Scalable Grid-Based Implementation for Membrane Computing

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Summary. We first present the formal semantics of a parallel rule-based formalism inspired by biological cells, and then provide a faithful parallel implementation of this computational model by using GridGain and taking care of various synchronization issues. Synchronization is achieved by using barriers and preconditions; both refer to the fact that a membrane can apply its rules only after it has received signals from the other related membranes. We develop a scalable parallel implementation using the MapReduce paradigm in GridGain which allows the splitting of a task into multiple subtasks, the parallel execution of these subtasks in parallel and the aggregation of the partial results into a single, final result. This implementation is very close to the formal description of this parallel model of membrane systems, a model which is computationally equivalent to Turing machines and able to provide polynomial solutions to NP-complete problems.

1 Introduction

Membrane systems are essentially parallel and nondeterministic computing models inspired by the compartments of (eukaryotic) cells and their biochemical reactions. The structure of a cell is represented by a set of hierarchically embedded membranes, all of which are contained inside a skin membrane. The molecular species (ions, proteins, etc.) floating inside cellular compartments are represented by multisets of objects described by means of symbols over a given alphabet. Objects can be modified or communicated between adjacent compartments. Chemical reactions are represented by evolution rules which operate on the objects, as well as on the compartmentalized structure (by dissolving, dividing, creating, or moving membranes).

Membrane systems (also called P systems) perform parallel computations in the following way: starting from an initial configuration (the initial membrane structure and the initial multisets of objects placed inside the membranes), a system evolves by applying the evolution rules of each membrane in a nondeterministic manner. A rule is applicable when all the objects which appear in its left hand side are available in the membrane where the rule is placed.

Since membrane systems aim to abstract computing ideas and models from the structure and the functioning of living cells, several extensions come from both biology (aiming to model more and more biological phenomena) and computer science (aiming to add new computing features). Their computing power and efficiency have been investigated using the approaches of formal languages, grammars, register machines and complexity theory. Membrane systems are presented together with many variants and examples in [7]. Several applications of these systems are presented in [5]. An updated bibliography can be found at the P systems web page http://ppage.psystems.eu. The state of the art is presented in the handbook published recently by Oxford University Press [8].

In this paper we present a paralel implementation of membrane systems by using GridGain [9], using a new appealing technology. The implementation is derived after studying some synchronization issues in membrane systems by defining their operational semantics and describing the parallel (sub)steps of their evolutions.

2 Operational Semantics of the Membrane Systems

The basic model of membrane computing is usually referred to as a transition membrane systems In this model, objects are represented using symbols from a given alphabet, and each symbol from this alphabet can appear inside a region in many different copies. A membrane system is composed of membranes which do not intersect, and which are all contained within a skin membrane. Each membrane can contain multisets of objects, evolution rules and other membranes. The objects inside a membrane evolve in a maximal parallel manner according to the evolution rules inside the same membrane. According to [7], maximal parallel "means that we assign objects to rules, non-deterministically choosing the objects and the rules, until no further assignment is possible."

First we present an abstract syntax for membrane systems, and then we a structural operational semantics of these systems by means of three sets of inference rules corresponding to maximal parallel rewriting, parallel communication, and parallel dissolving.

In general, operational semantics provide a way of rigorously describing the evolution of a computing system. Configurations are states of a transition system, and a computation consists of a sequence of transitions from one configuration to another, until a final configuration is reached (if the computation terminates, that is). Structural operational semantics provides a framework for defining a formal description of a computing system. In basic membrane systems, a computation is regarded as a sequence of parallel applications of rules in various membranes, followed by a communication step and a dissolving step. A structural operational semantics of membrane systems emphasizes the deductive nature of membrane computing by describing the transition steps through a set of inference rules. Considering a set $\mathcal{R}$ of inference rules of the form $\frac{premises}{conclusion}$, the evolution of a membrane system can be presented as a deduction tree.

A sequence of transition steps represents a *computation.* A computation is successful if this sequence is finite, namely there is no rule applicable to the objects present in the last committed configuration. In a halting committed configuration, the result of a successful computation is the total number of objects present either in the membrane considered as the output membrane, or in the outer region.

2.1 Configurations and Transitions

First we present an inductive definition of the membrane structure, the sets of configurations for a membrane system, and an intuitive definition for the transition systems, which is given by considering each transition step: maximal parallel rewriting, parallel communication, and parallel dissolving.

Let O be a finite alphabet of objects over which we consider the *free commutative monoid* O_c^*, whose elements are *multisets.* The empty multiset is denoted by *empty*. Objects can be enclosed in messages together with a target indication. We have *here* messages of typical form $(w, here)$, *out* messages (w, out), and *in* messages (w, in_L). For the sake of simplicity, hereinafter we consider that the messages with the same target indication merge into one message: $\prod_{i\in I}(v_i, here) = (w, here)$, $\prod_{i\in I}(v_i, in_L) = (w, in_L)$, $\prod_{i\in I}(v_i, out) = (w, out)$, with $w = \prod_{i\in I} v_i$, I a non-empty set, and $(v_i)_{i\in I}$ a family of multisets over O.

We use the mappings rules and $\mathsf{priority}$ to associate to a membrane label the set of evolution rules and the priority relation over rules (when this exists) : $\mathsf{rules}(L_i) = R_i$, $\mathsf{priority}(L_i) = \rho_i$, and the projections L and w which return from a membrane its label and its current multiset, respectively.

The *set* $\mathcal{M}(\Pi)$ *of membranes for a P system* Π, and the *membrane structures* are defined inductively, as follows:

- if L is a label, and w is a multiset over $O \cup (O \times \{here\}) \cup (O \times \{out\}) \cup \{\delta\}$, then $\langle\, L \mid w \,\rangle \in \mathcal{M}(\Pi)$; $\langle\, L \mid w \,\rangle$ is called a *simple (or elementary) membrane*, and it has the structure $\langle\rangle$;
- if L is a label, w is a multiset over $O \cup (O \times \{here\}) \cup (O \times \{in_{L(M_j)} \mid j \in [n]\}) \cup (O \times \{out\}) \cup \{\delta\}$, $M_1, \ldots, M_n \in \mathcal{M}(\Pi)$, $n \geq 1$, where each membrane M_i has the structure μ_i, then $\langle L|w; M_1, \ldots, M_n\rangle \in \mathcal{M}(\Pi)$; $\langle L|w; M_1, \ldots, M_n\rangle$ is called a *composite membrane* having the structure $\langle \mu_1, \ldots, \mu_n\rangle$.

