Sesqui-Pushout Rewriting:

Concurrency, Associativity and Rule Algebra Framework

Nicolas Behr (IRIF, Université de Paris)

Partially based upon previous work with:

Vincent Danos and Ilias Garnier (ENS Paris) Jean Krivine and Paul-André Melliès (Paris 07) Pawel Sobocinski (ECS Southampton) Gérard H.E. Duchamp (Paris 13) and Karol A. Penson (Paris 06) Giuseppe Dattoli and Silvia Licciardi (ENEA, Rome)

GCM 2019, Eindhoven Univ. of Technology, July 17 2019



INSTITUT
 DE RECHERCHE
 EN INFORMATIQUE
 FONDAMENTALE



· formal power series:

$$f(x) \in \mathbb{R}[[x]] \quad :\Leftrightarrow \quad f(x) = \sum_{n \ge 0} f_n x^n \quad (\text{with } f_n \in \mathbb{R} \text{ for all } n \in \mathbb{Z}_{\ge 0})$$

• two natural linear operators: \hat{x} and ∂_x

$$\hat{x}: \mathbb{R}[[x]] \to \mathbb{R}[[x]]: x^n \mapsto x^{n+1}, \quad \partial_x: \mathbb{R}[[x]] \to \mathbb{R}[[x]]: x^n \mapsto \begin{cases} 0 & \text{if } n = 0\\ nx^{n-1} & \text{if } n > 0 \end{cases}$$

· formal power series:

$$f(x) \in \mathbb{R}[[x]] \quad :\Leftrightarrow \quad f(x) = \sum_{n \ge 0} f_n x^n \quad (\text{with } f_n \in \mathbb{R} \text{ for all } n \in \mathbb{Z}_{\ge 0})$$

• two natural linear operators: \hat{x} and ∂_x

$$\hat{x}: \mathbb{R}[[x]] \to \mathbb{R}[[x]]: x^n \mapsto x^{n+1}, \quad \partial_x: \mathbb{R}[[x]] \to \mathbb{R}[[x]]: x^n \mapsto \begin{cases} 0 & \text{if } n = 0\\ nx^{n-1} & \text{if } n > 0 \end{cases}$$

• for all $p \in \mathbb{Z}_{>0}$ and $f(x), g(x) \in \mathbb{R}[[x]]$, "of course. . . "

$$\partial_x^p \left(f(x)g(x) \right) = \sum_{k=0}^p \binom{p}{k} \left(\partial_x^k f(x) \right) \left(\partial_x^{p-k}g(x) \right)$$

formal power series:

$$f(x) \in \mathbb{R}[[x]] \quad :\Leftrightarrow \quad f(x) = \sum_{n \ge 0} f_n x^n \quad (\text{with } f_n \in \mathbb{R} \text{ for all } n \in \mathbb{Z}_{\ge 0})$$

• two natural linear operators: \hat{x} and ∂_x

$$\hat{x}: \mathbb{R}[[x]] \to \mathbb{R}[[x]]: x^n \mapsto x^{n+1}, \quad \partial_x: \mathbb{R}[[x]] \to \mathbb{R}[[x]]: x^n \mapsto \begin{cases} 0 & \text{if } n = 0\\ nx^{n-1} & \text{if } n > 0 \end{cases}$$

• for all $p \in \mathbb{Z}_{>0}$ and $f(x), g(x) \in \mathbb{R}[[x]]$, "of course. . . "

$$\partial_x^p \left(f(x)g(x) \right) = \sum_{k=0}^p \binom{p}{k} \left(\partial_x^k f(x) \right) \left(\partial_x^{p-k}g(x) \right)$$

 \Rightarrow non-trivial "normal-ordering" type operator relation: (for $p, q \in \mathbb{Z}_{\geq 0}$)

$$\partial_x^p \hat{x}^q = \sum_{k=0}^{\min(p,q)} k! \binom{p}{k} \binom{q}{k} \hat{x}^{q-k} \partial_x^{p-k}$$

• non-trivial "normal-ordering" type operator relation: (for $p, q \in \mathbb{Z}_{\geq 0}$)

$$\begin{aligned} \partial_x^p \hat{x}^q &= \sum_{k=0}^{\min(p,q)} k! \binom{p}{k} \binom{q}{k} \hat{x}^{q-k} \partial_x^{p-k} \\ &= \sum_{k=0}^{\min(p,q)} \qquad \qquad \frac{1}{k!} \left(\frac{p!}{(p-k)!}\right) \left(\frac{q!}{(q-k)!}\right) \qquad \qquad \hat{x}^{q-k} \partial_x^{p-k} \end{aligned}$$

of ways to choose k objects from pools of p and q objects, disregarding order

 \Rightarrow WHY?

• non-trivial "normal-ordering" type operator relation: (for $p, q \in \mathbb{Z}_{\geq 0}$)

$$\partial_x^p \hat{x}^q = \sum_{k=0}^{\min(p,q)} k! \binom{p}{k} \binom{q}{k} \hat{x}^{q-k} \partial_x^{p-k}$$
$$= \sum_{k=0}^{\min(p,q)} \frac{1}{k!} \left(\frac{p!}{(p-k)!}\right) \left(\frac{q!}{(q-k)!}\right) \qquad \hat{x}^{q-k} \partial_x^{p-k}$$

of ways to choose k objects from pools of p and q objects, disregarding order

 \Rightarrow WHY?

somewhat surprising answer:

Because \hat{x} and ∂_x are the **canonical representations** of certain **rule algebra** elements associated to (discrete) **graph rewriting rules**!

Perspectives

category-theoretical graph rewriting theory

stochastic dynamical systems (CTMCs)

combinatorics

biochemical reaction systems and systems biology

cancer research

Perspectives



* concurrency theorem * associativity theorem * rule algebras



category-theoretical graph rewriting theory

stochastic dynamical systems (CTMCs)

combinatorics

biochemical reaction systems and systems biology

cancer research

The main construction:

- Recap: Sesqui-Pushout (SqPO) rewriting in adhesive categories
- · Main result I: a concurrency theorem for SqPO rewriting
- · Main result II: an associativity theorem for SqPO rule compositions
- Main result III: from SqPO rewriting to SqPO rule algebras

Application examples:

- · formal power series and the Heisenberg-Weyl algebra
- Main result IV: stochastic mechanics of continuous-time Markov chains for SqPO-type stochastic rewriting systems

The category-theoretical setup

Adhesive and extensive categories (cf. [1], Def. 3.1 ff)

A category C is said to be adhesive if

- (i) C has pushouts along monomorphisms,
- (ii) C has pullbacks, and if

(iii) pushouts along monomorphisms are van Kampen (VK) squares.

If **C** in addition possesses a **strict initial object** $\emptyset \in ob(\mathbf{C})$, i.e. an object s.th. $\forall X \in ob(\mathbf{C}) : \exists ! i_X : \emptyset \hookrightarrow X$ and all $X \to \emptyset$ are isos, the category is said to be **extensive**. It is called **finitary** [2] if every object Xhas only finitely many subobjects (up to iso).

• Examples for finitary adhesive extensive categories [2]:

- · FinSet, the category of (finite) sets and set functions
- FinGraph, the category of (finite) directed multigraphs and graph homomorphisms (and also colored/typed graphs, attributed graphs, hypergraphs,...)
- · different variants of categories of finite typed graphs (Kappa!)

[2] Karsten Gabriel et al. "Finitary *M*-adhesive categories". In: *Mathematical Structures in Computer Science* 24.04 (June 2014)

^[1] Stephen Lack and Pawel Sobociński. "Adhesive and quasiadhesive categories". In: RAIRO-Theoretical Informatics and Applications 39.3 (2005), pp. 511–545

Additional special requirements for the SqPO case

Final Pullback Complement (FPC) [3], [4]

Let C be a category. Given a commutative diagram



a pair of morphisms (d, b) is a final pullback complement (FPC) of a pair (c, a) if

- (i) (a,b) is a pullback of (c,d) (i.e. if the square marked (*) is a pullback square), and
- (ii) for each collection of morphisms (x, y, z, w) as in the diagram above, where (x, y) is pullback of (c, z) and where $a \circ w = x$, there exists a unique morphism w^* with $d \circ w^* = z$ and $w^* \circ y = b \circ w$.

 ^[3] Andrea Corradini et al. "Sesqui-Pushout Rewriting". In: Lecture Notes in Computer Science. Springer Berlin Heidelberg, 2006, pp. 30–45
 [4] Michael Löwe. "Polymorphic Sesqui-Pushout Graph Rewriting". In: Graph Transformation. Springer International Publishing, 2015, pp. 3–18

Additional special requirements for the SqPO case (detail)

Lemma (cf. [5], Fact 2, and [6], Lem. 2 and Prop. 2)

Let C be adhesive.

- Every pushout square along monomorphisms is also an FPC square.
- For an arbitrary morphism $f : A \to B$, (id_B, f) is an FPC of (f, id_A) and vice versa.
- · FPCs are unique up to isomorphism
- FPCs preserve monomorphisms*.

* If $C \xleftarrow{d} D \xleftarrow{b} A$ is the FPC of $C \xleftarrow{c} B \xleftarrow{a} A$ and if $a \in \text{mono}(\mathbb{C})$, then also $d \in \text{mono}(\mathbb{C})$ and vice versa (while $c \in \text{mono}(\mathbb{C})$ entails that $b \in \text{mono}(\mathbb{C})$ by stability of monomorphisms under pullbacks in an adhesive category \mathbb{C}).

[4] Michael Löwe. "Polymorphic Sesqui-Pushout Graph Rewriting". In: Graph Transformation. Springer International Publishing, 2015, pp. 3–18
 [5] Andrea Corradini et al. "Sesqui-Pushout Rewriting". In: Lecture Notes in Computer Science. Springer Berlin Heidelberg, 2006, pp. 30–45

[6] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Additional special requirements for the SqPO case (detail)

Lemma (cf. [5], Fact 2, and [6], Lem. 2 and Prop. 2)

Let C be adhesive.

