INSTITUT
DE RECHERCHE
EN INFORMATIQUE
FONDAMENTALE

Université Paris Cité

Fundamentals of Compositional Rewriting Theory

Topos Institute Colloquium, June 9, 2022

Nicolas Behr

CNRS, Université Paris Cité, IRIF (UMR 8243)

The long road towards
***compositional* categorical rewriting theory**

H. Ehrig, M. Pfender, and H.J. Schneider. Graph-grammars: an algebraic approach. In *Proceedings IEEE Conf. on Automata and Switching Theory*, pages 167–180, 1973.

Andrea Corradini, Ugo Montanari, Francesca Rossi, Hartmut Ehrig, Reiko Heckel, and Michael Löwe. Algebraic Approaches to Graph Transformation - Part I: Basic Concepts and Double Pushout Approach. In *Handbook of Graph Grammars and Computing by Graph Transformations, Volume 1: Foundations*, pages 163–246, 1997.

The long road towards
***compositional* categorical rewriting theory**

H. Ehrig, M. Pfender, and H.J. Schneider. Graph-grammars: an algebraic approach. In *Proceedings IEEE Conf. on Automata and Switching Theory*, pages 167–180, 1973.

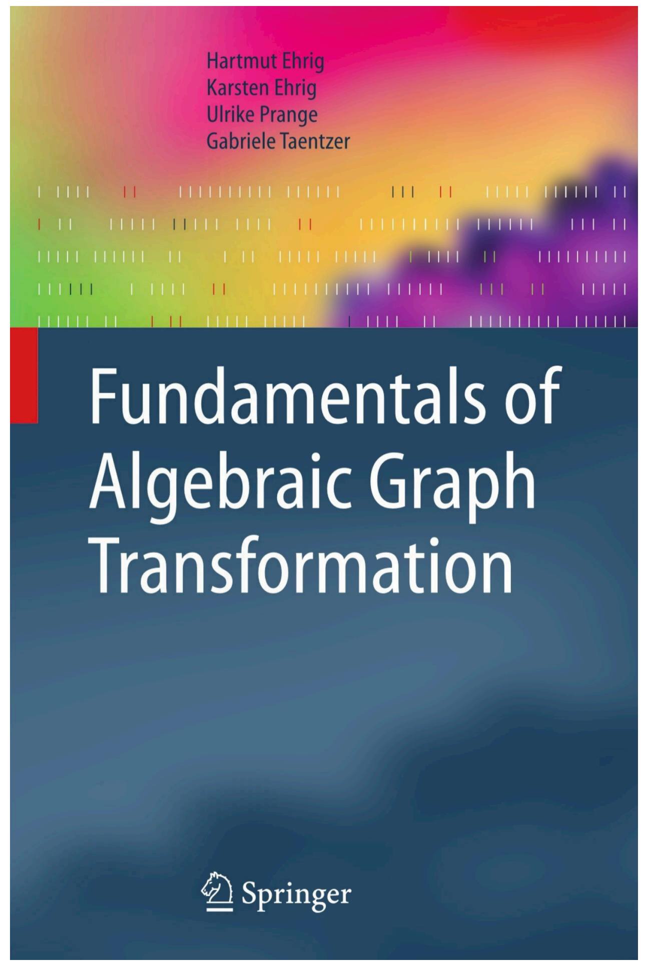
Andrea Corradini, Ugo Montanari, Francesca Rossi, Hartmut Ehrig, Reiko Heckel, and Michael Löwe. Algebraic Approaches to Graph Transformation - Part I: Basic Concepts and Double Pushout Approach. In *Handbook of Graph Grammars and Computing by Graph Transformations, Volume 1: Foundations*, pages 163–246, 1997.

Lack, S., Sobociński, P.: Adhesive Categories. In: FoSSaCS 2004. LNCS, vol. 2987, pp. 273–288 (2004). https://doi.org/10.1007/978-3-540-24727-2_20

Lack, S., Sobociński, P.: Adhesive and quasiadhesive categories. RAIRO - Theoretical Informatics and Applications **39**(3), 511–545 (2005). https://doi.org/10.1051/ita:2005028

Ehrig, H., et al.: Adhesive High-Level Replacement Categories and Systems. In: LNCS, vol. 3256, pp. 144–160 (2004). https://doi.org/10.1007/978-3-540-30203-2_12

The long road towards *compositional* categorical rewriting theory



H. Ehrig, M. Pfender, and H.J. Schneider. Graph-grammars: an algebraic approach. In *Proceedings IEEE Conf. on Automata and Switching Theory*, pages 167–180, 1973.

Andrea Corradini, Ugo Montanari, Francesca Rossi, Hartmut Ehrig, Reiko Heckel, and Michael Löwe. Algebraic Approaches to Graph Transformation - Part I: Basic Concepts and Double Pushout Approach. In *Handbook of Graph Grammars and Computing by Graph Transformations, Volume 1: Foundations*, pages 163–246, 1997.

Lack, S., Sobociński, P.: Adhesive Categories. In: FoSSaCS 2004. LNCS, vol. 2987, pp. 273–288 (2004). https://doi.org/10.1007/978-3-540-24727-2_20

Lack, S., Sobociński, P.: Adhesive and quasiadhesive categories. RAIRO - Theoretical Informatics and Applications **39**(3), 511–545 (2005). https://doi.org/10.1051/ita:2005028

Ehrig, H., et al.: Adhesive High-Level Replacement Categories and Systems. In: LNCS, vol. 3256, pp. 144–160 (2004). https://doi.org/10.1007/978-3-540-30203-2_12

The long road towards
***compositional* categorical rewriting theory**

Corradini, A., et al.: Sesqui-Pushout Rewriting. In: Graph Transformations. LNCS, vol. 4178, pp. 30–45. Springer Berlin Heidelberg (2006)

Corradini, A., et al.: AGREE – Algebraic Graph Rewriting with Controlled Embedding. In: Graph Transformation (ICGT 2015). LNCS, vol. 9151, pp. 35–51. Cham (2015). https://doi.org/10.1007/978-3-319-21145-9_3

Annegret Habel and Karl-Heinz Pennemann. Correctness of high-level transformation systems relative to nested conditions. *Mathematical Structures in Computer Science*, 19(02):245, 2009. DOI: https://doi.org/10.1017/s0960129508007202.

Ehrig, H., et al.: $\mathcal{M}$-adhesive transformation systems with nested application conditions. Part 1: parallelism, concurrency and amalgamation. MSCS **24**(04) (2014). https://doi.org/10.1017/s0960129512000357

Gabriel, K., et al.: Finitary $\mathcal{M}$-adhesive categories. MSCS **24**(04) (2014). https://doi.org/10.1017/S0960129512000321

Nicolas Behr, Jean Krivine, Jakob L. Andersen, Daniel Merkle (2021). Rewriting theory for the life sciences: A unifying theory of CTMC semantics. In: Theoretical Computer Science.

PDF Cite Video

Nicolas Behr, Russ Harmer, Jean Krivine (2021). Concurrency Theorems for Non-linear Rewriting Theories. In: arXiv preprint (long version including additional technical appendices of a paper with the same title accepted for ICGT 2021).

Preprint Cite Slides

Nicolas Behr, Joachim Kock (2021). Tracelet Hopf algebras and decomposition spaces. In: arXiv preprint.

Preprint Cite Slides Video

Nicolas Behr (2021). On Stochastic Rewriting and Combinatorics via Rule-Algebraic Methods. Invited Paper in Patrick Bahr (ed.): Proceedings 11th International Workshop on Computing with Terms and Graphs (TERMGRAPH 2020), Online, 5th July 2020, Electronic Proceedings in Theoretical Computer Science 334, pp. 11–28..

PDF Cite

Nicolas Behr, Jean Krivine (2021). Compositionality of Rewriting Rules with Conditions. Compositionality 3, 2 (2021)..

PDF Cite

Nicolas Behr, Maryam Ghaffari Saadat, Reiko Heckel (2020). Efficient Computation of Graph Overlaps for Rule Composition: Theory and Z3 Prototyping. In: B. Hoffmann and M. Minas: Proceedings of the Eleventh International Workshop on Graph Computation Models (GCM 2020), Online-Workshop, 24th June 2020, Electronic Proceedings in Theoretical Computer Science 330, pp. 126–144..

PDF Cite

Nicolas Behr, Pawel Sobocinski (2020). Rule Algebras for Adhesive Categories (invited extended jounral version). In: Logical Methods in Computer Science, Volume 16, Issue 3.

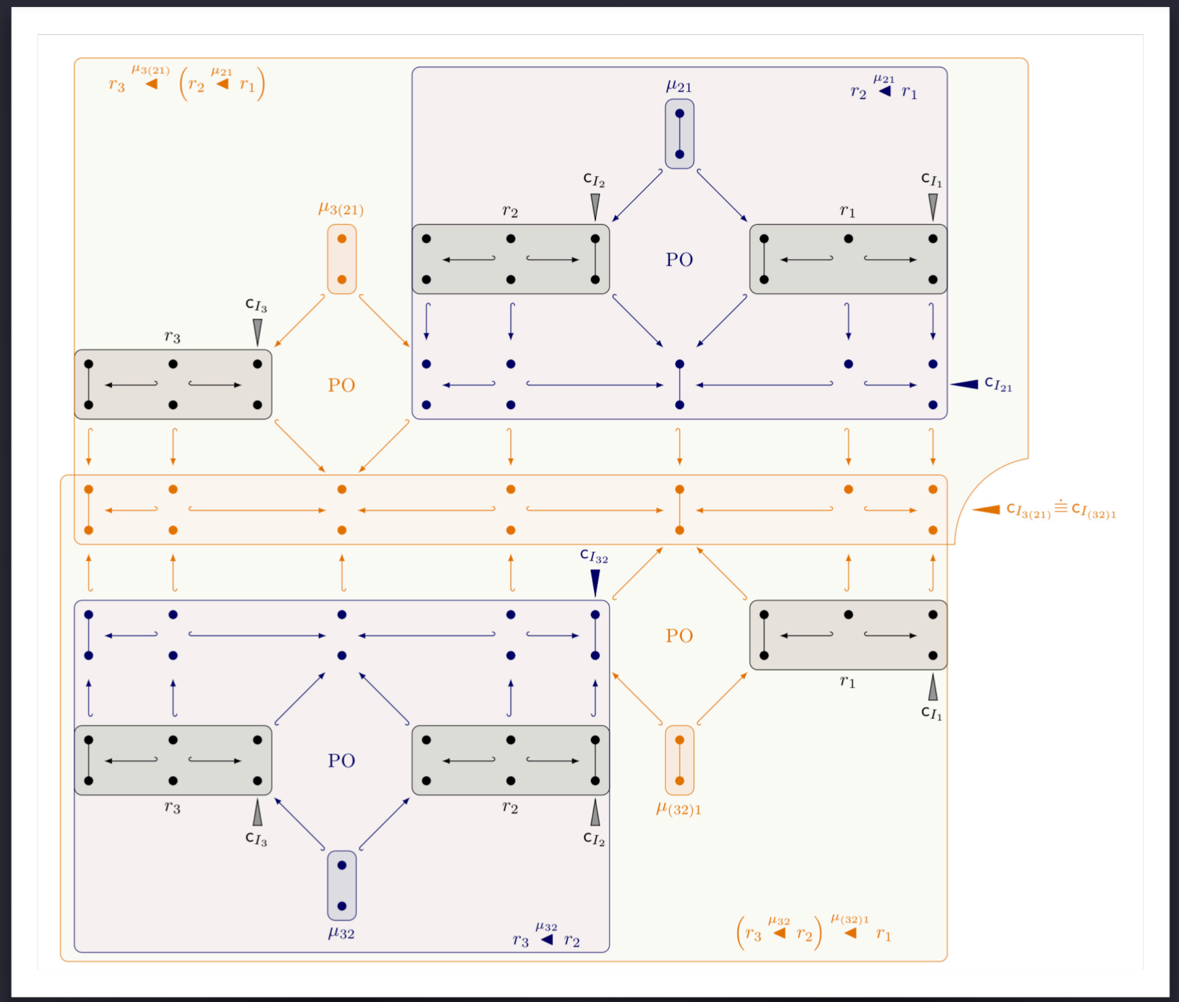
PDF Cite

Nicolas Behr, Vincent Danos, Ilias Garnier (2020). Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems. In: Logical Methods in Computer Science, Volume 16, Issue 3.

PDF Cite Slides

NEW YORK LICS
ACM/IEEE Logic in Computer Science
Columbia University • July 2016

NB et al.
2014 — 2021



Nicolas Behr (2019). Sesqui-Pushout Rewriting: Concurrency, Associativity and Rule Algebra Framework. Electronic Proceedings in Theoretical Computer Science, 309:23–52.

PDF Cite Slides

Nicolas Behr, Pawel Sobocinski (2018). Rule Algebras for Adhesive Categories. In: 27th EACSL Annual Conference on Computer Science Logic (CSL 2018), Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, Dagstuhl, Germany, *pp. 11:1–11:21*.

PDF Cite Slides

Nicolas Behr, Vincent Danos, Ilias Garnier, Tobias Heindel (2016). The algebras of graph rewriting. In: arXiv preprint.

Preprint PDF Cite Slides Video

Nicolas Behr, Vincent Danos, Ilias Garnier (2016). Stochastic mechanics of graph rewriting. In: Proceedings of the 31st Annual ACM/IEEE Symposium on Logic in Computer Science - LICS '16, ACM Press.

Preprint PDF Cite Slides

Nicolas Behr (2020). Tracelets and Tracelet Analysis Of Compositional Rewriting Systems. In: John Baez and Bob Coecke: Proceedings Applied Category Theory 2019 (ACT 2019), University of Oxford, UK, 15-19 July 2019, Electronic Proceedings in Theoretical Computer Science 323, pp. 44-71..

PDF Cite Slides Video

Fundamentals of Compositional Rewriting Theory★

Nicolas Behr[a,*], Russell Harmer[b], Jean Krivine[a]

[a] *Université Paris Cité, CNRS, IRIF, 8 Place Aurélie Nemours, Paris Cedex 13, 75205, France*
[b] *Université de Lyon, ENS de Lyon, UCBL, CNRS, LIP, 46 allée d'Italie, Lyon Cedex 07, 69364, France*

Fundamentals of Compositional Rewriting Theory★

Nicolas Behr[a,*], Russell Harmer[b], Jean Krivine[a]

[a] *Université Paris Cité, CNRS, IRIF, 8 Place Aurélie Nemours, Paris Cedex 13, 75205, France*
[b] *Université de Lyon, ENS de Lyon, UCBL, CNRS, LIP, 46 allée d'Italie, Lyon Cedex 07, 69364, France*

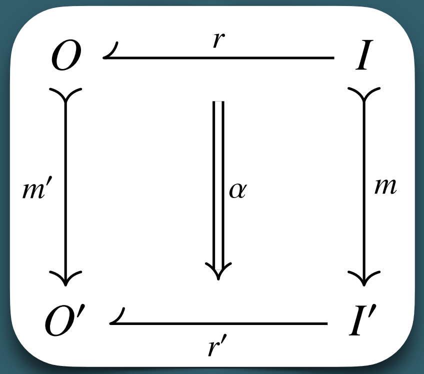
★ Special thanks to **Richard Garner**, **Paul-André Melliès** and **Noam Zeilberger !**

Fundamentals of Compositional Rewriting Theory⋆

Nicolas Behr[a,*], Russell Harmer[b], Jean Krivine[a]

[a] *Université Paris Cité, CNRS, IRIF, 8 Place Aurélie Nemours, Paris Cedex 13, 75205, France*
[b] *Université de Lyon, ENS de Lyon, UCBL, CNRS, LIP, 46 allée d'Italie, Lyon Cedex 07, 69364, France*

compositional rewriting double categories (crDCs)

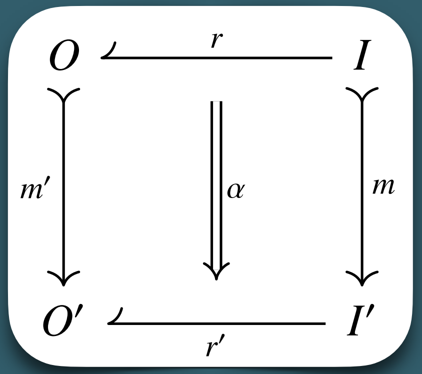


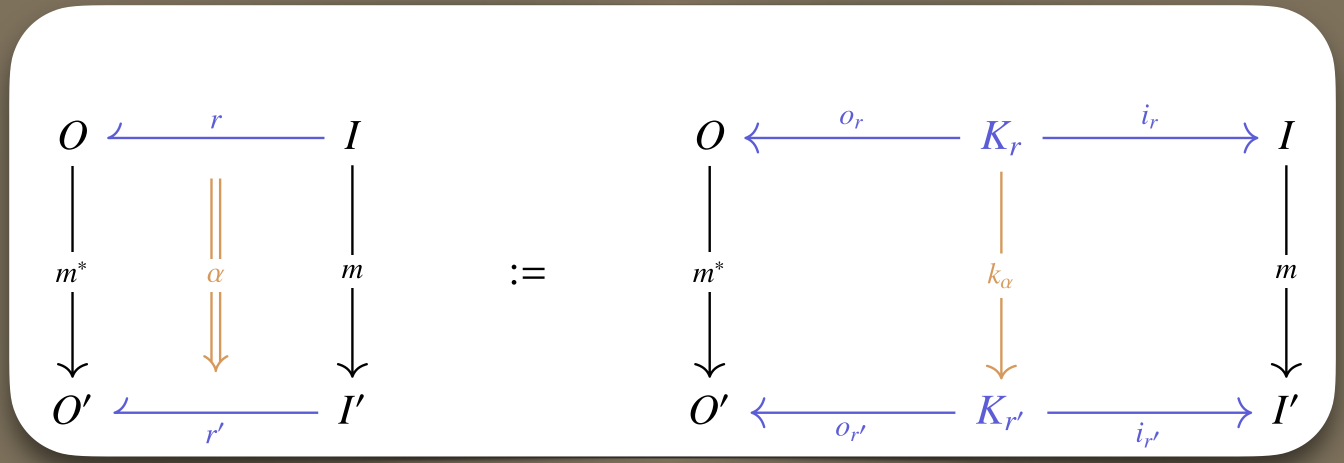

Fundamentals of Compositional Rewriting Theory★

Nicolas Behr[a,*], Russell Harmer[b], Jean Krivine[a]

