Analysis of the $\mathcal{M}$olecules of $\mathcal{K}$nowledge Model with the BioPepa Eclipse Plugin

Stefano Mariani
DISI, ALMA MATER STUDIORUM–Università di Bologna
via Sacchi 3, 47521 Cesena, Italy
Email: s.mariani@unibo.it

***Abstract*—In this brief technical report, we investigate the opportunity of exploiting biochemical processes simulation tools – in particular, BioPepa – to experiment about parameter tuning in chemical-like coordination models—in particular, $\mathcal{M}o\mathcal{K}$.**

I. INTRODUCTION

Natural systems gained increasing attention from the Computer Scientists community, mainly due to their ability to exhibit self-organising features appearing by emergence from a huge number of local, stochastic interactions. Such features are particularly attractive for the Coordination Models and Languages community, being its foremost goal to conceive models and build systems able to meaningfully coordinate a number of autonomous, independent, (possibly) distributed (software) entities so as to reach a shared goal [1]. Soon it became clear that some kind of support was needed to design such systems, in particular to effectively tune their parameters in order to achieve the desired self-* behaviours. Thus, many simulation and analysis tools have been proposed with the aim to ease the process of checking and predicting the behaviour of a nature-inspired software system prior to actual deployment [2].

In this brief technical report, I share my experience in using the BioPepa Eclipse plugin to investigate the $\mathcal{M}$olecules of $\mathcal{K}$nowledge model ($\mathcal{M}o\mathcal{K}$, for short) capabilities of exhibiting biochemical-like self-organising behaviours. To this end, Subsection I-A provides some background of the $\mathcal{M}o\mathcal{K}$ model, whereas Subsection I-B clears the goals of my investigation.

A. Background

The $\mathcal{M}o\mathcal{K}$ model is first of all a coordination model [3]. In particular, it is both a *knowledge -driven* and *-oriented* coordination model, which means that, on the one hand, coordination of interacting, autonomous agents happens not directly between their actions, but as a side effect of a proper management of the knowledge produced and consumed by such agents (*-driven* part), on the other hand, that the coordination process is focussed on coordinating the information to influence the agents, rather than coordinating the agents to influence the way in which information is stored (*-oriented* part).

The $\mathcal{M}o\mathcal{K}$ model is also a *biochemically-inspired*, tuple-based coordination model which exploits logic tuples to leverage user agents reasoning capabilities. As such, it has been deeply influenced by the *biochemical tuple space* coordination model proposed in [4]. Basically, tuples are seen as *reactants* floating in a chemical substance, user agents as *chemists* injecting, observing and withdrawing reactants, and the tuple space is no more merely a passive repository of information but an active environment acting as a *chemical dynamics simulator*, evolving tuples concentrations exactly as reactants evolve in a chemical substance due to *chemical reactions* [5]. As in chemistry then, other than the specific chemical reactions "installed" into the tuple space, what do matter for a successful model deployment is the tuning of the two most crucial parameters available, that is the *concentration* of reactants within the space and the *rate* of chemical reactions execution.

The main goals of the $\mathcal{M}o\mathcal{K}$ model are:

- to autonomously aggregate information chunks into *heaps of knowledge*
- to let information and knowledge autonomously *flow toward the interested users*, rather than be searched

The $\mathcal{M}o\mathcal{K}$ model has been formalized in [3], an early case study has been presented in [6] and further evaluated in [7]. Here follows a brief recap of such formalization, meant to ease understanding of the experimental plan presented in Section II.

$\mathcal{M}o\mathcal{K}$ Atoms.: Produced by a *source* and conveying an *atomic piece of information*, atoms should also store *ontological metadata* to ease automatic processing:

$$\texttt{atom(}src,val,attr\texttt{)}_c$$

$\mathcal{M}o\mathcal{K}$ Molecules.: $\mathcal{M}o\mathcal{K}$ heaps for information *aggregation*, molecules cluster together *semantically* related atoms:

$$\texttt{molecule(}Atoms\texttt{)}_c$$

$\mathcal{M}o\mathcal{K}$ Enzymes.: Enzymes represent the *reification* of (epistemic) knowledge-oriented *(inter-)actions*, and are meant to participate biochemical reactions to properly increase molecules' concentration[1]:

$$\texttt{enzyme(}Molecule\texttt{)}_c$$

$\mathcal{M}o\mathcal{K}$ $\mathcal{F}_{\mathcal{M}o\mathcal{K}}$ Function.: As a knowledge-oriented model, $\mathcal{M}o\mathcal{K}$ must have a way to determine the *semantic correlation* between information. Therefore, the *$\mathcal{M}o\mathcal{K}$ function* should be defined, taking two molecules and returning a value $m \in [0, 1]$:

[1] The term "molecule" will be used also for "atom" in the following.

$$\mathcal{F}_{\mathcal{M}o\mathcal{K}}\text{: } Molecule \times Molecule \longmapsto [0,1]$$

$\mathcal{M}o\mathcal{K}$ Reactions.: The behaviour of a $\mathcal{M}o\mathcal{K}$ system is determined by *biochemical reactions*, which stochastically drive molecules aggregation, as well as reinforcement, decay, and diffusion:

- Aggregation — Bounds together semantically related molecules
$$\texttt{molecule}(Atoms^1) + \texttt{molecule}(Atoms^2) \longmapsto^{r_{agg}} \texttt{molecule}(Atoms^1 \biguplus Atoms^2) + Residual(Atoms^1 \bigcup Atoms^2)$$
- Reinforcement — Consumes an enzyme to reinforce the related molecule
$$\texttt{enzyme}(Molecule^1) + Molecule^1_c \longmapsto^{r_{reinf}} Molecule^1_{c+1}$$
- Decay — Enforcing *time situatedness*, molecules should fade away as time passes
$$Molecule_c \longmapsto^{r_{decay}} Molecule_{c-1}$$
- Diffusion — Analogously, *space situatedness* is inspired by biology and therefore based upon *diffusion*
$$\{Molecule^1 \bigcup Molecules^1\}_{\sigma_i} + \{Molecules^2\}_{\sigma_{ii}} \longmapsto^{r_{diffusion}} \{Molecules^1\}_{\sigma_i} + \{Molecules^2 \bigcup Molecule^1\}_{\sigma_{ii}}$$