- · Every pushout square along monomorphisms is also an FPC square.
- For an arbitrary morphism $f : A \to B$, (id_B, f) is an FPC of (f, id_A) and vice versa.
- · FPCs are unique up to isomorphism
- FPCs preserve monomorphisms*.

* If $C \stackrel{d}{\leftarrow} D \stackrel{b}{\leftarrow} A$ is the FPC of $C \stackrel{c}{\leftarrow} B \stackrel{a}{\leftarrow} A$ and if $a \in \mathbf{mono}(\mathbf{C})$, then also $d \in \mathbf{mono}(\mathbf{C})$ and vice versa (while $c \in \mathbf{mono}(\mathbf{C})$ entails that $b \in \mathbf{mono}(\mathbf{C})$ by stability of monomorphisms under pullbacks in an adhesive category \mathbf{C}).

(I) Assumptions for compositional SqPO rewriting [7]

C is an adhesive category in which all FPCs along monomorphisms exist, and in which FPCs preserve monomorphisms.

[5] Michael Löwe. "Polymorphic Sesqui-Pushout Graph Rewriting". In: Graph Transformation. Springer International Publishing, 2015, pp. 3–18
[6] Andrea Corradini et al. "Sesqui-Pushout Rewriting". In: Lecture Notes in Computer Science. Springer Berlin Heidelberg, 2006, pp. 30–45
[7] Nicolas Behr, "Sesqui-Pushout Rewriting: Concurrency. Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Recap: Sesqui-Pushout rewriting

Sesqui-Pushout rewriting: linear productions and direct derivations

SqPO-type rewriting; compare [8]

Let C be an adhesive category satisfying Assumption (I). Denote by Lin(C) the set of isomorphism classes of so-called linear productions (i.e. of spans of monomorphisms),

$$\mathbf{Lin}(\mathbf{C}) := \{ p \equiv (O \xleftarrow{o} K \xrightarrow{i} I) \mid o, i \in \mathbf{mono}(\mathbf{C}) \} \nearrow_{\cong}$$

Note: Two productions $O \leftarrow K \rightarrow I$ and $O' \leftarrow K' \rightarrow I'$ are defined to be **isomorphic** if there exist isomorphisms $I \rightarrow I', K \rightarrow K'$ and $O \rightarrow O'$ that make the obvious diagram commute; we will not distinguish between isomorphic productions. As natural in this category-theoretical setting, the constructions presented in the following are understood as defined up to such isomorphisms.

Sesqui-Pushout rewriting: linear productions and direct derivations

SqPO-type rewriting; compare [8]

Given an object $X \in obj(\mathbb{C})$ and a linear production $p \in Lin(\mathbb{C})$, we denote the set of SqPO-admissible matches $\mathbf{M}_p^{SqPO}(X)$ as the set of monomorphisms $m : I \to X$. Then the diagram below is constructed by taking the **final pullback complement** marked **FPC** followed by taking the pushout marked **PO**:

We write $p_m(X) := X'$ for the object "produced" by the above diagram. The process is called (SqPO-) derivation of X along production p and admissible match m, and denoted $p_m(X) \notin \frac{SqPO}{p_m} X$.

New: SqPO-type rule composition [9]

Let $p_1, p_2 \in \text{Lin}(\mathbb{C})$, and let $\mathbf{m} = (I_2 \stackrel{m_2}{\longleftarrow} M_{21} \stackrel{m_1}{\longrightarrow} O_1)$ (with $m_1, m_2 \in \text{mono}(\mathbb{C})$) be an overlap of the output object O_1 of p_1 with the input object I_2 of p_2 . Take the pushout of \mathbf{m} (marked PO) to obtain the cospan $I_2 \stackrel{n_2}{\longrightarrow} N_{21} \stackrel{n_1}{\longleftarrow} O_1$.

Then **m** is called an **SqPO-admissible match of** p_2 into p_1 , denoted $\mathbf{m} \in \mathbf{M}_{p_2}^{SqPO}(p_1)$, if the **pushout** complement marked **POC** below exists:



In this case, the remaining parts of the diagram are formed by taking the final pullback complement marked **FPC** and the pushouts marked **PO**. If $\mathbf{m} \in \mathbf{M}_{p_2}^{SqPO}(p_1)$, we write $p_2 \overset{\mathbf{m}}{\preccurlyeq} p_1 \in \mathbf{Lin}(\mathbf{C})$ for the **composite** of p_2 with p_1 along the admissible match \mathbf{m} , defined as

$$p_2 \stackrel{\mathbf{m}}{\not\prec} p_1 := (O_{21} \stackrel{O_{21}}{\longleftarrow} K_{21} \stackrel{i_{21}}{\longrightarrow} I_{21}). \tag{3}$$

[8] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Double-Pushout (DPO), DPO[†] and Sesqui-Pushout (SqPO) rewriting

$$\operatorname{Lin}(\mathbf{C}) := \left\{ O \xleftarrow{o} K \xrightarrow{i} I \middle| o, i \in \operatorname{mono}(\mathbf{C}) \right\} \nearrow \cong$$
(4)

A rule application of a rule $r \in Lin(C)$ to an object X along a \mathbb{T} -admissible match m (resp. m^* for DPO^{\dagger}) is defined via the following type of commutative diagram (referred to as a direct derivation in the literature):

$$O \stackrel{r}{\longleftarrow} I \qquad O \stackrel{o}{\longleftarrow} K \stackrel{i}{\longrightarrow} I$$

$$m^{*} \downarrow \qquad \mathbb{T} \qquad \downarrow^{m} \qquad := \qquad m^{*} \stackrel{i}{\longleftarrow} (B) \qquad \downarrow \qquad (A) \qquad \downarrow^{m}$$

$$r_{m}(X) \xleftarrow{=} X \qquad \qquad r_{m}(X) \xleftarrow{=} \overline{K} \xrightarrow{----} X$$
(5)

The precise details and T-type admissibility are defined via

Type $\mathbb T$	nature of (B)	nature of (A)
DPO	РО	POC
DPO^{\dagger}	POC	РО
SqPO	РО	FPC

where POC indicates that these POCs must be constructible for admissible matches.

Key operation: rule compositions [10], [11]

Set of \mathbb{T} -type admissible matches of r_2 into r_1 for $\mathbb{T} \in \{DPO, SqPO\}$:

$$\mathbf{M}_{r_{2}}^{\mathbb{T}}(r_{1}) := \left\{ \mu_{21} = (I_{2} \leftarrow M_{21} \to O_{2}) \middle| n_{1}, n_{2} \text{ in } \mathbf{PO}(\mu_{21}) = (I_{2} \xrightarrow{n_{2}} N_{21} \xleftarrow{n_{1}} O_{1}) \\ \text{satisfy } n_{2} \in \mathbf{M}_{r_{2}}^{\mathbb{T}}(N_{21}) \land n_{1} \in \mathbf{M}_{r_{1}}^{\text{prof}}(N_{21}) \right\}.$$

$$(7)$$

For a \mathbb{T} -type admissible match $\mu_{21} = (I_2 \leftarrow M_{21} \rightarrow O_2) \in \mathbf{M}_{r_2}^{\mathbb{T}}(r_1)$, construct

From this diagram, one may compute (via pullback composition \circ of the two composable spans in the bottom row) a span of monomorphisms $(O_{21} \leftarrow I_{21}) \in \text{Lin}(\mathbb{C})$, which we define to be the \mathbb{T} -type composition of r_2 with r_1 along μ_{21} (for $\mathbb{T} \in \{DPO, SqPO\}$ as in (8)):

$$r_2^{\mu_{21}} \triangleleft_{\mathbb{T}} r_1 := (O_{21} \leftarrow I_{21}) = (O_{21} \leftarrow N_{21}) \circ (N_{21} \leftarrow I_{21}).$$
(9)

[10] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: 27th EACSL Annual Conference on Computer Science Logic (CSL 2018). Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum für Informatik, Sept. 2018, 11:1–11:21

[11] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

SqPO-type Concurrency Theorem

Let C be an adhesive category satisfying Assumption (I). Let $p_1, p_2 \in Lin(C)$ be two linear rules and $X_0 \in ob(C)$ an object.

· Synthesis: Given a two-step sequence of SqPO derivations

$$X_2 \stackrel{SqPO}{\underset{p_2,m_2}{\longrightarrow}} X_1 \stackrel{SqPO}{\underset{p_1,m_1}{\longrightarrow}} X_0, \tag{10}$$

with $X_1 := p_{1_{m_1}}(X_0)$ and $X_2 := p_{2_{m_2}}(X_1)$, there exists a SqPO-composite rule $q = p_2 \stackrel{\mathbf{n}}{\preccurlyeq} p_1$ for a unique $\mathbf{n} \in \mathbf{M}_{p_2}^{Sq}(p_1)$, and a unique SqPO-admissible match $n \in \mathbf{M}_q^{SqPO}(X)$, such that

$$q_n(X) \stackrel{SqPO}{\underbrace{q_n}{q_n}} X_0 \quad \text{and} \quad q_n(X_0) \cong X_2 \,.$$
 (11)

• Analysis: Given an SqPO-admissible match $\mathbf{n} \in \mathbf{M}_{p_2}^{sq}(p_1)$ of p_2 into p_1 and an SqPO-admissible match $n \in \mathbf{M}_q^{SqPO}(X)$ of the SqPO-composite $q = p_2 \overset{\mathbf{n}}{\leq} p_1$ into X, there exists a unique pair of SqPO-admissible matches $m_1 \in \mathbf{M}_{p_1}^{SqPO}(X_0)$ and $m_2 \in \mathbf{M}_{p_2}^{SqPO}(X_1)$ with $X_1 := p_{1_{m_1}}(X_0)$ such that

$$X_2 \xleftarrow{SqPO}{p_2, m_2} X_1 \xleftarrow{SqPO}{p_1, m_1} X_0 \quad \text{and} \quad X_2 \cong q_n(X).$$
 (12)

[12] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Main result II: SqPO-type associativity theorem [11] (new!)