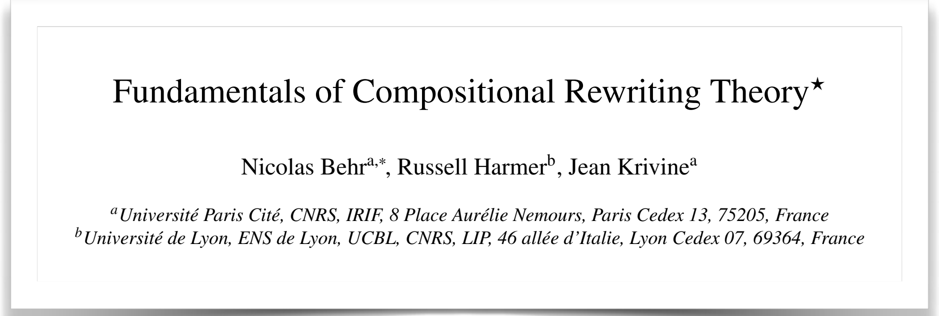
[a]Université Paris Cité, CNRS, IRIF, 8 Place Aurélie Nemours, Paris Cedex 13, 75205, France
[b]Université de Lyon, ENS de Lyon, UCBL, CNRS, LIP, 46 allée d'Italie, Lyon Cedex 07, 69364, France

compositional rewriting double categories (crDCs)





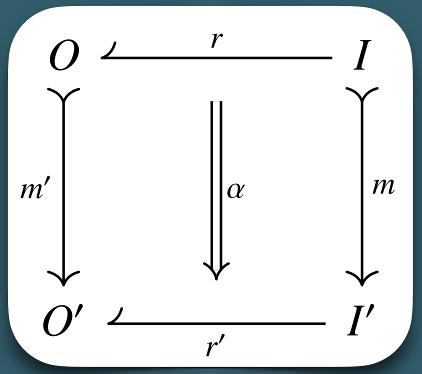
Explicit **rewriting semantics** (DPO, SqPO, …)

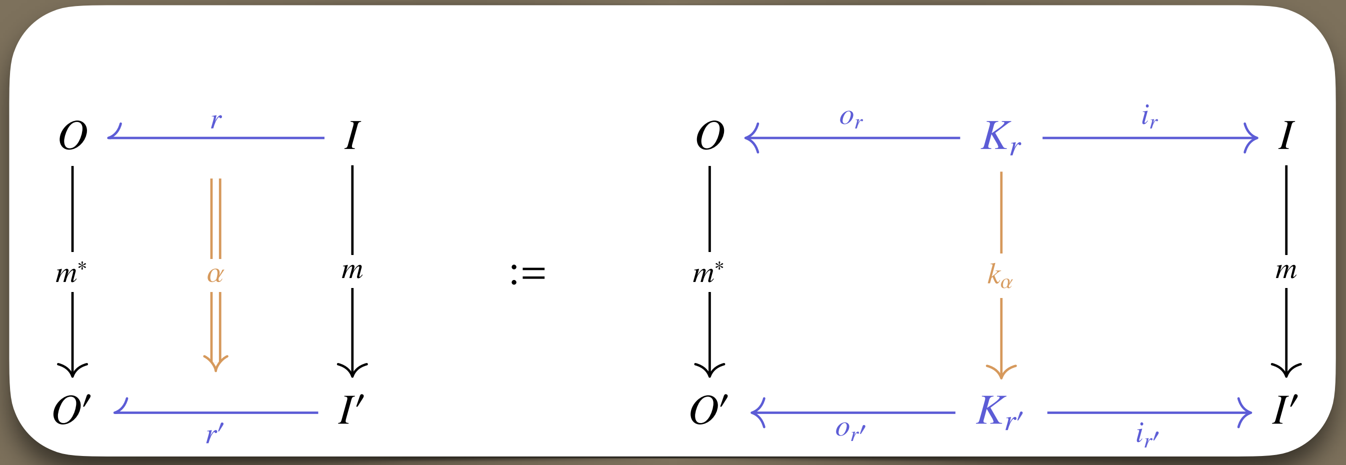

Fundamentals of Compositional Rewriting Theory*

Nicolas Behr[a,*], Russell Harmer[b], Jean Krivine[a]

[a]Université Paris Cité, CNRS, IRIF, 8 Place Aurélie Nemours, Paris Cedex 13, 75205, France
[b]Université de Lyon, ENS de Lyon, UCBL, CNRS, LIP, 46 allée d'Italie, Lyon Cedex 07, 69364, France

compositional rewriting double categories (crDCs)



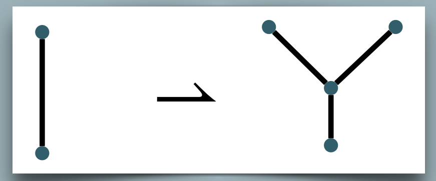


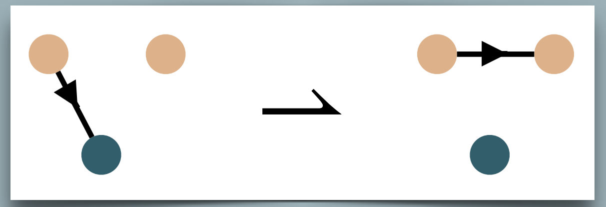
Explicit **rewriting semantics** (DPO, SqPO, …)


Fundamentals of Compositional Rewriting Theory*

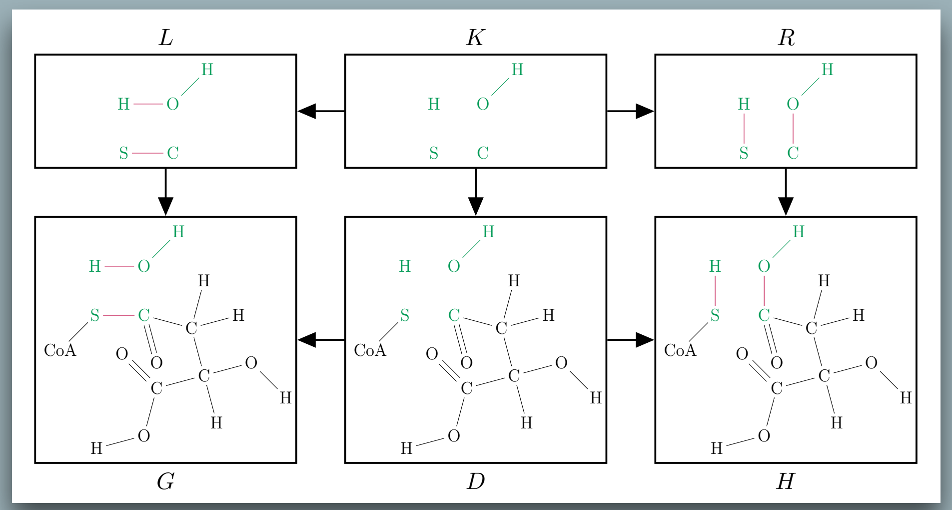
Nicolas Behr[a,*], Russell Harmer[b], Jean Krivine[a]

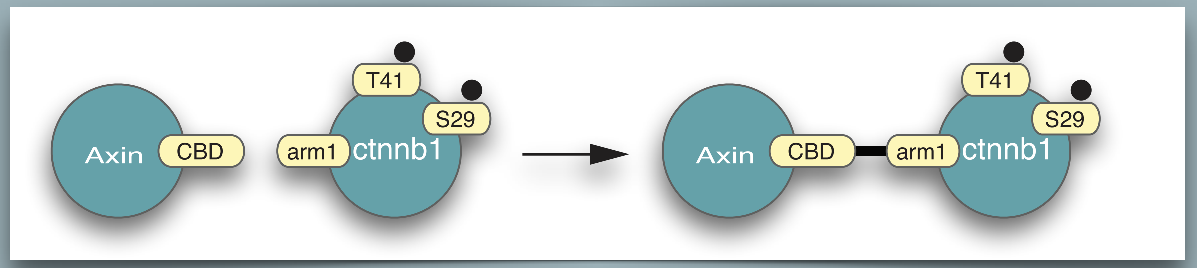
[a]Université Paris Cité, CNRS, IRIF, 8 Place Aurélie Nemours, Paris Cedex 13, 75205, France
[b]Université de Lyon, ENS de Lyon, UCBL, CNRS, LIP, 46 allée d'Italie, Lyon Cedex 07, 69364, France





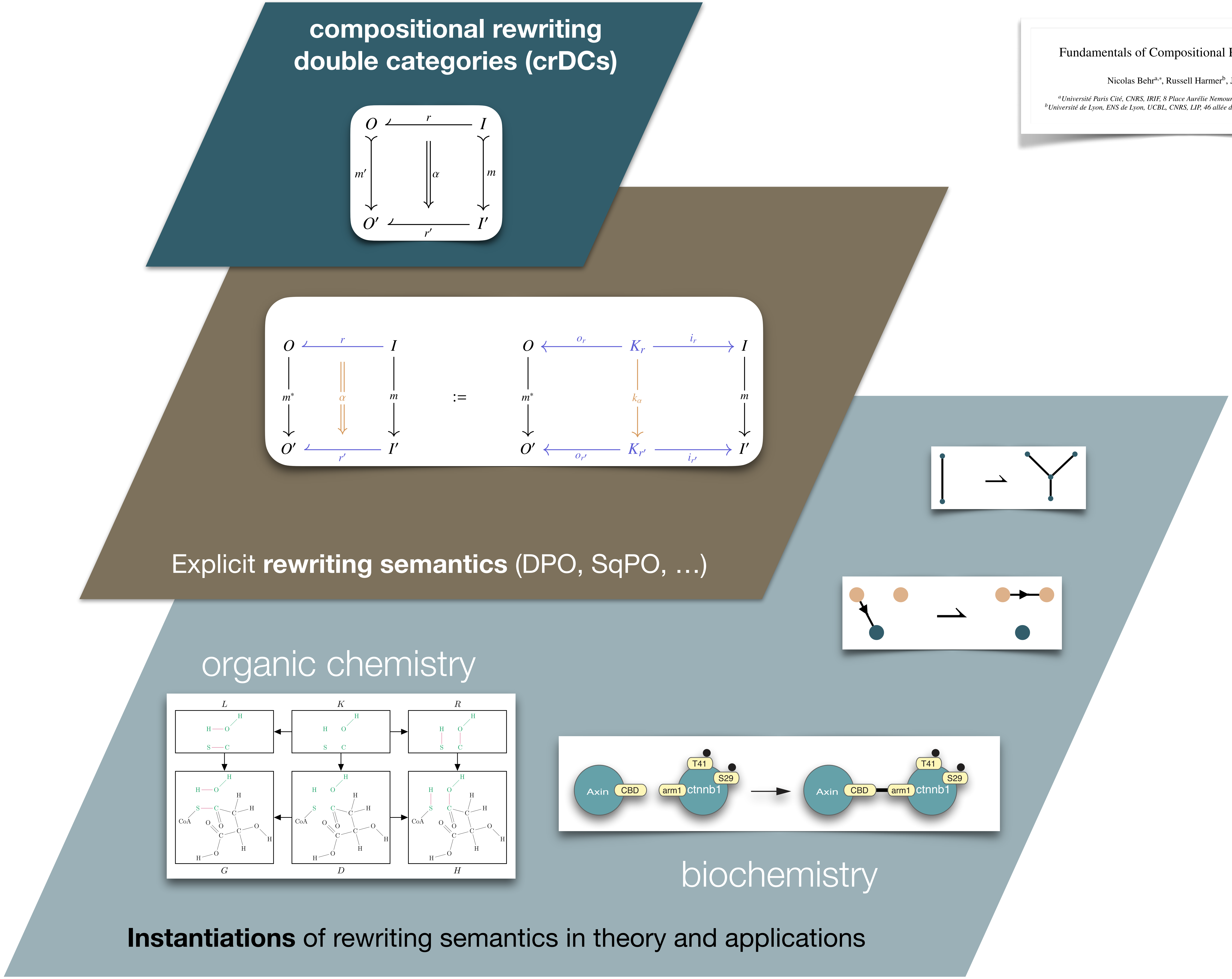
organic chemistry





biochemistry

Instantiations of rewriting semantics in theory and applications

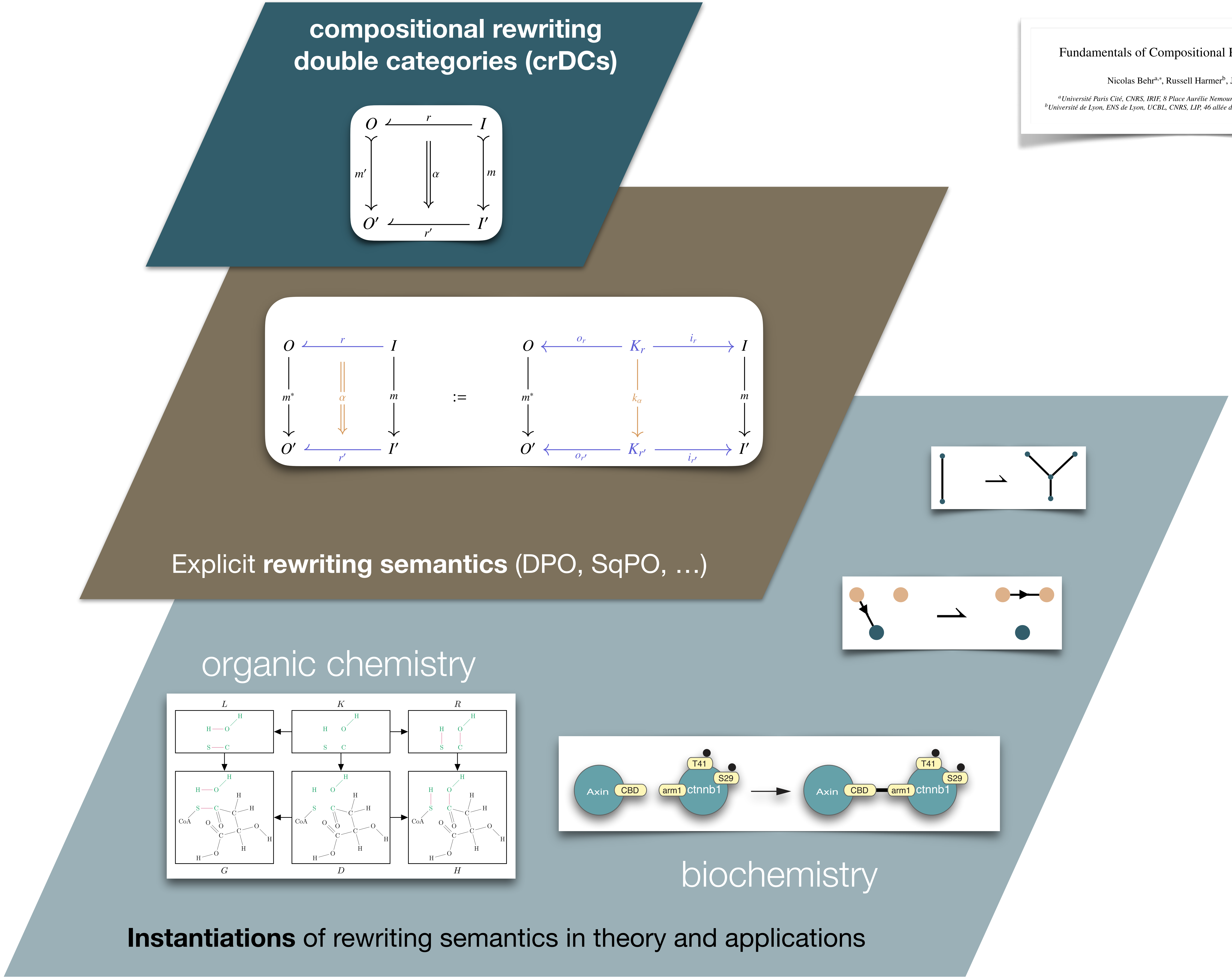


Fundamentals of Compositional Rewriting Theory*

Nicolas Behr[a,*], Russell Harmer[b], Jean Krivine[a]

[a]Université Paris Cité, CNRS, IRIF, 8 Place Aurélie Nemours, Paris Cedex 13, 75205, France
[b]Université de Lyon, ENS de Lyon, UCBL, CNRS, LIP, 46 allée d'Italie, Lyon Cedex 07, 69364, France