We conventionally suppose the existence of a set of sibling membranes denoted by $NULL$ such that $M, NULL = M = NULL, M$ and $\langle\, L \,|\, w\,;\, NULL \,\rangle = \langle\, L \,|\, w \,\rangle$. The use of $NULL$ significantly simplifies several definitions and proofs. Let $\mathcal{M}^*(\Pi)$ be the free commutative monoid generated by $\mathcal{M}(\Pi)$ with the operation $(\_,\_)$ and the identity element $NULL$. We define $\mathcal{M}^+(\Pi)$ as the set of elements from $\mathcal{M}^*(\Pi)$ without the identity element. Let M_+, N_+ range over non-empty sets of sibling membranes, M_i over membranes, M_*, N_* range over possibly empty multisets of sibling membranes, and L over labels. The membranes preserve the initial labeling, evolution rules and priority relation among them in all subsequent configurations.

Therefore in order to describe a membrane we consider its label and the current multiset of objects together with its structure.

A *configuration* for a P system $\varPi$ is a skin membrane which has no messages and no dissolving symbol δ, i.e., the multisets of all regions are elements in O_c^*. We denote by $\mathcal{C}(\varPi)$ the set of configurations for $\varPi$.

An *intermediate configuration* is an arbitrary skin membrane in which we may find messages or the dissolving symbol δ. We denote by $\mathcal{C}^\#(\varPi)$ the set of intermediate configurations. We have $\mathcal{C}(\varPi) \subseteq \mathcal{C}^\#(\varPi)$.

Each membrane system has an initial configuration which is characterized by the initial multiset of objects for each membrane and the initial membrane structure of the system. For two configurations C_1 and C_2 of $\varPi$, we say that there is a *transition* from C_1 to C_2, and write $C_1 \Rightarrow C_2$, if the following *steps* are executed in the given order:

1. *maximal parallel rewriting step*: each membrane evolves in a maximal parallel manner;
2. *parallel communication of objects through membranes* by sending and receiving messages;
3. *parallel membrane dissolving*, consisting in dissolving the membranes containing δ.

The last two steps take place only if there are messages or δ symbols resulting from the first step, respectively. If the first step is not possible, then neither are the other two steps; we say that the system has reached a *halting configuration.*

2.2 Maximal Parallel Rewriting Step

We briefly present an operational semantics for membrane systems, considering each of the three steps. First we formally define the maximal parallel rewriting $\overset{mpr}{\Longrightarrow}_L$ for a multiset of objects in one membrane, and we extend it to maximal parallel rewriting $\overset{mpr}{\Longrightarrow}$ over several membranes. Some preliminary notions are required.

Definition 1. *The irreducibility property w.r.t. the maximal parallel rewriting relation for multisets of objects, membranes, and for sets of sibling membranes is defined as follows:*

- *a multiset of messages and the dissolving symbol δ are* L**-irreducible***;*
- *a multiset of objects w is* L**-irreducible** *iff there are no rules in* $\mathsf{rules}(L)$ *applicable to w with respect to the priority relation* $\mathsf{priority}(L)$*;*
- *a simple membrane $\langle\, L \mid w \,\rangle$ is* **mpr-irreducible** *iff w is L-irreducible;*
- *a non-empty set of sibling membranes $M_1, \ldots, M_n$ is* **mpr-irreducible** *iff M_i is mpr-irreducible for every $i \in [n]$; $NULL$ is* **mpr-irreducible***;*
- *a composite membrane $\langle\, L \mid w\ ;\ M_1, \ldots, M_n \,\rangle$ is* **mpr-irreducible** *iff w is L-irreducible, and the set of sibling membranes $M_1, \ldots, M_n$ is mpr-irreducible.*

The priority relation is a form of control on the application of rules. In the presence of a priority relation, no rule of a lower priority can be used during the same evolution step when a rule with a higher priority is used, even if the two rules do not compete for the same objects. We formalize the conditions imposed by the priority relation on rule applications in the definition below.

Definition 2. *Let M be a membrane labeled by L, and w a multiset of objects. A non-empty multiset $R = (u_1 \to v_1, \ldots, u_n \to v_n)$ of evolution rules is (L, w)*-**consistent** *if:*

- $R \subseteq \mathsf{rules}(L)$,
- $w = u_1 \ldots u_n z$, *so each rule $r \in R$ is applicable on w,*
- $(\forall r \in R, \forall r' \in \mathsf{rules}(L))$ *r' applicable on w implies* $(r', r) \notin \mathsf{priority}(L)$ *(we have* $(r_1, r_2) \in \mathsf{priority}(L)$ *iff* $r_1 > r_2$ *),*
- $(\forall r', r'' \in R)$ $(r', r'') \notin \mathsf{priority}(L)$,
- *the dissolving symbol δ has at most one occurrence in the multiset $v_1 \ldots v_n$.*

Maximal parallel rewriting relations $\overset{mpr}{\Longrightarrow}_L$ and $\overset{mpr}{\Longrightarrow}$ are defined by the following inference rules:

For each $w = u_1 \ldots u_n z \in O_c^+$ such that z is L-irreducible, and (L, w)-consistent rules $(u_1 \to v_1, \ldots, u_n \to v_n)$,

$$(\mathbf{R_1})\ \frac{}{u_1 \ldots u_n z \overset{mpr}{\Longrightarrow}_L v_1 \ldots v_n z}$$

For each $w \in O_c^+$, $w' \in (O \cup Msg(O) \cup \{\delta\})_c^+$, and mpr-irreducible $M_* \in \mathcal{M}^*(\Pi)$,

$$(\mathbf{R_2})\ \frac{w \overset{mpr}{\Longrightarrow}_L w'}{\langle\, L \mid w\,;\, M_* \,\rangle \overset{mpr}{\Longrightarrow} \langle\, L \mid w'\,;\, M_* \,\rangle}$$