SqPO-type associativity theorem

Let C be an adhesive category satisfying Assumption (I). Then the SqPO-composition operation \dot{s} . on linear productions of C is associative in the following sense: given linear productions $p_1, p_2, p_3 \in Lin(C)$, there exists a bijective correspondence between pairs of SqPO-admissible matches $(\mathbf{m}_{21}, \mathbf{m}_{3(21)})$ and $(\mathbf{m}_{32}, \mathbf{m}_{(32)1})$ such that

$$p_{3} \overset{\mathbf{m}_{3(21)}}{\swarrow} \begin{pmatrix} \mathbf{m}_{21} \\ p_{2} \overset{\mathbf{m}_{21}}{\swarrow} p_{1} \end{pmatrix} \cong \begin{pmatrix} \mathbf{m}_{32} \\ p_{3} \overset{\mathbf{m}_{32}}{\swarrow} p_{2} \end{pmatrix} \overset{\mathbf{m}_{(32)1}}{\overset{\mathbf{m}_{32}}{\updownarrow}} p_{1}.$$
(13)

[12] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

SqPO-type associativity theorem proof (sketch) [13]

The **associativity property** in the **SqPO case** manifests itself in a form entirely analogous to the **DPO case** [12]:

The data provided along the path highlighted in **orange** below permits to uniquely compute the data provided along the path highlighted in **blue** and vice versa (with both sets of overlaps computing the **same "triple composite" production** that is encoded as the **composition of the three spans in the bottom front row**):



[13] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

[14] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: 27th EACSL Annual Conference on Computer Science Logic (CSL 2018). Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum für Informatik, Sept. 2018, 11:1–11:21 From SqPO-type rule compositions to SqPO-type rule algebras

Algebraically encoding non-determinism



A possibility to encode non-determinism:

map multiple possibilities of transitions ...

... into "sum of possibilities"

(via employing the notion of a vector space of states and of transitions as linear operators on this space)

The mathematical "blueprint": the Heisenberg-Weyl algebra



- pure state: a pool of *n* indistinguishable particles (of some type *X*)
- generic operations: remove *i* particles of type *X* from the pool, then add *o* particles of type *X* (with $i, o \in \mathbb{Z}_{\geq 0}$)
- · elementary operations:
 - pick a particle of type X at random and remove it
 - add a particle of type X
- ⇒ basic combinatorics:
 - · n possible ways to remove a particle
 - · 1 possible way to add a particle

The mathematical "blueprint": the Heisenberg-Weyl algebra

· from the theory of bosonic Fock spaces:

 $|n\rangle \stackrel{\frown}{=}$ **pure state** of *n* particles

 Ansatz: encode the elementary operations in terms of (representations of) the generators of the Heisenberg-Weyl algebra:

$$a \left| n \right\rangle := \begin{cases} n \left| n - 1 \right\rangle & \text{if } n > 0 \\ 0 & \text{else} \end{cases}$$
$$a^{\dagger} \left| n \right\rangle := \left| n + 1 \right\rangle \quad (n \ge 0)$$

· canonical commutation relations:

$$(aa^{\dagger} - a^{\dagger}a) |n\rangle = ((n+1) - (n)) |n\rangle = |n\rangle$$

 $\Leftrightarrow [a, a^{\dagger}] = aa^{\dagger} - a^{\dagger}a = \mathbb{1}$





Necessary additional structures for the SqPo rule algebra construction [14]

Initial objects

An object $\emptyset \in obj(\mathbb{C})$ of some category \mathbb{C} is said to be a **strict initial object** if for every object $X \in obj(\mathbb{C})$, there exists a unique morphism $\emptyset \to X$, and if any morphism $X \to \emptyset$ must be an isomorphism.

For example, the category Graph possesses a strict initial object (the empty graph).

^[14] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

^[15] Stephen Lack and Pawel Sobociński. "Adhesive and quasiadhesive categories". In: RAIRO-Theoretical Informatics and Applications 39.3 (2005), pp. 511-545

Necessary additional structures for the SqPo rule algebra construction [15]

Initial objects

An object $\emptyset \in obj(\mathbb{C})$ of some category \mathbb{C} is said to be a **strict initial object** if for every object $X \in obj(\mathbb{C})$, there exists a unique morphism $\emptyset \to X$, and if any morphism $X \to \emptyset$ must be an isomorphism.

For example, the category Graph possesses a strict initial object (the empty graph).

Extensive categories; [14], Lem. 4.1

An adhesive category C is an extensive category if and only if it possesses a strict initial object.

^[15] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

^[16] Stephen Lack and Pawel Sobociński. "Adhesive and quasiadhesive categories". In: RAIRO-Theoretical Informatics and Applications 39.3 (2005), pp. 511-545

Initial objects

An object $\emptyset \in obj(\mathbb{C})$ of some category \mathbb{C} is said to be a **strict initial object** if for every object $X \in obj(\mathbb{C})$, there exists a unique morphism $\emptyset \to X$, and if any morphism $X \to \emptyset$ must be an isomorphism.

For example, the category Graph possesses a strict initial object (the empty graph).

Extensive categories; [14], Lem. 4.1

An adhesive category C is an extensive category if and only if it possesses a strict initial object.

Assumption (II): Prerequisites for SqPO-type rule algebras

We assume that C is an adhesive category satisfying Assumption (I), and which is in addition finitary and possesses a strict initial object $\emptyset \in obj(C)$.

[16] Stephen Lack and Pawel Sobociński. "Adhesive and quasiadhesive categories". In: RAIRO-Theoretical Informatics and Applications 39.3 (2005), pp. 511-545

^[15] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Let δ : $Lin(C) \rightarrow \mathscr{R}_C$ be defined as an isomorphism from Lin(C) to the basis of a free \mathbb{R} -vector space $\mathscr{R}_C \equiv (\mathscr{R}_C, +, \cdot)$, such that

$$\mathscr{R}_{\mathbf{C}} := span_{\mathbb{R}}(\{\delta(p) \mid p \in \operatorname{Lin}(\mathbf{C})\}).$$
(14)

In order to clearly distinguish between elements of Lin(C) and basis vectors of \mathscr{R}_{C} , we introduce the notation

$$(O \stackrel{p}{\leftarrow} I) := \delta \left(O \stackrel{o}{\leftarrow} K \stackrel{i}{\rightarrow} I \right).$$
(15)

Let δ : $Lin(C) \rightarrow \mathscr{R}_C$ be defined as an isomorphism from Lin(C) to the basis of a free \mathbb{R} -vector space $\mathscr{R}_C \equiv (\mathscr{R}_C, +, \cdot)$, such that

$$\mathscr{R}_{\mathbf{C}} := span_{\mathbb{R}}(\{\delta(p) \mid p \in \operatorname{Lin}(\mathbf{C})\}).$$
(14)

In order to clearly distinguish between elements of Lin(C) and basis vectors of \mathscr{R}_C , we introduce the notation

$$(O \stackrel{p}{\leftarrow} I) := \delta \left(O \stackrel{o}{\leftarrow} K \stackrel{i}{\to} I \right).$$
(15)

Define the SqPO rule algebra product $\odot_{\mathscr{R}_C}$ on a category C that satisfies Assumption (II) as the binary operation

$$\odot_{\mathscr{R}_{\mathbf{C}}} : \mathscr{R}_{\mathbf{C}} \times \mathscr{R}_{\mathbf{C}} \to \mathscr{R}_{\mathbf{C}} : (R_1, R_2) \mapsto R_1 \odot_{\mathscr{R}_{\mathbf{C}}} R_2 ,$$
(16)

where for two basis vectors $R_i = \delta(p_i)$ encoding the linear rules $p_i \in Lin(\mathbb{C})$ (i = 1, 2),

$$R_2 \odot_{\mathscr{R}_{\mathbf{C}}} R_1 := \sum_{\mathbf{m} \in \mathbf{M}_{p_2}^{sq}(p_1)} \delta\left(p_2 \overset{\mathbf{m}}{\preccurlyeq} p_1\right).$$
(17)

[16] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Let δ : $Lin(C) \rightarrow \mathscr{R}_C$ be defined as an isomorphism from Lin(C) to the basis of a free \mathbb{R} -vector space $\mathscr{R}_C \equiv (\mathscr{R}_C, +, \cdot)$, such that

$$\mathscr{R}_{\mathbf{C}} := \operatorname{span}_{\mathbb{R}}(\{\delta(p) \mid p \in \operatorname{Lin}(\mathbf{C})\}).$$
(14)

In order to clearly distinguish between elements of Lin(C) and basis vectors of \mathscr{R}_C , we introduce the notation

$$(O \stackrel{p}{\leftarrow} I) := \delta \left(O \stackrel{o}{\leftarrow} K \stackrel{i}{\to} I \right).$$
(15)

Define the SqPO rule algebra product $\odot_{\mathscr{R}_C}$ on a category C that satisfies Assumption (II) as the binary operation

$$\Im_{\mathscr{R}_{\mathbf{C}}} : \mathscr{R}_{\mathbf{C}} \times \mathscr{R}_{\mathbf{C}} \to \mathscr{R}_{\mathbf{C}} : (R_1, R_2) \mapsto R_1 \odot_{\mathscr{R}_{\mathbf{C}}} R_2,$$
 (16)

where for two basis vectors $R_i = \delta(p_i)$ encoding the linear rules $p_i \in Lin(\mathbb{C})$ (i = 1, 2),

$$R_2 \odot_{\mathscr{R}_{\mathbf{C}}} R_1 := \sum_{\mathbf{m} \in \mathbf{M}_{p_2}^{sq}(p_1)} \delta\left(p_2 \overset{\mathbf{m}}{\lessdot} p_1\right).$$
(17)