$\mathcal{M}o\mathcal{K}$ Not-Yet-Formalised Abstractions.: Other aspects like topology, information production and consumption are addressed by:

- Compartments — the conceptual *loci* for all other $\mathcal{M}o\mathcal{K}$ abstractions, providing the notions of *locality* and *neighbourhood*
- Sources — each one associated to a compartment, $\mathcal{M}o\mathcal{K}$ sources are the origins of atoms, which are continuously injected at a given *rate*
- Catalysts — the abstraction for knowledge *prosumers*, who emit enzymes whenever they interact with their compartment

B. Goals

Being $\mathcal{M}o\mathcal{K}$ a biochemically-inspired model, the main goal here is to deeply investigate the two key parameters involved in biochemical reactions highlighted in Subsection I-A, that is, *concentration* and *rate*. In particular, how they "collaborate" to influence $\mathcal{M}o\mathcal{K}$ reactions effect on system dynamics according to different functional dependencies. Accordingly, Section II describes in details some of the "desiderata" the $\mathcal{M}o\mathcal{K}$ model should fulfill and which kind of experiments are planned to understand how such requirements can be met.

II. Experiments Plan

A. Single-Compartment

Sources injection.: Although $\mathcal{M}o\mathcal{K}$ sources are not among the already-formalised abstractions, they clearly play a crucial role in a $\mathcal{M}o\mathcal{K}$ system, being the ultimate "origin" of information. As such, they should:

- on the one hand, perpetually inject $\mathcal{M}o\mathcal{K}$ atoms within the system, since there is no way to know a-priori *when* some information will be useful
- on the other hand, not flood the system without any control, both in order to save memory and to avoid exponential proliferation of information

Injection rate tuning toward these two contrasting needs is experimentally investigate in Subsection III-A.

Atoms decay.: It may appear unclear why $\mathcal{M}o\mathcal{K}$ atoms should fade away as time passes, most of all because this way a $\mathcal{M}o\mathcal{K}$ system can lose information. Nevertheless, if the persistent nature of $\mathcal{M}o\mathcal{K}$ sources – which are not consumed by injection reaction and are not subject to decay – is taken into account, it is easy to see that information is never really lost, because there is always some way to "restore" it—e.g., by simply temporarily increase injection rate of the correspondent source.

Therefore, atoms decay becomes an effective way to resemble the relationship between information relevance and time flow. In many application scenarios in fact, information tends (on average) to lose potential relevance as time passes by: journalistic news do so, academic papers do so, even health records do so to some extent. Furthermore, decay enforce some kind of *negative feedback* which, together with a *positive* one, enables the *feedback loop* peculiar in natural systems.

How $\mathcal{M}o\mathcal{K}$ decay reaction should depend on time is investigated in Subsection III-A.

Enzymes reinforcement.: To properly engineer $\mathcal{M}o\mathcal{K}$ reinforcement reaction rate, we must keep in mind what enzymes are and what their main purpose is: representing a *situated interest* manifested by a user (catalyst) w.r.t. an information chunk (atom/molecule) which, therefore, should become more relevant—e.g., by increasing its concentration. With the word "situated" we mean that reinforcement gained by atoms should take into account *situatedness* of users (inter-)actions along a number of dimensions: time, space, who interacts, how and so on.

For these reasons, $\mathcal{M}o\mathcal{K}$ reinforcement reaction should:

- be prompt, that is rapidly increase atoms concentration despite decay
- limited both in time and space, since relevance should be a time & space related feature of information, as already said
- be related to the nature of the interaction performed by the user, e.g. a "pick" action could inject more enzymes and/or reinforce atoms with greater stoichiometry w.r.t. a "search" action.

Experimental results in tuning $\mathcal{M}o\mathcal{K}$ reinforcement reaction functional rate going along this line are shown in Subsection III-A.

B. Multi-Compartment

First of all, a little "disclaimer" has to be made. My original plans for multi-compartment investigation was to use the BioPepa tool to experiment with a very high number of

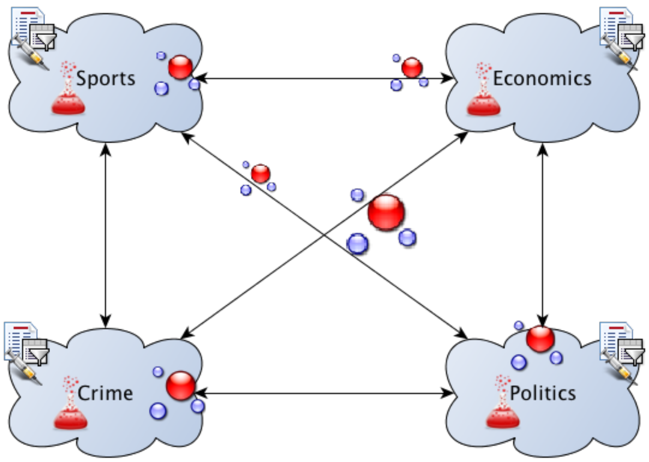

Fig. 1. Simple "topology" used for my multi-compartment experiments.

compartments, let's say a hundred and more, interconnected in the most random ways, to check if the "smart migration" pattern introduced in [7] could work and, if so, how diffusion rates could be tuned to drive such pattern behaviour. But, as soon as I read the paper on modeling biological compartments ([8]) and planned the first experiments, I understood that writing down a BioPepa specification for just ten compartments would be though, a hundred or so even infeasible.

