Nets with Mana: A Framework for Chemical Reaction Modelling

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Abstract. We use categorical methods to define a new flavor of Petri nets where transitions can only fire a limited number of times, specified by a quantity that we call mana. We do so with chemistry in mind, looking at ways of modelling the behavior of chemical reactions that depend on enzymes to work. We prove that such nets can be either obtained as a result of a comonadic construction, or by enriching them with extra information encoded into a functor. We then use a well-established categorical result to prove that the two constructions are equivalent, and generalize them to the case where the firing of some transitions can "regenerate" the mana of others. This allows us to represent the action of catalysts and also of biochemical processes where the byproducts of some chemical reaction are exactly the enzymes that another reaction needs to work.

Acknowledgements The first author was supported by the project MIUR PRIN 2017FTXR7S “IT-MaTTerS” and by the Independent Ethvestigator Program.

The second author was supported by the ESF funded Estonian IT Academy research measure (project 2014-2020.4.05.19-0001).

A video presentation of this paper can be found on Youtube at 9sxVBJs1okE.

1 Introduction

Albeit they have found great use outside their original domain, Petri nets were invented to describe chemical reactions [21]. The interpretation is as simple as it can get: places of the net represent types of compounds (be it atoms or molecules); tokens represent the amount of each combination we have available; transitions
represent reactions transforming compounds.

\[
\begin{array}{c}
\text{ATP} \\ \text{H}_2\text{O} \\ \text{P}^\text{\text{\textit{i}}}
\end{array} \quad \rightarrow \quad \begin{array}{c}
\text{ATP} \\ \text{H}_2\text{O} \\ \text{P}^\text{\textit{i}} \\
\end{array}
\]

\[
\begin{array}{c}
\text{ADP} \\ \text{P}^\text{\textit{i}}
\end{array}
\]

(1)

Still, things are not so easy in real-world chemistry: reactions often need “context” to happen, be it a given temperature, energy, presence of enzymes and catalysts. This is particularly true in biochemical processes, where enzymes of all sorts mediate rather complicated reactions. Importantly, these enzymes tend to degrade over time, resulting in reactions that do not keep happening forever [14]. This is one of the (many) reasons why organisms wither and die, but it is not captured by the picture above, where the transition can fire every time it is enabled.

Borrowing the terminology from the popular Turing machine Magic: The gathering [24, 7] we propose a possible solution to this problem by endowing transitions in a net with mana [23], representing the “viability” of reactions: once a reaction is out of mana, it cannot fire anymore.

Now, we could just represent mana by adding another place for each transition in a net. Indeed, this is the idea we will start with. Still, being accustomed to the yoga of type-theoretic reasoning, we are also aware that throwing everything in the same bucket is rarely a good idea: albeit mana can be a chemical compound, it is more realistic to consider it as conceptually separated from the reactions it catalyzes.

Resorting to categorical methods, we show how we can axiomatize the idea of mana in a better way. We do so by relaxing the definitions in the categorical approach to coloured nets already developed in [13], defining a functorial semantics representing the equipment of a net with mana. Then, we will prove how categorical techniques allow us to internalize such a semantics, exactly obtaining what we represented in the picture above.

Finally, we will show how the categorical semantics naturally leads to a further generalization, where transitions not only need mana to function but also provide byproducts that can be used as mana for other transitions. This allows us to represent catalysts\(^4\) (i.e. cards ‘adding \(\infty\) to the mana pool’, or more precisely mana that does not deteriorate over time) and in general nets apt to describe two-layered chemical processes, the first layer being the usual one represented by Petri nets and the second layer being the one of enzymes and catalysts being consumed and exchanged by different reactions.

\[^4\text{An unrelated categorical approach to nets with catalysts can be found in [2].}\]
2 Nets and their executions

Before presenting the construction itself, it is worth recappping the main points about categorical semantics for Petri nets. The definition of net commonly used in the categorical line of work is the following:

**Notation 1.** Let $S$ be a set; denote with $S^{\oplus}$ the set of finite multisets over $S$. Multiset sum will be denoted with $\oplus$, multiplication with $\odot$ and difference (only partially defined) with $\ominus$. $S^{\oplus}$ with $\oplus$ and the empty multiset is isomorphic to the free commutative monoid on $S$.

**Definition 1 (Petri net).** We define a Petri net as a couple functions $T \xrightarrow{s,t} S^{\oplus}$ for some sets $T$ and $S$, called the set of places and transitions of the net, respectively.

A morphism of nets is a couple of functions $f : T \rightarrow T'$ and $g : S \rightarrow S'$ such that the following square commutes, with $g^{\oplus} : S^{\oplus} \rightarrow S'^{\oplus}$ the obvious lifting of $g$ to multisets:

\[
\begin{array}{ccc}
S^{\oplus} & \xrightarrow{s} & T \xrightarrow{t} S^{\oplus} \\
S'^{\oplus} & \xleftarrow{s'} & T' \xrightarrow{t'} S'^{\oplus} \\
\end{array}
\]

Petri nets and their morphisms form a category, denoted Petri. The reader can find additional details in [18].

