A THEORY FOR MOLECULE STRUCTURES: THE MOLECULAR ONTHOLOGY THEORY

Stefania Bandini, Gianpiero Cattaneo, Paolo Stofella Dipartimento di Scienze dell'Informazione Università di Milano via Moretto da Brescia, 9 20133 Milano -ITALY- tel.+39-2-2772233

PRELIMINARY PAPER

1. INTRODUCTION

The main objective of this paper is to present a formal theory of the molecular onthology approach to the modelling of physical systems introduced by [5] and informally described in the same paper.

In qualitative modelling of physical systems [8] the use of molecular descriptions was introduced, but not developed, in [7] and also introduced in [2].

A theory for molecular structures will be presented here and it will be called "Molecular Onthology Theory" (MOT) [1].

First an Universe U will be defined as a set of a Places endowed with a family of adjacency relations $\{A_i^* : i \in I\}$.

The adjacency relations will be extended also on two sets of primitive elements, molecules (M) and obstacles (O). One and unique place in U is associated to any element of M and O and the collection of these places contitutes a configuration of a physical system.

In this structure, molecules and obstacles can move: a movement determines a change of the whole configuration. The movement of molecules is local and it is determined by the application of a set of local rules expanded by means of messages.

In this direction the specific example of the qualitative modelling of the behaviour of liquids will be presented in a bidimensional Universe with a priviledged direction of falling.

Finally, the semantics of expressions in a language for direct representation [6],[9],[10],[4] will denotate the configurations and the message function will provide the denotation of transformation expressions rules.

1

1.1 Places Universe

Let P a non empty set of elements p, q, r,.... \in P called places.

An oriented adjacency between places is an antireflexive and antisymmetric binary relation A^+ on P, $A^+ \subseteq P \times P$. Two places p, $q \in P$ are adjacent with respect to the orientation $^+$, with q as the next element of p, iff $A^+(p, q)$ (fig.1).



Figure 1 - The place p is adjacent to q

The adjacency relation with an orientation opposite to A^+ , denoted by A^- ,s, by definition, the transpose of A^+ . A non oriented adjacency relation A is the union of an oriented adjacency relation and its transpose ($A=A^+\cup A^-$); in this way p and q are adjacent iff they are in the oriented relation A^+ or in its transpose A^- . Notice that the adjacency relation A is symmetric and antireflexive.

Once given a set of places P, we define a universe of places U on P as a family $\{A_i^+: i \in I\}$, with index set $I = \{1, ..., k\}$, of oriented adjacency relations iff the next condition, called *the mutual exclusivity* holds: $\forall i, j \in I, i \neq j A_i^+$ (p, q) $\Rightarrow \neg A_j^+$ (p, q). We denote by $\alpha = \{A_i^+, A_i^- i \in I\}$ in the sequel.

The dimension of an universe of places is the cardinality of I. A general adjacency relation $A^* \subseteq (P \times P)$ is defined as follows: $A^* = \{\bigcup i (A^+_i \bigcup A^-_i)\}$.

Notice that the general adjacency relation A* is symmetric and antireflexive.

1.2 Molecules, obstacles, positions and configurations

Let M={m, n, ... } and O={o, r, ...} be two not empty sets whose elements are respectively called molecules and obstacles. Any pair (Π_c, Ω_c) where $\Pi_c \subseteq M \times P$

and $\Omega_c \subseteq O \times P$ is a possible configuration of the universe iff the following conditions are satisfied (for a formal description see [1]):

(1.m) a place cannot contain two molecules in the same configuration;

(2.m) a molecule cannot occupy two places in the same configuration;

(1.0) a place cannot contain two obstacles in the same configuration;

(2.0) an obstacle cannot occupy two places in the same configuration;

(1.m.o) a molecule and an obstacle cannot occupy the same place in a configuration.

The set Π_c (resp. Ω_c) is called the set of molecules (resp. obstacles) positions, the set of all possible configuration in U is denoted by Z.

<u>Non-compenetrability</u>: Conditions (1.m), (1.0), and (1.m.o) respectively define the non-compenetrability property between molecules, between obstacles and between obstacles and molecules.