So, in order to study the behaviour of $\mathcal{M}o\mathcal{K}$ diffusion reaction, all the experiments shown in Subsection II-A have been repeated in the simple multi-compartment setting shown in Fig. 1, in which any compartment can "communicate" with any other. The BioPepa specification used is the following:

```
// topology definition
location sports : size = 1, type = compartment;
location economics : size = 1, type = compartment;
location crime : size = 1, type = compartment;
location politics : size = 1, type = compartment;
```

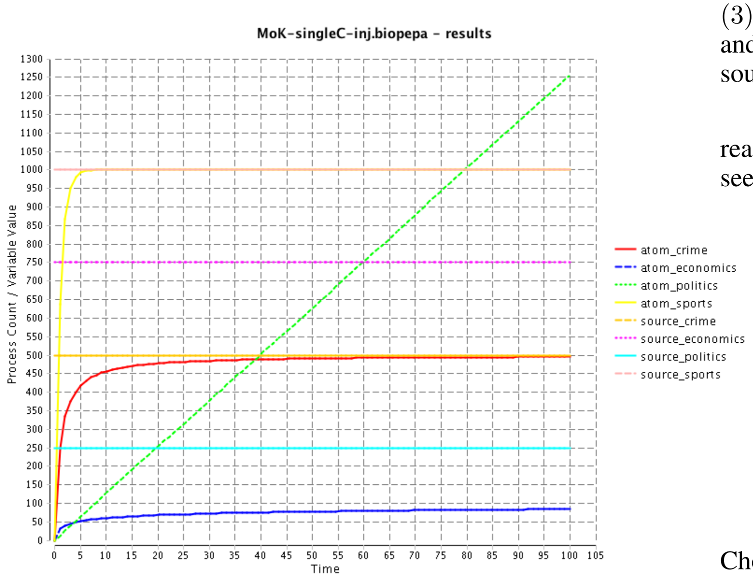

Fig. 2. Functional rates alternatives for $\mathcal{M}o\mathcal{K}$ sources. 30 Gillespie stochastic simulations have been performed.

Diffusion & injection.: The first set of experiments is devoted to study how $\mathcal{M}o\mathcal{K}$ diffusion reaction can affect sources' atoms injection behaviour. In particular, if some *spatial distribution* pattern can be reached and how functional rates should be designed to do so.

Diffusion & decay.: When adding diffusion to compartments in which injection and decay are already active, our main concern is that of keeping the same behaviours as those experimented in the single compartment scenario, that is, simply have a time-dependent decay, logarithmic in time and starting at a concentration value (for involved atoms) close as possible to sources own concentration.

Diffusion & reinforcement.: Since reinforcement is *local* by design, being $\mathcal{M}o\mathcal{K}$ enzymes unable to diffuse, our main concern regarding reinforcement reaction addition to diffusion and injection is to avoid interference. This means to design reinforcement's functional rate so as to preserve other chemical-like laws statistical behavior—that seen in the single compartment scenario.

III. Experiments Results

Stressing once again the incremental approach undertaken, in each of the following subsections is described one novel $\mathcal{M}o\mathcal{K}$ "behaviour" at a time, together with those previously defined, so as to end up with the (almost) full spectrum of cooperating behaviours.

A. *Single-Compartment Analysis*

Sources injection.: In the attempt to meet the requirements described in Subsection II-A, it seems three alternatives are possible:

1) making injection rates decreasing as time passes
2) enforce some "saturation" behaviour to stop injection
3) a combination of the two

Fig. 2 shows option (1) in blue, option (2) in yellow and option (3) in red. The green dashed line is for comparison purpose and plots the built-in fMA kinetic law. Horizontal lines are the sources, which participate injection reactions as activators.

Once discarded option (1), whose trend is too slow in reaching saturation compared to others, options (2) and (3) seem almost identical, but they aren't:

- option (2) in fact is saturation-driven only, which means that if at some point in time `atom_sports` will suddenly decrease in concentration – e.g. due to users interactions – they will go back to saturation-level as fast as possible, no matter how long their sources are within the system
- option (3) instead, by taking into account also the flow of time, makes the saturation process smoother, in particular, the longer `source_sports` are within the system the slower such process will be

Choosing among the two depends on the application-specific context in which the $\mathcal{M}o\mathcal{K}$ model is used, e.g., in $\mathcal{M}o\mathcal{K}$-`News` [6] option (3) is better, since in the news management scenario information loses relevance as time passes.

The BioPepa specification used to plot Fig. 2 is listed below.

```
// injection functional rates (sources => atoms)
injE = [source_economics/atom_economics * (1 / (1 + time))];
injS = [source_sports - atom_sports];
injC = [(1 / (1 + time)) * (source_crime - atom_crime)];
injP = [fMA(0.05)];

// sources inject atoms
source_economics =  (injE, 1) (+);
source_sports =     (injS, 1) (+);
source_crime =      (injC, 1) (+);
source_politics =   (injP, 1) (+);

// atoms are produced from sources (inj)
atom_economics =  (injE, 1) >>;
atom_sports =     (injS, 1) >>;
atom_crime =      (injC, 1) >>;
atom_politics =   (injP, 1) >>;

// System initial conditions
source_sports[1000] <*> source_economics[750] <*>
  source_crime[500] <*> source_politics[250] <*>
atom_sports[0] <*> atom_economics[0] <*> atom_crime[0] <*>
  atom_politics[0]
```

Atoms decay.: Time dependency alone is obviously not enough to have a meaningful decay behaviour: e.g., by using a fixed rate we end-up simply slowing down the saturation process enforced by sources injection reaction. Furthermore, as we already said, it is more interesting to study the interdependency between rates and concentration. Hence Fig. 3 shows basically three different combinations of time dependency and concentration dependency for *MoK* decay reaction—a fourth one (yellow line), non time-dependent, is given for comparison purpose:

i linear time dependency + relative concentration dependency (blue dashed line)
ii logarithmic time dependency + relative concentration dependency (red line)
iii linear time dependency + fixed rate, built-in fMA functional rate (green dashed line)