**Definition 2 (Markings and firings).** A marking for a net $T \xrightarrow{s,t} S^{\oplus}$ is an element of $S^{\oplus}$, representing a distribution of tokens in the net places. A transition $u$ is enabled in a marking $M$ if $M \ominus s(u)$ is defined. An enabled transition can fire, moving tokens in the net. Firing is considered an atomic event, and the marking resulting from firing $u$ in $M$ is $M \ominus s(u) \oplus t(u)$.

Category theory provides a slick definition to represent all the possible executions of a net – all the ways one can fire transitions starting from a given marking – as morphisms in a category. There are various ways to do this [18, 17, 22, 11, 12, 3], depending if we want to consider tokens as indistinguishable (common-token philosophy) or not (individual-token philosophy). In this work, we focus on chemical reactions. Since we consider atoms and molecules of the same kind to be physically indistinguishable, we will adopt the common-token perspective. In this case, the category of executions of a net is a commutative monoidal category – a monoidal category whose monoid of objects is commutative.
Definition 3 (Category of executions – common-token philosophy). Let $N : T \xrightarrow{s,t} S^\oplus$ be a Petri net. We can generate a free commutative strict monoidal category (FCSMC), $\mathcal{C}(N)$, as follows:

- The monoid of objects is $S^\oplus$. Monoidal product of objects $A, B$, denoted with $A \oplus B$, is given by the multiset sum;
- Morphisms are generated by $T$: each $u \in T$ corresponds to a morphism generator $(u, su, tu)$, pictorially represented as an arrow $su \rightarrow tu$; morphisms are obtained by considering all the formal (monoidal) compositions of generators and identities.

The readers can find a detailed description of this construction in [17].

As shown in the picture above, objects in $\mathcal{C}(N)$ represent markings of a net: $A \oplus A \oplus B$ means “two tokens in $A$ and one token in $B$”. Morphisms represent executions of a net, mapping markings to markings. A marking is reachable from another one if and only if there is a morphism between them.

The correspondence between Petri nets and their executions is categorically well-behaved, defining an adjunction between the category Petri and the category CSMC of commutative strict monoidal categories, with Definition 3 building the left-adjoint Petri $\rightarrow$ CSMC. The readers can find additional details in [17].

3 The internal mana construction

The idea presented in the introduction can naively be formalised by just attaching an extra input place to any transition in a net, representing the mana a given transition can consume. We call the following construction internal because it builds a category directly, in contrast with an external equivalent construction given in Definition 7.
Definition 4 (Internal mana construction). Let $N : T \to S \otimes$ be a Petri net, and consider $\mathcal{C}(N)$, its corresponding FCSMC. The internal mana construction of $N$ is given by the FCSMC $\mathcal{C}_M(N)$ generated as follows:

- The generating objects of $\mathcal{C}_M(N)$ are the coproduct of the generating objects of $\mathcal{C}(N)$ and $T$;
- For each generating morphism $A_1 \oplus \cdots \oplus A_n \to B_1 \oplus \cdots \oplus B_m$ in $\mathcal{C}(N)$, we introduce a morphism generator in $\mathcal{C}_M(N)$:

$$A_1 \oplus \cdots \oplus A_n \oplus u \to B_1 \oplus \cdots \oplus B_m$$

Notice that the writing above makes sense because $u$ is an element of $T$.

Because of the adjunction between Petri and CSMC, we can think every FCSMC as being presented by a Petri net. The category of Definition 4 is presented precisely by the net obtained from $N$ as we did in Section 1: the additional generating objects of $\mathcal{C}_M(N)$ represent the places containing the mana associated with each transition.

Example 1. Performing the construction in Definition 4 on the category of executions of the net on the left gives the category of executions of the net on the right, as we expect:

![Diagram of two nets with mana]

Proposition 1. The assignment $\mathcal{C}(N) \mapsto \mathcal{C}_M(N)$ defines a comonad\(^5\) in the category of FCMSCs and strict monoidal functors between them, FCSMC.

Proof. First of all, we have to prove that the procedure is functorial. For any strict monoidal functor $F : \mathcal{C}(N) \to \mathcal{C}(M)$ we define the action on morphisms $\mathcal{C}_M(F) : \mathcal{C}_M(N) \to \mathcal{C}_M(M)$ as the following monoidal functor:

- $\mathcal{C}_M(F)$ agrees with $F$ on generating objects coming from $\mathcal{C}(N)$. If $u$ is a generating morphism of $\mathcal{C}(N)$ and it is $Fu = f$, then $\mathcal{C}_M(F)u = f^N$, with $f^N$ being the multiset\(^6\) counting how many times each generating morphism of $\mathcal{C}(M)$ is used in $f$.

\(^5\) Given a category $\mathcal{C}$, a comonad on $\mathcal{C}$ is an endofunctor $S$ endowed with two natural transformations $\delta : S \Rightarrow S \circ S$ and $\epsilon : S \Rightarrow 1_\mathcal{C}$ such that $\delta$ is coassociative and has $\epsilon$ as a counit. More succinctly, a comonad is a comonoid in the monoidal category $[\mathcal{C}, \mathcal{C}]$ of endofunctors of $\mathcal{C}$. See [20, §5.3] for the definition and a variety of examples.