Once given a configuration $(\Pi_c, \Omega_c) \in \mathbb{Z}$ we introduce the set \mathbb{P}^m_c of places occupied by molecules, the set \mathbb{P}^o_c of places occupied by obstacles and the set \mathbb{P}^v_c of empty places at the configuration; in symbols (fig. 2) $\mathbb{P}^m_c = \{p \in \mathbb{P} \mid \exists (p, m) \in \Pi_c\}; \mathbb{P}^o_c = \{p \in \mathbb{P} \mid \exists (p, o) \in \Omega_c\}; \mathbb{P}^v_c = \mathbb{P} \setminus \mathbb{P}^m_c \cup \mathbb{P}^o_c$.



Figure 2 - A represents P^{m}_{c} , B represents P^{o}_{c} and C represents P^{v}_{c}

Let $T = \{t_0, t_1, ...\}$ be a discrete time set , whose elements are interpreted as time instants, with initial instant t_0 , i.e. a countable set endowed with a total order with respect to which it is lower bounded by the least element $t_0 \in T$.

A dynamic evolution in U is any family of pairs indexed by $t \in T$

$\{(\Pi_t, \Omega_t): t \in T\}$

such that every (Π_t, Ω_t) is a possible configuration (and so in particular $\Pi_t \subseteq M \times P$ and $\Omega_t \subseteq O \times P$) at t. In the sequel a possible configuration at t will be denoted by S_t .

 Π_t (resp. Ω_t) is the set of the places occupied by molecules (resp. obstacles) at the instant t. We set

$$\Pi = \{ (m, p, t) : (m, p) \in \Pi_t, t \in T \} \subseteq M \times P \times T$$

 $\Omega = \{(o, p, t) : (o, p) \in \Omega_t \ , t \in T\} \subseteq O \times P \times T$

and a dynamic evolution will also be denoted by (Π, Ω) .

For any instant t, adjacency relations between molecules, obstacles and places can be defined in a straightforward way, for instance, a molecule m and an obstacle o are adjacent in an instant i iff they occupy adjacent places in the given t: A_t^+ (m, o) iff (m, p, t) $\in \Pi \land (o, q, t) \in \Omega \land A^+(p, q)$, and so on.

1.4 Movement of molecules and obstacles

A molecule m moves in U passing from a place p at t to a place q adjacent to p at t+1 (the movement of a molecule is instantaneous - fig. 3) if and only if the following conditions are satisfied:

- i) A_t*(p, q) i.e., p and q are adjacent at t;
- ii) $(m, p, t) \in \Pi$ i.e., the molecule m occupies the place p at t;
- iii) $(m, q, t + 1) \in \Pi$ i.e., the molecule m occupies the place q at t+1.



Figure 3 - Movement of a molecule

Let us consider a molecule $m \in M$ which at t is in the position p, i.e. $(m, p, t) \in \Pi$; we say that this molecule doesn't move from p iff condition i) and iii) are not satisfied: $\neg \exists q \in P, A^*(p, q) \land (m, q, t+1) \in \Pi$; equivalently : $\forall q \in P, q \neq p \neg A^*(p, q) \lor \neg (m, q, t+1) \in \Pi$.

The consequence of this is:

(4.m) if a molecule occupies an insulated place (i.e. a place not adjacent to any other places) at t, then it doesn't move;

(4.0) if an obstacle occupies an insulated place at t, then it doesn't move.

Moreover, we do require that the following conditions hold:

(5.m) two adjacent molecules cannot interchange their positions;

(5.0) two adjacent obstacles cannot interchange their positions.

<u>Theorem 1.1</u>: Let $(m, p, t) \in \Pi \land (n, q, t) \in \Pi \land A^*(p, q)$. If m moves in q in the interval t, t+1, i.e. $(m, q, t+1) \in \Pi$ then $\exists r \in P \mid A^*(q, r)$ and n moves in r in the interval t, t+1, i.e. $(n, r, t+1) \in \Pi$.