The definition is extended to arbitrary (finite) linear combinations of basis vectors by bilinearity, whence for $p_i, p_j \in \text{Lin}(\mathbb{C})$ and $\alpha_i, \beta_j \in \mathbb{R}$,

$$\left(\sum_{i} \alpha_{i} \cdot \delta(p_{i})\right) \odot_{\mathscr{R}_{\mathbf{C}}} \left(\sum_{j} \beta_{j} \cdot \delta(p_{j})\right) := \sum_{i,j} (\alpha_{i} \cdot \beta_{j}) \cdot \left(\delta(p_{i}) \odot_{\mathscr{R}_{\mathbf{C}}} \delta(p_{j})\right).$$
(18)

[16] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Let δ : $Lin(C) \rightarrow \mathscr{R}_C$ be defined as an isomorphism from Lin(C) to the basis of a free \mathbb{R} -vector space $\mathscr{R}_C \equiv (\mathscr{R}_C, +, \cdot)$, such that

$$\mathscr{R}_{\mathbf{C}} := span_{\mathbb{R}}(\{\delta(p) \mid p \in \operatorname{Lin}(\mathbf{C})\}).$$
(14)

In order to clearly distinguish between elements of Lin(C) and basis vectors of \mathscr{R}_{C} , we introduce the notation

$$(O \stackrel{p}{\leftarrow} I) := \delta \left(O \stackrel{o}{\leftarrow} K \stackrel{i}{\to} I \right).$$
(15)

Define the SqPO rule algebra product $\odot_{\mathscr{R}_C}$ on a category C that satisfies Assumption (II) as the binary operation

$$\Im_{\mathscr{R}_{\mathbf{C}}} : \mathscr{R}_{\mathbf{C}} \times \mathscr{R}_{\mathbf{C}} \to \mathscr{R}_{\mathbf{C}} : (R_1, R_2) \mapsto R_1 \odot_{\mathscr{R}_{\mathbf{C}}} R_2,$$
 (16)

where for two basis vectors $R_i = \delta(p_i)$ encoding the linear rules $p_i \in Lin(\mathbb{C})$ (i = 1, 2),

$$R_2 \odot_{\mathscr{R}_{\mathbf{C}}} R_1 := \sum_{\mathbf{m} \in \mathbf{M}_{p_2}^{q_2}(p_1)} \delta\left(p_2 \overset{\mathbf{m}}{\preccurlyeq} p_1\right).$$
(17)

The definition is extended to arbitrary (finite) linear combinations of basis vectors by bilinearity, whence for $p_i, p_j \in \text{Lin}(\mathbb{C})$ and $\alpha_i, \beta_j \in \mathbb{R}$,

$$\left(\sum_{i} \alpha_{i} \cdot \delta(p_{i})\right) \odot_{\mathscr{R}_{\mathbf{C}}} \left(\sum_{j} \beta_{j} \cdot \delta(p_{j})\right) := \sum_{i,j} (\alpha_{i} \cdot \beta_{j}) \cdot \left(\delta(p_{i}) \odot_{\mathscr{R}_{\mathbf{C}}} \delta(p_{j})\right).$$
(18)

We call $\mathscr{R}_{C}^{sq} \equiv (\mathscr{R}_{C}, \odot_{\mathscr{R}_{C}})$ the SqPO-type rule algebra over the finitary adhesive and extensive category C. [16] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: *arXiv preprint* 1904.08357 (2019)

Theorem

For every category C satisfying Assumption (II), the associated SqPO-type rule algebra $\mathscr{R}_{C}^{sq} \equiv (\mathscr{R}_{C}, \odot_{\mathscr{R}_{C}})$ is an associative unital algebra, with unit element $R_{\varnothing} := (\varnothing \Leftarrow \varnothing)$.

Let C = FinGraph be the category of finite directed multigraphs, with \emptyset the empty graph. Then with $\odot \equiv \odot_{\mathscr{R}_C}$, we find for example

$$\delta(\varnothing \leftrightarrow \varnothing \hookrightarrow \bullet) \odot \delta(\bullet \bullet \leftrightarrow \varnothing \hookrightarrow \varnothing)$$

$$= \sum_{\substack{\mathbf{m} \in \{(\bullet \leftrightarrow \varnothing \hookrightarrow \bullet), (\bullet \leftrightarrow \bullet \to \bullet), \\ (\bullet \to \bullet \to \bullet)\}}} \delta\left((\varnothing \leftrightarrow \varnothing \hookrightarrow \bullet) \overset{\mathbf{m}}{\not{\leftarrow}} (\bullet \bullet \leftrightarrow \varnothing \hookrightarrow \varnothing)\right)$$

$$= \delta(\bullet \leftrightarrow \leftrightarrow \varnothing \hookrightarrow \bullet) + 2\delta(\bullet \leftrightarrow \varnothing \hookrightarrow \varnothing).$$
(19)

The result of the composition thus captures the combinatorial insight that there are two contributions that evaluate to an isomorphic rule algebra element.
Example: some SqPO-type rule compositions in FinGraph

Let C = FinGraph be the category of finite directed multigraphs, with \emptyset the empty graph. Then with $\odot \equiv \odot_{\mathscr{R}_C}$, we find for example

$$\delta(\varnothing \leftrightarrow \varnothing \hookrightarrow \bullet) \odot \delta(\bullet \bullet \leftrightarrow \varnothing \hookrightarrow \varnothing)$$

$$= \sum_{\substack{\mathbf{m} \in \{(\bullet \leftrightarrow \varnothing \hookrightarrow \bullet), (\bullet \leftrightarrow \bullet \to \bullet), \\ (\bullet \leftarrow \bullet \to \bullet)\} \\ = \delta(\bullet \bullet \leftrightarrow \varnothing \hookrightarrow \bullet) + 2\delta(\bullet \leftrightarrow \varnothing \hookrightarrow \varnothing).}} \delta\left((\varnothing \leftrightarrow \varnothing \hookrightarrow \varnothing), \overset{\mathbf{m}}{\Leftrightarrow} (\bullet \bullet \leftrightarrow \varnothing \hookrightarrow \varnothing)\right)$$
(19)

The result of the composition thus captures the combinatorial insight that there are two contributions that evaluate to an isomorphic rule algebra element.

More generally, one finds the following structure of compositions of rule algebra elements based upon "discrete" graph rewriting rules: letting • $^{\oplus n}$ denote the *n*-vertex graph without edges (for $n \ge 0$), one finds (for $p, q, r, s \ge 0$)

$$\delta(\bullet^{\oplus p} \longleftrightarrow \varnothing \hookrightarrow \bullet^{\oplus q}) \odot \delta(\bullet^{\oplus r} \longleftrightarrow \varnothing \hookrightarrow \bullet^{\oplus s})$$

$$= \sum_{k=0}^{\min(q,r)} k! \binom{q}{k} \binom{r}{k} \delta(\bullet^{\oplus (p+r-k)} \longleftrightarrow \varnothing \hookrightarrow \bullet^{\oplus (q+s-k)}).$$
(20)

Canonical representation of \mathscr{R}^{sq}_{C}

Let C be a category satisfying Assumption (II), with a strict initial object $\emptyset \in ob(C)$, and let \mathscr{R}^{sq}_{C} be its associated rule algebra of SqPO type. Denote by \hat{C} the free \mathbb{R} -vector space spanned by basis vectors $|X\rangle$ indexed by isomorphism classes of objects,

$$\hat{\mathbf{C}} := span_{\mathbb{R}}(\{|X\rangle|X \in obj(\mathbf{C})_{\cong}\}) \equiv (\hat{C}, +, \cdot).$$
(21)

Then the **canonical representation** $\rho_{\mathbf{C}}^{sq} : \mathscr{R}_{\mathbf{C}}^{sq} \to End_{\mathbb{R}}(\hat{\mathbf{C}})$ of $\mathscr{R}_{\mathbf{C}}^{sq}$ is defined as a morphism from the SqPO-type rule algebra $\mathscr{R}_{\mathbf{C}}^{sq}$ to endomorphisms of $\hat{\mathbf{C}}$, with

$$\rho_{\mathbf{C}}^{sq}(\boldsymbol{\delta}(p))|X\rangle := \begin{cases} \sum_{m \in \mathbf{M}_{p}^{SqPO}(X)} |p_{m}(X)\rangle & \text{if } \mathbf{M}_{p}^{SqPO}(X) \neq \emptyset \\ 0_{\hat{\mathbf{C}}} & \text{otherwise,} \end{cases}$$
(22)

and extended to arbitrary elements of \mathscr{R}^{sq}_{C} and of \hat{C} by linearity.