\(^6\) This makes sense since $\mathcal{C}(M)$ is free, hence decomposition of morphisms in terms of (monoidal) compositions of generators and identities is unique modulo the axioms of monoidal categories, which do not introduce nor remove generating objects.
– $\mathcal{C}_M(F)$ agrees with $F$ on generating morphisms.

Identities and compositions are clearly respected, making $\mathcal{C}_M(\_)$ an endofunctor in $\text{FCSMC}$. As a counit, on each component $N$ we define the strict monoidal functor $\epsilon_N : \mathcal{C}_M(N) \to \mathcal{C}(N)$ sending:

– Generating objects coming from $\mathcal{C}(N)$ to themselves, and every other generating object to the monoidal unit.
– Generating morphisms to themselves.

The procedure is natural in the choice of $N$, making $\epsilon$ into a natural transformation $\mathcal{C}_M(\_ \to \text{id}_{\text{FCMC}}$.

As for the comultiplication, on each component $N$ we define the strict monoidal functor $\delta_N : \mathcal{C}_M(\mathcal{C}_M(N)) \to \mathcal{C}_M(\mathcal{C}_M(N))$ sending:

– Generating objects coming from $\mathcal{C}(N)$ to themselves, every other generating object $u$ is sent to $u \oplus u$.
– Generating morphisms are again sent to themselves.

The naturality of $\delta$ and the comonadicity conditions are a straightforward check.

4 The external mana construction

As we stressed in Section 1, the construction as in Definition 4 has the disadvantage of throwing everything in the same bucket: in performing it, we do not keep any more a clear distinction between the different layers of our chemical reaction networks, given by mana and compounds.

In the spirit of [13], we now recast the mana construction externally, as Petri nets with a semantics attached to them. A semantics for a Petri net is a functor from its category of executions to some other monoidal category $\mathcal{S}$.

A huge conceptual difference is that in [13] this functor was required to be strict monoidal. This point of view backed up the interpretation that a semantics “attaches extra information to tokens”, to be used by the transitions somehow. In here, we require this functor to be lax-monoidal: lax-monoidal amounts to saying that we can attach non-local information to tokens: tokens may “know” something about the overall state of the net and the laxator represents the process of “tokens joining knowledge”.

In terms of mana construction, we want to endow each token with a local “knowledge” of how much mana each transition has available. Laxating amounts to consider ensembles of tokens together – as entangled, if you wish – where their knowledge is merged.

A lax monoidal functor between two monoidal categories $(\mathcal{C}, \boxtimes J), (\mathcal{D}, \otimes, I)$ is a functor $F : \mathcal{C} \to \mathcal{D}$ endowed with maps $m : FA \otimes FB \to F(A \boxtimes B)$ and $u : I \to FJ$ satisfying suitable coherence conditions; see [16, Def. 3.1]. If $m, u$ are isomorphisms in $\mathcal{D}$, $F$ is called strong monoidal. If just $u$ is an isomorphism, $F$ is called normal monoidal.
**Example 2.**

If token $a$ knows that transition $u$ has 3 mana left, and token $b$ knows that transitions $u$ and $v$ have 1 and 8 mana left, respectively, then tokens $a$ and $b$, considered together, know that transitions $u$ and $v$ have $3 + 1 = 4$ and $0 + 8 = 8$ mana left, respectively.

**Definition 5 (Non-local semantics – common-token philosophy).** Let $N$ be a Petri net and let $S$ be a monoidal category. A **Petri net with a non-local commutative semantics** is a couple $(N, N^\#)$, with $N^\#$ a lax-monoidal functor $\mathbb{C}(N) \to S$. A morphism $(N, N^\#) \to (M, M^\#)$ of Petri nets with commutative semantics is a strict monoidal functor $\mathbb{C}(N) \overset{F}{\rightarrow} \mathbb{C}(M)$.

We denote the category of Petri nets with non-local commutative semantics with $\text{Petri}_S$.

We now provide an external version of the mana construction.

**Notation 2.** We denote with $\text{Span}$ the bicategory of sets, spans and span morphisms between them. Recall that a morphism $A \to B$ in $\text{Span}$ consists of a set $S$ and a pair of functions $A \leftarrow S \rightarrow B$. When we need to notationally extract this information from $f$, we write $A \leftarrow S_f \rightarrow B$. We sometimes consider a span as a morphism $f : S_f \to A \times B$, thus we may write $f(s) = (a, b)$ for $s \in S_f$ with $f_1(s) = a$ and $f_2(s) = b$. Recall moreover that a 2-cell in $\text{Span}$ $f \Rightarrow g$ is a function $\theta : S_f \rightarrow S_g$ such that $f = g \circ \theta$.