Part 1: Motivation



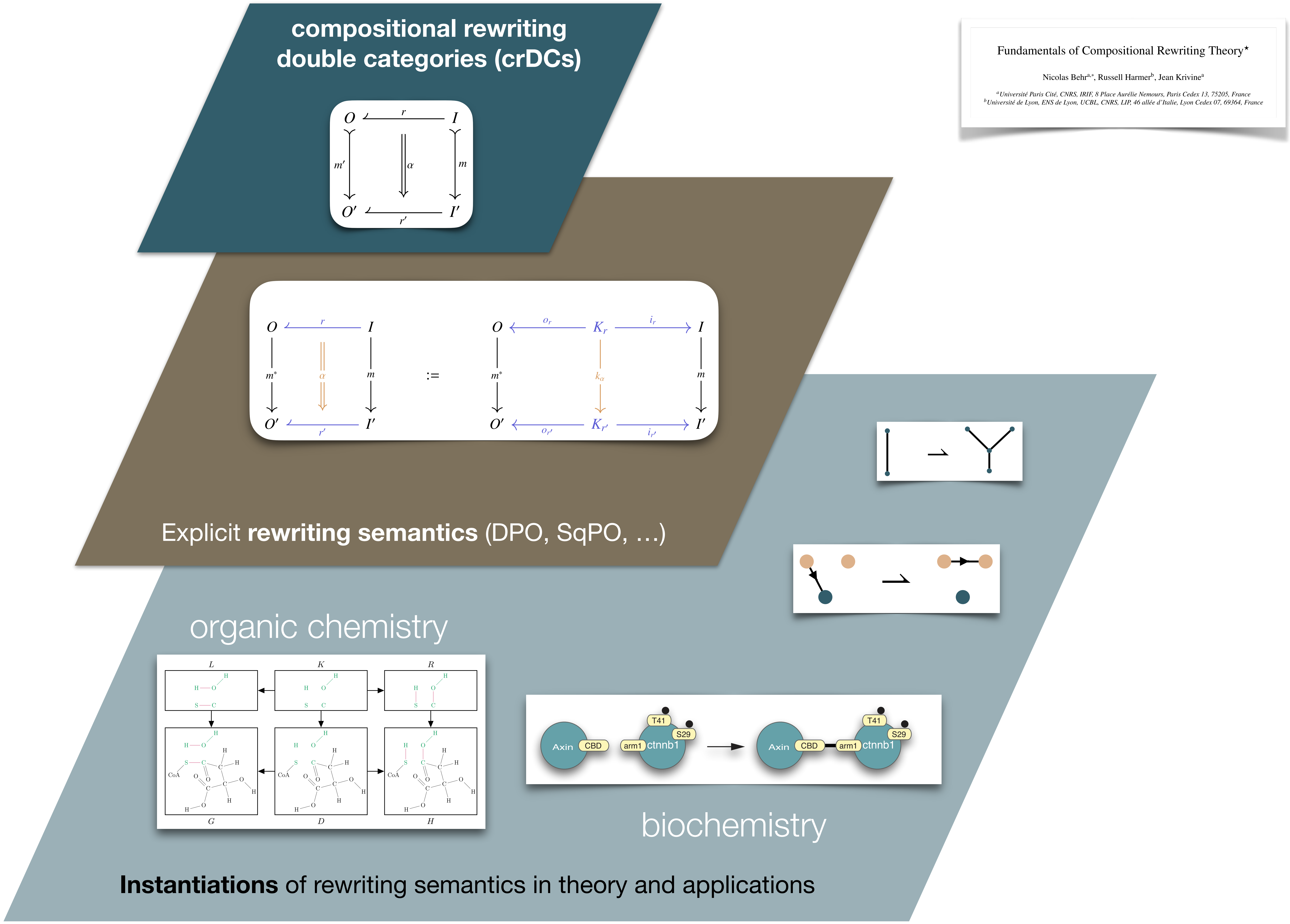
Fundamentals of Compositional Rewriting Theory*

Nicolas Behr[a,*], Russell Harmer[b], Jean Krivine[a]

[a]Université Paris Cité, CNRS, IRIF, 8 Place Aurélie Nemours, Paris Cedex 13, 75205, France
[b]Université de Lyon, ENS de Lyon, UCBL, CNRS, LIP, 46 allée d'Italie, Lyon Cedex 07, 69364, France

Part 1: Motivation

Part 2: FCRT



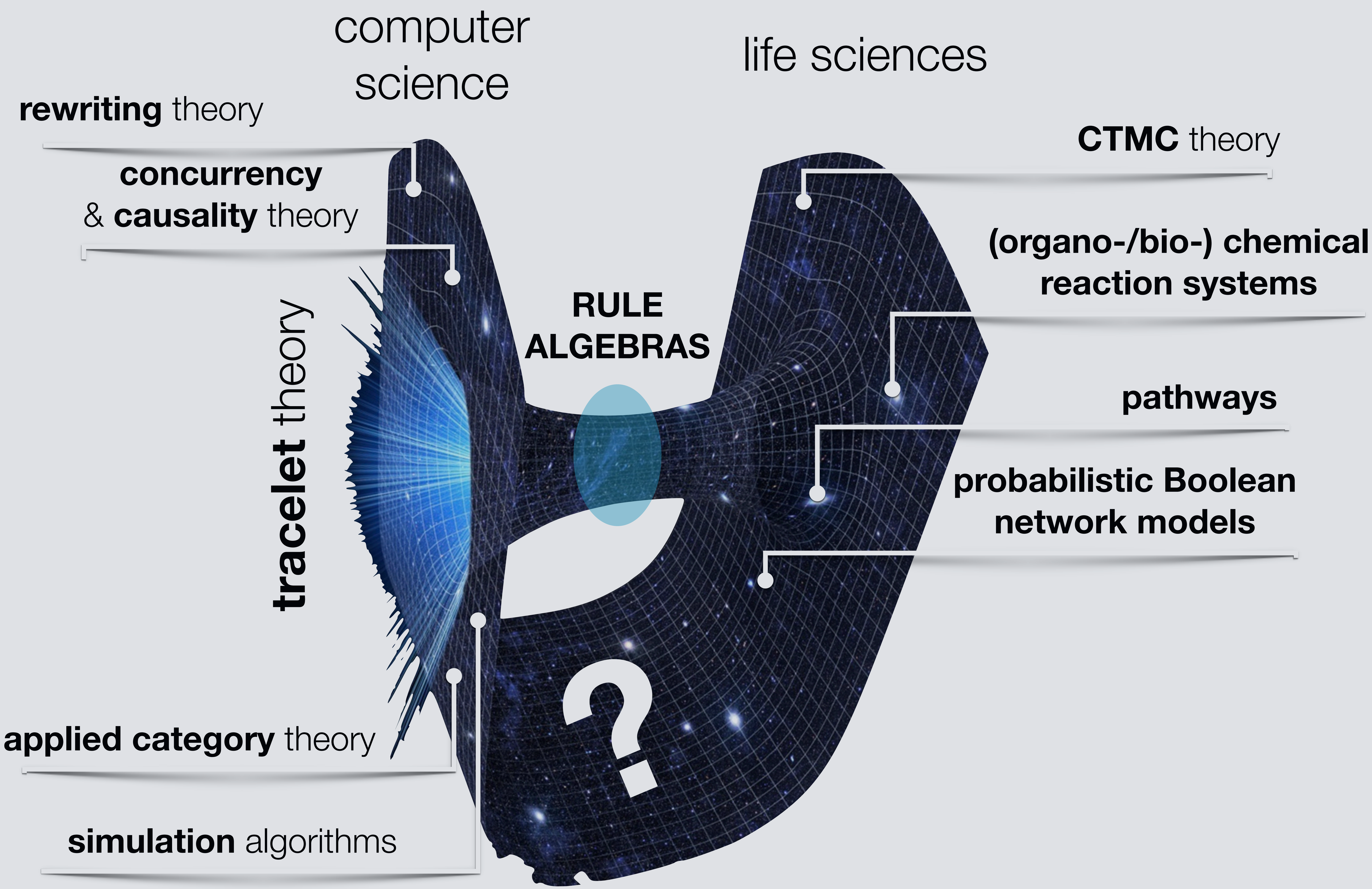
Part 1: Motivation

Part 2: FCRT

Part 3: CoREACT

PART 1: MOTIVATION

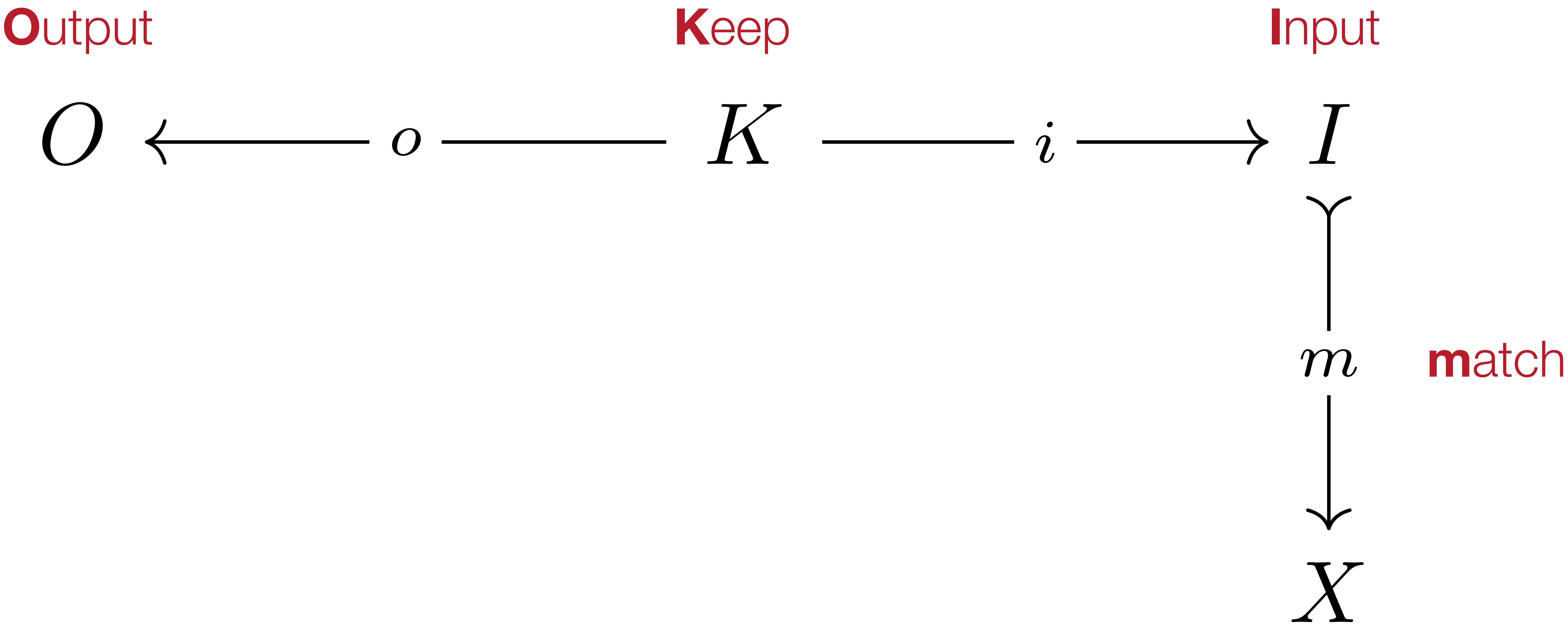
What is compositional rewriting theory?



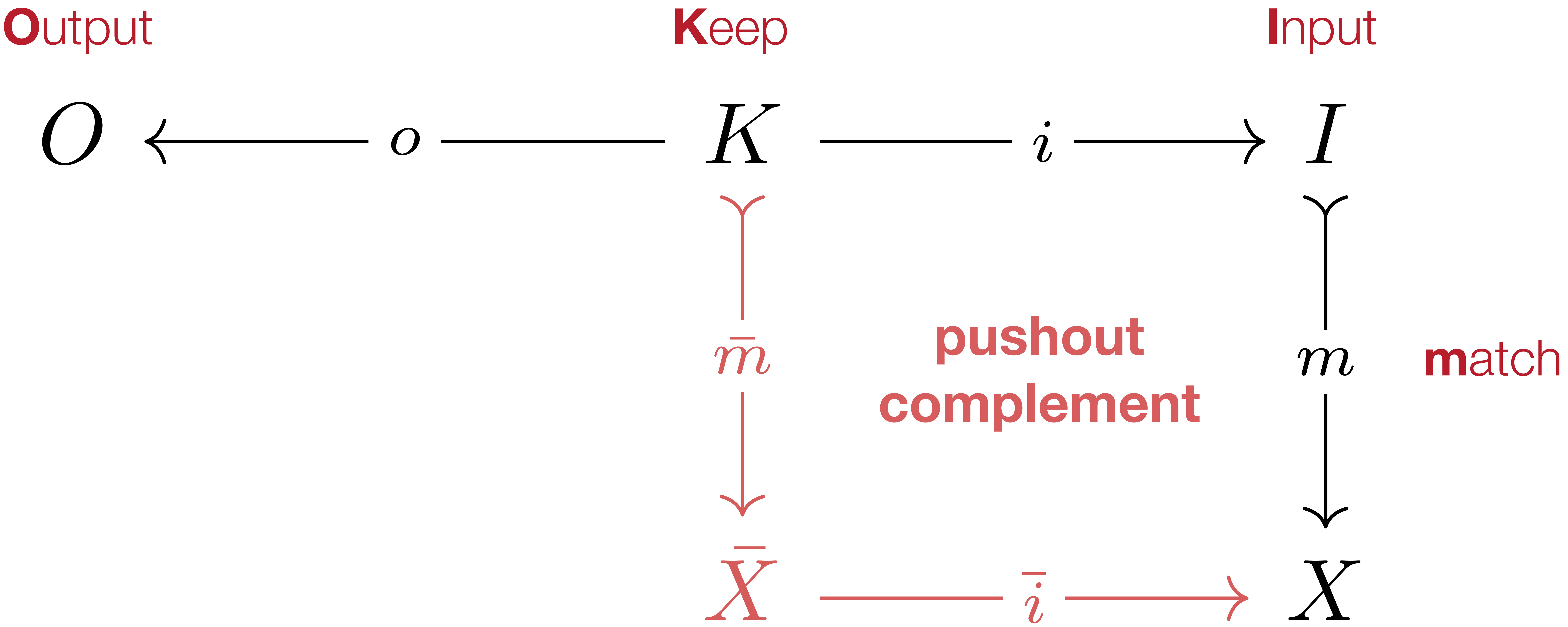
PART 1: MOTIVATION

What is compositional rewriting theory?