For each L-irreducible $w \in O_c^*$, and $M_+, M'_+ \in \mathcal{M}^+(\Pi)$,

$$(\mathbf{R_3})\ \frac{M_+ \overset{mpr}{\Longrightarrow} M'_+}{\langle\, L \mid w\,;\, M_+ \,\rangle \overset{mpr}{\Longrightarrow} \langle\, L \mid w\,;\, M'_+ \,\rangle}$$

For each $w \in O_c^+$, $w' \in (O \cup Msg(O) \cup \{\delta\})_c^+$, $M_+, M'_+ \in \mathcal{M}^+(\Pi)$,

$$(\mathbf{R_4})\ \frac{w \overset{mpr}{\Longrightarrow}_L w', M_+ \overset{mpr}{\Longrightarrow} M'_+}{\langle\, L \mid w\,;\, M_+ \,\rangle \overset{mpr}{\Longrightarrow} \langle\, L \mid w'\,;\, M'_+ \,\rangle}$$

For each $M, M' \in \mathcal{M}(\Pi)$, and $M_+, M'_+ \in \mathcal{M}^+(\Pi)$,

$$(\mathbf{R_5})\ \frac{M \overset{mpr}{\Longrightarrow} M', M_+ \overset{mpr}{\Longrightarrow} M'_+}{M, M_+ \overset{mpr}{\Longrightarrow} M', M'_+}$$

For each $M, M' \in \mathcal{M}(\Pi)$, and mpr-irreducible $M_+ \in \mathcal{M}^+(\Pi)$,

$$(\mathbf{R_6})\ \frac{M \overset{mpr}{\Longrightarrow} M'}{M, M_+ \overset{mpr}{\Longrightarrow} M', M_+}$$

We note that $\overset{mpr}{\Longrightarrow}$ for simple membranes can be described by rule $(\mathbf{R_2})$ with $M_* = NULL$.

Remark 1. M is mpr-irreducible iff there does not exist M' such that $M \overset{mpr}{\Longrightarrow} M'$.

Proposition 1. *Let Π be a membrane system. If $C \in \mathcal{C}(\Pi)$ and $C' \in \mathcal{C}^{\#}(\Pi)$ such that $C \overset{mpr}{\Longrightarrow} C'$, then C' is mpr-irreducible.*

The formal definition of $\overset{mpr}{\Longrightarrow}$ given above corresponds to the intuitive description of maximal parallelism. The nondeterminism is given by the associativity and commutativity of the concatenation operation over objects used in $\mathbf{R_1}$. The parallelism of the evolution rules in a membrane is also given by $\mathbf{R_1}$: $u_1 \ldots u_n z \overset{mpr}{\Longrightarrow}_L v_1 \ldots v_n z$ says that the rules of the multiset $(u_1 \to v_1, \ldots, u_n \to v_n)$ are applied simultaneously. The fact that the membranes evolve in parallel is described by rules $\mathbf{R_3}-\mathbf{R_6}$.

2.3 Parallel Communication of Objects

We say that a multiset w is *here-free/out-free/in$_L$-free* if it does not contain any *here/out/in$_L$* messages, respectively. For w a multiset of objects and messages, we introduce the operations obj, here, out, and in$_L$ as follows:

$$\begin{aligned}
&\mathsf{obj}(w) \text{ is obtained from } w \text{ by removing all messages,}\\
&\mathsf{here}(w) = \begin{cases} empty & \text{if } w \text{ is } here\text{-free,}\\ w'' & \text{if } w = w'(w'', here) \wedge w' \text{ is } here\text{-free;}\end{cases}\\
&\mathsf{out}(w) = \begin{cases} empty & \text{if } w \text{ is } out\text{-free,}\\ w'' & \text{if } w = w'(w'', out) \wedge w' \text{ is } out\text{-free;}\end{cases}\\
&\mathsf{in}_L(w) = \begin{cases} empty & \text{if } w \text{ is } in_L\text{-free,}\\ w'' & \text{if } w = w'(w'', in_L) \wedge w' \text{ is } in_L\text{-free.}\end{cases}
\end{aligned}$$

We consider the extension of the operator w (previously defined over membranes) to non-empty sets of sibling membranes by setting $\mathsf{w}(NULL) = empty$ and $\mathsf{w}(M_1, \ldots, M_n) = \mathsf{w}(M_1) \ldots \mathsf{w}(M_n)$.

We recall that the messages with the same target merge in one larger message.

Definition 3. *The* **tar-irreducibility** *property for membranes and for sets of sibling membranes is defined as follows:*

- *a simple membrane $\langle\ L \mid w\ \rangle$ is* **tar-irreducible** *iff w is here-free and $L \neq Skin \vee (L{=}Skin \wedge w$ out-free);*
- *a non-empty set of sibling membranes $M_1, \ldots, M_n$ is* **tar-irreducible** *iff M_i is tar-irreducible for every $i \in [n]$; $NULL$ is* **tar-irreducible***;*

- *a composite membrane* $\langle\, L \mid w \,;\, M_1, \ldots, M_n \,\rangle$*,* $n \geq 1$*, is* **tar-irreducible** *iff:* w *is here-free and* $in_{L(M_i)}$*-free for every* $i \in [n]$*,* $L \neq Skin \vee (L = Skin \wedge$ w *is out-free),* $\mathsf{w}(M_i)$ *is out-free for all* $i \in [n]$*, and the set of sibling membranes* $M_1, \ldots, M_n$ *is tar-irreducible;*

Notation. We treat messages of the form $(w', here)$ as a particular communication inside a membrane, and we substitute $(w', here)$ by w'. We denote by $\overline{w}$ the multiset obtained by replacing $(\mathsf{here}(w), here)$ with $\mathsf{here}(w)$ in w. For instance, if $w = a\,(bc, here)\,(d, out)$ then $\overline{w} = abc\,(d, out)$, where $\mathsf{here}(w) = bc$. We note that $\mathsf{in}_L(\overline{w}) = \mathsf{in}_L(w)$, and $\mathsf{out}(\overline{w}) = \mathsf{out}(w)$.