1.5 Changes of configuration in the universe



Figure 4- Configuration change

Once given a dynamic evolution (Π, Ω) in U let us introduce the following sets: $\Sigma_m = \{\Pi_t : t \in T\}$ which represents the molecules dynamics $\Sigma_0 = \{\Omega_t : t \in T\}$ which represents the obstacles dynamics $\Sigma_{-} = \{S_t : t \in T\}$ which represents the system dynamics It is possible to consider Σ as the representation of the dynamic evolution of the system in T, in which configurations S_t are the states of that evolution. S_{t0} is the initial state of Σ . Let $[t_0, t_0+n]$ denote the discrete time interval between t_0 and t_0+n , $\{t_0, t_0+1, ..., t_0+n\}$, we define dynamic process the $[t_0, t_0+n]$ - segment of the system dynamics, i.e. the collection of states $\Sigma(n) := \{S_{t0}, S_{t0+1}, ..., S_{t0+n}\} \subseteq \Sigma$

Let $\Gamma = \{g_1, ..., g_n\}$ be a fixed finite set of configurations representing desired system states, called **goal**. A **succesfull dynamic process** (SDP) of a dynamic evolution (Π, Ω) is a dynamic process Σ (n), in which the final state belongs to the set of fixed goals:

$$SDP = \Sigma(n) | S_{t0+n} \in \Gamma$$

1.6 States of molecules

The passage from a configuration S_t to a configuration S_{t+1} , is called configuration change (fig. 4); the configuration change is due to the application of some local behaviour rules which are defined once that a particular type of molecules is considered and they give their instantiation. For any fixed initial configuration S_{t0} the local behaviour rules determines, with an iterative step by step application, in a unique way a dynamic process Σ depending from the choice of S_{t0} .

A particular type of molecules is in general characterized by a set $X = \{s_1, ..., s_n\}$ of possible individual states. The local behaviour rules are formalized by a function μ : (M, X) × P × α × S_t → Bool× S_{t+1}, called message, where Bool = {Success, Fail}. The application of this function determines the configuration change if μ = Success, S_{t+1} for a particular molecule.

The simulation of a process is a dynamic evolution in which an initial state, a set of local behaviour rules and a set of goals is provided.

In the next section we will see an example for a computational model for processes simulation for molecules of liquid, in a bidimensional universe, with associated proper states and transition rules, and behaviour rules.

2. THE CASE OF LIQUIDS

Modelling liquids behaviour in a qualitative way is one of the most dealt with example in literature [7],[3],[2]. In this section an example of liquids modelling using MOT will be presented: it is limited to a bidimensional finite universe with a falling direction (gravity).

After a brief description of the main features of this universe, the notion of state of molecules of liquid and the set of state transition rules will be given.

The dynamic behaviour of liquids will be defined by a set of local behaviour conditions applied by means of messages exchange expressed as a functional application. General assumptions here assumed are:

. each molecule represents an arbitrary indivisible quantity of liquid;

. in this model speed and pressure are not considered;

. viscosity and flexibility are not considered.

2.1 The universe of liquids

In this section the description of obstacles (with associated the status of "solid molecules") and of liquid molecules will be given. The universe U of places is bidimensional (fig.5) since two oriented adjacency relations are defined on it: (the oriented rightwards-adjacency relation and the downwards one, denoted resp. by A^{\rightarrow} , A^{\downarrow} , whereas their transpose, denoted by A^{\leftarrow} , A^{\uparrow} are resp. the leftwards-adjacency and the upwards-adjacency.



Figure 5 - Bidimensional universe

 $M=\{m, n, ...\}$ and $O=\{o, r, ...\}$ are two non empty sets whose elements are respectively called liquid molecules and solid obstacles. Also in this case, $\Pi_c \subseteq M \times P$ and $\Omega_c \subseteq O \times P$ are the set of liquid molecules positions and of solid obstacles positions whose elements satisfy conditions (1.m), (2.m), (1.o), (2.o) and (1.m.o) (fig.6).



Let A^{\downarrow}_{t} (fig. 7) be the relation of downwards-adjacency at t; for instance, either between molecules : $A^{\downarrow}_{t}(m, n)$, where m, $n \in M$, or between empty places: $A^{\downarrow}_{t}(p, q)$, where p, $q \in P^{v}_{t}$, or between molecules and places: $A^{\downarrow}_{t}(m, q)$, where $m \in M \land q \in P^{v}_{t}$, and so on.