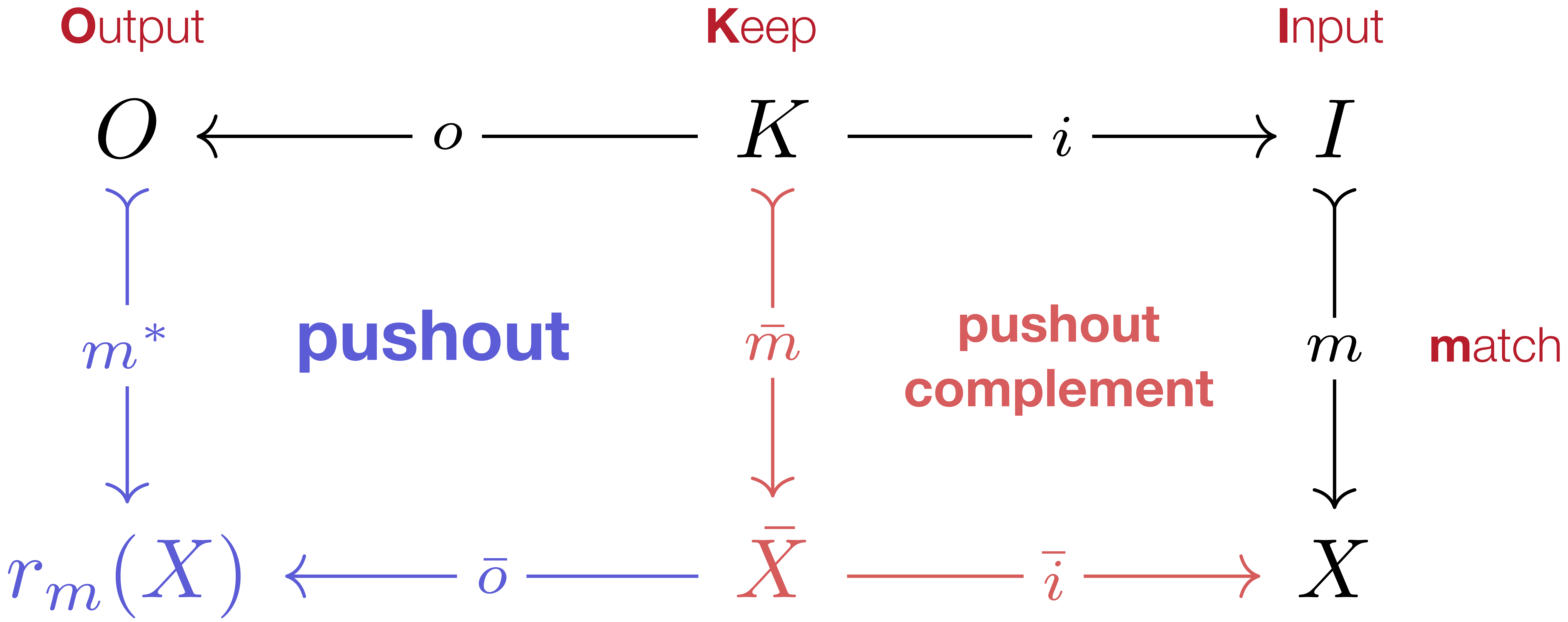
Double Pushout (DPO) rewriting



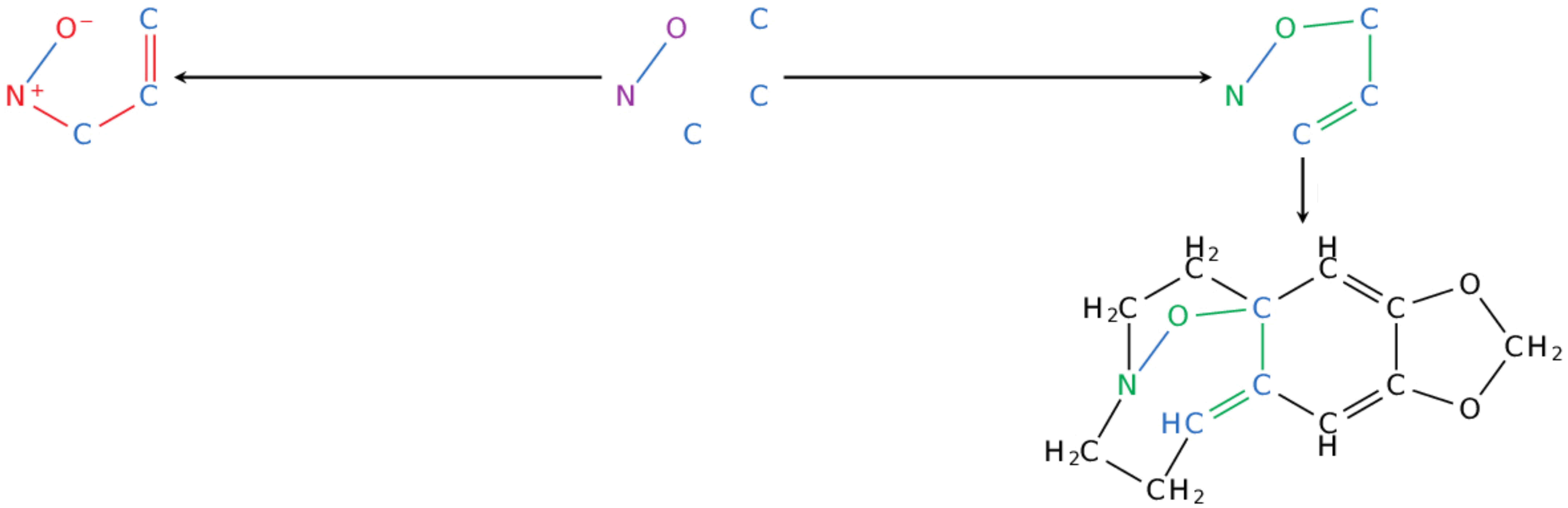
Double Pushout (DPO) rewriting



Double Pushout (DPO) rewriting

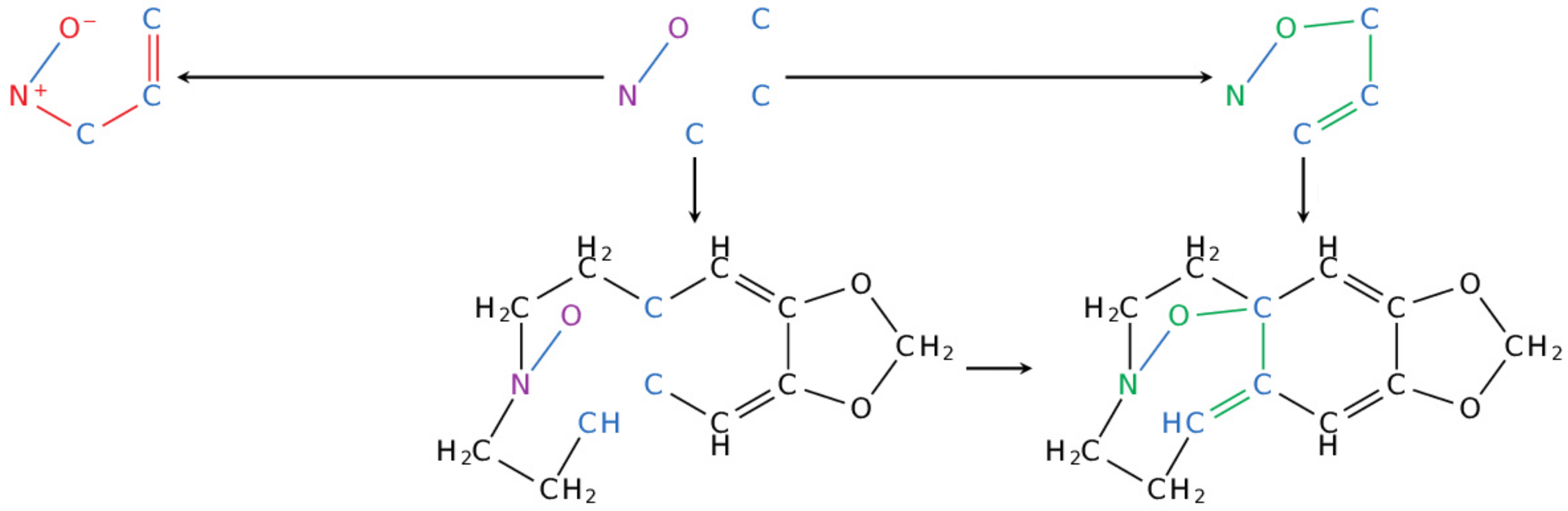


Organic chemistry via DPO-type rewriting (!)



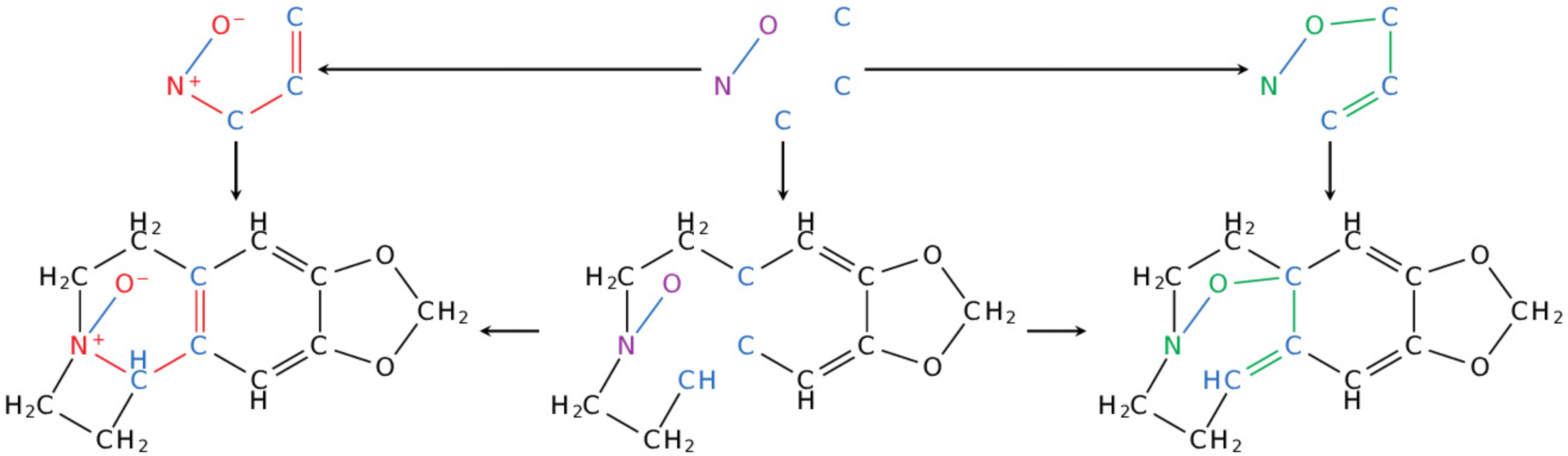
Source: *Algorithmic Cheminformatics Group, SDU Odense*

Organic chemistry via DPO-type rewriting (!)



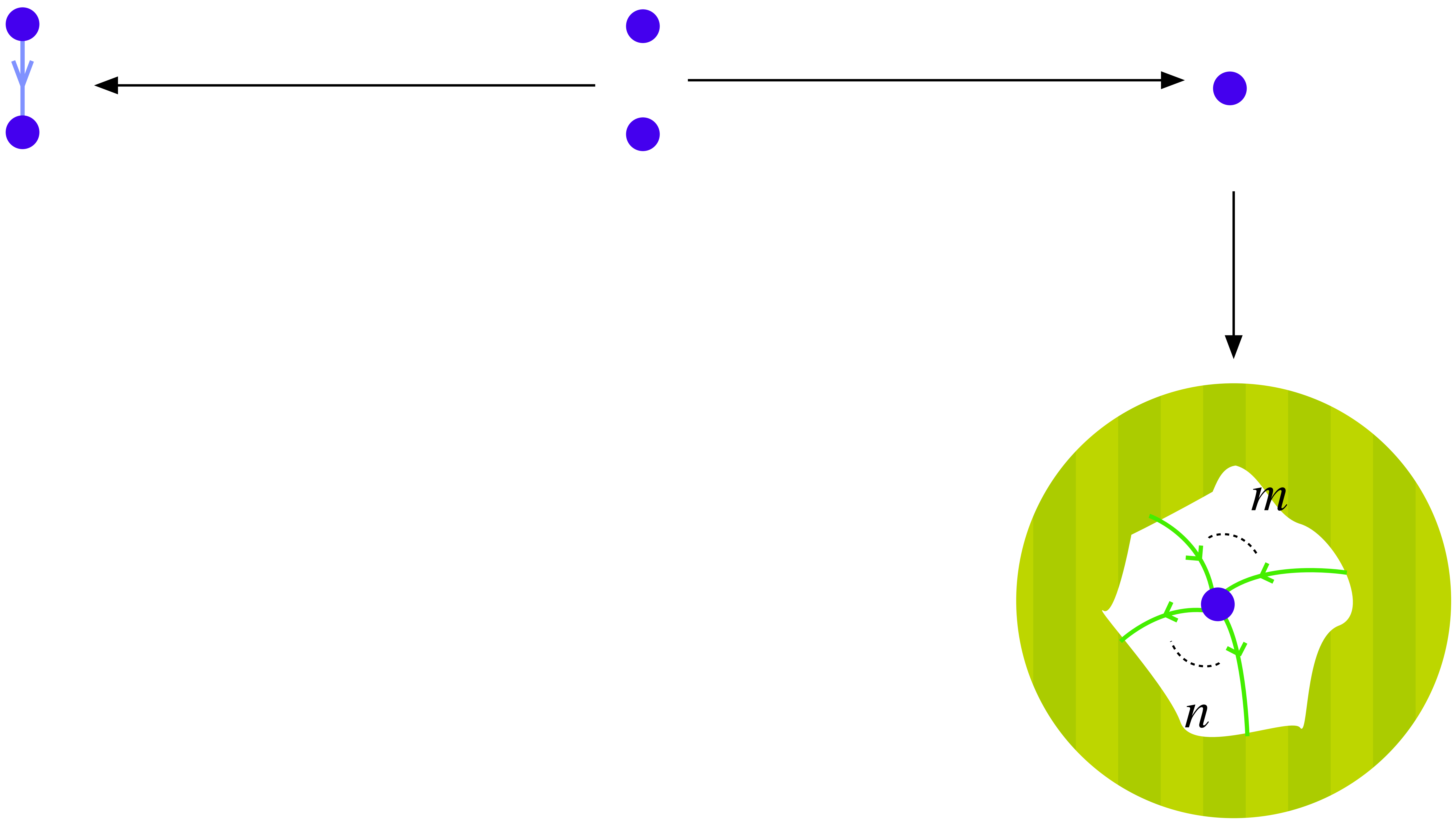
Source: *Algorithmic Cheminformatics Group, SDU Odense*

Organic chemistry via DPO-type rewriting (!)

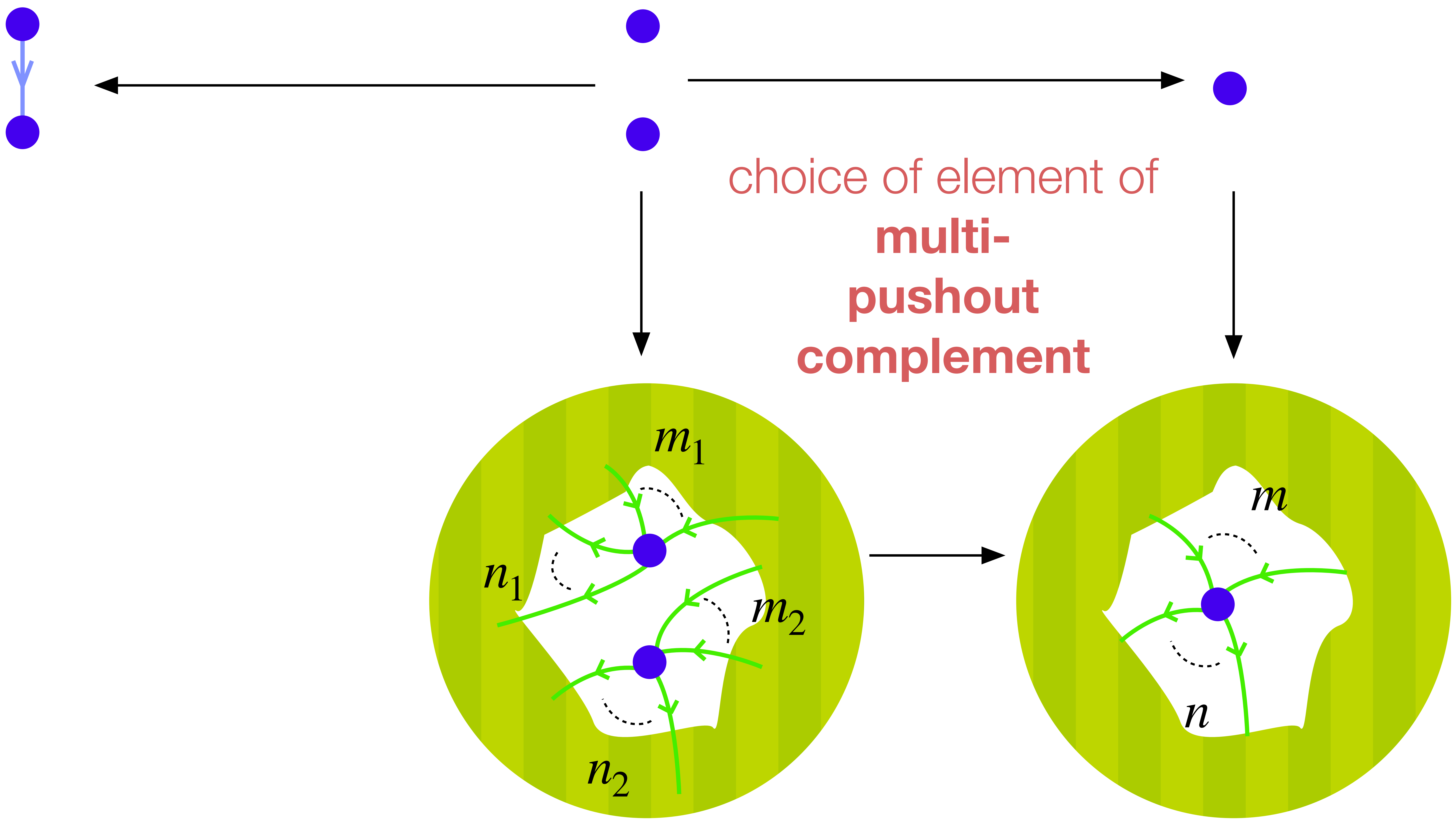


Source: *Algorithmic Cheminformatics Group, SDU Odense*

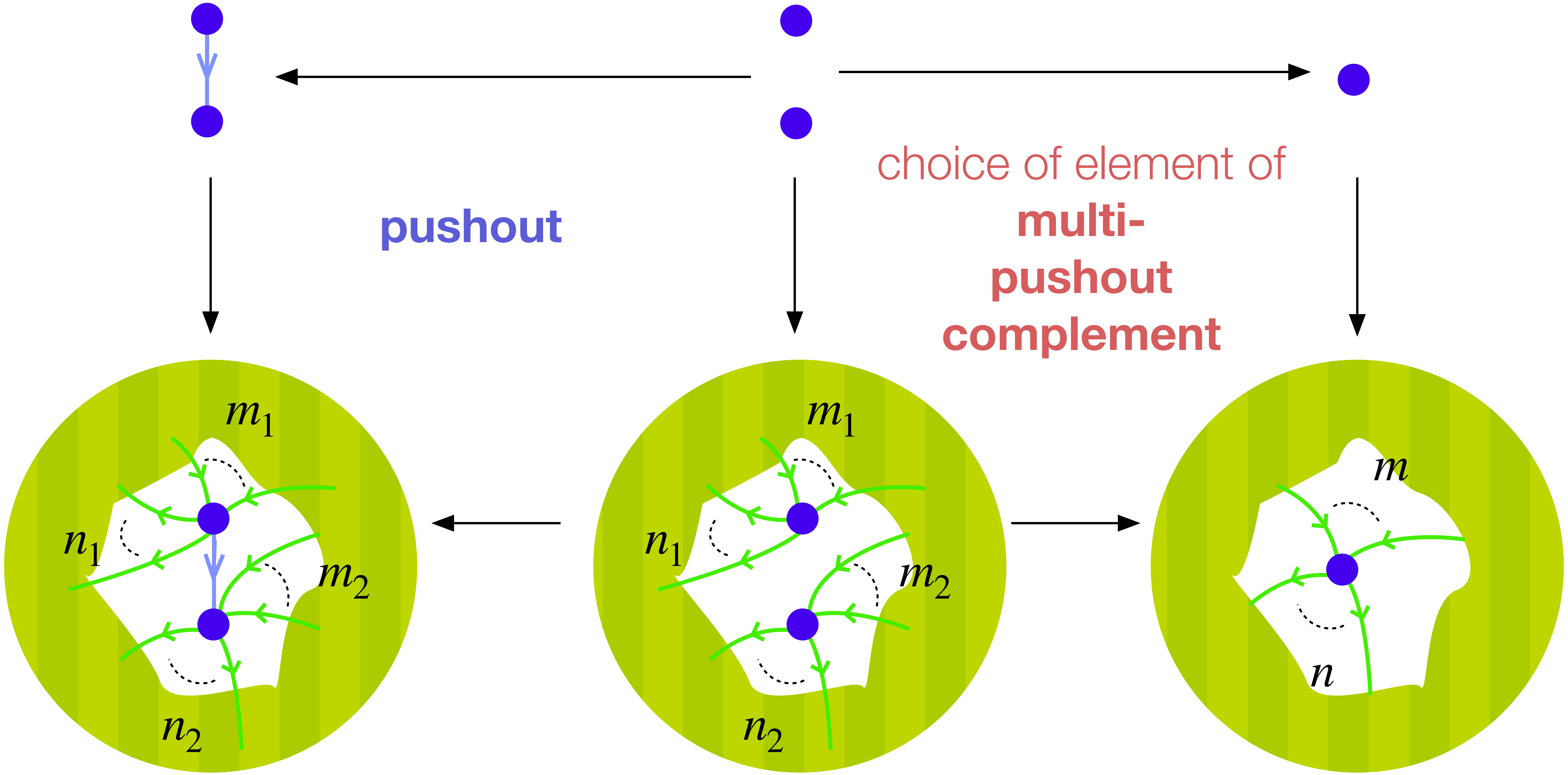
non-linear Double Pushout (DPO) rewriting



non-linear Double Pushout (DPO) rewriting



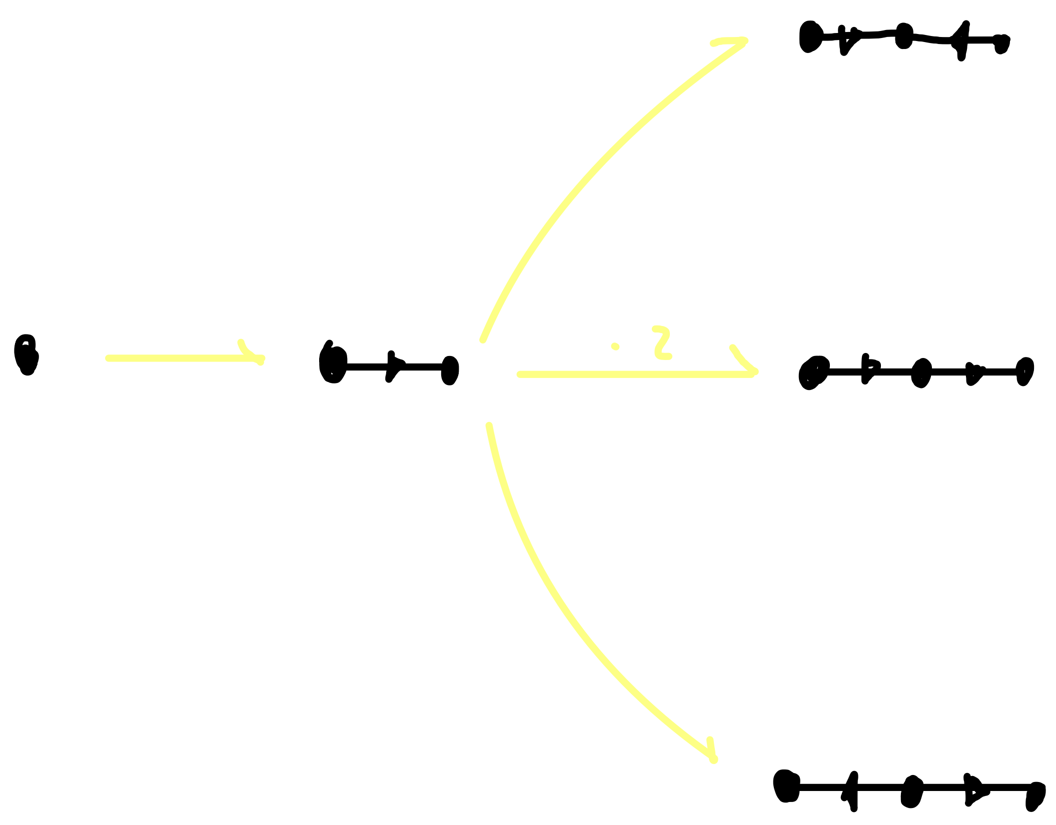
non-linear Double Pushout (DPO) rewriting