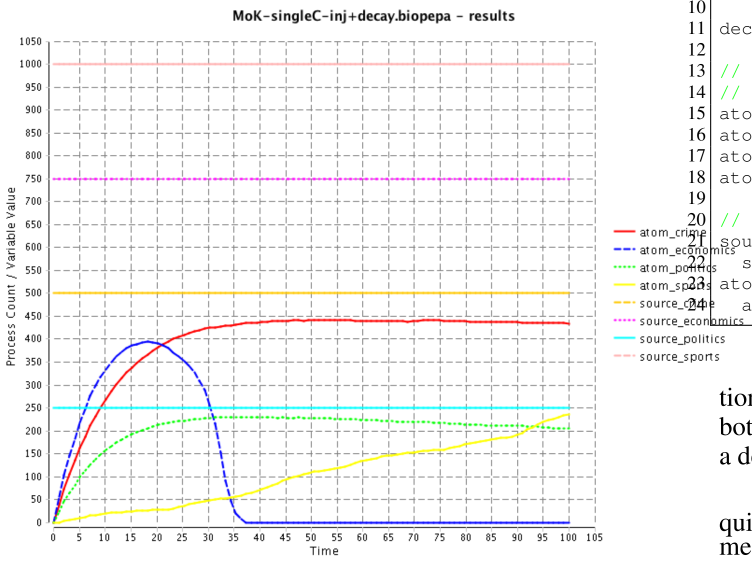

Fig. 3. Functional rates alternatives for *MoK* decay reaction. 30 Gillespie stochastic simulations have been performed.

Option (3) for sources injection reaction is assumed—see Subsection III-A.

Suddenly discarding option (i) and the fourth one due to their weird trend, options (ii) and (iii) seem viable solutions but also identical. Fig. 4 shows they're not identical at all, by plotting a longer time horizon. As we expected from the above description, option (ii) follows a logarithmic trend whereas option (iii) follows a linear one instead. Furthermore, as highlighted by the BioPepa specification listed below, also their dependency on concentrations is quite different.

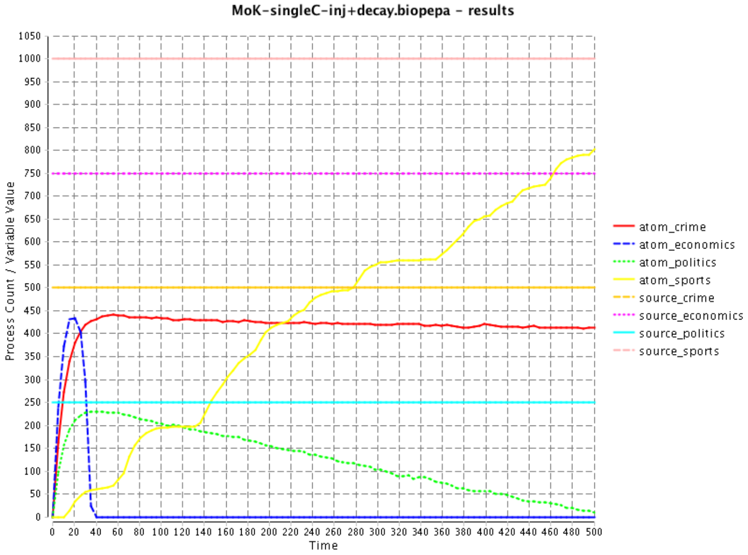

Fig. 4. Functional rates alternatives for *MoK* decay reaction. 30 Gillespie stochastic simulations have been performed.

```
// sources specification
...

// decay dynamic rates (atoms => _)
decayS = [H(atom_sports) * source_sports / atom_sports];
decayE = [H(atom_economics) *
            source_economics / atom_economics *
            time];
decayC = [H(atom_crime) * source_crime / atom_crime *
            log(1+time)];
decayP = [H(atom_politics) * fMA(der) * time];

// atoms are produced from sources (inj)
// and subject to decay (decay)
atom_sports =     (injS, 1) >> + (decayS, 1) <<;
atom_economics =  (injE, 1) >> + (decayE, 1) <<;
atom_crime =      (injC, 1) >> + (decayC, 1) <<;
atom_politics =   (injP, 1) >> + (decayP, 1) <<;

// System initial conditions
source_sports[1000] <*> source_economics[750] <*>
  source_crime[500] <*> source_politics[250] <*>
atom_sports[0] <*> atom_economics[0] <*> atom_crime[0] <*>
  atom_politics[0]
```

Notice usage of the Heaviside function, to prevent application of the reaction when there are no more atoms. Said that, both options are surely viable and, as for the case of injection, a decision should be made according to the application at hand.

Enzymes reinforcement.: Despite the three different requirements we highlighted in Subsection II-A, *MoK* reinforcement reaction functional rate was quite simple to design, as it can bee seen in the BioPepa specification listed below.

```
// sources specification
...
```

```

// decay specification
...

// reinforcement dynamic rates (enzymes => atoms)
feedS = [H(enzyme_sports) * (source_sports / atom_sports)];
feedE = [H(enzyme_economics) *
            (source_economics / atom_economics)];
feedC = [H(enzyme_crime) * (source_crime / atom_crime)];

// atoms are produced from sources (inj),
// subject to decay (decay)
// and reinforcement (feed)
atom_sports =     (injS, 1) >> + (decayS, 1) << +
                    (feedS, 10) >>;
atom_economics =  (injE, 1) >> + (decayE, 1) << +
                    (feedE, 10) >>;
atom_crime =      (injC, 1) >> + (decayC, 1) << +
                    (feedC, 10) >>;
atom_politics =   (injP, 1) >> + (decayP, 1) <<;

// enzymes "feed" atoms
enzyme_sports =     (feedS, 1) <<;
enzyme_economics =  (feedE, 1) <<;
enzyme_crime =      (feedC, 1) <<;

// System initial conditions
source_sports[1000] <*> source_economics[750] <*>
  source_crime[500] <*> source_politics[250] <*>
atom_sports[0] <*> atom_economics[0] <*> atom_crime[0] <*>
  atom_politics[0] <*>
enzyme_sports[300] <*> enzyme_economics[300] <*>
  enzyme_crime[300]
```