The **parallel communication relation** $\overset{tar}{\Longrightarrow}$ is defined by the following inference rules:

For each tar-irreducible $M_* \in \mathcal{M}^*(\Pi)$ and multiset w such that
$\mathsf{here}(w) \neq empty$, or $L = Skin \wedge \mathsf{out}(w) \neq empty$, or there exists $M_i \in M_*$ with
$\mathsf{in}_{L(M_i)}(w)\mathsf{out}(\mathsf{w}(M_i)) \neq empty$,

$$(\mathbf{C_1})\,\frac{}{\langle\, L \mid w \,;\, M_* \,\rangle \overset{tar}{\Longrightarrow} \langle\, L \mid w' \,;\, M'_* \,\rangle}$$

where

$$w' = \begin{cases} \mathsf{obj}(\overline{w})\,\mathsf{out}(\mathsf{w}(M_*)) & \text{if } L = Skin, \\ \mathsf{obj}(\overline{w})\,(\mathsf{out}(w), out)\,\mathsf{out}(\mathsf{w}(M_*)) & \text{otherwise;} \end{cases}$$

and

$$\mathsf{w}(M'_i) = \mathsf{obj}(\mathsf{w}(M'_i))\,\mathsf{in}_{\mathsf{L}(M_i)}(w), \text{ for all } M_i \in M_*$$

For each $M_1, \ldots, M_n, M'_1, \ldots, M'_n \in \mathcal{M}^+(\Pi)$, and multiset w,

$$(\mathbf{C_2})\,\frac{M_1, \ldots, M_n \overset{tar}{\Longrightarrow} M'_1, \ldots, M'_n}{\langle\, L \mid w \,;\, M_1, \ldots, M_n \,\rangle \overset{tar}{\Longrightarrow} \langle\, L \mid w'' \,;\, M''_1, \ldots, M''_n \,\rangle}$$

where

$$w'' = \begin{cases} \mathsf{obj}(\overline{w})\,\mathsf{out}(\mathsf{w}(M'_1, \ldots, M'_n)) \;\; \text{if } L = Skin, \\ \mathsf{obj}(\overline{w})\,(\mathsf{out}(w), out)\,\mathsf{out}(\mathsf{w}(M'_1, \ldots, M'_n)) \\ \text{otherwise;} \end{cases}$$

and each M''_i is obtained from M'_i by replacing its resources with

$$\mathsf{w}(M''_i) = \mathsf{obj}(\overline{\mathsf{w}(M'_i)})\,\mathsf{in}_{\mathsf{L}(M'_i)}(w), \text{ for all } i \in [n]$$

For each $M, M' \in \mathcal{M}(\Pi)$, and tar-irreducible $M_+ \in \mathcal{M}^+(\Pi)$,

$$(\mathbf{C_3})\,\frac{M \overset{tar}{\Longrightarrow} M'}{M, M_+ \overset{tar}{\Longrightarrow} M', M_+}$$

For each $M \in \mathcal{M}(\Pi)$, $M_+ \in \mathcal{M}^+(\Pi)$,

$$(\mathbf{C_4})\frac{M \overset{tar}{\Longrightarrow} M', M_+ \overset{tar}{\Longrightarrow} M'_+}{M, M_+ \overset{tar}{\Longrightarrow} M', M'_+}$$

Remark 2. M is tar-irreducible iff there does not exist M' such that $M \overset{tar}{\Longrightarrow} M'$.

Proposition 2. *Let Π be a membrane system. If $C \in \mathcal{C}^{\#}(\Pi)$ with messages and $C \overset{tar}{\Longrightarrow} C'$, then C' is tar-irreducible.*

2.4 Parallel Membrane Dissolving

If the special symbol δ occurs in the multiset of objects of a membrane labeled by L, that membrane is dissolved, its evolution rules and the associated priority relation are lost, and its contents (objects and membranes) is added to the contents of the surrounding membrane. We say that a multiset w is *δ-free* if it does not contain the special symbol δ.

Definition 4. *The δ-**irreducibility** property for membranes and for sets of sibling membranes is defined as follows:*

- *a simple membrane is δ-**irreducible** iff it has no messages;*
- *a non-empty set of sibling membranes $M_1, \ldots, M_n$ is δ-**irreducible** iff every membrane M_i is δ-irreducible, for $1 \le i \le n$; $NULL$ is δ-**irreducible**;*
- *a composite membrane $\langle\, L \mid w \,;\, M_+ \,\rangle$ is δ-**irreducible** iff w has no messages, M_+ is δ-irreducible, and $w(M_+)$ is δ-free;*

Parallel dissolving relation $\overset{\delta}{\Longrightarrow}$ is defined by the following inference rules:

For each $M_* \in \mathcal{M}^*(\Pi)$, δ-irreducible $\langle\, L_2 \mid w_2\delta \,;\, M_* \,\rangle$, and label L_1,

$$(\mathbf{D_1})\frac{}{\langle\, L_1 \mid w_1 \,;\, \langle\, L_2 \mid w_2\delta \,;\, M_* \,\rangle \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L_1 \mid w_1 w_2 \,;\, M_* \,\rangle}$$

For each $M_+ \in \mathcal{M}^+(\Pi)$, $M'_* \in \mathcal{M}^*(\Pi)$, δ-free multiset w_2, multisets w_1, w'_2, and labels L_1, L_2

$$(\mathbf{D_2})\frac{\langle\, L_2 \mid w_2 \,;\, M_+ \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L_2 \mid w'_2 \,;\, M'_* \,\rangle}{\langle\, L_1 \mid w_1 \,;\, \langle\, L_2 \mid w_2 \,;\, M_+ \,\rangle \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L_1 \mid w_1 \,;\, \langle\, L_2 \mid w'_2 \,;\, M'_* \,\rangle \,\rangle}$$

