantics* $[[U]]$ of $U \in \boldsymbol{RECE}$ is $\bigcup_{G \in FCV[U]} [[G]]$, for any maximal volley G, i.e. if $G \subseteq G' \in \boldsymbol{FCV}[U]$ and
$(s,t) \in [[G']]$ then $G = G'$. Closure $[[U]]^*$ and reachability and computation are defined as in Definition 1.7. □

In Definition 4.6, if $x \in {}^\bullet G$ then $\overline{{}^\bullet G}(x) \neq \omega$, because the volley G is enabled in the state s thus $\overline{{}^\bullet G}(x)$ is 0 or 1. If $x \notin {}^\bullet G^\bullet$ then $\overline{{}^\bullet G}(x) = 0$ and $\overline{G^\bullet}(x) = 0$ hence $\neg\overline{{}^\bullet G}(x) = 1$, thus $t(x) = s(x)$ (strictly, "=" means equivalence). Evidently, formula $(s(x) \wedge \neg\overline{{}^\bullet G}(x)) \vee \overline{G^\bullet}(x)$ is equivalent to $(s(x) \Rightarrow \overline{{}^\bullet G}(x)) \Rightarrow \overline{G^\bullet}(x)$. Note also that description of semantics by means of this propositional formula is justified by the property of reaction systems: presence of token ("entity") at a node absorbs another token arriving in this node. Another property of reaction systems, the lack of conflicts between different reactions, takes place in reaction c-e structures due to the lack of inconsistent firing components in $G \in \boldsymbol{FCV}[U]$.

Example 4.1 (reaction c-e structure assembling a chemical molecule)

A description of creating some chemical molecules presents the reaction system

$$A = (\{C, H, O, U, V, W, X, Y, Z\}, \{r1, r2, r3, r4, r5, r6\}),$$

starting with initial state $\{C, H, O\}$ and with reactions defined as follows:

$r1 = (\{C, H\}, \varnothing, \{U\})$ U contains molecule CH (methylidyne)
$r2 = (\{U, C, H\}, \varnothing, \{V\})$ V contains molecule C_2H_2 (acetylene)
$r3 = (\{V, H\}, \varnothing, \{W\})$ W contains molecule C_2H_3 (ethylenyl)
$r4 = (\{W, H\}, \varnothing, \{X\})$ X contains molecule C_2H_4 (ethylene)
$r5 = (\{X, H, O\}, \varnothing, \{Y\})$ Y contains molecule C_2H_5O (ethoxide)
$r6 = (\{Y, H\}, \varnothing, \{Z\})$ Z contains molecule C_2H_5OH (ethanol)

A diagram of the final result, that is the ethanol molecule, is in Fig. 4 and a certain translation of this reaction system into a reaction c-e structure is depicted in Fig. 5. Successive steps of the reaction system evolution are the following:

$res_{r1}(\{C, H, O\}) = \{U\}$ (since $\{C, H\} \subseteq \{C, H, O\}$ and $\varnothing \cap \{C, H, O\} = \varnothing$)
$res_{r2}(\{C, H, O\}) = res_{r3}(\{C, H, O\}) = res_{r4}(\{C, H, O\}) = res_{r5}(\{C, H, O\}) =$
$res_{r6}(\{C, H, O\}) = \varnothing$ thus
$res_A(\{C, H, O\}) = \{U\}$

$res_{r1}(\{C, H, O, U\}) = \{U\}$ (since $\{C, H\} \subseteq \{C, H, O, U\}$ and
$\varnothing \cap \{C, H, O, U\} = \varnothing$)
$res_{r2}(\{C, H, O, U\}) = \{V\}$ (since $\{C, H, U\} \subseteq \{C, H, O, U\}$ and
$\varnothing \cap \{C, H, O, U\} = \varnothing$)
$res_{r3}(\{C, H, O, U\}) = res_{r4}(\{C, H, U\}) = res_{r5}(\{C, H, O, U\}) =$
$res_{r6}(\{C, H, O, U\}) = \varnothing$ thus
$res_A(\{C, H, O, U\}) = \{U, V\}$