The reason is that we should take into account the other MoK reactions cooperating with reinforcement, so as to effectively achieve our desired behaviour. In particular, Fig. 5 shows:

- promptness of reinforcement, due to triggering of reinforcement reaction with a high rate as soon as enzymes are available
- time-boundedness, due to depletion of enzymes which stops the reinforcement reaction to trigger

Notice that, to simulate users interaction happening at a given point in time, we added the term e.g. `H(time-300)` as a multiplicative factor in reinforcement functional rate.

As regards the last desiderata for MoK reinforcement reaction, that is dependency from the nature of the interaction which caused enzymes release, Fig. 6 and Fig. 7 clearly highlight how an increment to enzymes concentration and atoms stoichiometry, respectively, affect reinforcement trend. In particular, Fig. 6 shows how an increment in enzymes concentration by a factor 2 directly causes a increment in reinforcement reaction duration by the same factor, whereas the atoms concentration "peak" reached is not affected at all. On the contrary, Fig. 7 shows that an increment in atoms stoichiometry within MoK reinforcement reaction by a factor 2 causes a much higher peak in atoms concentration, whereas reinforcement duration is not affected.

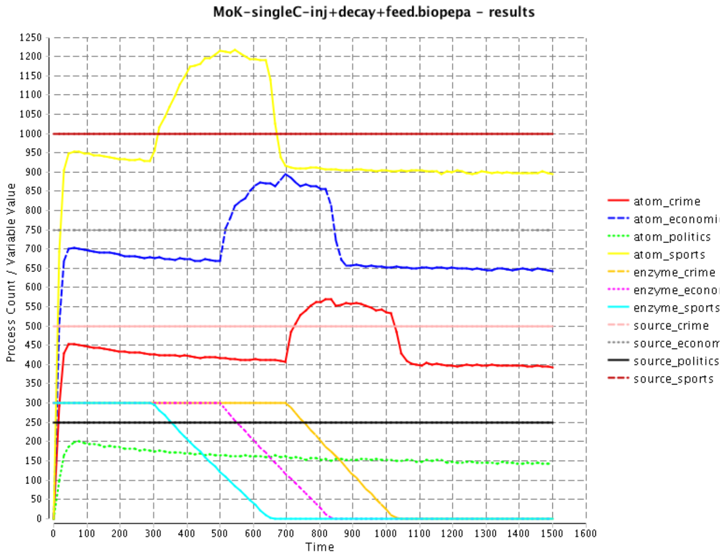

Fig. 5. MoK reinforcement reaction behaviour. 30 Gillespie stochastic simulations have been performed.

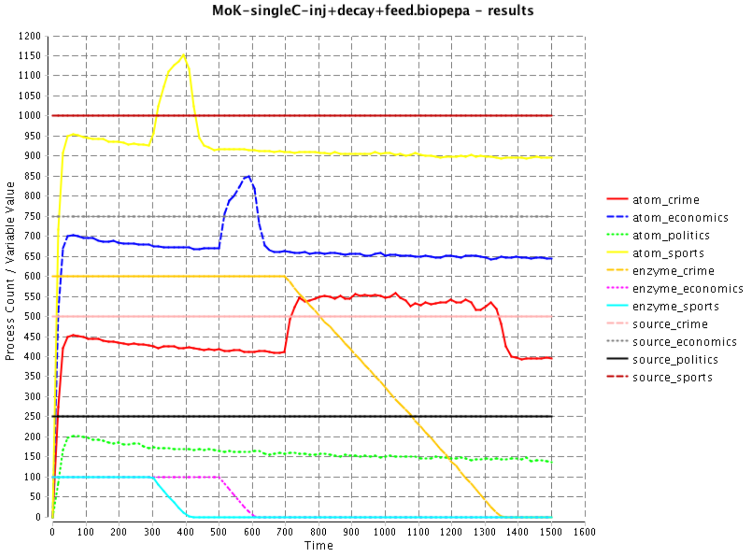

Fig. 6. Enzymes concentration increment effect on MoK reinforcement reaction behaviour. 30 Gillespie stochastic simulations have been performed.

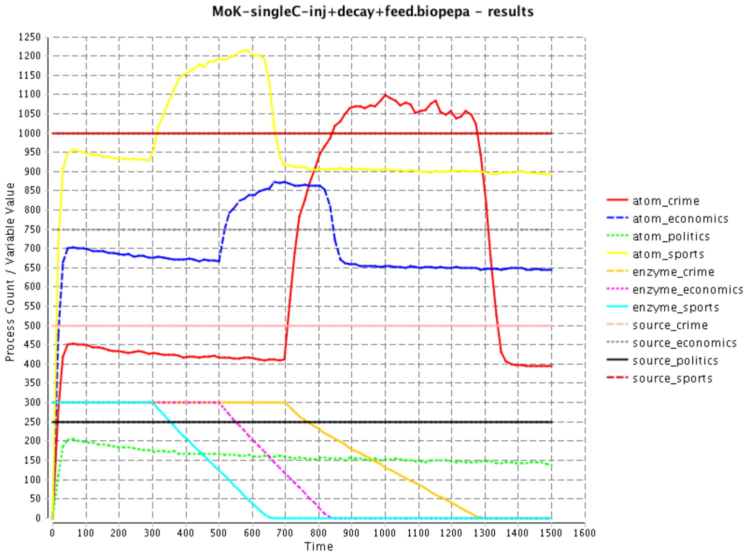

Fig. 7. Atoms stoichiometry increment effect onMoK reinforcement reaction behaviour. 30 Gillespie stochastic simulations have been performed.