An aggregate of solid obstacles OA_t is a maximal set of adjacent solid obstacles at tand it is called object (fig. 8):

 $\forall o \in OA_t \exists r \in OA_t \exists p, q \in P \mid (o, p, t) \in \Pi \land (r, p, t) \in \Pi \land A^*_t (p, q).$



Figure 8

2.4 Notion of state of molecules of liquid

The state space of a liquid molecule $m \in M$ is a boolean set $X=\{L,B\}$ where L means free and B means bound (fig 9).



Figure 9

A molecule $m \in M$ is free at t iff an empty place downwards-adjacent to it exists (fig. 10):

(i)
$$\exists p \in P^{v}, A^{\downarrow}(m, p)$$

or if a free molecule downwards-adjacent to it exists:

(ii) $\exists n \in M \Rightarrow A^{\downarrow}_{t}(m, n) \land n=L.$



Figure 10 - Free molecules

A molecule $m \in M$ at t is **bound** iff a solid obstacle is downwards-adjacent to it (fig. 11):

i)
$$\exists o \in O, A^{\downarrow}_{t}(m, o)$$

or if a bound molecule is downwards-adjacent to it:

(ii)
$$\exists n \in M \Rightarrow A^{\downarrow}(m, n) \land n=B$$
.



Figure 11 - Bound molecules

<u>State transition rules</u>: Liquid molecules can change their state with the following set $R=\{r_1, r_2\}$ of state transition rules:

 r_1 . A free molecule at t becomes bound at t+1 iff:

either (i) $A_{t+1}^{\downarrow}(m, n) \land n=B;$ or (ii) $A_{t+1}^{\downarrow}(m, o) \land o \in O.$

 r_2 . A bound molecule at t becomes free at t+1 iff:

either (i) $A^{\downarrow}_{t+1}(m, p) \land p \in P^{v}_{t+1};$

or (ii) $A_{t+1}^{\downarrow}(m, n) \wedge n=L$.

2.3 Liquid molecules movement and configuration change

In the movement of liquid molecules in U the particular falling direction plays a fundamental role: it acts at t only on free molecules and determines a vertical falling. Bound molecules can move only if sollecited by other molecules. In this case the falling direction directly determines the transition state rules.



Figure 12 - Molecule m is on molecule n

The message function for liquids behaviour is as expressed:

 $\mu: (M,X) \times P \times \alpha \times S_t \rightarrow \text{Bool} \times S_{t+1}$

where M is the set of molecules, P is the set of places, $\alpha = \{A^{\uparrow}, A^{\downarrow}, A^{\rightarrow}, A^{\leftarrow}\}$. S_t and S_{t+1} are the possible configurations at instant t and t+1, respectively.

In fig.14 the mechanism of returning message is illustrated.

As in general, in the universe of liquids, the simulation of a dynamical evolution in U where an initial and a final state are given as yield by the application of μ .



Figure 14

Function μ (m, π , α , S_t) : Bool, S_{t+1}

```
begin
if m=L
begin
       if A^{\downarrow}_{t}(m, p) and p \in P^{v}_{t}
       then m moves; \mu = Success, S_{t+1};
       <u>if</u> A^{\downarrow}_{t}(m, n) <u>and</u> n = L <u>and</u> \mu (n, \pi, A^{\downarrow}, S_{t}) = Success, S_{t+1}
       <u>then</u> m moves; \mu = Success, S<sub>t+1</sub>;
                   \underline{if} A^{\downarrow}_{t}(m, n) \underline{and} n = B
                   for x random { A^{\uparrow}, A^{\downarrow}, A^{\rightarrow}, A^{\leftarrow} }
                   if \mu (n, q, x, S<sub>t</sub>) = Success, S<sub>t+1</sub>
                    then m moves; \mu = Success, S<sub>t+1</sub>; exit;
                    else m doesn't move; S_{t+1} = S_t; \mu = Fail, S_{t+1};
end;
if m=B
begin
       if \alpha(m, p) and p \in P^{v}_{t} and not ON(p, r)
       then m moves; \mu = Success, S<sub>t+1</sub>;
       if \alpha(m, n) and n = L and \mu(n, \pi, A^{\downarrow}, S_t) = Success, S_{t+1}
       then m moves; \mu = Success, S<sub>1+1</sub>;
       if \alpha(m, n) and n = B
       for x random { A^{\uparrow}, A^{\downarrow}, A^{\rightarrow}, A^{\leftarrow} }
                    if \mu (n, \pi, x, S<sub>t</sub>) = Success, S<sub>t+1</sub>
                    then m moves; \mu = Success, S<sub>t+1</sub>; exit;
                    else m doesn't move; S_{t+1} = S_t; \mu = Fail, S_{t+1};
end;
```