Note: ρ_{C}^{sq} being a representation of the unital associative algebra \mathscr{R}_{C}^{sq} entails the two properties

$$\rho_{\mathbf{C}}^{sq}(R_{\varnothing}) = \mathbb{1}_{End_{\mathbb{R}}(\widehat{\mathbf{C}})}, \qquad \rho_{\mathbf{C}}^{sq}\left(R_{1} \odot_{\mathscr{R}_{\mathbf{C}}} R_{2}\right) = \rho_{\mathbf{C}}^{sq}\left(R_{1}\right)\rho_{\mathbf{C}}^{sq}\left(R_{2}\right).$$
(23)

[16] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Canonical representations of the SqPO-type rule algebras – illustrative example [17]

Define
$$\rho \equiv \rho_{\text{FinGraph}}^{sq}$$
. Let
 $\hat{D} := \rho(\delta(\emptyset \leftrightarrow \emptyset \hookrightarrow \bullet)), \quad \hat{X} := \rho(\delta(\bullet \leftrightarrow \emptyset \hookrightarrow \emptyset)), \quad |n\rangle := |\bullet^{\oplus n}\rangle (n \ge 0).$
(24)

^[17] P Blasiak et al. "Boson normal ordering via substitutions and Sheffer-Type Polynomials". In: Physics Letters A 338.2 (2005), pp. 108–116; Pawel Blasiak, Gerard HE Duchamp, et al. "Combinatorial Algebra for second-quantized Quantum Theory". In: Advances in Theoretical and Mathematical Physics 14.4 (2010), pp. 1209–1243; Pawel Blasiak and Philippe Flajolet. "Combinatorial Models of Creation-Annihilation". In: Séminaire Lotharingien de Combinatoire 65. B65c (2011), pp. 1–78

^[18] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Canonical representations of the SqPO-type rule algebras – illustrative example [17]

Define
$$\rho \equiv \rho_{\operatorname{FinGraph}}^{sq}$$
. Let
 $\hat{D} := \rho(\delta(\varnothing \leftrightarrow \varnothing \hookrightarrow \bullet)), \qquad \hat{X} := \rho(\delta(\bullet \leftrightarrow \varnothing \hookrightarrow \varnothing)), \qquad |n\rangle := |\bullet^{\oplus n}\rangle (n \ge 0).$
(24)

One may verify that

$$\hat{D}|0\rangle = 0_{\widehat{\mathbf{FinGraph}}}, \quad \hat{D}|n\rangle = n|n-1\rangle \ (n>0), \qquad \hat{X}|n\rangle = |n+1\rangle.$$
(25)

The above data furnishes a **representation** of the famous **Heisenberg-Weyl algebra** that is of fundamental importance in combinatorics and physics (see e.g. [17]). An isomorphic representation is given by the linear operators \hat{x} (**multiplication by** *x*) and ∂_x (**derivation by** *x*) acting on the \mathbb{R} -vector space spanned by **monomials** x^n , with

$$\partial_x x^0 = 0, \quad \partial_x x^n = n x^{n-1}, \qquad \hat{x} x^n = x^{n+1}.$$
 (26)

^[17] P Blasiak et al. "Boson normal ordering via substitutions and Sheffer-Type Polynomials". In: *Physics Letters A* 338.2 (2005), pp. 108–116; Pawel Blasiak, Gerard HE Duchamp, et al. "Combinatorial Algebra for second-quantized Quantum Theory". In: Advances in Theoretical and Mathematical Physics 14.4 (2010), pp. 129–1243; Pawel Blasiak and Philippe Flajolet. "Combinatorial Models of Creation-Annihilation". In: Sciminaire Lotharingien de Combinatoire 65. B65c (2011), pp. 1–78

^[18] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Canonical representations of the SqPO-type rule algebras – illustrative example [17]

Define
$$\rho \equiv \rho_{\text{FinGraph}}^{sq}$$
. Let
 $\hat{D} := \rho(\delta(\emptyset \leftrightarrow \emptyset \hookrightarrow \bullet)), \qquad \hat{X} := \rho(\delta(\bullet \leftrightarrow \emptyset \hookrightarrow \emptyset)), \qquad |n\rangle := |\bullet^{\oplus n}\rangle (n \ge 0).$
(24)

One may verify that

$$\hat{D}|0\rangle = 0_{\widehat{\mathbf{FinGraph}}}, \quad \hat{D}|n\rangle = n|n-1\rangle \ (n>0), \qquad \hat{X}|n\rangle = |n+1\rangle.$$
(25)

The above data furnishes a **representation** of the famous **Heisenberg-Weyl algebra** that is of fundamental importance in combinatorics and physics (see e.g. [17]). An isomorphic representation is given by the linear operators \hat{x} (**multiplication by** *x*) and ∂_x (**derivation by** *x*) acting on the \mathbb{R} -vector space spanned by **monomials** x^n , with

$$\partial_x x^0 = 0, \quad \partial_x x^n = n x^{n-1}, \qquad \hat{x} x^n = x^{n+1}.$$
 (26)

However, the action of \hat{D} and \hat{X} is of course defined on **all** states $|G\rangle$ with $G \in obj(\mathbf{FinGraph})$, so that we may e.g. compute the following "**derivative of a graph**":

$$\hat{D} | \bullet \bullet \bullet \bullet \diamond \rangle = 2 | \bullet \bullet \bullet \diamond + | \bullet \bullet \diamond$$
(27)

^[17] P Blasiak et al. "Boson normal ordering via substitutions and Sheffer-Type Polynomials". In: *Physics Letters A* 338.2 (2005), pp. 108–116; Pawel Blasiak, Gerard HE Duchamp, et al. "Combinatorial Algebra for second-quantized Quantum Theory". In: Advances in Theoretical and Mathematical Physics 14.4 (2010), pp. 1209–1243; Pawel Blasiak and Philippe Flajolet. "Combinatorial Models of Creation-Annihilation". In: Sciminaire Lotharingien de Combinatoire 65. B65c (2011), pp. 1–78

^[18] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Continuous-time Markov chains via stochastic mechanics of SqPO-type rule algebras

Stochastic transition systems and continuous time Markov chain (CTMC) theory

• Standard CTMC theory [18]: one way to describe the CTMC's dynamics is to give a probability distribution (with S the set of pure states)

$$|\Psi(t)\rangle := \sum_{S \in \mathbf{S}} p_S(t)|S\rangle$$
 (28)

of being in one of the pure states (represented by basis vectors $|S\rangle$), and specifying the **Master equation** (aka **Kolmogorov forward equation**)

$$\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle, \qquad (29)$$

where *H* is the evolution operator.

 How precisely *H* is determined for a given system will be intimately related to the concept of rule algebras in our formalism!



The "stochastic mechanics" viewpoint

Benefits:

 \exists a full-blown formalism [19][20] aka "stochastic mechanics" [21] for studying CTMCs:

• Observables 𝒪 are linear operators under which each pure state is an Eigenstate,

$$\mathscr{O}|S\rangle = \mathscr{O}_{\mathscr{O}}(S)|S\rangle.$$
 (30)

 Expectation values of observables are computed by introducing the "dual projection vector"

$$\langle |S\rangle := 1 \quad \forall S \in \mathbf{S}, \tag{31}$$

such that for any state probability distribution $|\Psi(t)
angle$

$$\mathbb{E}_{|\Psi(t)\rangle}(\mathscr{O}) \equiv \langle \mathscr{O} \rangle(t) := \langle |\mathscr{O}|\Psi(t)\rangle.$$
(32)

⇒ evolution of expectation values of observables via Master equation:

$$\frac{d}{dt}\langle \mathcal{O}\rangle(t) = \langle \mathcal{O}H\rangle(t).$$
(33)

• Additional property of the evolution operator H:

$$\langle |e^{tH}|\Psi(0)\rangle \stackrel{!}{=} 1 \quad \Rightarrow \quad \langle |H=0, \qquad (34)$$

i.e. H preserves normalizations.

 \Rightarrow analogue of the **Ehrenfest equation** of quantum mechanics:

$$\frac{d}{dt} \langle \mathcal{O} \rangle(t) = \langle [\mathcal{O}, H] \rangle(t) \,, \tag{35}$$

where [A,B] := AB - BA is the **commutator**

- [19] M Doi. "Second quantization representation for classical many-particle system". In: Journal of Physics A: Mathematical and General 9.9 (Sept. 1976), pp. 1465–1477
- [20] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Stochastic mechanics of graph rewriting". In: Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016) (2016), pp. 46–55
- [21] John Baez and Jacob D Biamonte. Quantum Techniques in Stochastic Mechanics. WORLD SCIENTIFIC, May 2017

Let C be a category satisfying Assumption (II), and which in addition possesses a countable set of isomorphism classes of objects $obj(C)_{\cong}$. Let \hat{C} denote the free \mathbb{R} -vector space indexed by iso-classes of objects of C. We define the space Prob(C) as the space of sub-probability distributions in the following sense:

$$Prob(\mathbf{C}) := \left\{ \left| \Psi \right\rangle = \sum_{o \in obj(\mathbf{C})_{\cong}} \psi_o \left| o \right\rangle \left| \forall o \in obj(\mathbf{C})_{\cong} : \psi_o \in \mathbb{R}_{\geqslant 0} \land \sum_{o \in obj(\mathbf{C})_{\cong}} \psi_o \leqslant 1 \right. \right\}$$
(36)

Let $Stoch(\mathbf{C}) := End_{\mathbb{R}}(Prob(\mathbf{C}))$ be the space of endomorphisms of $Prob(\mathbf{C})$, with elements referred to as sub-stochastic operators.