B. Multi-Compartment Analysis

Diffusion & injection.: As an early specification of MoK diffusion functional rate, a simple consideration can be done: analogously to what we have done with injection, we would like to have some degree of control upon how much a given compartment diffuse toward another. In particular, it is reasonable to assume "destination" compartment to contain at most a fraction of "source" compartment atoms, at least if no other MoK reactions are working. Therefore, a saturation behaviour can be enforced on diffusion reaction as follows:

```
// sources specification
...

// diffusion weight
DW = 0.75;

// diffusion functional rates (a@x => a@y)
diffSE = [DW * as@sports - as@economics];
diffSC = [DW/2 * as@sports - as@crime];
diffSP = [DW/3 * as@sports - as@politics];
diffES = [DW * ae@economics - ae@sports];
diffEC = [DW * ae@economics - ae@crime];
diffEP = [DW * ae@economics - ae@politics];
diffCS = [DW * ac@crime - ac@sports];
diffCE = [DW * ac@crime - ac@economics];
diffCP = [DW * ac@crime - ac@politics];
diffPS = [DW * ap@politics - ap@sports];
diffPE = [DW * ap@politics - ap@economics];
diffPC = [DW * ap@politics - ap@crime];

// atoms are produced from sources (inj)
// and can diffuse (diff)
as =  (injS, 1) >> as@sports
        + (diffSE[sports->economics], 1) (.) as
        + (diffSC[sports->crime], 1) (.) as
        + (diffSP[sports->politics], 1) (.) as;
ae =  (injE, 1) >> ae@economics
        + (diffES[economics->sports], 1) (.) ae
        + (diffEC[economics->crime], 1) (.) ae
        + (diffEP[economics->politics], 1) (.) ae;
ac =  (injC, 1) >> ac@crime
        + (diffCS[crime->sports], 1) (.) ac
        + (diffCE[crime->economics], 1) (.) ac
        + (diffCP[crime->politics], 1) (.) ac;
ap =  (injP, 1) >> ap@politics
        + (diffPS[politics->sports], 1) (.) ap
        + (diffPE[politics->economics], 1) (.) ap
        + (diffPC[politics->crime], 1) (.) ap;

// System initial conditions
ss@sports[1000] <*> se@economics[750] <*> sc@crime[500] <*>
  sp@politics[250] <*>
as@sports[0] <*> as@economics[0] <*> as@crime[0] <*>
  as@politics[0] <*>
ae@economics[0] <*> ae@sports[0] <*> ae@crime[0] <*>
  ae@politics[0] <*>
ac@crime[0] <*> ac@sports[0] <*> ac@economics[0] <*>
  ac@politics[0] <*>
ap@politics[0] <*> ap@sports[0] <*> ap@economics[0] <*>
  ap@crime[0]
```

The result of such BioPepa specification is shown in Fig. 8.

As can be seen, a higher DW value leads to an higher saturation value in destination compartment, conveniently expressed as a fraction of source compartment atoms concentration.

Diffusion & decay.: Adding MoK diffusion reaction to our usual network of compartments in which both injection and decay behaviours are active, leads to a strange "malfunctioning" we didn't expect—Fig. 9. In particular, atoms strive to survive and succeed only in their origin compartment. Nevertheless, their concentration is anyway far from the desired saturation level achieved in the single compartment case.

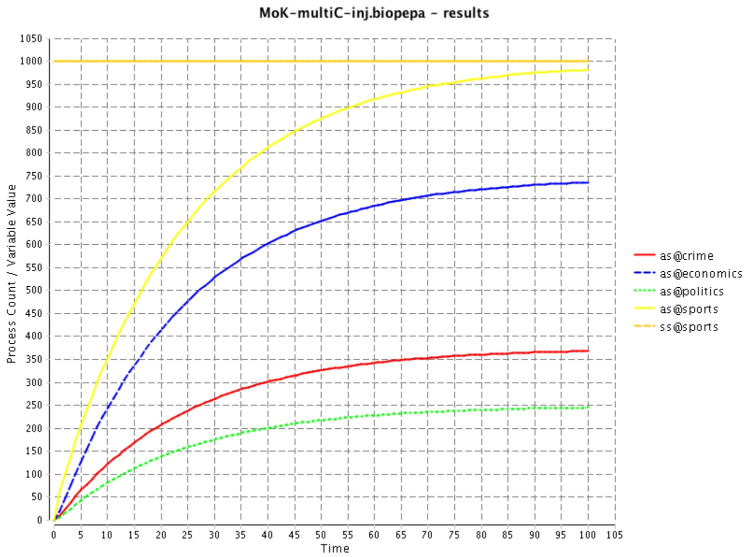

Fig. 8. DW parameter influence on MoK diffusion reaction. Only other MoK behaviour active is injection. Usual 30 Gillespie stochastic simulations have been performed.