For each $M_+ \in \mathcal{M}^+(\Pi)$, $M'_* \in \mathcal{M}^*(\Pi)$, multisets w_1, w_2, w'_2, and labels L_1, L_2

$$(\mathbf{D_3})\frac{\langle\, L_2 \mid w_2\delta \,;\, M_+ \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L_2 \mid w'_2\delta \,;\, M'_* \,\rangle}{\langle\, L_1 \mid w_1 \,;\, \langle\, L_2 \mid w_2\delta \,;\, M_+ \,\rangle \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L_1 \mid w_1 w'_2 \,;\, M'_* \,\rangle}$$

For each $M_+ \in \mathcal{M}^+(\Pi)$, $M'_*, N'_* \in \mathcal{M}^*(\Pi)$, δ-irreducible $\langle\, L \mid w \,;\, N_+ \,\rangle$, and multisets w', w'',

$$(\mathbf{D_4})\frac{\langle\, L \mid w \,;\, M_+ \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L \mid w' \,;\, M'_* \,\rangle}{\langle\, L \mid w \,;\, M_+, N_+ \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L \mid w' \,;\, M'_*, N_+ \,\rangle}$$

$$(\mathbf{D_5})\,\frac{\langle\, L \mid w\ ;\ M_+ \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L \mid ww'\ ;\ M'_* \,\rangle\langle\, L \mid w\ ;\ N_+ \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L \mid ww''\ ;\ N'_* \,\rangle}{\langle\, L \mid w\ ;\ M_+, N_+ \,\rangle \overset{\delta}{\Longrightarrow} \langle\, L \mid ww'w''\ ;\ M'_*, N'_* \,\rangle}$$

Remark 3. M is δ-irreducible iff there does not exist M' such that $M \overset{\delta}{\Longrightarrow} M'$.

Proposition 3. *Let Π be a membrane system. If $C \in \mathcal{C}^{\#}(\Pi)$ is tar-irreducible and $C \overset{\delta}{\Longrightarrow} C'$, then C' is δ-irreducible.*

It is worth noting that $C \in \mathcal{C}(\Pi)$ iff C is tar-irreducible and δ-irreducible. According to the standard description in membrane computing, a *transition step* between two configurations $C, C' \in \mathcal{C}(\Pi)$ is given by: $C \Rightarrow C'$ iff C and C' are related by one of the following relations:

either $C \overset{mpr}{\Longrightarrow}; \overset{tar}{\Longrightarrow} C'$,
or $C \overset{mpr}{\Longrightarrow}; \overset{\delta}{\Longrightarrow} C'$,
or $C \overset{mpr}{\Longrightarrow}; \overset{tar}{\Longrightarrow}; \overset{\delta}{\Longrightarrow} C'$.

The three alternatives in defining $C \Rightarrow C'$ are given by the existence of messages and dissolving symbols along the system evolution. Starting from a configuration without messages and dissolving symbols, we apply the "mpr" rules and get an intermediate configuration which is mpr-irreducible; if we have messages, then we apply the "tar" rules and get an intermediate configuration which is tar-irreducible; if we have dissolving symbols, then we apply the dissolving rules and get a configuration which is δ-irreducible. If the last configuration has no messages or dissolving symbols, then we say that the transition relation $\Rightarrow$ is well-defined as an evolution step between the first and last configurations.

Proposition 4. *The relation $\Rightarrow$ is well-defined over the entire set $\mathcal{C}(\Pi)$ of configurations.*

Examples of inference trees, as well as the proofs of the results are presented in [1] and [2].

3 Synchronization Issues in Implementing P Systems

It is evident from the operational semantics that there are several synchronization aspects related to the evolution of a membrane system.

The relationship between the synchronous and the asynchronous in computing systems, particularly in massively-parallel and multiprocessor computing systems, will remain a challenging topic for many years to come. There are reasons to think that the asynchronous approach has some advantages; however the synchronous methodology prevails in the modern computing systems architecture. As if this is not enough, different fields treat the concepts of synchrony and asynchrony somewhat differently. The main terms (parallelism, concurrency, time) should be clarified in order to discuss the synchronous and asynchronous issues. In our approach we work with a "causal" time (defined as the partial order on some events resulting from their cause-effect relationships) rather a physical time (defined as an independent physical variable related to a clock). The concept of causal time was formulated initially by Aristotle (If nothing happens, no time); it can be useful in systems dealing with events defining cause-effect relationships. The abstract model of a finite state machine corresponds to the model of an asynchronous system evolving in logical time; a possible conversion to a synchronous approach is given by a barrier synchronization (as an engineering solution) in order to manage unpredictable variations of the delays introduced by real physical components. An algorithm (its program) consists of a sequence of steps which perform some actions. Asynchrony is usually treated as the dependence of the number of steps required to obtain the result on the input data. In the case of a fully sequential algorithm (program), such treatment of asynchrony is important only for performance evaluation. Parallel algorithms and programs present new and challenging tasks. Certain steps of an algorithm can be performed concurrently. Representing an algorithm (program) in the form suitable for concurrent implementation is reduced to the cause-effect relationships between the operations (processes, commands) in the algorithm. Thus a parallel specification is a procedure for introducing logical time into the algorithm. An implementation of a global synchronous system can be given by delivering a termination signal from the processors (processes) of the system. Difficulties appear when several processes have a shared resource, and non-synchronized events may occur. A possible solution of a synchronous implementation that eliminates the problems of physical asynchrony is as follows:

- every process can be in two phases: active and passive;
- a process can run only when active;
- to transit from passive to active a process has to receive a signal;
- after an active process executes, it signals other passive processes;

Initially we activate some processes, which after their executions signal passive processes. This repeats until all processes have terminated. Following this scenario, deadlock can occur if the process dependency graph contains cycles. In this scenario, process can be synchronized using a barrier. A *process barrier* is an concurrent abstraction through which multiple processes can be synchronized. Thus a passive process can be considered a process that is waiting at the barrier, and by passing the barrier it becomes an active one.

We can apply this type of synchronization to membrane systems, by allowing a membrane to evolve only after it has passed the barrier. To model this, we use a set of antecedents and a set of descendants for each membrane when describing the system. To apply its rules, a membrane needs to receive signals from all of its antecedents. After it applies its rules, the membrane signals all of its descendants. The set of antecedents specifies how many times a signal needs to be received from each membrane. The set of descendants specifies the membranes that need to be signaled after the application of rules.