$res_{r1}(\{C, H, O, U, V\}) = \{U\}$ (since $\{C, H\} \subseteq \{C, H, O, U, V\}$ and
$\varnothing \cap \{C, H, O, U, V\} = \varnothing$)
$res_{r2}(\{C, H, O, U, V\}) = \{V\}$ (since $\{C, H, U\} \subseteq \{C, H, O, U, V\}$ and
$\varnothing \cap \{C, H, O, U, V\} = \varnothing$)
$res_{r3}(\{C, H, O, U, V\}) = \{W\}$ (since $\{H, V\} \subseteq \{C, H, O, U, V\}$ and
$\varnothing \cap \{C, H, O, U, V\} = \varnothing$)
$res_{r4}(\{C, H, O, U, V\}) = res_{r5}(\{C, H, O, U, V\}) = res_{r6}(\{C, H, O, U, V\}) = \varnothing$ thus
$res_A(\{C, H, O, U, V\}) = \{U, V, W\}$

$res_{r1}(\{C, H, O, U, V, W\}) = \{U\}$ (since $\{C, H\} \subseteq \{C, H, O, U, V, W\}$ and $\varnothing \cap \{C, H, O, U, V, W\} = \varnothing$)
$res_{r2}(\{C, H, O, U, V, W\}) = \{V\}$ (since $\{C, H, U\} \subseteq \{C, H, O, U, V, W\}$ and $\varnothing \cap \{C, H, O, U, V, W\} = \varnothing$)

$res_{r3}(\{C,H,O,U,V,W\}) = \{W\}$ (since $\{H,V\} \subseteq \{C,H,O,U,V,W\}$ and $\varnothing \cap \{C,H,O,U,V,W\} = \varnothing$)
$res_{r4}(\{C,H,O,U,V,W\}) = \{X\}$ (since $\{H,W\} \subseteq \{C,H,O,U,V,W\}$ and $\varnothing \cap \{C,H,O,U,V,W\} = \varnothing$)
$res_{r5}(\{C,H,O,U,V,W\}) = res_{r6}(\{C,H,O,U,V,W\}) = \varnothing$ thus
$res_A(\{C,H,O,U,V,W\}) = \{U,V,W,X\}$

$res_{r1}(\{C,H,O,U,V,W,X\}) = \{U\}$ (since $\{C,H\} \subseteq \{C,H,O,U,V,W,X\}$ and $\varnothing \cap \{C,H,O,U,V,W,X\} = \varnothing$)
$res_{r2}(\{C,H,O,U,V,W,X\}) = \{V\}$ (since $\{C,H,U\} \subseteq \{C,H,O,U,V,W,X\}$ and $\varnothing \cap \{C,H,O,U,V,W,X\} = \varnothing$)
$res_{r3}(\{C,H,O,U,V,W,X\}) = \{W\}$ (since $\{H,V\} \subseteq \{C,H,O,U,V,W,X\}$ and $\varnothing \cap \{C,H,O,U,V,W,X\} = \varnothing$)
$res_{r4}(\{C,H,O,U,V,W,X\}) = \{X\}$ (since $\{H,W\} \subseteq \{C,H,O,U,V,W,X\}$ and $\varnothing \cap \{C,H,O,U,V,W,X\} = \varnothing$)
$res_{r5}(\{C,H,O,U,V,W,X\}) = \{Y\}$ (since $\{H,O,X\} \subseteq \{C,H,O,U,V,W,X\}$ and $\varnothing \cap \{C,H,O,U,V,W,X\} = \varnothing$)
$res_{r6}(\{C,H,O,U,V,W,X\}) = \varnothing)$ thus
$res_A(\{C,H,O,U,V,W,X\}) = \{U,V,W,X,Y\}$

