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Local reversibility in a Calculus of Covalent Bonding

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ABSTRACT

We introduce a process calculus with a new prefixing operator that allows us to model locally controlled reversibility. Actions can be undone spontaneously, as in other reversible process calculi, or as pairs of concerted actions, where performing a weak action forces undoing of another action. The new operator in its full generality allows us to model out-of-causal order computation, where causes are undone before their effects are undone, which goes beyond what typical reversible calculi can express. However, the core calculus, which uses only the reduced form of the new operator, is well behaved as it satisfied causal consistency. We demonstrate the usefulness of the calculus by modelling the hydration of formaldehyde in water into methanediol, an industrially important reaction, where the creation and breaking of some bonds are examples of locally controlled out-of-causal order computation.

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1. Introduction

There are many different computation tasks which involve undoing of previously performed steps or actions. Consider a computation where the action a causes the action b , written $a < b$, and where the action c occurs independently of a and b . There are three executions of this computation that preserve *causality*, namely abc , acb and cab . We note that a always comes before b . There are several conceptually different ways of undoing these actions [38]. *Backtracking* is undoing in precisely the reverse order in which they happened. So, $\text{undo } b \text{ undo } c \text{ undo } a$ is a backtrack of the execution acb . *Reversing* is a more general form of undoing: here actions can be undone in any order provided causality is preserved (meaning that causes cannot be undone before effects). For example, $\text{undo } c \text{ undo } b \text{ undo } a$ is a reversal of acb for the events a , b and c above.

There are networks of reactions in biochemistry, however, where actions are undone seemingly *out-of-causal order*. The creation and breaking of molecular bonds between the proteins involved in the ERK signalling pathway is a good example of this phenomenon [29]. Let us assume for simplicity that the creation of molecular bonds is represented by actions a , b , c where, as above, $a < b$ and c is independent of a and b . In the ERK pathway, the molecular bonds are broken in the following order: $\text{undo } a$, $\text{undo } b$, $\text{undo } c$, which seems to undo the cause a before the effect b .

We introduced informally a novel and purely local in character mechanism for undoing of computation in short papers [16,17]. Here, we build a process calculus around this mechanism and give it operational semantics. We then discuss various properties that hold in the calculus. Most importantly, we show that out-of-causal order computation can be modelled in the calculus. Hence, in general, the *causal consistency* property [7] does not hold. There are reachable states that can only be arrived at by a mixture of forward and reverse steps. However, we argue that causal consistency holds in a restricted version of our calculus, thus the full calculus is in effect a “conceptual” extension of a causally consistent reversible process calculus.

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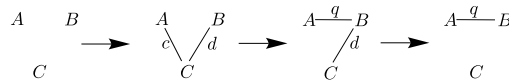


Fig. 1. A catalytic reaction.

The benefits of the calculus are shown by modelling hydration of formaldehyde in water. The molecules of formaldehyde and water are modelled as compositions of carbon, oxygen and hydrogen atoms. When composed in parallel, the molecules react and the reactions are represented by sequences of transitions of *concerted actions*. We are able to represent different forms of reversibility, including out-of-causal order reversibility, and computation can proceed in any directions without external control.

The novel features of our calculus are introduced via an example of a simple catalytic reaction. Consider two molecules A and B that are only able to bond if assisted by a catalyst C . Once A and B are bonded with the catalyst C , A bonds with B and, at the same time, the bond between A and C is broken. Finally, the bond between B and C is broken. This is illustrated in Fig. 1.

We assume $A \stackrel{def}{=} (a; p).A'$, $B \stackrel{def}{=} (b; p).B'$ and $C \stackrel{def}{=} (a, b).C'$, where A' , B' and C' represent further potential behaviour of the molecules A , B and C . We use a new prefix operator $(s; p).P$ where s is a sequence of actions or executed actions and p is a *weak action*. Initially the actions in s take place, and then p takes place. The molecules A , B and C can bond by performing synchronously the matching actions according to the communication function $\gamma(a, a) = c$, $\gamma(b, b) = d$ and $\gamma(p, p) = q$, producing thus new actions c , d and q respectively. A weak action p can be left out in $(s; p).P$ (as in B and C above). In general, the actions of s in $(s; p).P$ can take place in any order, very much like in [8,29], and the new feature is that p can happen only if all actions in s have already taken place. Once p takes place, one of the executed actions in s must be undone immediately: this is our new mechanism for triggering reverse computation. We shall model these two almost simultaneous events as a transition of concerted actions. This is a realistic representation of the mechanism of covalent bonding, the most common type of chemical bonding between atoms, hence we call our calculus a *Calculus of Covalent Bonding*.

Returning to our example, we represent the system of molecules A , B and C as $((a; p).A' \mid (b; p).B' \mid (a, b).C') \setminus \{a, b, p\}$, where \mid is the parallel composition and \setminus the restriction as in ACP [1]. We note that A and B cannot interact initially since $\gamma(a, b)$ is not defined. They can however both interact with C :

$$(a; p).A' \mid (b; p).B' \mid (a, b).C' \xrightarrow{c[1]} (a[1]; p).A' \mid (b; p).B' \mid (a[1], b).C' \xrightarrow{d[2]} (a[1]; p).A' \mid (b[2], p).B' \mid (a[1], b[2]).C'$$

Numbers 1 and 2 are the *communication keys* [25,26]: they indicate which pairs of actions have bonded. Molecules A and B can now bond on p (with the key 3), producing the action $q[3]$. This causes immediately the breaking of the bond $c[1]$, which means undoing of the action a in A and action a in C (and still leaving A and B bonded). We model such an event of creating a bond and simultaneously breaking another bond by a pair of *concerted actions*:

$$(a[1]; p).A' \mid (b[2], p).B' \mid (a[1], b[2]).C' \xrightarrow{\{q[3], c[1]\}} (a; p[3]).A' \mid (b[2], p[3]).B' \mid (a, b[2]).C'$$

The bond with the key 3 on the weak action p in A is unstable, and thus gets *promoted* to a stable and stronger bond on a and p , which is modelled by the following rewrite:

$$(a; p[3]).A' \mid (b[2], p[3]).B' \mid (a, b[2]).C' \Rightarrow (a[3]; p).A' \mid (b[2], p[3]).B' \mid (a, b[2]).C'$$

Finally, the catalyst dissolves the bond with B :

$$(a[3]; p).A' \mid (b[2], p[3]).B' \mid (a, b[2]).C' \xrightarrow{d[2]} (a[3]; p).A' \mid (b, p[3]).B' \mid (a, b).C'$$

We note that A and B are now bonded although the synchronisation function did not allow it to happen initially. The main consequence of this is that the bond between $a[3]$ and $p[3]$ is *irreversible*, namely it cannot be undone. Looking at the pattern of doing and undoing of bonds we obtain $c[1]d[2]q[3]c[1]d[2]$. Since creation of bonds c and d causes the bond q , we have here an example of an out-of-causal order computation.

The calculus CCB is given *Structural Operational Semantics* (SOS for short) style semantics. This includes novel SOS rules for concerted actions and three rewrite rules that prescribe when bonds on weak actions can be promoted to strong action bonds. We show that CCB is a well behaved calculus by proving a number of useful properties. For example, the sub-calculus with the simple prefixing operator $(s).P$ satisfies causal consistency. We show that the full calculus allows us to represent out-of-causal order computation patterns via the hydration of formaldehyde in water case study.

Next we summarise the main items of related work.

1.1. Related work

Scientists started to investigate the speed of chemical reactions and the rates achieved as soon as the concept of chemical reactions was first developed. The behaviour of a system of compounds over time can be modelled using a set of

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