Using this mechanism, we can control the relative evolution speed of the antecedents of a membrane. This approach allows to specify that a certain membrane can repeat its step several times before sending its signal to the descendents. In this way we can have a *parameterized synchronization* between membranes, and this aspect could be very useful in modeling biological phenomena. The evolution of a membrane can be described by the following steps which are repeated until no rule can be applied.

1. collect signals from all the antecedents;
2. apply the rules after receiving all the signals;
3. signal all descendants.

4 A Grid-Based Implementation of P Systems

We present here a grid implementation of membrane systems in which we emphasize the notion of computation and synchronization. We employ a synchronization mechanism based on certain preconditions expressing the consistency of the global state of the system. This synchronization mechanism has been introduced to control the dependency relation between membranes. We propose a synchronous model of execution used to coordinate membrane evolution.

To achieve scalability we make use of the grid paradigm *MapReduce*. The paradigm is defined by two main steps: *map*, and *reduce*. The map step allows splitting a task into multiple jobs that execute in parallel on the grid nodes. The reduce step aggregates the result of each job, and returns the task result.

Thus the simulation of a membrane system can be viewed as a grid task. The jobs associated with this task define the execution of each membrane. Hence the number of jobs is equal to the number of membranes. To model the proposed synchronization mechanism between membranes, a communication between jobs is required.

We have selected GridGain [9] as our grid platform because it provides all the required features, and it is easily deployed on multiple platforms. GridGain is a Java-based open source grid computing infrastructure, released under LGPL license. It provides a zero deployment model, meaning that a node can be deployed by running a script, or by creating a node instance. A valuable feature of the system is its support for advanced load balancing and scheduling by providing early and late load balancing that are defined by load balancing and collision (scheduling) resolution. Another important feature is pluggable fault-tolerance with several popular implementations available out-of-the-box. It allows the failover of logic and not only the data. The most notable features of GridGain that we use are: tasks and jobs modeled according to the MapReduce paradigm, communication between grid jobs, and on-demand class loading.

The main steps of the simulation are: (1) Build a membrane system from an specification file; (2) Using the generated membrane system, construct and execute a grid job: (i) *Map*: create a job for each membrane; (ii) *Reduce*: gather all the

```
public class Membrane {
  private List<MembraneLabel> childrenLabels;
  private List<Rule> rules;
  private HashMultiset contents;
  private HashMultiset incomingObjects;
  private MembraneLabel label;
  private MembraneLabel parentLabel;
  private HashMap<MembraneLabel, Integer> antecedents;
  private List<MembraneLabel> descendants;
  private int appliedRules;//number of applied rules in this
      step

  public Membrane()
  //test if the membrane contains a multiset
  public boolean contains(HashMultiset multiset)
  //store a  multiset that resulted in this evolution step
  public void enqueMultiset(HashMultiset multiset)
  //add the objects that resulted in this evolution step
  public void endEvolution()
  //return the list of applicable rules
  public List<Rule> getApplicableRules()
}
```

Fig. 1. Membrane Class

responses from the jobs and create the resulting membrane system.
The simulation repeats step 2 as long as a rule is applied. Each generated job contains an object that describes a membrane from the system. The job is responsible for the correct simulation of the evolution of the membrane. Thus it needs to synchronize with other membranes, and also to apply different rules. The result of the job consists of the final state of the simulated membrane. We have used a modular design for the entities of the system in which we separated the objects defining the *grid behavior* from those defining the *membrane systems*. Thus we implement several abstractions that model various notions such as: *membranes*, *rules*, membrane *objects*, etc. For the grid behavior we define the following concepts: *task*, *job*, *barrier*.

In Figure 1 we describe the members and main methods of class Membrane. The object is responsible only for operations that modify the contents of a membrane. The evolution logic is implemented using the Rule and EvolutionVisitor objects. To model the rules of a membrane system we used a extensible approach. Each rule can be seen as a list of constraints; a constraint is responsible for checking if its precondition is valid (via method *check*), and for applying its postcondition on a membrane (via method *apply*).

```
public class Rule extends RuleConstraint {
  List<RuleConstraint> constraints;

  public Rule()
  public void apply(Membrane membrane) {
    for (RuleConstraint constraint : constraints) {
      constraint.apply(membrane);
    }
  }
  public boolean check(Membrane membrane) {
    boolean isApplicable = true;
    Iterator<RuleConstraint> iter = constraints.iterator();
    while (isApplicable && iter.hasNext()) {
      isApplicable = isApplicable && iter.next().check(membrane)
          ;
    }
    return isApplicable;
  }
}
```

Fig. 2. Rule Class

From a software engineering perspective, the rule follows the composite pattern. In Appendix[1], we present the RuleConstraint class and in how a constraint multiset can be implemented. The main methods of the Rule class are presented in Figure 2. Using these abstractions we can easily implement rules with various ingredients, only by describing constraints and aggregating them into a new type of Rule. The evolution of a membrane is performed by the EvolutionVisitor object described. The method *localMembraneEvolution* defines the logic of a single step of evolution. A step is simulated by the repeated application of rules.

A grid task is defined by the class PsTask, which follows the MapReduce paradigm. The method *split* takes as input a membrane system, and for each membrane creates a job that will be executed on the grid. The method *reduce* receives a list of job results that contain membranes, and assembles them in a membrane system.

A grid job is described by the PsJob object (in Appendix). This object contains a membrane which holds the data, and a barrier used for synchronization. The main method of this class is *execute*, in which the evolution of a membrane is executed. The evolution consists of a three-step loop: (i) wait at the barrier for incoming signals, (ii) after receiving the signals, apply the rules, and (iii) after applying the rules, signal the descendants. The result of the job is a maximally parallel step of the membrane.