Observe that there is nothing in the previous definition of $\text{Span}$ that requires the objects to be mere sets; in particular, we will later employ the following variation on Notation 2:

**Definition 6 (Spans of pointed sets).** Define a bicategory $\text{Span}_\bullet$ of spans of pointed sets objects the pointed sets, $(A, a)$ where $a \in A$ is a distinguished element; composition of spans is as expected.

**Remark 1.** This is in turn just a particular case of a more general construction: let $\mathcal{C}$ be a category with pullbacks; then, there is a bicategory $\text{Span}\mathcal{C}$ having 1-cells the spans $A \leftarrow X \to B$ of morphisms of $\mathcal{C}$, and where a pullback of their adjacent legs defines the composition of 1-cells. Evidently, $\text{Span} = \text{Span}(\text{Set})$ and $\text{Span}_\bullet = \text{Span}(\text{Set}_\bullet)$, where $\text{Set}_\bullet$ is the category of pointed sets $(A, a)$ and maps that preserve the distinguished elements of the domain and codomain. See [9, §2] and [8] for a way more general perspective on bicategories of the form $\text{Span}\mathcal{C}$ and the universal property of the $\text{Span}$ construction.

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8 See [6, Def. 1.1] for the definition of bicategory; intuitively, in a bicategory, one has objects (0-cells), 1-cells and 2-cells, and composition of 1-cells is associative and unital up to some specified invertible 2-cells $F(GH) \cong (FG)H$ and $F1 \cong F \cong 1F$. 

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Nets with Mana: A Framework for Chemical Reaction Modelling
Definition 7 (External mana construction). Given a Petri net $N : T \xrightarrow{\delta} S^\oplus$, define the following functor $N^\sharp : \mathcal{C}(N) \to \text{Span}$:

- Each object $A$ of $\mathcal{C}(N)$ is mapped to the set $T^\oplus$, the set of multisets over the transitions of $N$;
- Each morphism $A \xrightarrow{f} B$ is sent to the span $N^\sharp f$ defined as:

$$T^\oplus \xleftarrow{\oplus f^\oplus} T^\oplus = T^\oplus$$

With $f^\oplus$ being the multiset counting how many times each generating morphism of $\mathcal{C}(M)$ is used in $f$.

Proposition 2. The functor of Definition 7 is lax monoidal. Functors as in Definition 7 form a subcategory of $\text{Petri}^{\text{Span}}$, which we call $\text{Petri}^\mathcal{M}$.

Proof. Functor laws are obvious: $\text{id}_N^\sharp$ is the empty multiset for each object $A$, hence $N^\sharp \text{id}_A = \text{id}_{T^\oplus}$. This correspondence preserves composition since

$$
\begin{array}{ccc}
T^\oplus & \xrightarrow{-\oplus g^\oplus} & T^\oplus \\
\downarrow & & \downarrow \\
T^\oplus & \xrightarrow{\oplus f^\oplus} & T^\oplus \\
\end{array}
\quad
\begin{array}{ccc}
T^\oplus & \xrightarrow{-\oplus g^\oplus} & T^\oplus \\
\downarrow & & \downarrow \\
T^\oplus & \xrightarrow{-\oplus f^\oplus} & T^\oplus \\
\end{array}
\quad
\begin{array}{ccc}
T^\oplus & \xrightarrow{-\oplus f^\oplus} & T^\oplus \\
\downarrow & & \downarrow \\
T^\oplus & \xrightarrow{-\oplus g^\oplus} & T^\oplus \\
\end{array}
$$

The laxator is the morphism $S^\oplus \times S^\oplus \xrightarrow{\otimes} S^\oplus$ that evaluates two multisets to their sum, embedded in a span. The naturality condition for the laxator reads:

$$
\begin{array}{ccc}
T^\oplus \times T^\oplus & \xrightarrow{N^\sharp f \times N^\sharp g} & T^\oplus \times T^\oplus \\
\downarrow & & \downarrow \\
T^\oplus & \xrightarrow{N^\sharp(f \otimes g)} & T^\oplus \\
\end{array}
$$

And the two morphisms from $T^\oplus \times T^\oplus \to T^\oplus$ are:

$$
\begin{array}{ccc}
T^\oplus \times T^\oplus & \xrightarrow{-\oplus f^\oplus \times -\oplus g^\oplus} & T^\oplus \\
\downarrow & & \downarrow \\
T^\oplus \times T^\oplus & \xrightarrow{(-\oplus f^\oplus) \times (-\oplus g^\oplus)} & T^\oplus \\
\downarrow & & \downarrow \\
T^\oplus \times T^\oplus & \xrightarrow{-\oplus f^\oplus \otimes g^\oplus} & T^\oplus \\
\end{array}
= 
\begin{array}{ccc}
T^\oplus \times T^\oplus & \xrightarrow{-\oplus f^\oplus \times -\oplus g^\oplus} & T^\oplus \\
\downarrow & & \downarrow \\
T^\oplus \times T^\oplus & \xrightarrow{(-\oplus f^\oplus) \times (-\oplus g^\oplus)} & T^\oplus \\
\downarrow & & \downarrow \\
T^\oplus \times T^\oplus & \xrightarrow{-\oplus f^\oplus \otimes g^\oplus} & T^\oplus \\
\end{array}
$$