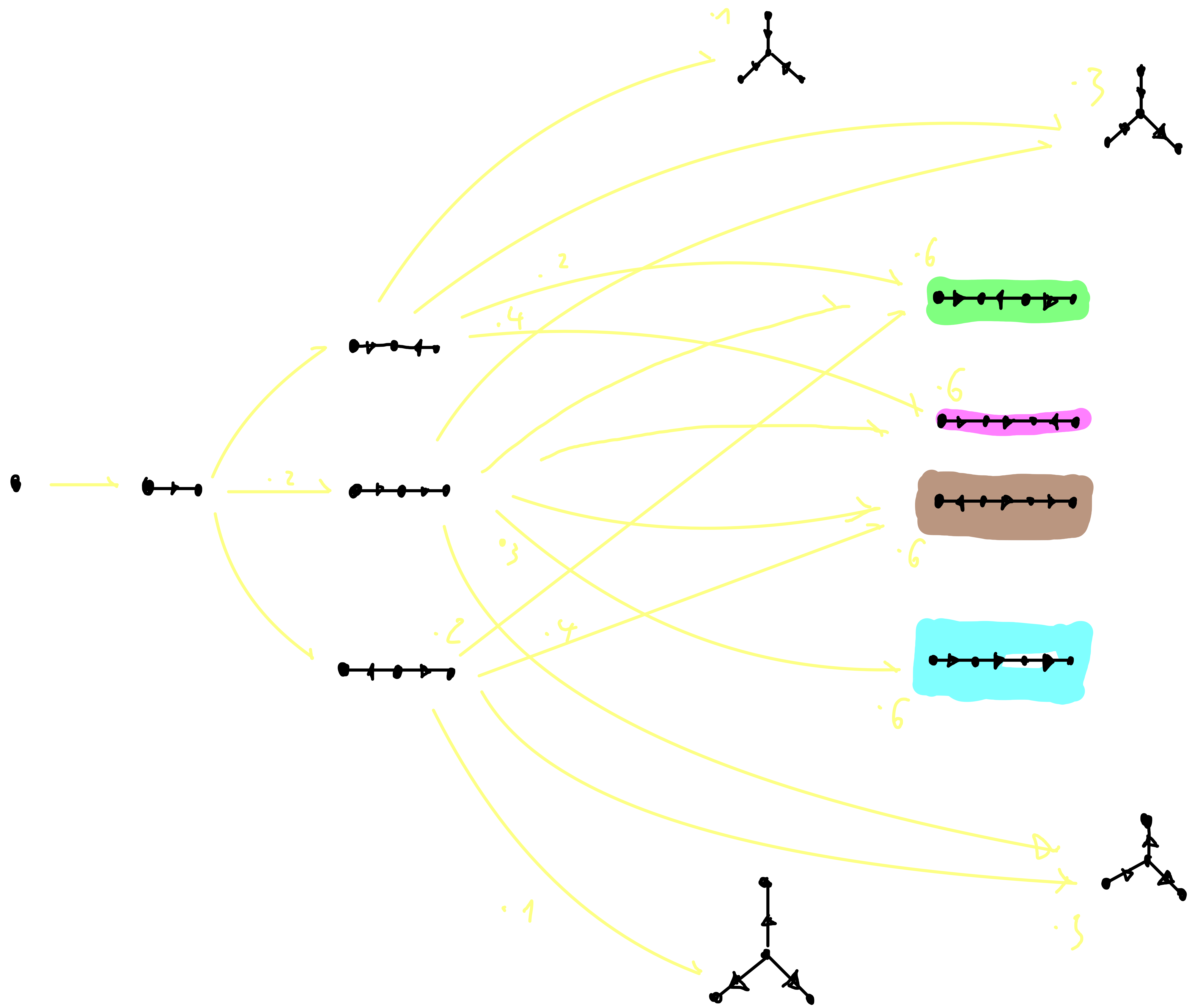
non-linear Double Pushout (DPO) rewriting

non-linear Double Pushout (DPO) rewriting

non-linear Double Pushout (DPO) rewriting



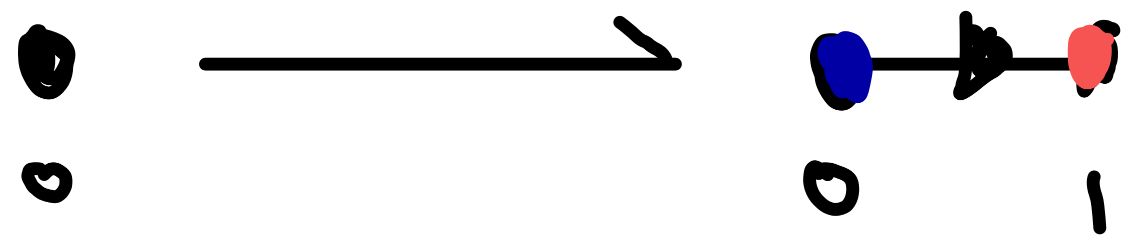
non-linear Double Pushout (DPO) rewriting



non-linear Sesqui-Pushout (SqPO) rewriting

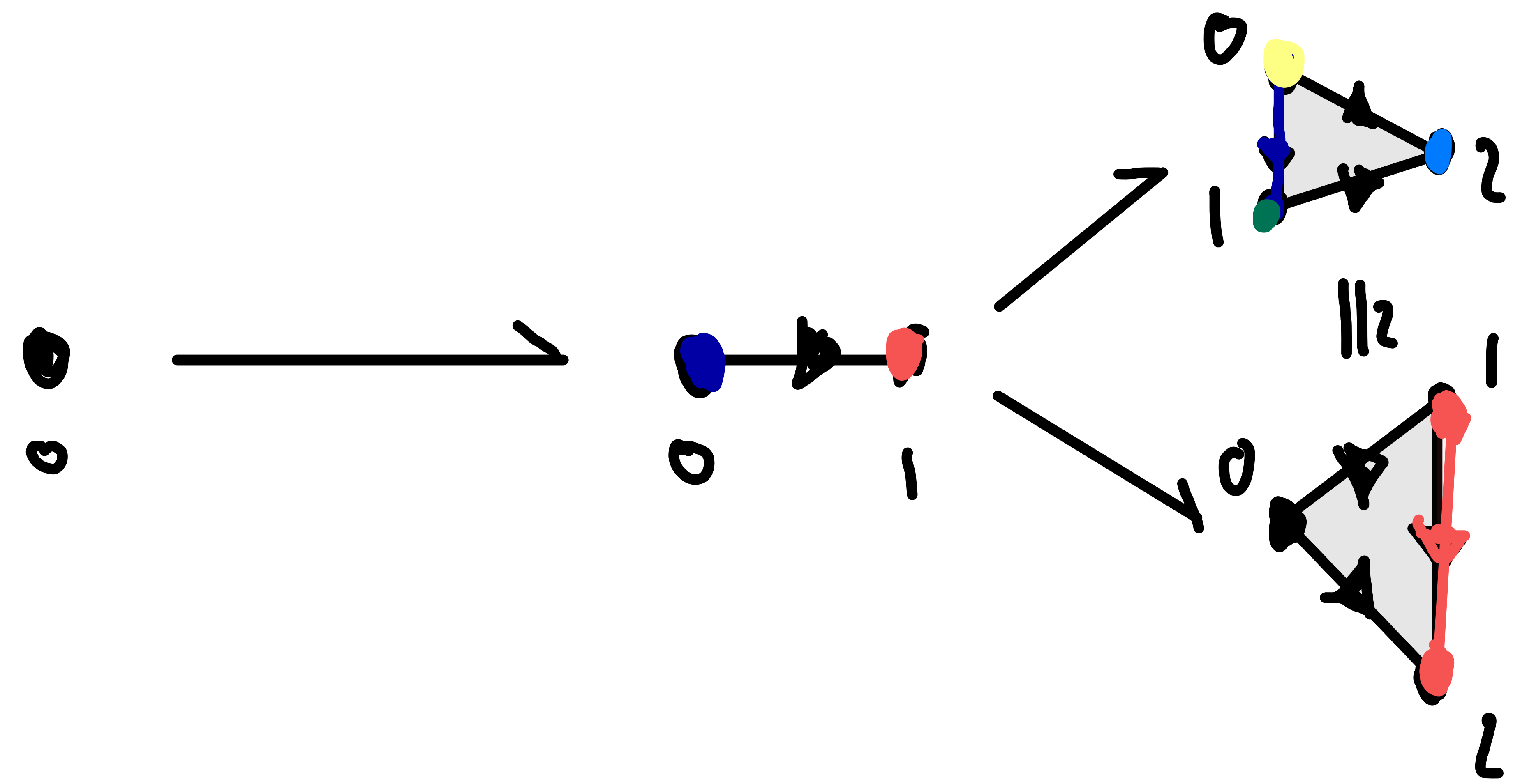
Corradini, A., et al.: Sesqui-Pushout Rewriting. In: Graph Transformations. LNCS, vol. 4178, pp. 30–45. Springer Berlin Heidelberg (2006)

non-linear Sesqui-Pushout (SqPO) rewriting



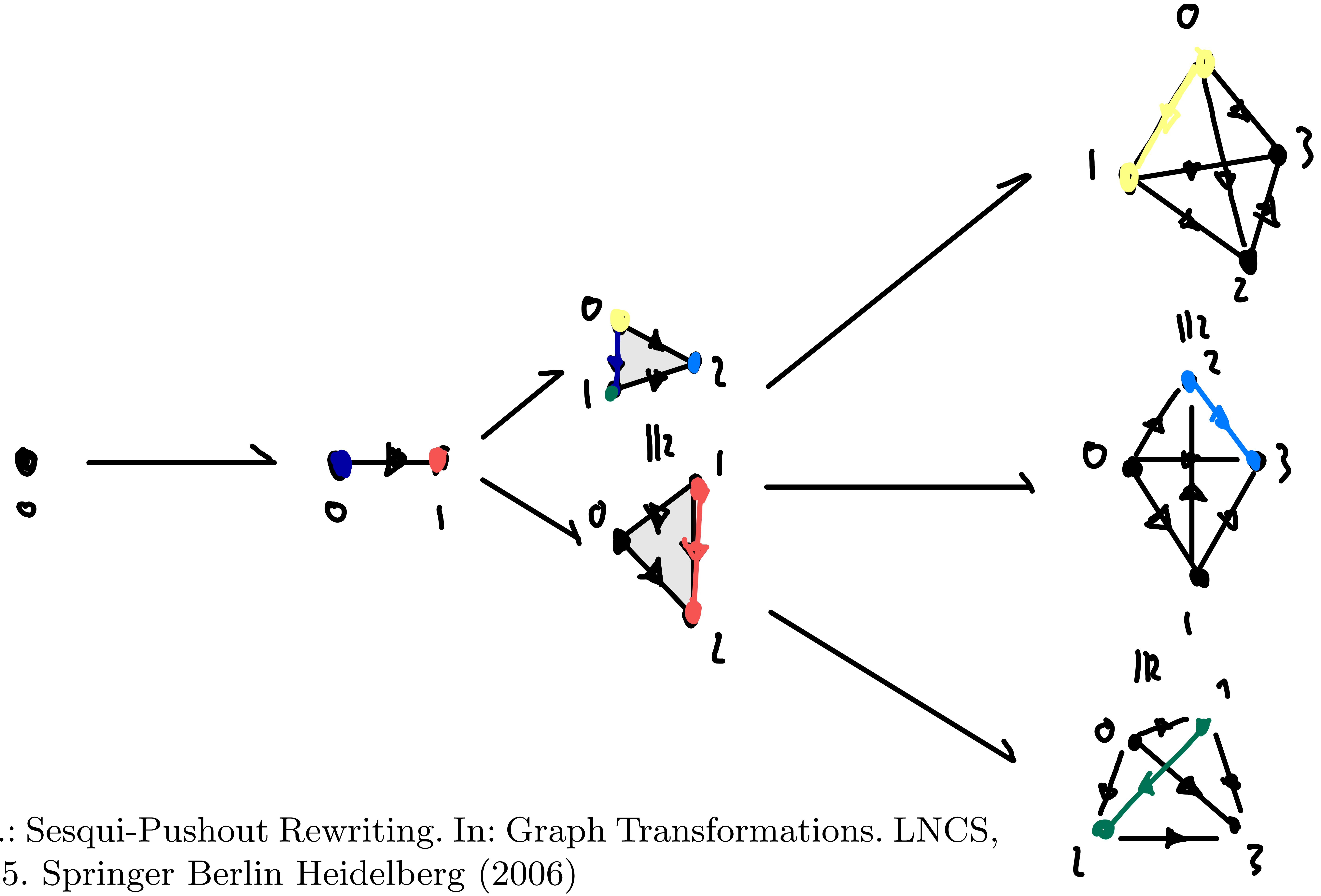
Corradini, A., et al.: Sesqui-Pushout Rewriting. In: Graph Transformations. LNCS, vol. 4178, pp. 30–45. Springer Berlin Heidelberg (2006)

non-linear Sesqui-Pushout (SqPO) rewriting

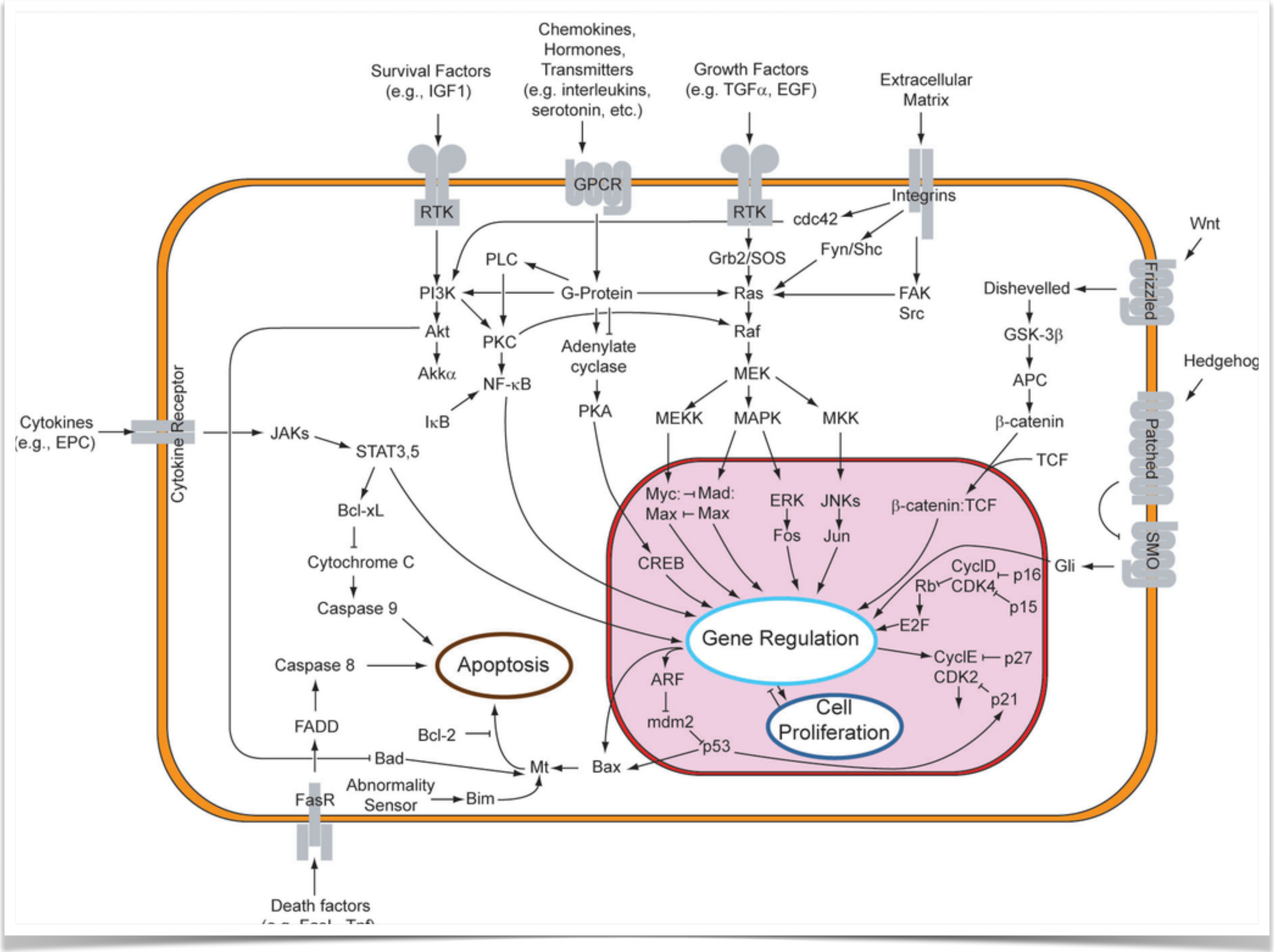


Corradini, A., et al.: Sesqui-Pushout Rewriting. In: Graph Transformations. LNCS, vol. 4178, pp. 30–45. Springer Berlin Heidelberg (2006)