Definition

Then a continuous-time Markov chain (CTMC) is specified in terms of a tuple of data $(|\Psi(0)\rangle, H)$, where $|\Psi(0)\rangle \in Prob(\mathbb{C})$ is the initial state, and where $H \in End_{\mathbb{R}}(\mathscr{S}_{\mathbb{C}})$ is the infinitesimal generator or Hamiltonian of the CTMC (with $\mathscr{S}_{\mathbb{C}}$ the space of real-valued sequences indexed by elements of $obj(\mathbb{C})_{\cong}$ and with finite coefficients). *H* is required to be an infinitesimal (sub-)stochastic operator, which entails that for $H \equiv (h_{o,o'})_{o,o' \in obj(\mathbb{C})_{\cong}}$ and for all $o, o' \in obj(\mathbb{C})_{\cong}$,

$$(i) \ h_{o,o} \leq 0, \ (ii) \ \forall o \neq o': \ h_{o,o'} \geq 0, \ (iii) \ \sum_{o'} h_{o,o'} = 0.$$
(36)

Then this data encodes the evolution semi-group $\mathscr{E} : \mathbb{R}_{\geq 0} \to Stoch(\mathbb{C})$ as the (point-wise minimal non-negative) solution of the Kolmogorov backwards or master equation:

$$\frac{d}{dt}\mathscr{E}(t) = H\mathscr{E}(t), \ \mathscr{E}(0) = \mathbb{1}_{Stoch(\mathbf{C})} \Rightarrow \ \forall t, t' \in \mathbb{R}_{\ge 0} : \mathscr{E}(t)\mathscr{E}(t') = \mathscr{E}(t+t')$$
(37)

Consequently, the **time-dependent state** $|\Psi(t)\rangle$ of the system is given by

$$\forall t \in \mathbb{R}_{\geq 0} : |\Psi(t)\rangle = \mathscr{E}(t) |\Psi(0)\rangle.$$
(38)

[22] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)



Definition

Let $\mathscr{O}_{\mathbb{C}} \subset End_{\mathbb{R}}(S_{\mathbb{C}})$ denote the space of observables, defined as the space of diagonal operators,

$$\mathscr{O}_{\mathbf{C}} := \{ O \in End_{\mathbb{R}}(S_{\mathbf{C}}) \mid \forall X \in obj(\mathbf{C})_{\cong} : O \mid X \rangle = \omega_O(X) \mid X \rangle, \ \omega_O(X) \in \mathbb{R} \}.$$
(39)

We furthermore define the so-called **projection operation** $\langle | : S_C \to \mathbb{R}$ via extending by linearity the definition of $\langle |$ acting on basis vectors of $\hat{\mathbf{C}}$,

$$\forall X \in obj(\mathbf{C})_{\cong} : \quad \langle |X\rangle := 1_{\mathbb{R}}.$$
(40)

These definitions induce a notion of **correlators** of observables (also referred to as (mixed) moments), defined for $O_1, \ldots, O_n \in \mathcal{O}_{\mathbf{C}}$ and $|\Psi\rangle \in Prob(\mathbf{C})$ as

$$\langle O_1, \dots, O_n \rangle_{|\Psi\rangle} := \langle |O_1, \dots, O_n |\Psi\rangle = \sum_{X \in obj(\mathbf{C})_{\cong}} \psi_X \cdot \omega_{O_1}(X) \cdots \omega_{O_n}(X).$$
(41)

[23] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Observables [22]

Definition

Let $\mathscr{O}_{\mathbb{C}} \subset End_{\mathbb{R}}(S_{\mathbb{C}})$ denote the space of **observables**, defined as the space of **diagonal operators**,

$$\mathscr{O}_{\mathbf{C}} := \{ O \in End_{\mathbb{R}}(S_{\mathbf{C}}) \mid \forall X \in obj(\mathbf{C})_{\cong} : O \mid X \rangle = \omega_O(X) \mid X \rangle, \ \omega_O(X) \in \mathbb{R} \}.$$
(39)

We furthermore define the so-called **projection operation** $\langle | : S_C \to \mathbb{R}$ via extending by linearity the definition of $\langle |$ acting on basis vectors of $\hat{\mathbf{C}}$,

$$\forall X \in obj(\mathbf{C})_{\cong} : \quad \langle |X\rangle := 1_{\mathbb{R}}.$$
(40)

These definitions induce a notion of **correlators** of observables (also referred to as (mixed) moments), defined for $O_1, \ldots, O_n \in \mathscr{O}_{\mathbb{C}}$ and $|\Psi\rangle \in Prob(\mathbb{C})$ as

$$\langle O_1, \dots, O_n \rangle_{|\Psi\rangle} := \langle |O_1, \dots, O_n |\Psi\rangle = \sum_{X \in obj(\mathbf{C})_{\cong}} \psi_X \cdot \omega_{O_1}(X) \cdots \omega_{O_n}(X).$$
(41)

Note:Depending on the concrete case, the eigenvalue $\omega_O(X)$ in $O|X\rangle = \omega_O(X)|X\rangle$ may e.g. coincide with the number of occurrences of a pattern in the object *X*.

^[23] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Theorem

Let **C** be a category satisfying **Assumption (II)**. Let $\{(O_j \rightleftharpoons I_j) \in \mathscr{R}^{sq}_{\mathbf{C}}\}_{j \in \mathscr{J}}$ be a (finite) set of rule algebra elements, and $\{\kappa_j \in \mathbb{R}_{\geq 0}\}_{j \in \mathscr{J}}$ a collection of non-zero parameters (called **base rates**). Then one may construct the Hamiltonian *H* of the associated CTMC from this data according to

$$H := \hat{H} + \bar{H}, \quad \hat{H} := \sum_{j \in \mathscr{J}} \kappa_j \cdot \rho_{\mathbf{C}}^{sq} \left(O_j \stackrel{p_j}{\Leftarrow} I_j \right), \quad \bar{H} := -\sum_{j \in \mathscr{J}} \kappa_j \cdot \mathbb{O}_{I_j}^{sq}.$$
(42)

Here, the notation \mathbb{O}_M^{sq} for arbitrary objects $M \in obj(\mathbb{C})$ denotes the **observables** (sometimes referred to as **motif counting observables**) for the resulting CTMC of SqPO-type, with

$$\mathbb{O}_{M}^{sq} := \rho_{\mathbf{C}}^{sq} \left(\delta \left(M \stackrel{id_{M}}{\longleftarrow} M \stackrel{id_{M}}{\longrightarrow} M \right) \right).$$
(43)

We furthermore have the SqPO-type jump-closure property, whereby for all $(O \leftarrow I) \in \mathscr{R}_{C}^{sq}$

$$\langle | \rho_{\mathbf{C}}^{sq}(O \stackrel{p}{\leftarrow} I) = \langle | \mathbb{O}_{I}^{sq}.$$
(44)

Observable moment evolution equations

Proposition ([23], Prop. 3.35): For linear operators A, B ∈ End_K(𝒱) (with 𝒱 a K-vector space) and λ a formal variable,

$$e^{\lambda A}Be^{-\lambda A} = e^{ad_{\lambda A}}B,\qquad(45)$$

where

$$ad_AB := [A,B] = AB - BA, ad_A^0B := B.$$

[5] Brian C. Hall. Lie Groups, Lie Algebras, and Representations. Springer International Publishing, 2015

^[6] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Stochastic mechanics of graph rewriting". In: Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016) (2016), pp. 46–55

^[7] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: arXiv preprint 1904.07313 (2019)

Observable moment evolution equations

Proposition ([23], Prop. 3.35): For linear operators A, B ∈ End_K(𝒱) (with 𝒱 a K-vector space) and λ a formal variable,

$$e^{\lambda A}Be^{-\lambda A} = e^{ad_{\lambda A}}B,\qquad(45)$$

where

$$ad_AB := [A,B] = AB - BA$$
, $ad_A^0B := B$.

• **Application:** suppose *H* is an evolution operator, and let

$$\underline{\lambda} \cdot \underline{\mathscr{O}} \equiv \sum_i \lambda_i \mathscr{O}_i$$

denote a formal linear combination of observables \mathcal{O}_i .

- [5] Brian C. Hall. Lie Groups, Lie Algebras, and Representations. Springer International Publishing, 2015
- [6] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Stochastic mechanics of graph rewriting". In: Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016) (2016), pp. 46–55
- [7] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: arXiv preprint 1904.07313 (2019)

• Define the moment-generating function $\mathscr{M}(t;\underline{\lambda})$ of the CTMC as

$$\mathscr{M}(t;\underline{\lambda}) := \left\langle e^{\underline{\lambda} \cdot \underline{\mathscr{O}}} \right\rangle(t),$$

whence formally

$$\left[\partial_{\lambda_{i_1}}^{n_1}\cdots\partial_{\lambda_{i_k}}^{n_k}\mathscr{M}(t;\underline{\lambda})\right]\Big|_{\underline{\lambda}\to\underline{0}}=\langle \mathscr{O}_{i_1}^{n_1}\cdots \mathscr{O}_{i_k}^{n_k}\rangle(t).$$

Observable moment evolution equations

Proposition ([23], Prop. 3.35): For linear operators A, B ∈ End_K(𝒴) (with 𝒴 a K-vector space) and λ a formal variable,

$$e^{\lambda A}Be^{-\lambda A} = e^{ad_{\lambda A}}B,\qquad(45)$$

where

$$ad_AB := [A,B] = AB - BA, ad_A^0B := B.$$

• **Application:** suppose *H* is an evolution operator, and let

$$\underline{\lambda} \cdot \underline{\mathscr{O}} \equiv \sum_i \lambda_i \mathscr{O}_i$$

denote a formal linear combination of observables \mathcal{O}_i .

• Define the moment-generating function $\mathcal{M}(t; \underline{\lambda})$ of the CTMC as

$$\mathscr{M}(t;\underline{\lambda}) := \left\langle e^{\underline{\lambda} \cdot \underline{\mathscr{O}}} \right\rangle(t),$$

whence formally

$$\left[\partial_{\lambda_{i_1}}^{n_1}\cdots\partial_{\lambda_{i_k}}^{n_k}\mathscr{M}(t;\underline{\lambda})\right]\Big|_{\underline{\lambda}\to\underline{0}}=\langle \mathscr{O}_{i_1}^{n_1}\cdots \mathscr{O}_{i_k}^{n_k}\rangle(t).$$

Formal all-order moment evolution equation [24] [25]:

$$\begin{split} \frac{d}{dt}\mathscr{M}(t;\underline{\lambda}) &= \left\langle \left| e^{\underline{\lambda}\cdot\underline{\mathscr{O}}} H \right| \Psi(t) \right\rangle \\ &= \left\langle \left| \left(e^{\underline{\lambda}\cdot\underline{\mathscr{O}}} H e^{-\underline{\lambda}\cdot\underline{\mathscr{O}}} \right) e^{\underline{\lambda}\cdot\underline{\mathscr{O}}} \right| \Psi(t) \right\rangle \\ &= \left\langle \left| \left(e^{ad_{\underline{\lambda}\cdot\underline{\mathscr{O}}}} H \right) e^{\underline{\lambda}\cdot\underline{\mathscr{O}}} \right| \Psi(t) \right\rangle. \end{split}$$

[5] Brian C. Hall. Lie Groups, Lie Algebras, and Representations. Springer International Publishing, 2015

^[6] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Stochastic mechanics of graph rewriting". In: Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016) (2016), pp. 46–55

^[7] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: arXiv preprint 1904.07313 (2019)

Let **FinGraph** be the finitary restriction of the category **Graph**, and denote by $\emptyset \in$ **FinGraph** the strict initial object (the empty graph).