[1] Available online at `www.gcn.us.es/12bwmc_proceedings`

```
public class PsTask{
  public MembraneSystem reduce(List results){
    MembraneSystem result = new MembraneSystem();
    int appliedRules = 0;
    for (GridJobResult gridJobResult : results) {
      Membrane data = gridJobResult.getData();
      result.getMembranes().put(data.getLabel(), data);
      appliedRules += data.getAppliedRules();
    }
    result.setAppliedRules(appliedRules);
    return result;
  }
  protected List<GridJob> split(MembraneSystem arg){
    List<PsJob> jobs = new ArrayList<PsJob>();
    for(Membrane mbr : arg.getMembranes().values()){
      jobs.add(new PsJob(mbr));
    }
    return jobs;
  }
}
```

Fig. 3. PsTask Class

Membrane synchronization is achieved by using a special form of barrier. The barrier waits to be signaled from each antecedent membrane a specified number of times. After this, it releases the job that called the method *waitAt*. The barrier also listens for termination signals. When it receives such a signal it informs the waiting job that it should finish its execution.

5 Example

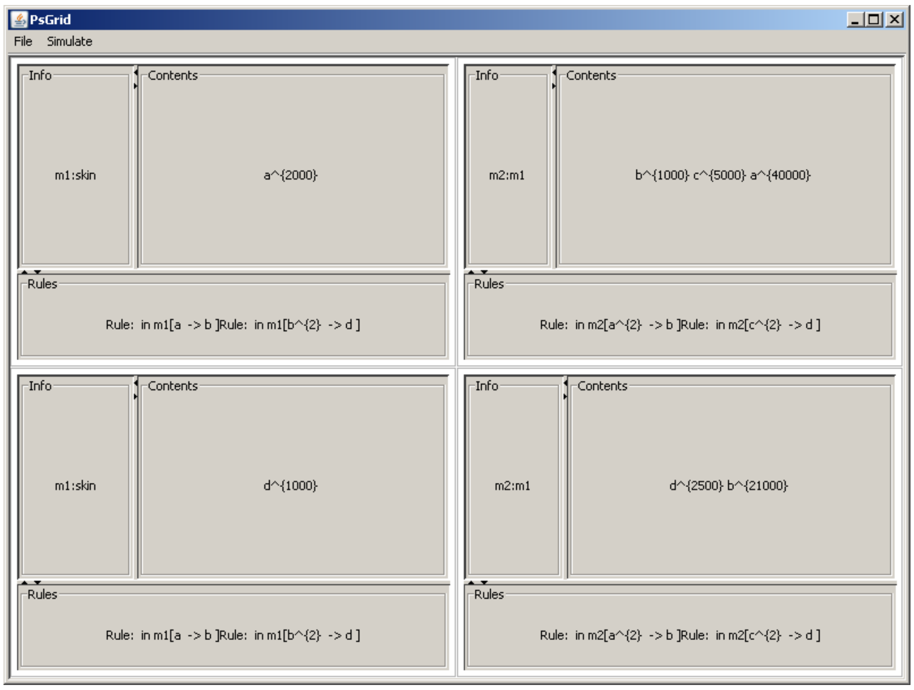
We provide a simple example to illustrate the developed simulator. The system is composed of two membranes $m1$, $m2$. Membrane $m1$ contains a^{2000} and has rules $a \to b$, and $b^2 \to d$, while membrane $m2$ contains $a^{40000}b^{1000}c^{5000}$ and has rules $a^2 \to b$, and $c^2 \to d$. The signaling part is denoted by the contents of *wait*, and *signal*. Those include a sequence of membranes and the number of times they have to signal. Notice that $m2$ has to wait to be signaled by $m1$ two times before it can apply a rule. The parent of $m2$ is $m1$, which is the skin membrane.

```
/* PsGrid input file */
membrane m1 /*name of the membrane*/ :
       skin /*name of the parent*/{
  children {
    m1  /*name of children*/
  }
  contents {
    a^{2000}/*contents of the membrane*/
  }
  rules {
    /*rules of the membrane*/
    [a^{1} ==> b^{1}]
    [b^{2} ==> d^{1}]
  }
  wait{
    /*the antecedents*/
  }
  signal{
    m2 /*the descendants*/
  }
}
membrane m2 : m1{
  children {
  }
  contents {
    a^{40000}b^{1000}c^{5000}
  }
  rules {
    [a^{2} ==> b^{1}]
    [c^{2} ==> d^{1}]
  }
  wait{
    m1^{2}
  }
  signal{
  }
}
```

We also present the log from each node of the grid. The log shows the order in which membrane jobs arrive at each node, and the actions they execute. The number of rule applications executed in a certain step is written at the end of the lines (after #). Notice that the job ends if it receives a terminate signal, or if the membrane did not apply any rules in this step.

```
[20:26:56,843][INFO ][gridgain-#6%null%][PsJob] Received membrane with
    contents :m1:[a^{2000} ] [[Rule: in m1[a -> b ], Rule: in m1[b^{2}
     -> d ]]] #0
[20:26:56,843][INFO ][gridgain-#10%null%][PsJob] Received membrane with
    contents :m2:[b^{1000} c^{5000} a^{40000} ] [[Rule: in m2[a^{2} -> b
     ], Rule: in m2[c^{2} -> d ]]] #0
[20:26:56,843][INFO ][gridgain-#10%null%][PsJob] Waiting at barrier:m2
[20:26:56,843][INFO ][gridgain-#6%null%][PsJob] Waiting at barrier:m1
[20:26:56,843][INFO ][gridgain-#6%null%][PsJob] Passing the barrier:m1
[20:26:56,875][INFO ][gridgain-#6%null%][PsJob] Sending signal to
    descendants
[20:26:56,890][INFO ][gridgain-#6%null%][PsJob] After evolution :m1:[b
    ^{2000} ] [[Rule: in m1[a -> b ], Rule: in m1[b^{2} -> d ]]] #2000
[20:26:56,890][INFO ][gridgain-#6%null%][PsJob] Waiting at barrier:m1
[20:26:56,890][INFO ][gridgain-#6%null%][PsJob] Passing the barrier:m1
[20:26:56,890][INFO ][gridgain-#10%null%][PsJob] Passing the barrier:m2
[20:26:56,906][INFO ][gridgain-#6%null%][PsJob] Sending signal to
    descendants
[20:26:56,921][INFO ][gridgain-#6%null%][PsJob] After evolution :m1:[d
    ^{1000} ] [[Rule: in m1[a -> b ], Rule: in m1[b^{2} -> d ]]] #1000
[20:26:56,921][INFO ][gridgain-#6%null%][PsJob] Waiting at barrier:m1
[20:26:56,921][INFO ][gridgain-#6%null%][PsJob] Passing the barrier:m1
[20:26:56,921][INFO ][gridgain-#6%null%][PsJob] Sending signal to
    descendants
```

```
[20:26:56,921][INFO ][gridgain-#6%null%][PsJob] After evolution :m1:[d
    ^{1000} ] [[Rule:  in m1[a  -> b ], Rule:  in m1[b^{2}  -> d ]]] #0
[20:26:57,062][INFO ][gridgain-#10%null%][PsJob] Sending signal to
    descendants
[20:26:57,062][INFO ][gridgain-#10%null%][PsJob] After evolution :m2:[d
    ^{2500} b^{21000} ] [[Rule:  in m2[a^{2}  -> b ], Rule:  in m2[c^{2}
    -> d ]]] #22500
[20:26:57,062][INFO ][gridgain-#10%null%][PsJob] Waiting at barrier:m2
[20:26:57,062][INFO ][gridgain-#10%null%][PsJob] Passing the barrier:m2
[20:26:57,062][INFO ][gridgain-#10%null%][PsJob] Sending signal to
    descendants
[20:26:57,062][INFO ][gridgain-#10%null%][PsJob] After evolution :m2:[d
    ^{2500} b^{21000} ] [[Rule:  in m2[a^{2}  -> b ], Rule:  in m2[c^{2}
    -> d ]]] #0
```