which evidently coincide. Interaction with the associators, unitors and symmetries of the monoidal structure is guaranteed by the fact that they are all identities in $\mathcal{C}(N)$.
The external mana construction has the advantage of keeping the reaction layer and the mana layer separated completely. In this setting, we say that a marking of the net is a couple \((X, u)\), with \(X\) an object of \(\mathcal{C}(N)\) and \(u \in T^\oplus\) representing the initial distribution of mana for our transitions. A transition \(X \xrightarrow{f} Y\) is again a generating morphism of \(\mathcal{C}(N)\), and we say that it is enabled if \(N \hat{\delta} f_1\) hits \(u\), or, more explicitly, if \(u \ominus f N\) is defined. Since \(f N\) for \(f\) a morphism generator is defined to be 0 everywhere and 1 on \(f\), this amounts to say that \(f\) is enabled when \(u(f) - 1 \geq 0\). In that case, the resulting marking after the firing is \((Y, u(f) - 1)\): Each firing just decreases the mana of the firing transition by 1.

Example 3. Consider the net

\[
\begin{array}{c}
\text{compound A} \\
\text{compound B} \\
\text{compound C}
\end{array}
\]

In the marking \((A \oplus B, 2)\), the transition is enabled. The resulting marking will be \((C, 1)\). The transition is not enabled in the marking \((A \oplus B, 0)\) or \((A, 4)\).

4.1 Internalization

Having given two different definitions of endowing a net with mana, it seems fitting to say how the two are connected. As we already stressed, we abide by the praxis already established in [13] and prove that the external and internal mana constructions describe the same thing from different points of view:

**Theorem 1.** Let \((N, N^\#)\) be an object of \(\text{Petri}^N\). The category \(\mathcal{C}_M(N)\) of Definition 4 is isomorphic to the category of elements \(\int N^\#\). Explicitly:

- **Objects of** \(\int N^\#\) **are couples** \((X, x)\) **where** \(X\) **is a object of** \(\mathcal{C}_M(N)\) **and** \(x \in N^\# X\).
- **Morphisms** \((X, x) \to (Y, y)\) **of** \(\int N^\#\) **are morphisms** \((f, s)\) **with** \(f : X \to Y\) **of** \(\mathcal{C}_M(N)\) **and** \(s\) **such that** \(N^\# f s = (x, y)\).

**Proof.** First of all, we need to define a commutative strict monoidal structure on \(\int N^\#\). Given the particular shape of \(N^\#\), the objects of its category of elements are pairs where the first component is a multiset on the places of \(N\) and the second one is a multiset on its transition. Hence we can define:

\[(C, x) \boxtimes (D, y) := (C \oplus D, x \oplus y)\]

---

9 The category of elements of a functor \(F : \mathcal{C} \to \text{Set}\) is defined having objects the pairs \((C, x)\), where \(x \in FC\), and morphisms \((C, x) \to (C', x')\) the morphisms \(u : C \to C'\) such that \(Fu\) sends \(x\) into \(x'\). See [4, p. 12.2], where this is called the Grothendieck construction performed on \(F\). Here we need to tweak this construction in order for it to make sense for lax functors valued in \(\text{Span}\), using essentially the same technique in [19].
(Note that in order to obtain an element in \( N^\sharp(C \oplus D) \), we have implicitly applied the laxator \( \oplus : N^\sharp C \times N^\sharp D \to N^\sharp(C \oplus D) \) to the elements in the second coordinate.) Commutativity of \( \otimes \) follows from the commutativity of \( \oplus \).

On morphisms, if we have \((A_1, x_1) \xrightarrow{(f_1, s_1)} (B_1, y_1)\) and \((A_2, x_2) \xrightarrow{(f_2, s_2)} (B_2, y_2)\) then it is \( N^\sharp f_1 s_1 = (x_1, y_1) \) and \( N^\sharp f_2 s_2 = (x_2, y_2) \), and hence by naturality of the laxator \( N^\sharp(f_1 \oplus f_2)(s_1, s_2) = ((x_1 \oplus x_2), (y_1 \oplus y_2)) \), allowing us to set \( f_1 \otimes f_2 = f_1 \oplus f_2 \). Associators and unitors are defined as in \( \mathcal{E}(N) \).

Now we prove freeness: by definition, objects are a free monoid generated by couples \((p, I)\) and \((I, u)\) with \( p \) a generating object of \( \mathcal{C}(N) \) (a place of \( N \)), \( u \) a generating morphism of \( \mathcal{C}_M(N) \) (a transition of \( N \)), and \( I \) the tensor unit. These generators are in bijection with the coproduct of places and transitions of \( N \). As such, the monoid of objects of \( \int N^\sharp \) is isomorphic to the one of \( \mathcal{C}_B(N) \).