Let **FinGraph** be the finitary restriction of the category **Graph**, and denote by $\emptyset \in$ **FinGraph** the strict initial object (the empty graph).

We define a stochastic SqPO rewriting system based upon rules encoding vertex creation/deletion (v_{\pm}) and edge creation/deletion (e_{\pm}):

$$v_{+} := (\bullet \leftarrow \varnothing \to \varnothing) \qquad v_{-} := (\varnothing \leftarrow \varnothing \to \bullet) e_{+} := (\bullet \to \bullet \leftarrow \bullet \to \bullet \to \bullet) \qquad e_{-} := (\bullet \to \leftarrow \bullet \to \bullet \to \bullet \to \bullet)$$
(46)

Let **FinGraph** be the finitary restriction of the category **Graph**, and denote by $\emptyset \in$ **FinGraph** the strict initial object (the empty graph).

We define a stochastic SqPO rewriting system based upon rules encoding vertex creation/deletion (v_{\pm}) and edge creation/deletion (e_{\pm}):

$$v_{+} := (\bullet \leftarrow \varnothing \to \varnothing) \qquad v_{-} := (\varnothing \leftarrow \varnothing \to \bullet) e_{+} := (\bullet \to \bullet \leftarrow \bullet \to \bullet \to \bullet) \qquad e_{-} := (\bullet \bullet \leftarrow \bullet \to \bullet \to \bullet \to \bullet)$$
(46)

Together with a choice of **base rates** $v_{\pm}, \varepsilon_{\pm} \in \mathbb{R}_{\geq 0}$ and an **initial state** $|\Psi(0)\rangle \in Prob(\mathbf{FinGraph})$, this data defines a stochastic rewriting system with Hamiltonian $H := \hat{H} + \bar{H}$,

$$\hat{H} = \mathbf{v}_{+}\mathbf{V}_{+} + \mathbf{v}_{-}\mathbf{V}_{-} + \boldsymbol{\varepsilon}_{+}E_{+} + \boldsymbol{\varepsilon}_{-}E_{-}
\bar{H} = -\mathbf{v}_{+}\mathbb{O}_{\varnothing} - \mathbf{v}_{-}\mathbb{O}_{\bullet} - \boldsymbol{\varepsilon}_{+}\mathbb{O}_{\bullet\bullet} - \boldsymbol{\varepsilon}_{-}\mathbb{O}_{\bullet\bullet\bullet\bullet},$$
(47)

where $V_{\pm} := \rho_{\mathrm{FinGraph}}^{sq}(\delta(v_{\pm}))$ and $E_{\pm} := \rho_{\mathrm{FinGraph}}^{sq}(\delta(e_{\pm})).$

^[26] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Vertex-counting observable dynamics:

• Exponential moment generating function of the observable $O_V := \mathbb{O}_{\bullet}$.

$$M_{V}(t;\lambda) := \langle |e^{\lambda O_{V}}|\Psi(t)\rangle \qquad (t \ge 0, \lambda \text{ formal})$$
(48)

Vertex-counting observable dynamics:

• Exponential moment generating function of the observable $O_V := \mathbb{O}_{\bullet}$.

$$M_{V}(t;\lambda) := \langle | e^{\lambda O_{V}} | \Psi(t) \rangle \qquad (t \ge 0, \lambda \text{ formal})$$
(48)

• formal evolution equation for $M_V(t; \lambda)$:

$$\frac{\partial}{\partial t}M_{V}(t;\lambda) = \langle |e^{\lambda O_{V}}H|\Psi(t)\rangle = \langle |\left(e^{\lambda O_{V}}He^{-\lambda O_{V}}\right)e^{\lambda O_{V}}|\Psi(t)\rangle = \langle |\left(e^{ad_{\lambda O_{V}}}H\right)e^{\lambda O_{V}}|\Psi(t)\rangle.$$
(49)

Vertex-counting observable dynamics:

• Exponential moment generating function of the observable $O_V := \mathbb{O}_{\bullet}$.

$$M_{V}(t;\lambda) := \langle | e^{\lambda O_{V}} | \Psi(t) \rangle \qquad (t \ge 0, \lambda \text{ formal})$$
(48)

• formal evolution equation for $M_V(t; \lambda)$:

$$\frac{\partial}{\partial t}M_{V}(t;\lambda) = \langle |e^{\lambda O_{V}}H|\Psi(t)\rangle = \langle |\left(e^{\lambda O_{V}}He^{-\lambda O_{V}}\right)e^{\lambda O_{V}}|\Psi(t)\rangle$$

$$= \langle |\left(e^{ad_{\lambda O_{V}}}H\right)e^{\lambda O_{V}}|\Psi(t)\rangle.$$
(49)

• Since by definition $\langle | H = 0$, it remains to compute the adjoint action $ad_{O_V}(H)$ of O_V on H:

$$ad_{O_V}(H) = \mathbf{v}_+[O_V, V_+] + \mathbf{v}_-[O_V, V_-] + \varepsilon_+[O_V, E_+] + \varepsilon_-[O_V, E_-]$$

= $\mathbf{v}_+V_+ - \mathbf{v}_-V_-$ (50)

Note: the result that $[O_V, E_{\pm}] = 0$ has a very simple **intuitive meaning**: in applications of the linear rules e_{\pm} , the number of vertices remains unchanged, whence the vanishing of the commutator.

Vertex-counting observable dynamics:

• Exponential moment generating function of the observable $O_V := \mathbb{O}_{\bullet}$.

$$M_{V}(t;\lambda) := \langle |e^{\lambda O_{V}} |\Psi(t) \rangle \qquad (t \ge 0, \lambda \text{ formal})$$
(48)

• formal evolution equation for $M_V(t; \lambda)$:

$$\frac{\partial}{\partial t} M_V(t;\lambda) = \langle |e^{\lambda O_V} H |\Psi(t)\rangle = \langle |\left(e^{\lambda O_V} H e^{-\lambda O_V}\right) e^{\lambda O_V} |\Psi(t)\rangle$$

$$= \langle |\left(e^{ad_{\lambda O_V}} H\right) e^{\lambda O_V} |\Psi(t)\rangle.$$
(49)

Combining these results with the SqPO-type jump-closure property, we finally arrive at

$$\frac{\partial}{\partial t}M_{V}(t;\lambda) = \mathbf{v}_{+}\left(e^{\lambda}-1\right)\langle|V_{+}e^{\lambda O_{V}}|\Psi(t)\rangle + \mathbf{v}_{-}\left(e^{-\lambda}-1\right)\langle|V_{-}e^{\lambda O_{V}}|\Psi(t)\rangle$$

$$\frac{^{(44)}}{=}\mathbf{v}_{+}\left(e^{\lambda}-1\right)\langle|e^{\lambda O_{V}}|\Psi(t)\rangle + \mathbf{v}_{-}\left(e^{-\lambda}-1\right)\langle|O_{V}e^{\lambda O_{V}}|\Psi(t)\rangle$$

$$= \left(\mathbf{v}_{+}\left(e^{\lambda}-1\right)+\mathbf{v}_{-}\left(e^{-\lambda}-1\right)\frac{\partial}{\partial\lambda}\right)M_{V}(t;\lambda).$$
(50)

Vertex-counting observable dynamics:

• Exponential moment generating function of the observable $O_V := \mathbb{O}_{\bullet}$.

$$M_{V}(t;\lambda) := \langle | e^{\lambda O_{V}} | \Psi(t) \rangle \qquad (t \ge 0, \lambda \text{ formal})$$
(48)

• Supposing for simplicity an initial state $|\Psi(0)\rangle = |G_0\rangle$ (for $G_0 \in obj(\mathbf{Graph}_{fin})$ some graph with N_V vertices and N_E edges), we find that $M_V(0;\lambda) = \exp(\lambda N_V)$. The resulting initial value problem may be solved in closed-form via **semi-linear normal-ordering** techniques known from the combinatorics literature [26] (see also [27], [28]), and we obtain (for $t \ge 0$)

$$M_V(t;\lambda) = \exp\left(\frac{\nu_+}{\nu_-}(e^{\lambda}-1)(1-e^{-\nu_-t})\right) \left(1+(e^{\lambda}-1)e^{-\nu_-t}\right)^{N_V}.$$
(49)

In the limit $t \to \infty$, the moment-generating function becomes that of a **Poisson-distribution** (of parameter v_+/v_-), thus confirming the aforementioned intuition that the vertex-counting observable has the dynamical behavior of a so-called **birth-death process** (see e.g. [29]).