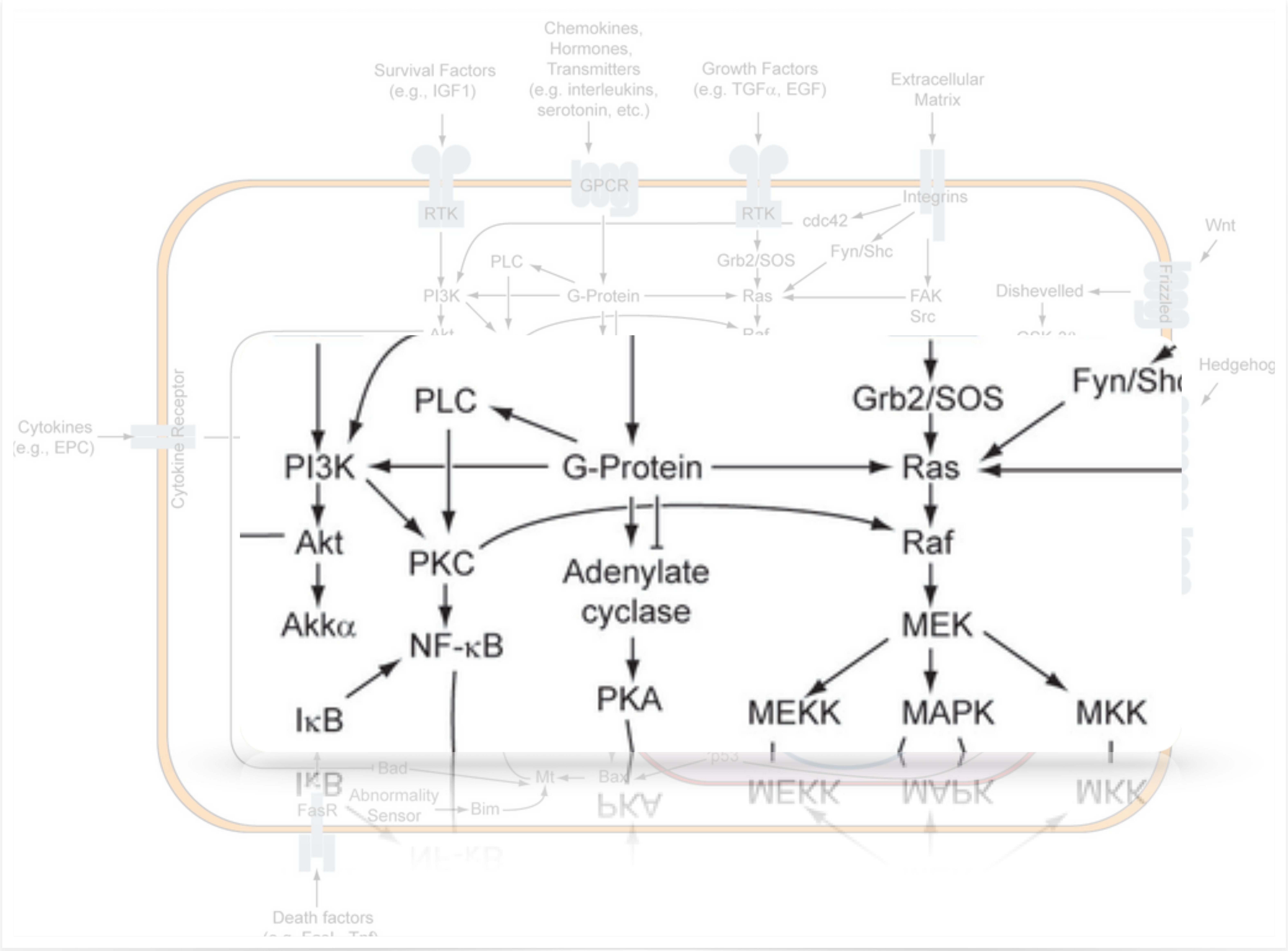
non-linear Sesqui-Pushout (SqPO) rewriting



Corradini, A., et al.: Sesqui-Pushout Rewriting. In: Graph Transformations. LNCS, vol. 4178, pp. 30–45. Springer Berlin Heidelberg (2006)

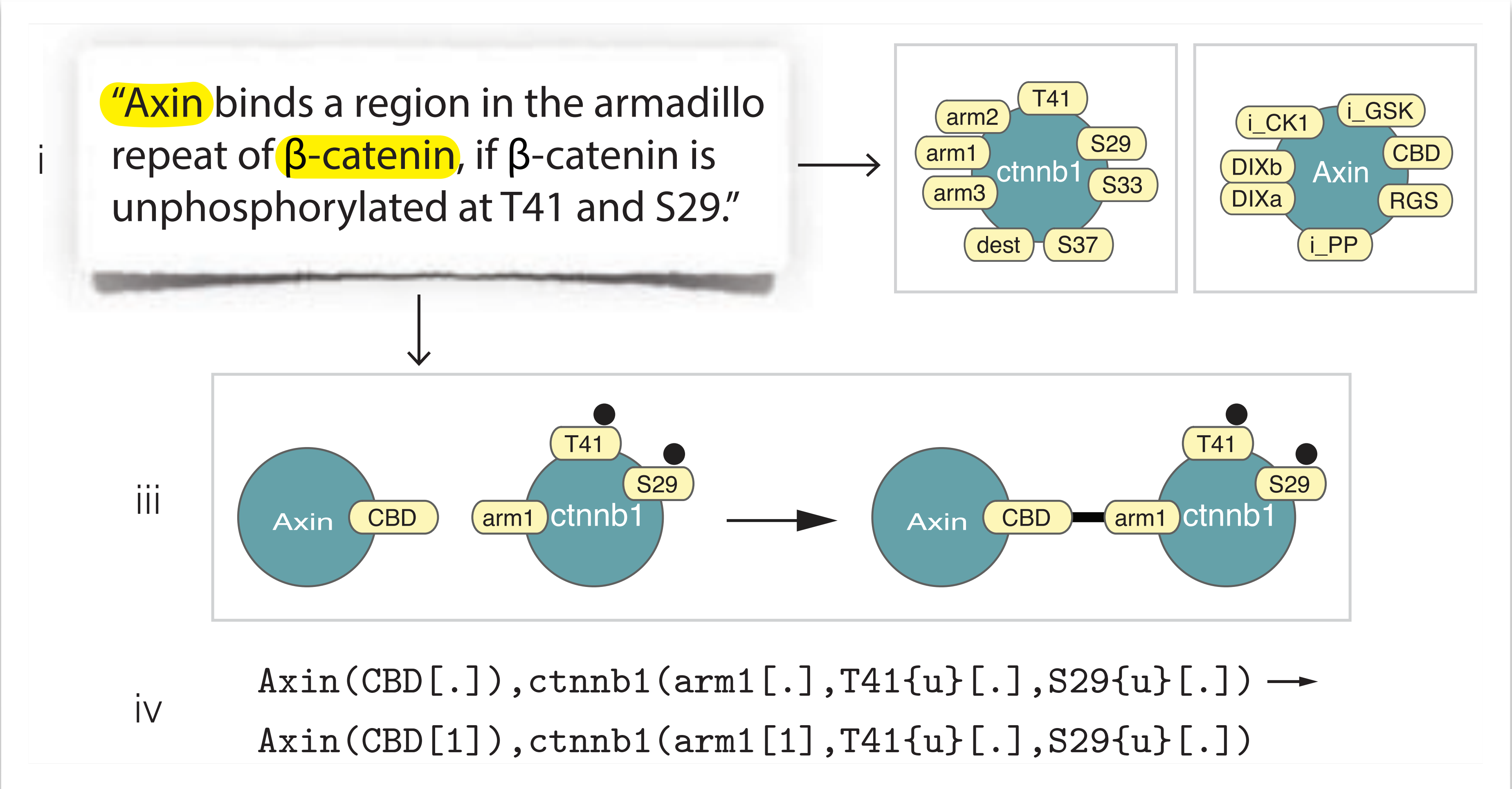


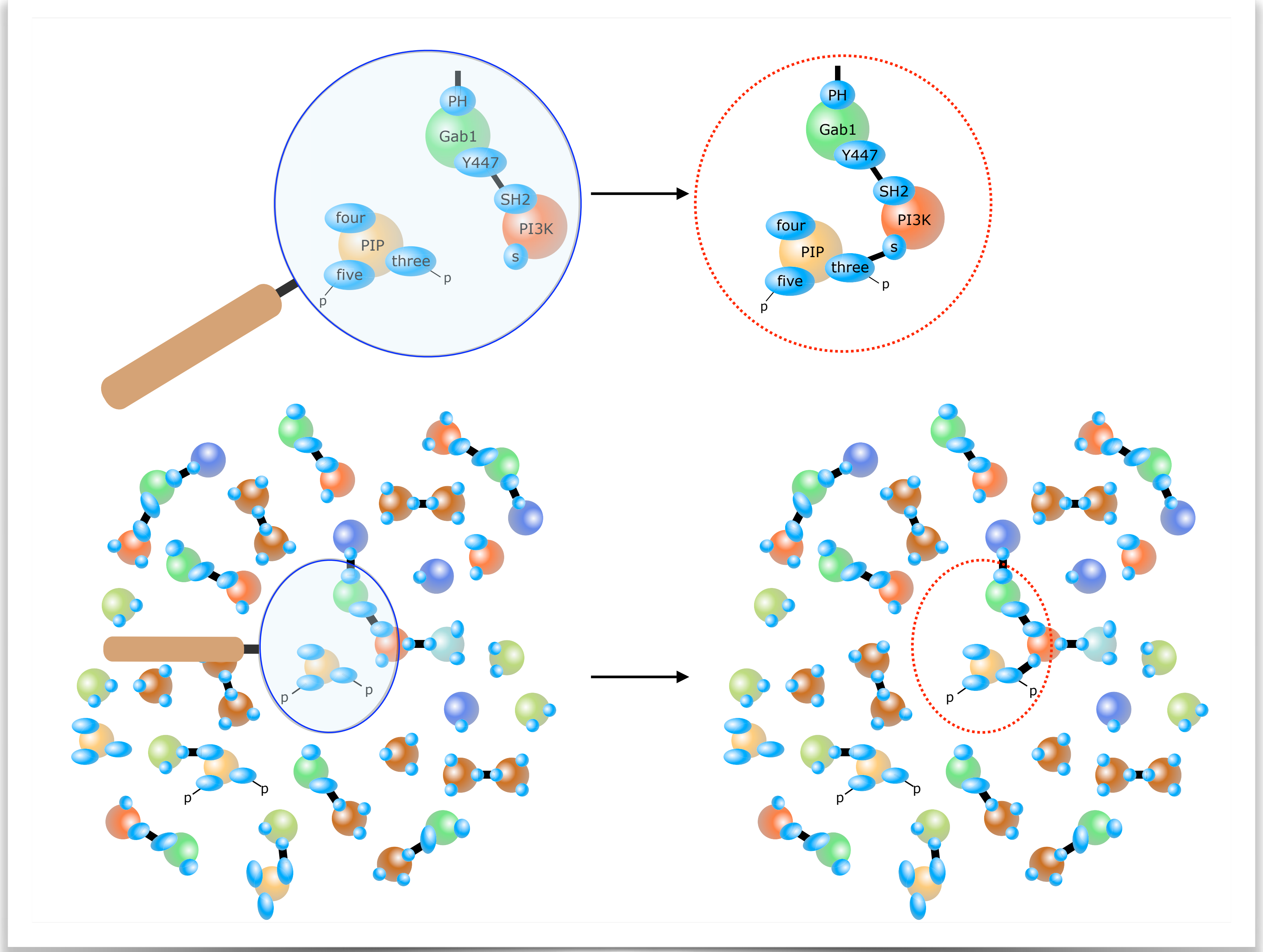
source: *Stochastic graph rewriting and (executable) knowledge representation for molecular biology*, J. Krivine (lecture notes)

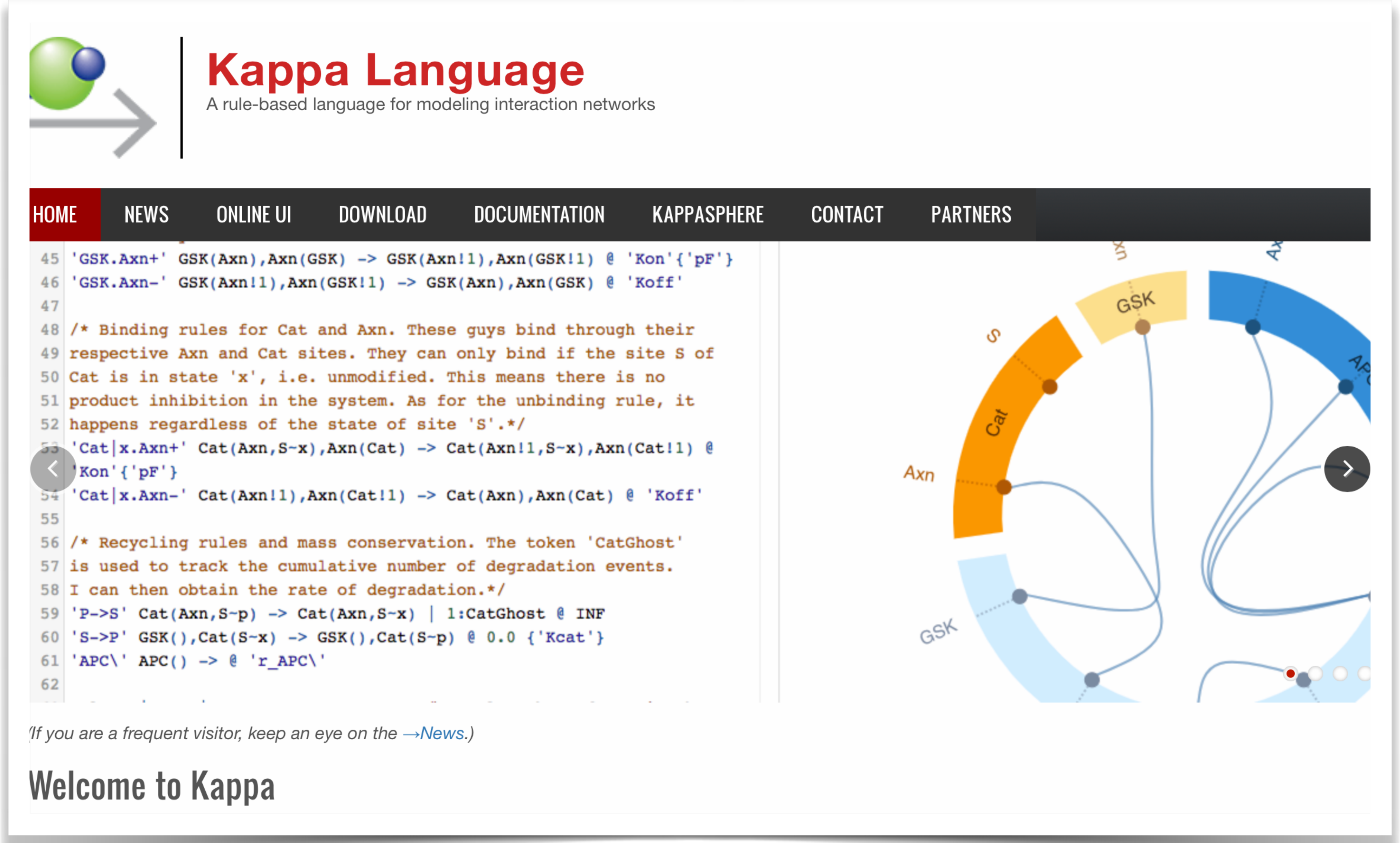


source: *Stochastic graph rewriting and (executable) knowledge representation for molecular biology*, J. Krivine (lecture notes)