end.

3. DIRECT REPRESENTATION AND LIQUIDS UNIVERSE

As suggested in [6] we can see a class of languages larger than that in which the unique semantic primitive is the application of an function to an argument [10]: it is possible to introduce a general notion of representation language (\mathcal{L}_r) as a language with an associated semantic theory, a calculus which associates language expressions to individuals, relations, actions, configurations, etc. of the world the language itself expresses knowledge about. In this way, a semantic theory which defines the meaning of the expressions as a language makes a formal language a representation language.

A representation language $\mathcal{L}_r < C$, G> is defined by a set C of possible configurations on a vocabulary P of primitive symbols and by a set G of grammar rules to produce new configurations on the basis of some given.

A model for \mathcal{L}_r is given by a finite set of entities as primitive symbols meaninigs, an interpretation function which associates any symbol to the particular meaning and, for each grammar rule by a semantic rule which defines the meaning of a configuration in terms of aggregation of the meanings of its parts [12].

This general notion of language can also be used for direct representation languages: the most meaningful notion in a direct representation language $\mathfrak{f}_r < C$, G> is the notion of <u>configuration</u>: in \mathfrak{f}_r a configuration represents a particular situation where each element is given once and all its relations with other elements are concurrently present.

In our example primitive symbols of our language \mathcal{J}_r are three:

which represent an obstacle $o \in O$,



which represents a free molecule of liquid $m \in M_L$ and

which represents a bound molecule $m \in M_V$.

Configurations transformations can be defined in terms of productions in a contextual bidimensional grammar.

An arbitrary number of adjacent obstacles is called object; in \mathbf{a}_r an expression in which a certain number of adjacent obstacles will denote an object.

13

In the implementation of our example an object's library of meaningful tools to deal with liquids has been built. For instance:



represents a generic container.

Each configuration $S_t \in C$ of this symbols is an expression of \mathcal{F}_r . For instance:



represents a container with bound molecules of liquid and a free molecule going into it. A tap represents a source [1] yielding free molecules which fall (they occupy the empty downwards-adjacent place):



The configuration change from $S_t \in C$ to $S_{t+1} \in C$ occurs with the application of μ . The simulation of a process is defined by a sequence of configurations with an initial state and a set of final states representing desired goals. In this way an operational semantics is associated with grammar rules. Intermediate states can be occur in according whith general MOT conditions.

3.1 From the universe to the bidimensional array

Bidimensional universe U introduced in section 2 is represented in a computational system by a bidimensional array called **World**. It is possible to establish a correspondence between the objects of MOT: to each place $p \in P$ the pair < i, j > is associated with, $i, j \in N$ and with $i \in 0...max$ i and $j \in 0...max$ j.