- [26] G. Dattoli et al. "Evolution operator equations: Integration with algebraic and finite-difference methods: Applications to physical problems in classical and quantum mechanics and quantum field theory". In: Riv. Nuovo Cim. 20N2 (1997), pp. 1–133; P Blasiak et al. "Boson normal ordering via substitutions and Sheffer-Type Polynomials". In: Physics Letters A 338.2 (2005), pp. 108–116; Pawel Blasiak and Philippe Flajolet. "Combinatorial Models of Creation-Annihilation". In: Seminaire Lotharingien de Combinatoria 65.B65c (2011), pp. 1–78; Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: arXiv:1712.06575 (2017)
- [27] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories (invited extended journal version)". In: arXiv preprint 1807.00785v2 (2019)
- [28] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: arXiv preprint 1904.07313 (2019)
- [29] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: arXiv:1712.06575 (2017)
- [30] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

Edge-counting observable dynamics:

For sake of illustration, consider the evolution equation for the expectation value of the edge-counting observable O_E := 0_{●→→●}, which reads (analogue of the so-called Ehrenfest equation)

$$\frac{\partial}{\partial t}\langle |O_E|\Psi(t)\rangle = \langle |O_EH|\Psi(t)\rangle = \langle |(HO_E + [O_E,H])|\Psi(t)\rangle.$$
(50)

Edge-counting observable dynamics:

For sake of illustration, consider the evolution equation for the expectation value of the edge-counting observable O_E := 0_{●→→●}, which reads (analogue of the so-called Ehrenfest equation)

$$\frac{\partial}{\partial t} \langle | O_E | \Psi(t) \rangle = \langle | O_E H | \Psi(t) \rangle = \langle | (H O_E + [O_E, H]) | \Psi(t) \rangle.$$
(50)

• Recalling that $\langle | H = 0$, it remains to compute the commutator $[O_E, H]$:

$$\begin{aligned} [O_E, H] &= \mathbf{v}_+ [O_E, V_+] + \mathbf{v}_- [O_E, V_-] + \mathbf{\varepsilon}_+ [O_E, E_+] + \mathbf{\varepsilon}_- [O_E, V_-] \\ &= \mathbf{v}_+ \cdot 0 - \mathbf{v}_- (E_-^{0,1} + E_-^{1,0}) + \mathbf{\varepsilon}_+ E_+ - \mathbf{\varepsilon}_- E_- \\ E_-^{0,1} &= \rho_{\mathbf{FinGraph}}^{sq} \left(\delta \left(\underbrace{\bullet}_s \leftarrow \underbrace{\bullet}_s \to \underbrace{\bullet}_s \right) \right), \quad E_-^{1,0} = \rho_{\mathbf{FinGraph}}^{sq} \left(\delta \left(\underbrace{\bullet}_s \leftarrow \underbrace{\bullet}_s \to \underbrace{\bullet}_s \right) \right). \end{aligned}$$
(51)

Edge-counting observable dynamics:

For sake of illustration, consider the evolution equation for the expectation value of the edge-counting observable O_E := 0,→→→, which reads (analogue of the so-called Ehrenfest equation)

$$\frac{\partial}{\partial t}\langle |O_E|\Psi(t)\rangle = \langle |O_EH|\Psi(t)\rangle = \langle |(HO_E+[O_E,H])|\Psi(t)\rangle.$$
(50)

• Recalling that $\langle | H = 0$, it remains to compute the commutator $[O_E, H]$:

$$[O_E, H] = \mathbf{v}_+[O_E, V_+] + \mathbf{v}_-[O_E, V_-] + \mathbf{\varepsilon}_+[O_E, E_+] + \mathbf{\varepsilon}_-[O_E, V_-]$$

$$= \mathbf{v}_+ \cdot 0 - \mathbf{v}_-(E_-^{0,1} + E_-^{1,0}) + \mathbf{\varepsilon}_+ E_+ - \mathbf{\varepsilon}_- E_-$$

$$E_-^{0,1} = \rho_{\mathbf{FinGraph}}^{sq} \left(\delta \left(\underbrace{\bullet}_{s} \leftarrow \underbrace{\bullet}_{s} \to \underbrace{\bullet}_{s} \to \underbrace{\bullet}_{s} \right) \right), \quad E_-^{1,0} = \rho_{\mathbf{FinGraph}}^{sq} \left(\delta \left(\underbrace{\bullet}_{s} \leftarrow \underbrace{\bullet}_{s} \to \underbrace{\bullet}_{s} \to \underbrace{\bullet}_{s} \right) \right).$$
(51)

• It then remains to apply the jump-closure property together with the identity $\mathbb{O}_{\bullet\bullet} = O_V(O_V - 1)$ in order to obtain the evolution equation

$$\frac{\partial}{\partial t}\langle |O_E|\Psi(t)\rangle = \varepsilon_+ \langle |O_V(O_V-1)|\Psi(t)\rangle - (\varepsilon_- + 2\nu_-)\langle |O_E|\Psi(t)\rangle.$$
(52)



Summary and outlook



Thank you!

- John Baez and Jacob D Biamonte. Quantum Techniques in Stochastic Mechanics. WORLD SCIENTIFIC, May 2017.
- Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: *arXiv preprint* 1904.08357 (2019).
- Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: *arXiv preprint 1904.07313* (2019).
- Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: *arXiv preprint 1904.07313* (2019).
- Nicolas Behr, Vincent Danos, and Ilias Garnier. "Stochastic mechanics of graph rewriting". In: Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016) (2016), pp. 46–55.
- Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: arXiv:1712.06575 (2017).
- Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: 27th EACSL Annual Conference on Computer Science Logic (CSL 2018). Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum für Informatik, Sept. 2018, 11:1–11:21.

- Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories (invited extended journal version)". In: *arXiv* preprint 1807.00785v2 (2019).
- Pawel Blasiak, Gerard HE Duchamp, et al. "Combinatorial Algebra for second-quantized Quantum Theory". In: Advances in Theoretical and Mathematical Physics 14.4 (2010), pp. 1209–1243.
- Pawel Blasiak and Philippe Flajolet. "Combinatorial Models of Creation-Annihilation". In: Séminaire Lotharingien de Combinatoire 65.B65c (2011), pp. 1–78.
- P Blasiak et al. "Boson normal ordering via substitutions and Sheffer-Type Polynomials". In: *Physics Letters A* 338.2 (2005), pp. 108–116.
- Andrea Corradini et al. "Sesqui-Pushout Rewriting". In: *Lecture Notes in Computer Science*. Springer Berlin Heidelberg, 2006, pp. 30–45.
- G. Dattoli et al. "Evolution operator equations: Integration with algebraic and finite-difference methods: Applications to physical problems in classical and quantum mechanics and quantum field theory". In: *Riv. Nuovo Cim.* 20N2 (1997), pp. 1–133.
- M Doi. "Second quantization representation for classical many-particle system". In: Journal of Physics A: Mathematical and General 9.9 (Sept. 1976), pp. 1465–1477.
- Karsten Gabriel et al. "Finitary *M*-adhesive categories". In: *Mathematical Structures in Computer Science* 24.04 (June 2014).
- Brian C. Hall. Lie Groups, Lie Algebras, and Representations. Springer International Publishing, 2015.
- Stephen Lack and Paweł Sobociński. "Adhesive and quasiadhesive categories". In: *RAIRO-Theoretical Informatics and Applications* 39.3 (2005), pp. 511–545.

- Michael Löwe. "Polymorphic Sesqui-Pushout Graph Rewriting". In: *Graph Transformation*. Springer International Publishing, 2015, pp. 3–18.
- James R. Norris. Markov Chains. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press, 1998.

SqPO-type concurrency theorem – proof of the synthesis part [29]



(i) Obtain the span $\mathbf{n} = (I_2 \leftarrow M_{21} \rightarrow O_1)$ via pulling back the cospan $(I_2 \rightarrow X_1 \leftarrow O_1)$.

(ii) construct N_{21} via taking the pushout of **n**, which induces a unique arrow $N_{21} \rightarrow X_1$ (that is a **monomorphism** due to effectiveness of pushouts in adhesive categories).

SqPO-type concurrency theorem – proof of the synthesis part [29]



- (iii) Take the pullbacks of the spans $\overline{K}_i \to X_1 \leftarrow N_{21}$ (for i = 1, 2), obtaining the squares (2') and (3').
- (iv) By virtue of pushout-pullback decomposition, the squares (2) and (2') are pushouts.
- (v) Invoking vertical FPC-pullback decomposition, the squares (3) and (3') are FPCs.
- (vi) Let $O_{21} := \mathbf{PO}(O_2 \leftarrow K_2 \rightarrow K'_2)$ and $I_{21} := \mathbf{PO}(O_1 \leftarrow K_1 \rightarrow K'_1)$. Then via vertical FPC-pushout decomposition the squares (1) and (1') are FPCs and $I_{21} \rightarrow X_0$ is a monomorphism, while via pushout-pushout decomposition the squares (4) and (4') are pushouts.

[30] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

SqPO-type concurrency theorem – proof of the synthesis part [29]



- (vii) Take **pullbacks** $K_{21} = \mathbf{PB}(K'_2 \to N_{21} \leftarrow K'_1)$ and $\overline{K}_{21} = \mathbf{PB}(\overline{K}_2 \to X_1 \leftarrow \overline{K}_1)$, which by universality of pullbacks induces a unique arrow $K_{21} \to \overline{K}_{21}$.
- (viii) Via pullback-pullback decomposition, the squares $\Box(K_{21}, \overline{K}_{21}, \overline{K}_i, K'_i)$ (for i = 1, 2) are pullbacks.
- (ix) Since the square $\Box(K'_1, \overline{K}_1, X_1, N_{21})$ is a pushout, via the **van Kampen property** the square $\Box(K_{21}, \overline{K}_{21}, \overline{K}_2, K'_2)$ is a **pushout**.

[30] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)
SqPO-type concurrency theorem – proof of the synthesis part [29]



- (x) Since pushouts along monos are also FPCs, it follows via horizontal composition of FPCs that the square $\Box(K_{21}, \overline{K}_{21}, X_1, N_{21})$ is an FPC.
- (xi) The pushout square $\Box(K'_1, \overline{K}_1, X_1, N_{21})$ is also an FPC, so via **horizontal decomposition of FPCs** the square $\Box(K_{21}, \overline{K}_{21}, \overline{K}_1, K'_1)$ is an **FPC**.

[30] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)

SqPO-type concurrency theorem – proof of the synthesis part [29]



(xiii) The claim follows by invoking **pushout composition** and **horizontal FPC composition** in order to obtain the **pushout square** $\Box(K_{21}, \overline{K}_{21}, X_2, O_{21})$ and the **FPC square** $\Box(K_{21}, \overline{K}_{21}, X_0, I_{21})$.

back to main text

^[30] Nicolas Behr. "Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework". In: arXiv preprint 1904.08357 (2019)