Rewriting in the life sciences: **bioinformatics**

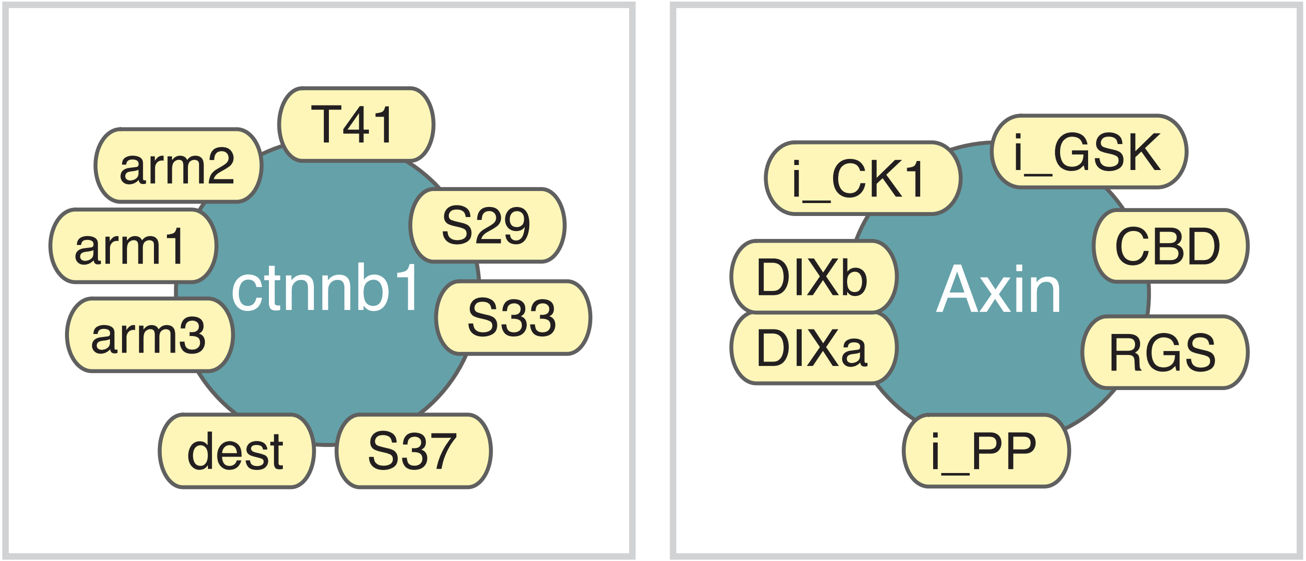




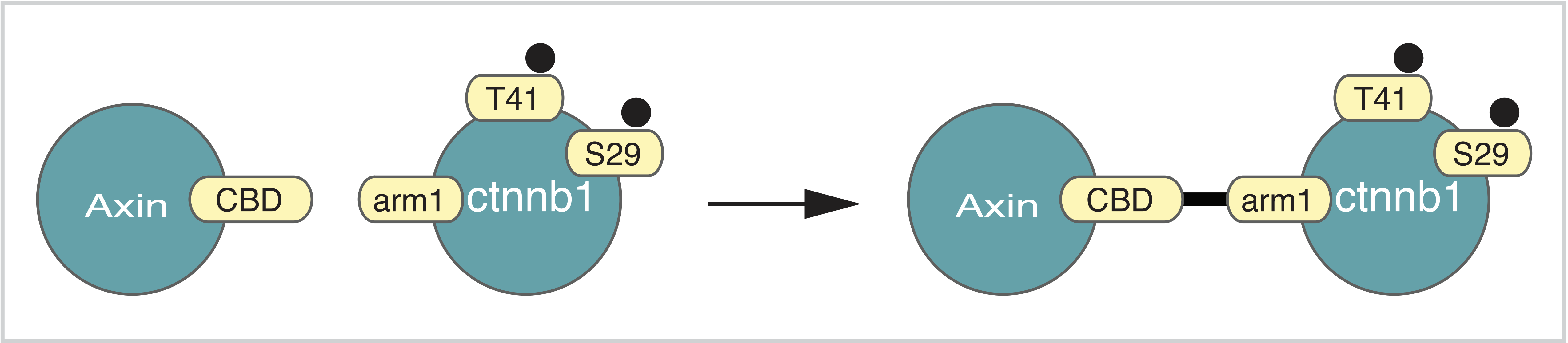


source: *The Kappa platform for rule-based modeling*, Boutillier, P., Maasha, M., Li, X., Medina-Abarca, H.F., Krivine, J., Feret, J., Cristescu, I., Forbes, A.G. and Fontana, W., 2018, *Bioinformatics*, *34*(13), pp.i583-i592.

i “Axin binds a region in the armadillo repeat of β-catenin, if β-catenin is unphosphorylated at T41 and S29.”

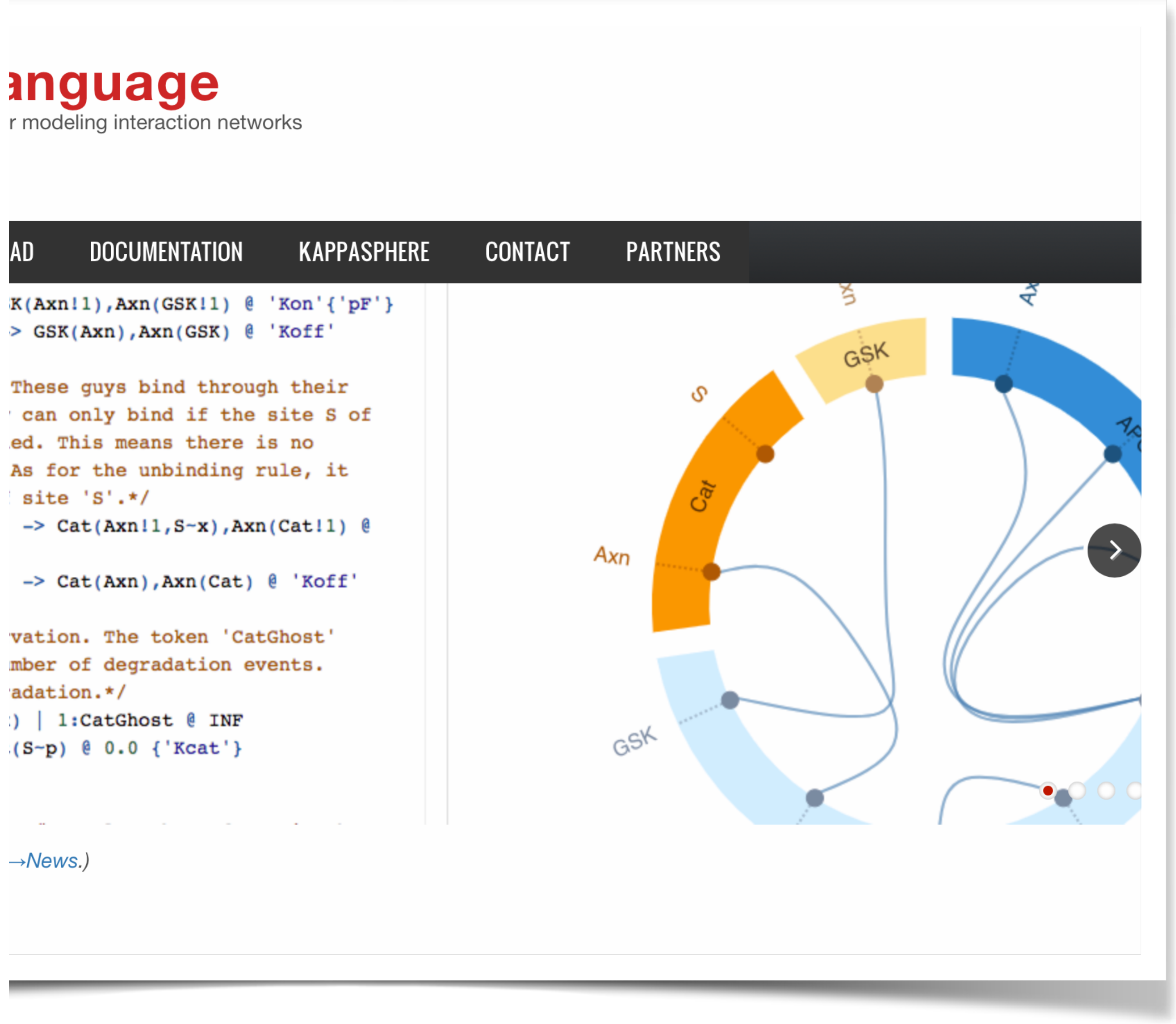


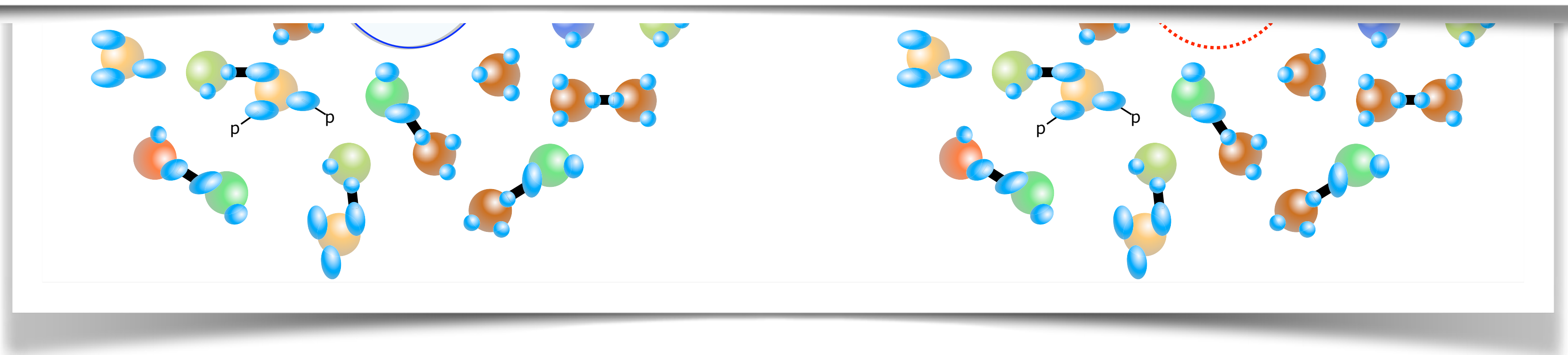
iii



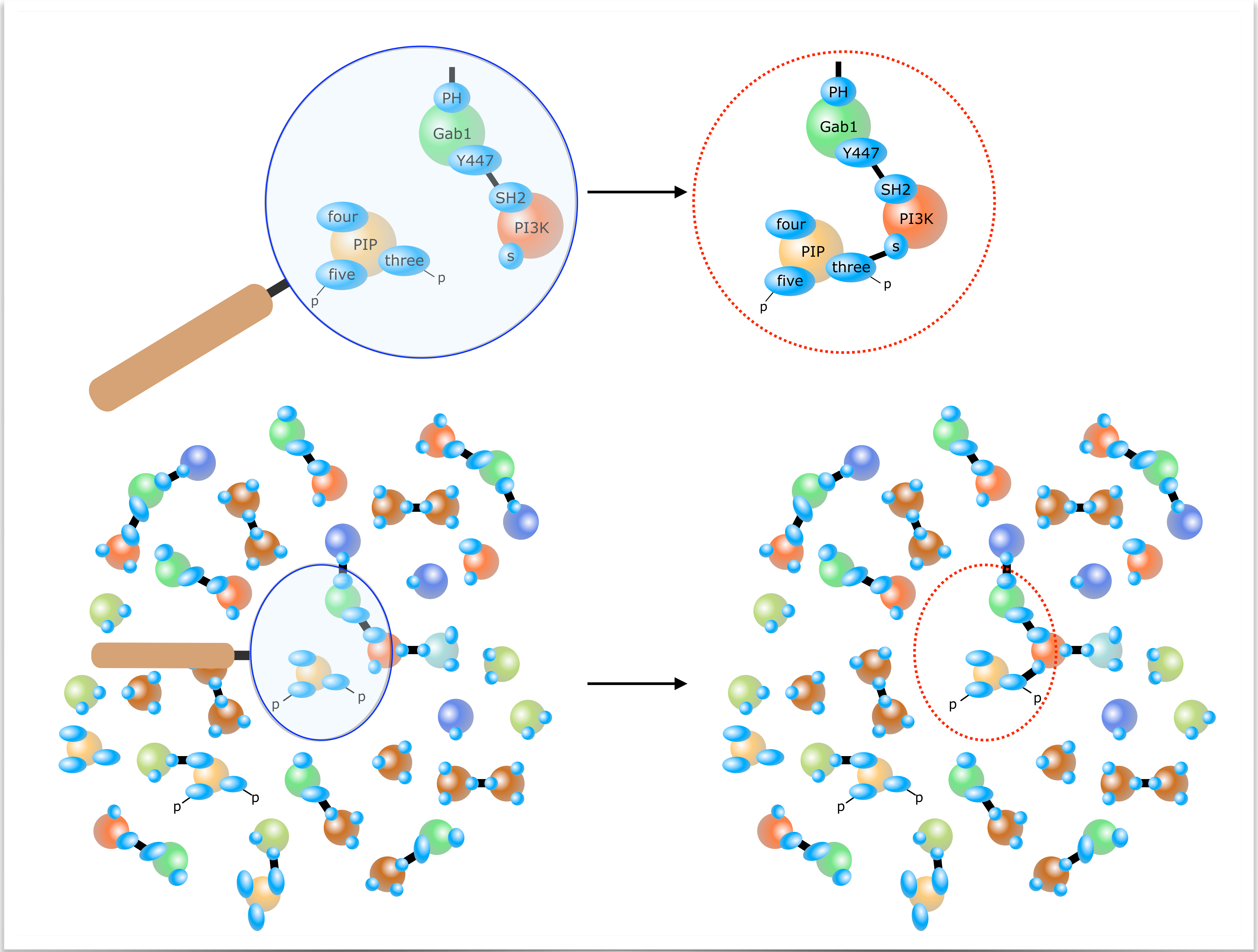
iv

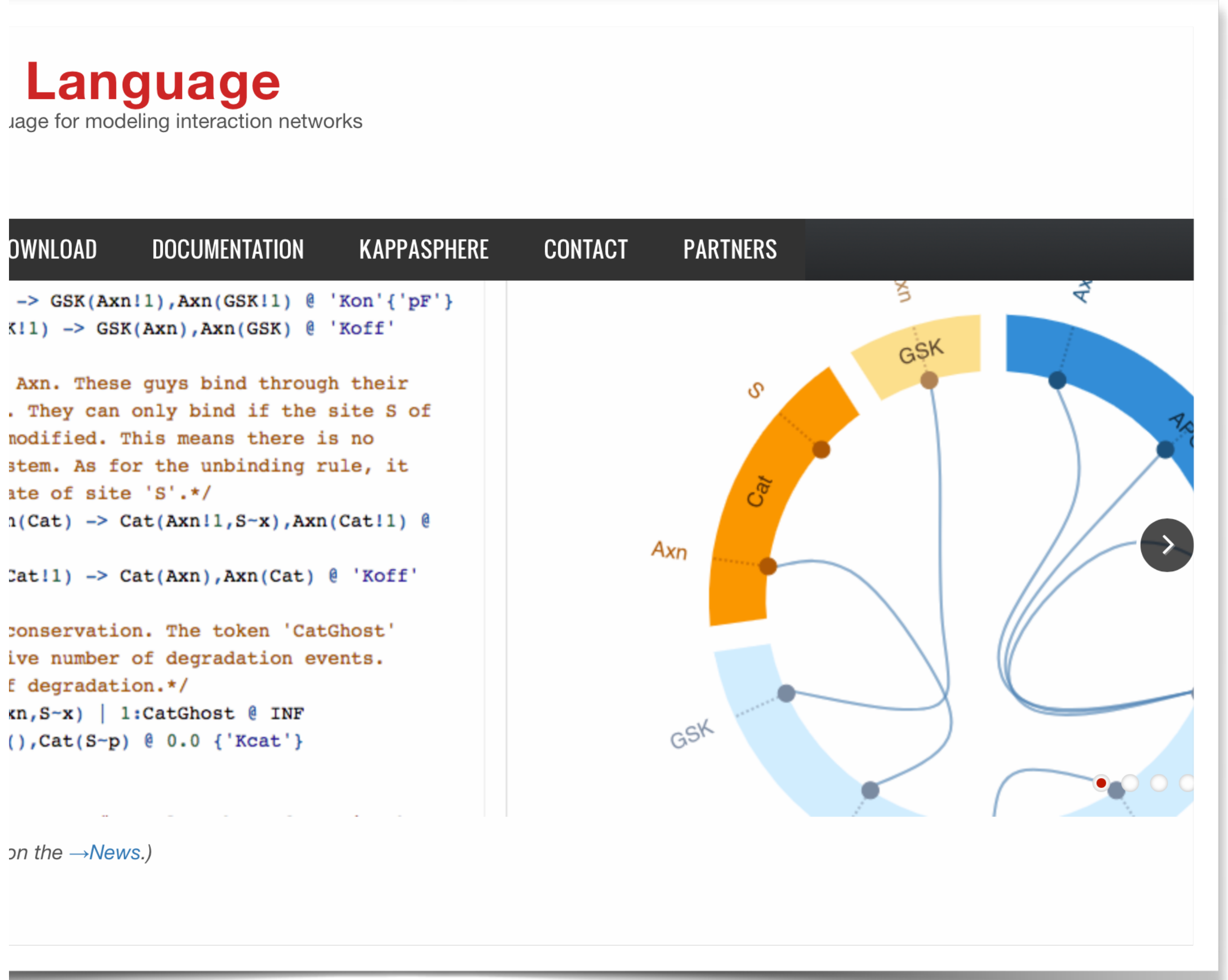
```
Axin(CBD[.]),ctnnb1(arm1[.],T41{u}[.],S29{u}[.]) →
Axin(CBD[1]),ctnnb1(arm1[1],T41{u}[.],S29{u}[.])
```



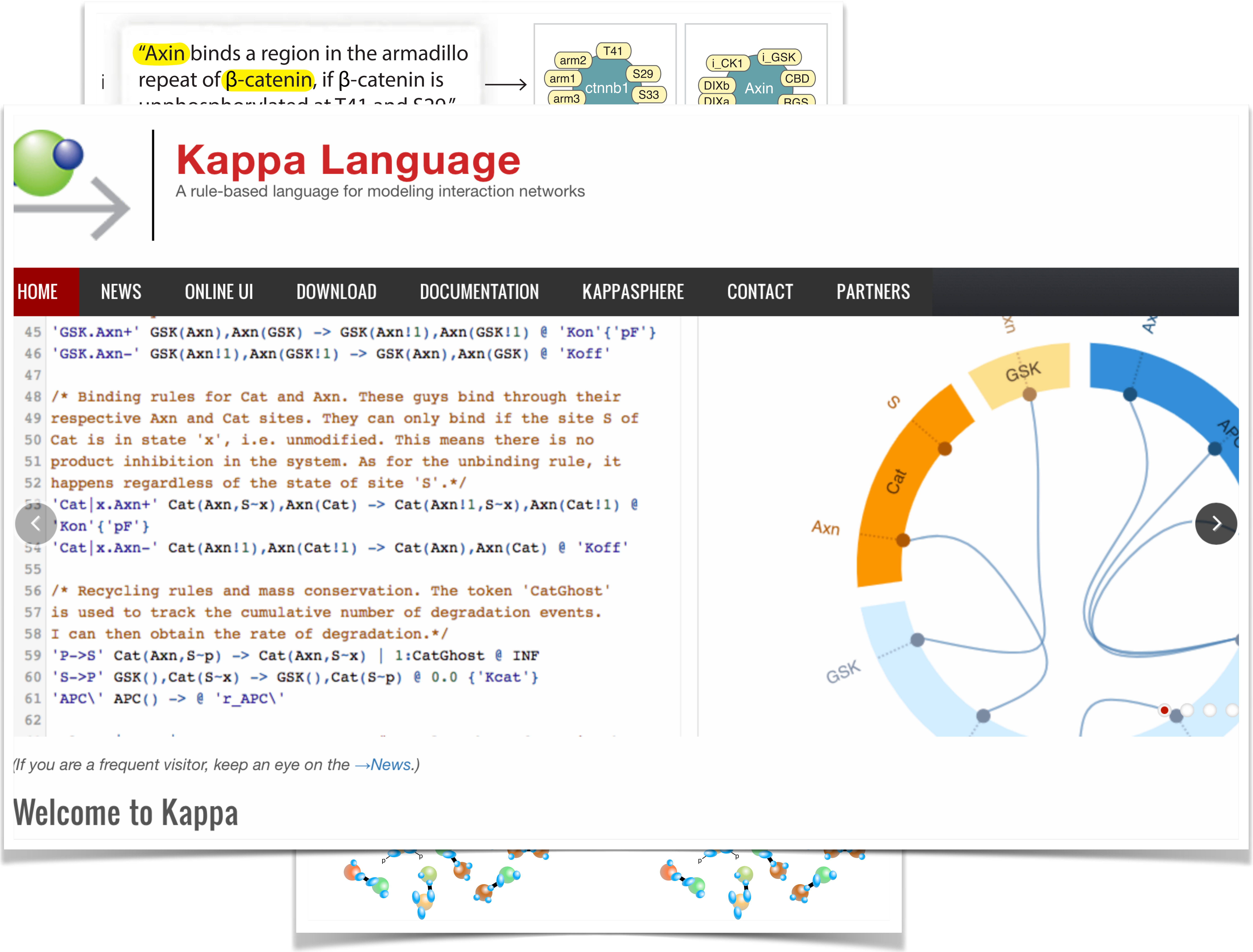


source: *The Kappa platform for rule-based modeling*, Boutillier, P., Maasha, M., Li, X., Medina-Abarca, H.F., Krivine, J., Feret, J., Cristescu, I., Forbes, A.G. and Fontana, W., 2018, *Bioinformatics*, *34*(13), pp.i583-i592.