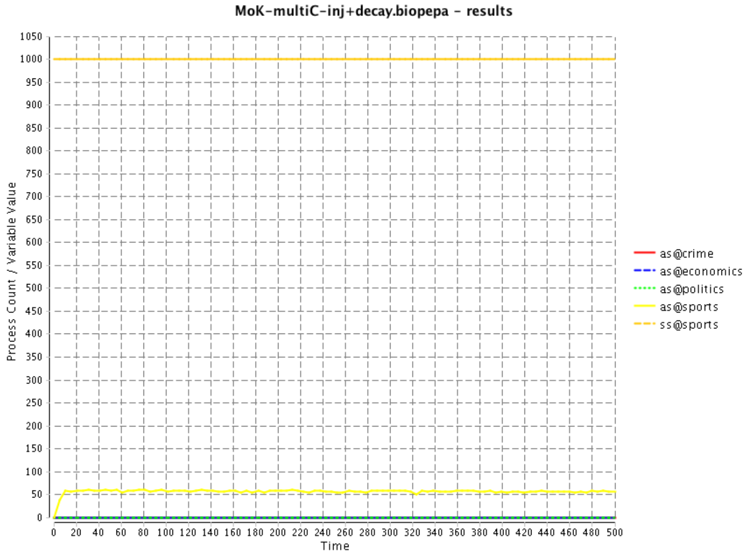

Fig. 9. Usual setting augmented with diffusion.

Such issue can be resolved quite easily by slightly modifying MoK decay functional rates, as shown by the BioPepa specification listed below.

```
// saturation & time weights
...
SATd = 0.75;
TIMEd = 1 - SATd;
// time exponential weight
EXP = 1.5;

// decay dynamic rates (atoms => _)
decaySS = [H(as@sports) * (
            (1 - SATd) * ss@sports / as@sports +
            TIMEd * log(1+time)^EXP
          )];
decaySE = [H(as@economics) * (
            (1 - SATd) * ss@sports / as@economics +
            TIMEd * log(1+time)^EXP
          )];
decaySC = [H(as@crime) * (
```

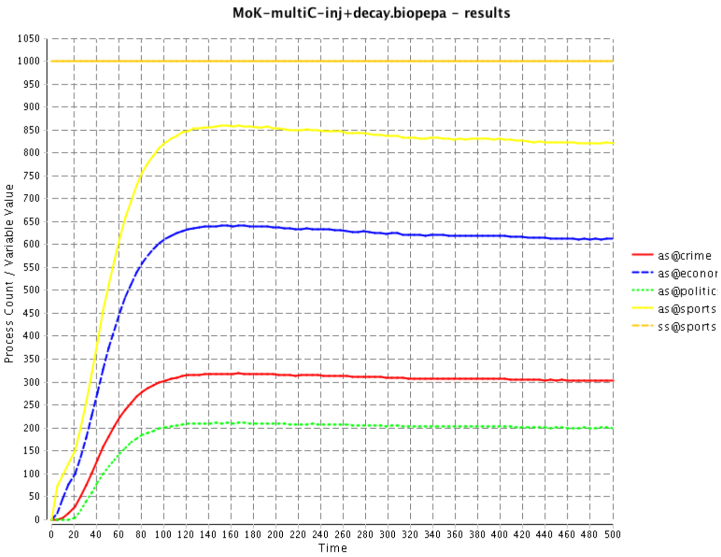

Fig. 10. *MoK* diffusion together with injection and decay, correct parameters tuning.

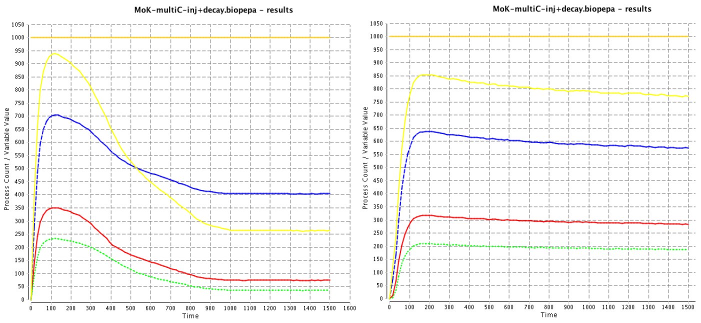

Fig. 11. Too high saturation weight (on the left) vs. correct saturation weight (no the right).

```
            (1 - SATd) * ss@sports / as@crime +
            TIMEd * log(1+time)^EXP
          )];
decaySP = [H(as@politics) * (
            (1 - SATd) * ss@sports / as@politics +
            TIMEd * log(1+time)^EXP
          )];
...
```

We can see that such new decay functional rate simply introduces two *weights* to tune saturation vs. time-dependancy. In particular, if SATd increases then atoms decay will depend more on relative concentration of decaying atoms w.r.t. sources. On the contrary, increasing TIMEd leads to a smoother curve and later saturation. After a bit of parameters tuning, the trend plotted in Fig. 10 can be achieved. Notice that, further increasing saturation parameter SATd leads to a worse behaviour, as shown by Fig. 11.In particular, although injection saturation is reached sooner, then decay abruptly comes in rapidly depleting atoms concentration, without following the "logarithmic-time" trend desired.

As a last note, although only sports atoms are shown in this subsection, others follow the same trend, so have been left out to ease plots understanding.

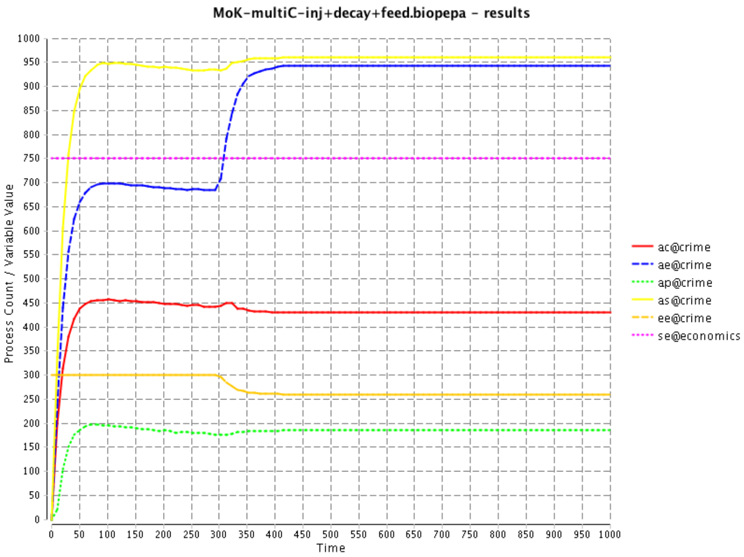

Fig. 12. Not only enzymes are not depleted, but also some interference with other reactions is clearly highlighted.