$res_{r1}(\{C,H,O,U,V,W,X,Y\}) = \{U\}$ (since $\{C,H\} \subseteq \{C,H,O,U,V,W,X,Y\}$ and $\varnothing \cap \{C,H,O,U,V,W,X,Y\} = \varnothing$)
$res_{r2}(\{C,H,O,U,V,W,X,Y\}) = \{V\}$ (since $\{C,H,U\} \subseteq \{C,H,O,U,V,W,X,Y\}$ and $\varnothing \cap \{C,H,O,U,V,W,X,Y\} = \varnothing$)
$res_{r3}(\{C,H,O,U,V,W,X,Y\}) = \{W\}$ (since $\{H,V\} \subseteq \{C,H,O,U,V,W,X,Y\}$ and $\varnothing \cap \{C,H,O,U,V,W,X,Y\} = \varnothing$)
$res_{r4}(\{C,H,O,U,V,W,X,Y\}) = \{X\}$ (since $\{H,W\} \subseteq \{C,H,O,U,V,W,X,Y\}$ and $\varnothing \cap \{C,H,O,U,V,W,X,Y\} = \varnothing$)
$res_{r5}(\{C,H,O,U,V,W,X,Y\}) = \{Y\}$ (since $\{H,O,X\} \subseteq \{C,H,O,U,V,W,X,Y\}$ and $\varnothing \cap \{C,H,O,U,V,W,X,Y\} = \varnothing$)
$res_{r6}(\{C,H,O,U,V,W,X,Y\}) = \{Z\}$ (since $\{H,Y\} \subseteq \{C,H,O,U,V,W,X,Y\}$ and $\varnothing \cap \{C,H,O,U,V,W,X,Y\} = \varnothing$) thus
$res_A(\{C,H,O,U,V,W,X,Y\}) = \{U,V,W,X,Y,Z\}$

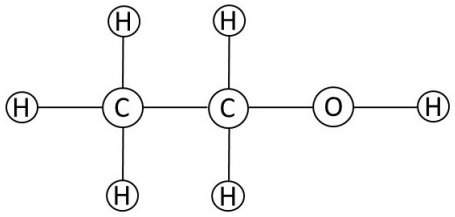

Figure 4: Diagram of ethanol. C, H, O - symbols of Carbon, Hydrogen and Oxygen atoms.

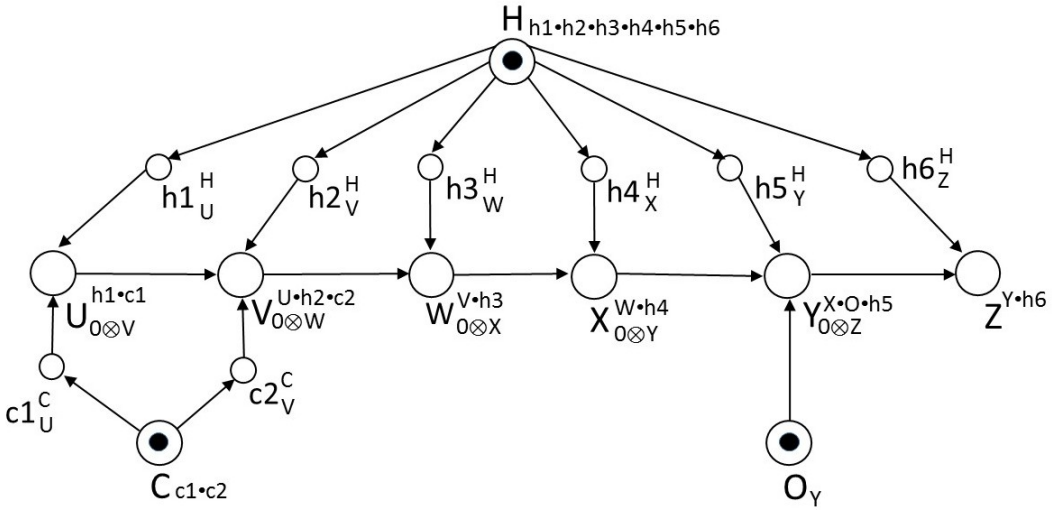

Figure 5: A c-e structure with initial state $s(C) = s(H) = s(O) = 1$ (and empty remaining nodes) imitating behaviour of reaction system A specified in Example 4.1. Regarding it as a translation of A, note that nodes $c1, c2, h1, h2, h3, h4, h5, h6$ are some "artifacts" of this fairly liberal translation and have no counterparts in A. Intuitively, they might be seen as holding single atoms of elements C and H.

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