The set P^v, of empty places in a configuration is

 $P^{v}_{t} = \{ \langle i, j \rangle | \langle i, j \rangle \in P \land World(i, j) = NIL \}.$

where World is a predicate assigned to the pair (i, j) denoting an object and retourning NIL if no objects occupy the position in the array denoted by the pair $\langle i,j \rangle$. Each molecule is an instance of the flavor MOLECULE (see the Object Oriented programming techniques adopted for the implementation of the model [1],[11] in a given configuration. The set P^m , of molecules in a configuration is

 $P^{m}_{i} = \{ \langle i, j \rangle \mid \langle i, j \rangle \in P \land is_molecule(World(i, j)) \}$

where is_molecule is a predicate which asserts that the object in the position individuated by $\langle i, j \rangle$ is a molecule. The same holds for the set P^{0}_{t} of obstacles:

 $P_{t}^{o} = \{\langle i, j \rangle \mid \langle i, j \rangle \in P \land is_obstacle(World(i, j))\}$

The adjacency relation A* is so represented:

 $A^*(\langle i, j \rangle, \langle h, k \rangle) \Leftrightarrow (i = h \land |(j-k)| = 1) \lor (j=k \land |(i-h)| = 1)$

Molecules of liquid and obtacles are represented on a bidimensional graphic video by pixel matrixes 4×4 as schematicly illustrated in fig. 15.



Figure 15

4. CONCLUSIONS

On the basis of proposed Molecular Ontology Theory applied to liquids and of representation choices of \mathcal{F}_r a program for the qualitative simulation of liquids behaviour [11],[5] has been implemented. It is presently installed at the laboratory of Artificial Intelligence and Robotics of Euratom (Ispra) and a set of experiments has been successfully executed. The program allows to run the simulation of molecules of liquids in the basis of conditions and properties of the MOT.

The system on which the program has been implemented is the LISP Machine Symbolics 3600 which has a set of tools particularly useful for Object Oriented programming techniques, the Flavor System.

The implementation of the example of liquids has been a very important experience to consolidate the possibilities of proposed MOT. A generalized workstation based on MOT, not only circumscripted to the liquids-world, is the new project we are working on.

REFERENCES

- [1] Bandini, S., <u>Un Modello Computazionale per Strutture di Molecole nella Fisica</u> <u>Naive</u>, Tesi di Dottorato di Ricerca, Università di Milano (in italian), 1988
- [2] Collins, J.W., <u>Reasoning about Fluids Via Molecular Collections</u>, in Forbus, K.D., (ed.) <u>Proceedings of Qualitative Physics Workshop</u>, University of Urbana, Urbana, 1987
- [3] Forbus, K.D., <u>Qualitative Process Theory</u>, AI-TR-789, MIT, 1981
- [4] Funt, B.V.; <u>Problem Solving with Diagrammatic Representations</u>, Artificial Intelligence Journal, n.13, 1980
- [5] Gardin, F., B.Meltzer, P.Stofella, <u>The Analogical Representation</u> of Liquids in Naive Physics, Proceedings ECAI 7, Brighton, 1986
- [6] Hayes, P.J., <u>Some Problems and Non-problems in Representation</u> <u>Theory</u>, Proc. AISB Summer Conference, University of Sussex, Brighton, 1974, also in Brachman, R.J., H.J.Levesque (eds.), "Readings in Knowledge Representation", Morgan & Kaufman Pu.Inc., Los Altos, 1985
- [7] Hayes, P.J., <u>Naive Physics I: Ontology for Liquids</u>, in Hobbs, J.R., R.C. Moore, (eds.) <u>Formal Theories of the Commonsense World</u>, Ablex Publishing Co., Norwood, NJ, 1985
- [8] Hobbs, J.R., R.C. Moore, (eds.) Formal Theories of the Commonsense World, Ablex Publishing Co., Norwood, NJ, 1985
- [9] Meltzer, B., L.Gambardella, F.Gardin, <u>Analogical Representation</u> in <u>Reasoning Systems</u>, Internal Report, AI & Robotics Lab., EURATOM, Ispra, 1985
- [10] Sloman, A., <u>Interactions Between Philosophy and Artificial Intelligence</u>, Artificial Intelligence Journal, n.2, 1971
- [11] Stofella, P., <u>La Rappresentazione Analogica dei Liquidi nella Naive Physics</u>, Tesi di Laurea in Scienze dell'Informazione, Dipartimento di Scienze dell'Informazione, Università degli Studi di Milano, 1986
- [12] Tarski, A., <u>The Semantic Conception of Truth and the Foundations of</u> <u>Semantics</u>, Philos. and Phenom. Research, IV, 1944