Diffusion & reinforcement.: Again, simply adopting the same functional rate used in the single compartment scenario leads to an unexpected, undesirable behaviour, depicted in Fig. 12. Not only enzymes are not completely depleted as we expect, but also some interference with other reactions is clearly highlighted: in particular, the concentrations of sports and crime atoms in crime compartment experiments some undesirable fluctuation. After some experiments changing reinforcement reaction functional rate dependencies, we found that only by adding another parameter to our model – actually, the fourth – the above issue could be successfully faced. Therefore, the BioPepa specification has been adjusted as follows:

```
// feed factor > 1
FF = 2;

// reinforcement functional rates (enzymes => atoms)
feedEC = [H(time-300) * H(ee@crime) *
             (se@economics / (ae@crime * FF))];

// atoms are [...] and to reinforcement (feed)
ae =  (injE, 1) >> ae@economics
        + (diffES[economics->sports], 1) (.) ae
        ...
        + (feedEC, 10) >> ae@crime;

// enzymes "feed" atoms
ee =  (feedEC, 1) << ee@crime;

// System initial conditions
ss@sports[1000] <*> ... <*> ee@crime[300]
```

In practice, a scaling factor is used to weight the influence of the atoms to be reinforced w.r.t. the concentration of the corresponding source in the compartment the latter belongs to.

Doing so leads to the behaviour depicted in Fig. 13, in which both no interference with other reactions happens as well as the correct reinforcement is given to involved atoms—e.g., they can go beyond sources' own threshold.

IV. Conclusion

Whereas Section III commented on single experiments results, describing expected outcomes, issues arose and how

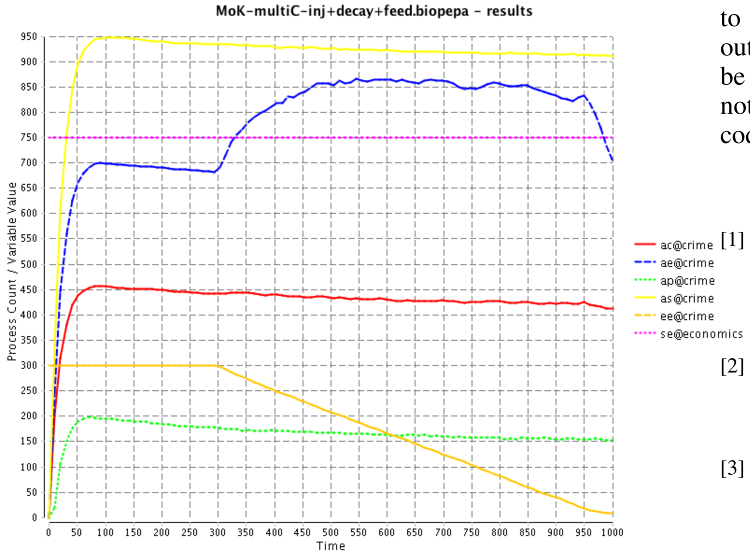

Fig. 13. With the adjusted reinforcement functional rate, we get no interference and the desired reinforcement trend.

I dealt with them in the attempt to get as close as possible to $\mathcal{M}o\mathcal{K}$ desired behaviour, in this section I will briefly comment the overall experience of using the BioPepa tool to experiment with the different $\mathcal{M}o\mathcal{K}$ model behaviours.

First of all, another disclaimer about experiments planning. As the reader may notice, $\mathcal{M}o\mathcal{K}$ aggregation reaction has been completely left out from the experiments plan. This is due to some kind of incompatibility between the modeling expressive power of BioPepa and $\mathcal{M}o\mathcal{K}$ aggregation reaction. In particular, aggregation demands for the capability to link a *possibly unbounded number* of atoms into a single molecule, which is something BioPepa cannot model effectively—because it wasn't meant to do so, obviously.

Furthermore, $\mathcal{M}o\mathcal{K}$ injection behaviour was not part of the initial experimental plan, as well as it is not part of the current formalisation of the $\mathcal{M}o\mathcal{K}$ model. But, as soon as the first experiments were done, suddenly it became clear that the way in which $\mathcal{M}o\mathcal{K}$ sources adds atoms to the system can deeply influence subsequent behaviour of all other $\mathcal{M}o\mathcal{K}$ reactions. Therefore, a first result concerning the $\mathcal{M}o\mathcal{K}$ model has been achieved, that is, precisely to recognize relevance and centrality of the injection behaviour. Thanks to this result, probably a $\mathcal{M}o\mathcal{K}$ injection reaction will be formalized and become part of the $\mathcal{M}o\mathcal{K}$ model set of *core reactions*.

Another important result achieved is related to $\mathcal{M}o\mathcal{K}$ reinforcement reaction. Prior to run experiments, I expected $\mathcal{M}o\mathcal{K}$ reinforcement reaction to require a long and painful tuning process, mostly due to its central role within the $\mathcal{M}o\mathcal{K}$ model. So it was surprising to see that despite the simple functional rate used, much of the tuning simply involves changing reinforcement stoichiometry and enzymes concentration, not the functional rate mathematical expression at all.

These considerations mainly arose during single-compartment experiments. As regards the multi-compartment plan of experiments, as I said the original goal was to experiment with *a plethora* of compartments, but it turned out to be a bad idea. Nevertheless, from the experiments carried out in the simpler setting of a 4-compartments network, it can be argued that even a much more complicated setting will not change the $\mathcal{M}o\mathcal{K}$ model behaviour—solely the "pain" of coding it.

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