On morphisms, notice that every morphism in \( \int N^\sharp \) can be written univocally – modulo the axioms of a commutative strict monoidal category – as a composition of monoidal products of identities and morphisms of the form \((A, u) \xrightarrow{(f, u)} (B, u')\), with \( f \) a morphism generator in \( \mathcal{C}(N) \) and \( u = u' \oplus f^\text{hl} \).

The isomorphism between \( \int N^\sharp \) and \( \mathcal{C}_B(N) \) follows by observing that the following mappings between objects and morphism generators are bijections:

\[
(A, u) \mapsto A \oplus u
\]

\[
(A, u) \xrightarrow{(f, u)} (B, u') \mapsto A \oplus u \xrightarrow{f} B \oplus u'
\]

**Example 4.** The internalization of the net in Example 3 gives exactly the net of Example 1.

## 5 Extending the mana construction

Focusing more on the external mana construction of Definition 7, we realize that it is somehow restrictive: it makes sense to map each generating object of an FCSMC \( \mathcal{C}_M(N) \) to the set of multisets over the transitions of \( N \). This construction captures the idea of endowing each transition with an extra place representing its mana. On the other hand, the only requirement we would expect on morphisms is that, to fire, a transition must consume mana only from its mana pool. In Definition 7 we do much more than this, hardcoding that “one firing = one mana” in the structure of the functor.

The act of replacing the mapping on morphisms in Definition 7 with the following span provides a reasonable generalization of the previous perspective:

\[
\begin{array}{c}
\text{T}^\oplus \\
\xleftarrow{\oplus (\alpha \circ f^\text{hl})} \\
\xrightarrow{\oplus (\beta f)} \text{T}^\oplus
\end{array}
\]

with \( \alpha \) and \( \beta f \) arbitrary multisets. In doing so, the only thing we are disallowing in our new definition is for transitions to consume mana of other transitions: each transition may use only the mana in its pool. Still, it is now possible for transitions to:
Nets with Mana: A Framework for Chemical Reaction Modelling

– Fire without consuming mana;
– Consume more than 1 unit of mana to fire;
– Produce mana – also for other transitions – upon firing.

These are all good conditions in practical applications. The first models chemical reactions that do not need any additional compound to work; the second aims to model reactions that need more than one molecule of a given compound to work; the third models both catalysts – which completely regenerate their mana at the end of the reactions they aid – and reactions that produce, as byproducts, enzymes needed by other reactions.

**Example 5.** It is worth giving an explicit description of how the internalized version of a net, as in our attempted generalized definition, looks like. In the picture below, each transition has its mana, but now this mana does not have to be necessarily used, as for transition $u_1$, or can be used more than once, as for transition $u_2$. Furthermore, transitions such as $u_3$ regenerate their mana after firing (catalysts), while transitions such as $u_2$ and $u_4$ produce mana for each other in a closed loop. $u_4$ also produces more than one kind of mana as a byproduct of its firing. It is worth noticing that this formalism allows to model nets that never run out of mana, and that we think of as “self-sustaining” [14].

When looking at technicalities, unfortunately, things are not so easy. Defining $\alpha$ and the family $\beta_f$ so that functorial laws are respected is tricky. Luckily enough, we do not need to do so explicitly. Indeed, we can generalize the internal mana-net construction of Definition 4 to the following one, that subsumes nets as in Example 5:

**Definition 8 (Generalized internal mana construction).** Let $N : T \xrightarrow{\alpha_f} S^\oplus$ be a Petri net, and consider $\mathcal{C}(N)$, its corresponding FCSMC. A *generalized internal mana construction* for $N$ is any FCSMC $\mathcal{C}_M(N)$ such that:

– The generating objects of $\mathcal{C}_M(N)$ are the coproduct of the generating objects of $\mathcal{C}(N)$ and $T$;
– Generating morphisms

$$A_1 \oplus \cdots \oplus A_n \xrightarrow{u_f} B_1 \oplus \cdots \oplus B_m$$

in $\mathcal{C}(N)$ are in bijection with generating morphisms in $\mathcal{C}_M(N)$:

$$A_1 \oplus \cdots \oplus A_n \oplus U_1 \xrightarrow{u_f} U_2 \oplus B_1 \oplus \cdots \oplus B_m$$
With \( U_1 \) a multiset over \( T \) being 0 on any \( u' \neq u \), and \( U_2 \) being an arbitrary multiset over \( T \).

Notice moreover that, for each generalized mana-net \( G \), we obtain a strict monoidal functor \( F : G \rightarrow C \) as in Proposition 1: we send generating objects of \( C \) to themselves, all the other generating objects to the monoidal unit and generating morphisms to themselves. We keep calling \( F \) the counit of \( G \), even if it won’t be in general true that we still get a comonad.

Counits can be turned into functors \( C \rightarrow \text{Span} \) using a piece of categorical artillery called the Grothendieck construction (or the category of elements construction).