Info: m1:skin
Contents: a^{2000}
Rules: Rule: in m1[a -> b]Rule: in m1[b^{2} -> d]

Info: m2:m1
Contents: b^{1000} c^{5000} a^{40000}
Rules: Rule: in m2[a^{2} -> b]Rule: in m2[c^{2} -> d]

Info: m1:skin
Contents: d^{1000}
Rules: Rule: in m1[a -> b]Rule: in m1[b^{2} -> d]

Info: m2:m1
Contents: d^{2500} b^{21000}
Rules: Rule: in m2[a^{2} -> b]Rule: in m2[c^{2} -> d]

Fig. 4. PsGrid Screen After Executing the Example

The simulator has a simple but flexible graphical interface. A screen-shot after executing a simulation is presented in Figure 4. The first row presents the initial configuration of the membrane system. The second row presents the contents of the membranes after the simulation.

Even though this example is simple, the implementation can benefit from several features of GridGain, and provide a complex parallel implementation of membrane systems. The main points are that the implementation is faithful to the formal description of the membrane systems, and it is also scalable to a high number of membranes (which is the case in cell biology simulations).

6 Conclusion

Hierarchies are often used in modeling and simulation for computational biology. A hierarchical perspective of the cell considers components structured into classes of similar kinds, e.g. golgi, ER, and nucleus form organelles, i.e. membrane-bound compartments of the cell. New models of membrane systems need to be simulated on complex hardware systems in order to provide a valuable feedback to biologists. Membrane computing is a branch of natural computing using an explicit hierarchical description coming exactly from the structure and functioning of the living cell. The main areas where membrane computing has been used as a modeling framework (biology and bio-medicine, linguistics, economics, computer science, etc.) are presented in [5]. In that volume, several implementations (mainly using sequential computational environments) for simulating various types of cell-like membrane systems are presented in [6]. We consider that the simulation of P systems with sequential computers is a complex task because membrane systems are intrinsically parallel and nondeterministic computational devices, and their computation trees are difficult to store and handle with one processor. Therefore it is necessary to look for parallel and scalable implementations able to simulate as close as possible the formal description of the membrane systems.

In this paper we present a faithful parallel implementation of membrane systems using GridGain, emphasizing on the synchronization problems appearing in membrane computing. Thus we hope to offer a more suitable simulator for membrane systems, opening a new possibility of using membrane computing as a parallel and nondeterministic modeling framework for addressing structural and dynamical aspects of complex systems modeling phenomena in cell biology where huge number of elements are used (some phenomena are presented in [5]).

In the papers devoted to membrane systems it is not mentioned how the membranes (or groups of membranes) interact or synchronize. The usual thinking is that membrane systems are synchronized locally (a step of a membrane is given by the parallel application of rules), and behave asynchronously at the global level. We emphasize here the global aspects, by adding a form of parameterized barrier synchronization between membranes.

There are several software simulators for P systems; however almost all of them are on sequential hardware, and so they do not match the parallel nature of P systems. A parallel implementation of P systems (one of the very few, if not the unique working in a parallel hardware setting) is presented in [4]. It uses a cluster of 64 dual processors, and an MPI library in order to describe the communication and synchronization of parallel processes. In that parallel simulator, the rules are implemented as threads. At the system initialization phase, one thread is created for each rule. Within one membrane, several rules can be applied concurrently.

This parallelism between rule applications within one membrane is modeled with multithreading. Rule applications are performed in terms of rounds. To synchronize each thread (rule) within the system, two barriers implemented as mutexes are associated with a thread. At the beginning of each round, the barrier that the rule thread is waiting on is released by the primary controlling thread. After the rule application is done, the thread waits for the second barrier, and the primary thread locks the first barrier. During the following round it would repeat the above procedure, releasing and locking alternating barriers. Since many rules are executing concurrently and they are sharing resources, a mutual exclusion algorithm is necessary.

The communication and synchronization between membranes is implemented using the Message Passing Interface library of functions for parallel computation. The execution is performed in terms of rounds. At the end of each round, every membrane exchanges messages with all its children and parent before proceeding to the next round. Another concern is the termination detection problem. When the system is no longer active, there is no rule in any membrane that is applicable, all the membranes must be able to be informed, and to terminate. Once the skin membrane detects the termination, it broadcasts this information to all the other membranes. Thereafter, the system terminates and the output is written to a specified file. Fundamental distributed algorithms in the framework of membrane systems are presented in [3].

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