**Theorem 2 (Grothendieck construction, [19]).** Let \( C \) be a category. Then, there is an equivalence \( \text{Cat}/C \cong \text{Cat}[C,\text{Span}] \), with \( \text{Cat}[C,\text{Span}] \) being the category of lax functors \( C \rightarrow \text{Span} \). A functor \( F : D \rightarrow C \) defines a functor \( \Gamma F : C \rightarrow \text{Span} \) as follows:

- On objects, \( C \) is mapped to the set \( \{ D \in D \mid FD = C \} \);
- On morphisms, \( C \xrightarrow{f} C' \) is mapped to the span
  \[
  \{ D \in C \mid FD = C \} \xleftarrow{g \in D \mid Ff = g} \{ D \in C \mid FD = C' \}
  \]

The other way around, regarding \( C \) as a locally discrete bicategory and letting \( F : C \rightarrow \text{Span} \) be a lax functor, \( F \) maps to the functor \( \Sigma F \), from the pullback (in \( \text{Cat} \)) below:

\[
\begin{array}{ccc}
\int F & \longrightarrow & \text{Span}_* \\
\Sigma F \downarrow & & \downarrow U \\
C & \longrightarrow & \text{Span} \\
\end{array}
\]

where \( \text{Span}_* \) is the bicategory of spans between pointed sets, and \( U \) is the forgetful functor.

More concretely, \( \int F \) is defined as the category (all 2-cells are identities, due to the 2-discreteness of \( C \)) having

- 0-cells of \( \int F \) are couples \((X, x)\) where \( X \) is a 0-cell of \( C \) and \( x \in FX \);
- 1-cells \((X, x) \rightarrow (Y, y)\) of \( \int F \) are couples \((f, s)\) where \( f : X \rightarrow Y \) is a 1-cell of \( C \) and \( s \in SFf \) with \( Ff(s) = (x, y) \). Representing a span as a function \((S, s) \rightarrow (X \times Y, (x, y))\) between (pointed) sets, a morphism is a pair \((f, s)\) such that \( Ff : s \mapsto (x, y) \).

Finally, the categories \( \int F \) and \( D \) are isomorphic.

This result is a particular case of a more general correspondence between slice categories and lax normal functors to the category of profunctors [15], which is well-known in category theory and dates back to Bénabou [6, 5]. It gives an entirely abstract way to switch from/to and define internal/external semantics for mana-nets. Indeed, with a proof partly similar to the one carried out in our Theorem 1, we can show that:
Proposition 3. Monoidality of $\mathcal{C}_M(N) \xrightarrow{\Gamma} \mathcal{C}(N)$ implies $\Gamma F$ is lax-monoidal.

We can thus define the external semantics of a generalized mana-net by applying $\Gamma$ to $F$. A generalization of Theorem 1 then holds by definition.

Summing up, we showed that the mana-net construction can be generalized to more practical applications and the correspondence between a “naïve” internal semantics and a “type-aware” external one is still preserved. The evident price we have to pay for our generalization is that our external semantics is now not just lax-monoidal but lax-monoidal-lax.

6 Conclusion and future work

In this work, we introduced a new notion of Petri net where transitions come endowed with “mana”, a quality representing how many times a transition will be able to fire before losing its effectiveness. We believe this may be especially useful in modelling chemical processes mediated by enzymes that degrade over time.

Importantly, we showed how a categorical point of view on the matter allows to give two different definitions: A naïve, “hands-on” one, that we called internal, and a type-aware, functorial one, that we called external, which we proved to be two sides of the same coin.

Indeed, the equivalence between internal and external semantics is the consequence of a much more profound result in category theory, connecting slice categories and categories of lax monoidal functors. We were able to rely on this result to generalize our mana-nets further, while keeping the equivalence between the internal and external points of view.

We believe that further generalizations of the external semantics presented here may prove valuable to produce categorical semantics for nets with inhibitor arcs [1]. An inhibitor arc is an input arc to a transition that is enabled only when there are no tokens in their place. This concept is powerful enough to turn Petri nets into a Turing-complete model of computation [25, 26].

Indeed, we notice that by relaxing Definition 7 to allow any span $T^\oplus \to T^\oplus$, we can model situations where a transition can fire just if it has no mana (e.g., we can map transition $f$ to a span that is only defined when its source multiset has value 0 on $f$). The similarities in behaviour with inhibitor arcs are evident and constitute a direction of future work that we will surely pursue. The various technicalities involved are nevertheless tricky and necessitate a careful investigation.

Another direction of future work is about implementing the ideas at this moment presented using already available category theory libraries, such as [10].

References

[1] T. Agerwala. “Complete model for representing the coordination of asynchronous processes”. 1974 (cit. on p. 13).
J. C. Baez, J. Foley, and J. Moeller. “Network Models from Petri Nets with Catalysts”. In: Compositionality 1 (2019), p. 4 (cit. on p. 2).

J. C. Baez, F. Genovese, J. Master, and M. Shulman. Categories of Nets. 2021. arXiv: 2101.04238 [cs, math] (cit. on p. 3).

M. Barr and C. Wells. Category theory for computing science. Vol. 49. Prentice Hall New York, 1990 (cit. on p. 9).

J. Bénabou and T. Streicher. “Distributors at work”. Lecture notes written by Thomas Streicher. 2000 (cit. on p. 12).

J. Bénabou. “Introduction to Bicategories”. In: J. Bénabou, R. Davis, A. Dold, J. Isbell, S. MacLane, U. Oberst, and J. -. Roos. Reports of the Midwest Category Seminar. Vol. 47. Berlin, Heidelberg: Springer Berlin Heidelberg, 1967, pp. 1–77 (cit. on pp. 7, 12).

A. Churchill, S. Biderman, and A. Herrick. “Magic: The gathering is Turing complete”. In: arXiv preprint arXiv:1904.09828 (2019) (cit. on p. 2).

R. M. Dawson, R. Paré, and D. A. Pronk. “Universal properties of Span”. In: Theory and Applications of Categories 13.4 (2004), pp. 61–85 (cit. on p. 7).

R. Dawson, R. Paré, and D. Pronk. “The span construction”. In: Theory Appl. Categ 24.13 (2010), pp. 302–377 (cit. on p. 7).

F. Genovese, A. Gryzlov, J. Herold, A. Knispel, M. Perone, E. Post, and A. Videla. Idris-Ct: A Library to Do Category Theory in Idris. 2019. arXiv: 1912.06191 [cs, math] (cit. on p. 13).

F. Genovese, A. Gryzlov, J. Herold, M. Perone, E. Post, and A. Videla. Computational Petri Nets: Adjunctions Considered Harmful. 2019. arXiv: 1904.12974 [cs, math] (cit. on p. 3).

F. Genovese and J. Herold. “Executions in (Semi-)Integer Petri Nets Are Compact Closed Categories”. In: Electronic Proceedings in Theoretical Computer Science 287 (2019), pp. 127–144 (cit. on p. 3).

F. Genovese and D. I. Spivak. “A Categorical Semantics for Guarded Petri Nets”. In: Graph Transformation. Ed. by F. Gadducci and T. Kehrer. Vol. 12150. Lecture Notes in Computer Science. Cham: Springer International Publishing, 2020, pp. 57–74 (cit. on pp. 2, 6, 9).

J. Letelier, J. Soto-Andrade, F. Guinez, A. Cornish-Bowden, and M. Cárdenas. “Organizational invariance and metabolic closure: Analysis in terms of M; R systems”. In: Journal of theoretical biology 238 (2006), pp. 949–61 (cit. on pp. 2, 11).

F. Loregian. “Coend Calculus”. In: London Mathematical Society Lecture Note Series 468 (2021). ISBN 9781108746120 (cit. on p. 12).

S. M. Marcelo Aguiar. Monoidal Functors, Species and Hopf Algebras. Centre de Recherches Mathématiques Monograph Series 29. American Mathematical Society, 2010 (cit. on p. 6).

J. Master. “Petri Nets Based on Lawvere Theories”. In: Mathematical Structures in Computer Science 30.7 (2020), pp. 833–864. arXiv: 1904.09091 (cit. on pp. 3, 4).
[18] J. Meseguer and U. Montanari. “Petri Nets Are Monoids”. In: Information and Computation 88.2 (1990), pp. 105–155 (cit. on p. 3).
[19] D. Pavlović and S. Abramsky. “Specifying Interaction Categories”. In: Category Theory and Computer Science. Ed. by E. Moggi and G. Rosolini. Red. by G. Goos, J. Hartmanis, and J. van Leeuwen. Vol. 1290. Lecture Notes in Computer Science. Berlin, Heidelberg: Springer Berlin Heidelberg, 1997, pp. 147–158 (cit. on pp. 9, 12).
[20] P. Perrone. Notes on Category Theory with examples from basic mathematics. 2019. eprint: arXiv:1912.10642 (cit. on p. 5).
[21] C. Petri and W. Reisig. Petri Net. Scholarpedia. 2008. url: http://www.scholarpedia.org/article/Petri_net (cit. on p. 1).
[22] V. Sassone. “On the Category of Petri Net Computations”. In: TAPSOFT ’95: Theory and Practice of Software Development. Ed. by P. D. Mosses, M. Nielsen, and M. I. Schwartzbach. Red. by G. Goos, J. Hartmanis, and J. Leeuwen. Vol. 915. Berlin, Heidelberg: Springer Berlin Heidelberg, 1995, pp. 334–348 (cit. on p. 3).
[23] Wikipedia. Magic (Game Terminology). 2020. url: https://en.wikipedia.org/wiki/Magic_(game_terminology) (cit. on p. 2).
[24] Wikipedia. Magic: The Gathering. 2020. url: https://en.wikipedia.org/wiki/Magic:_The_Gathering (cit. on p. 2).
[25] D. A. Zaitsev. “Universal Petri Net”. In: Cybernetics and Systems Analysis 48.1 (2012), pp. 498–511 (cit. on p. 13).
[26] D. A. Zaitsev. “Toward the Minimal Universal Petri Net”. In: IEEE Transactions on Systems, Man, and Cybernetics: Systems 44.1 (2014), pp. 47–58 (cit. on p. 13).