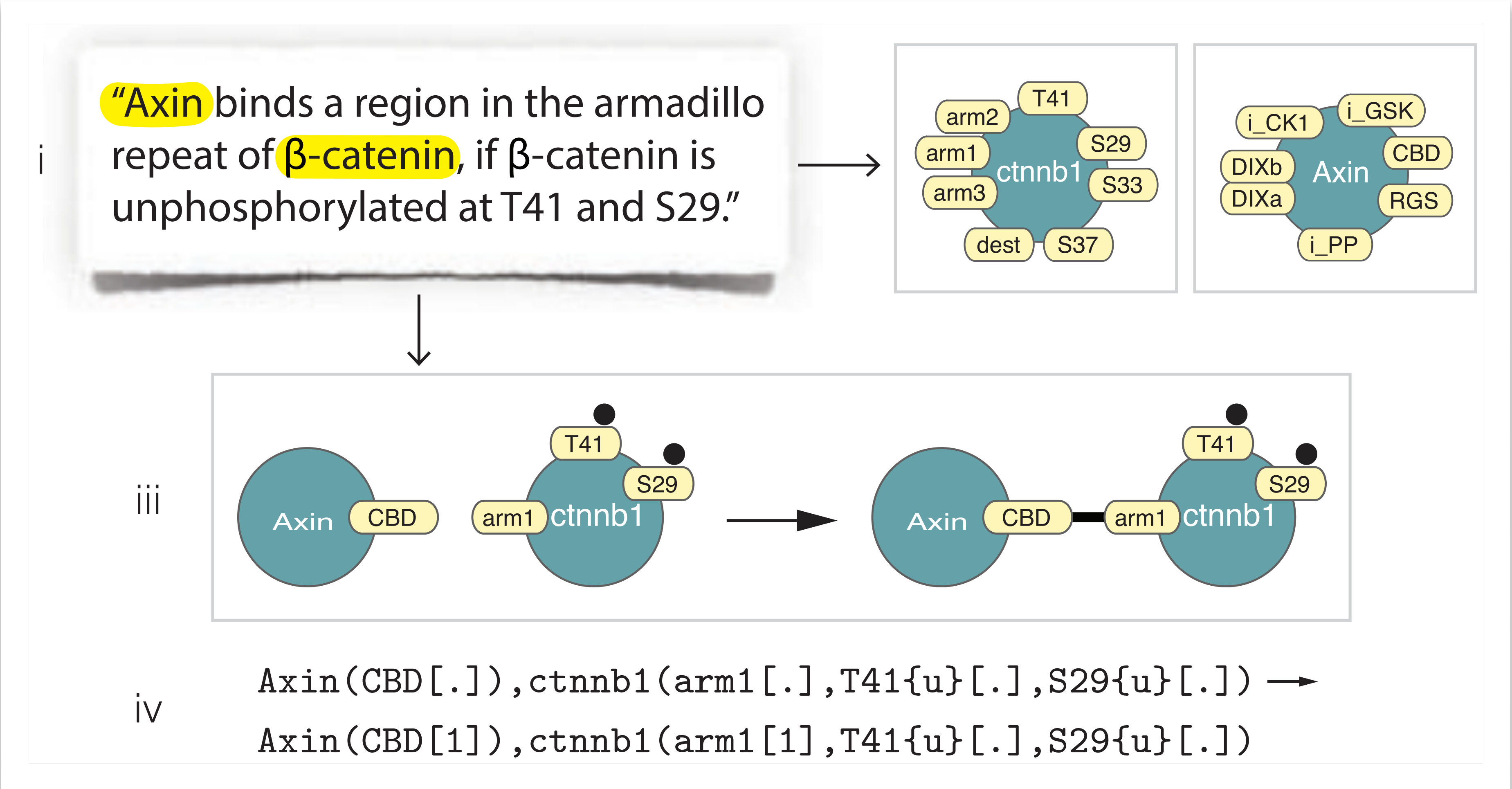


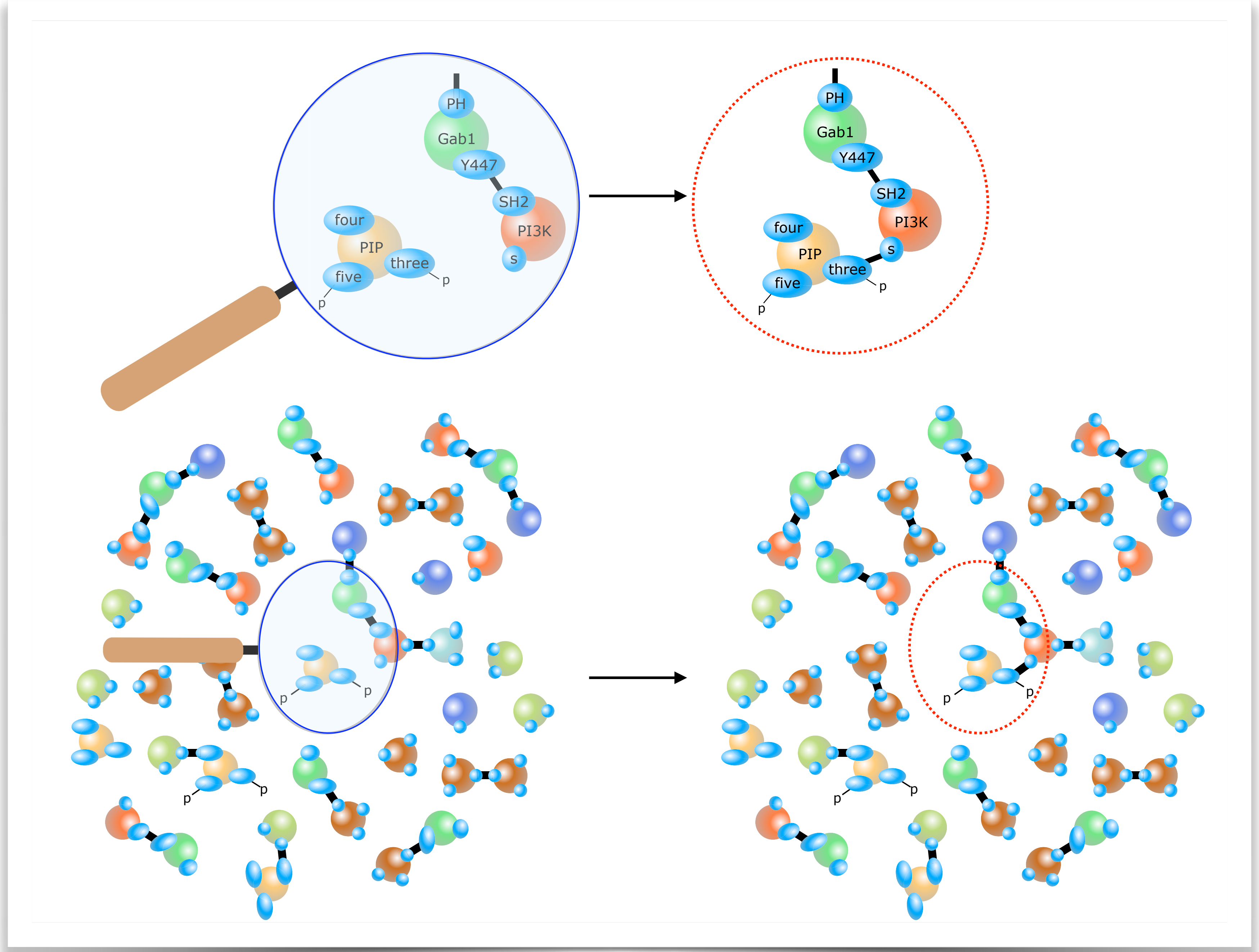
source: *The Kappa platform for rule-based modeling*, Boutillier, P., Maasha, M., Li, X., Medina-Abarca, H.F., Krivine, J., Feret, J., Cristescu, I., Forbes, A.G. and Fontana, W., 2018, *Bioinformatics*, *34*(13), pp.i583-i592.

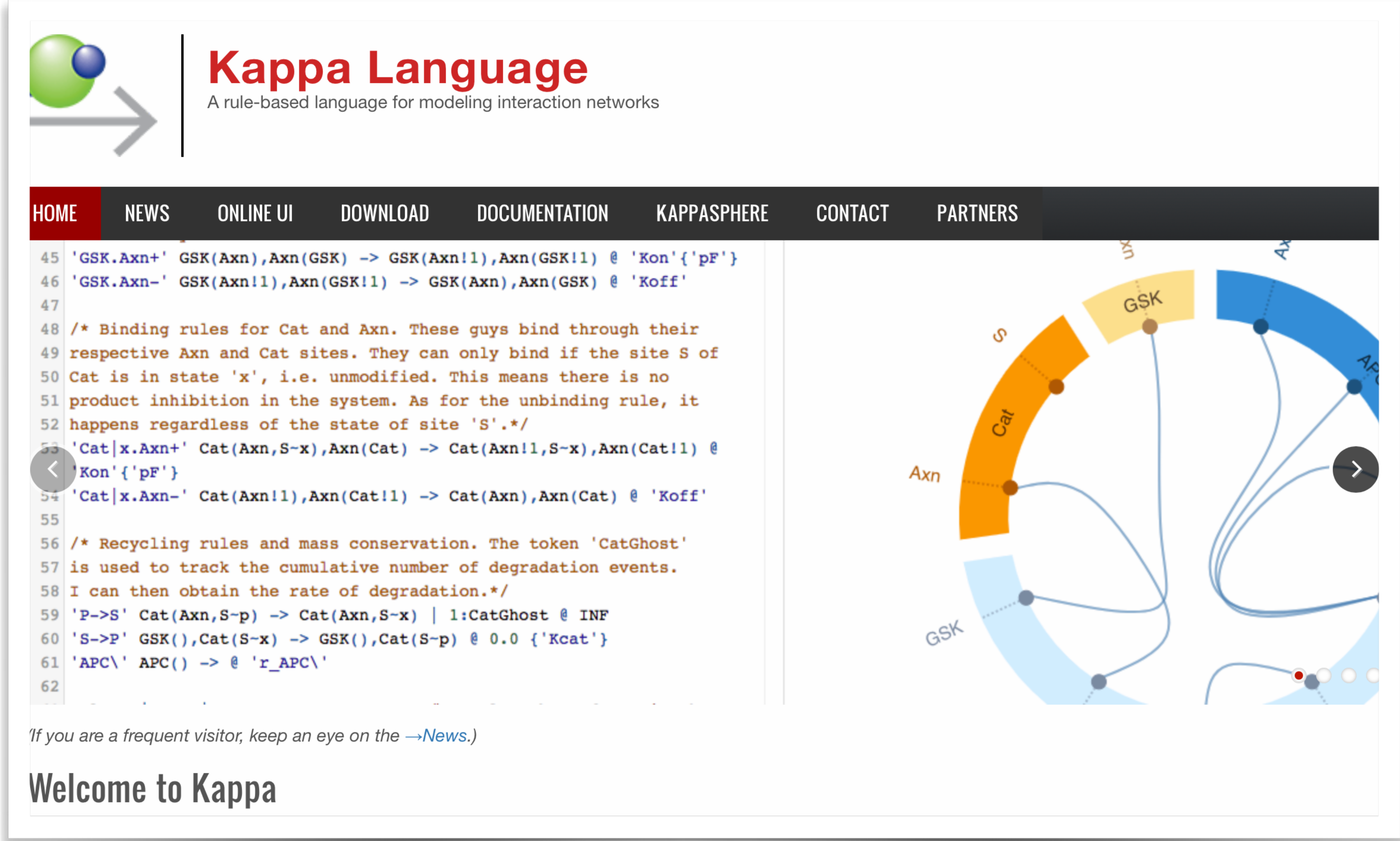


source: *The Kappa platform for rule-based modeling*, Boutillier, P., Maasha, M., Li, X., Medina-Abarca, H.F., Krivine, J., Feret, J., Cristescu, I., Forbes, A.G. and Fontana, W., 2018, *Bioinformatics*, *34*(13), pp.i583-i592.

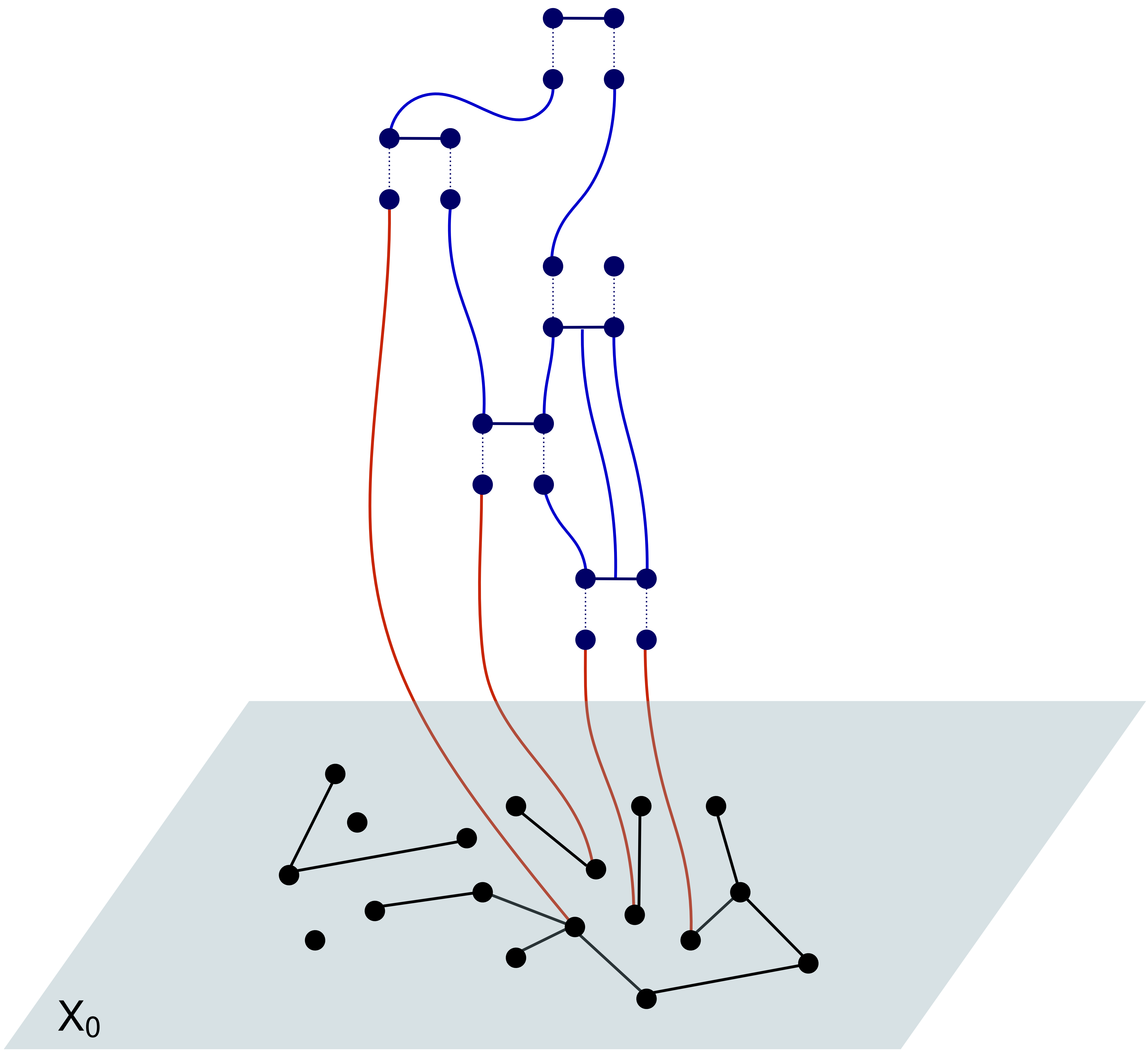
Rewriting in the life sciences: **bioinformatics**

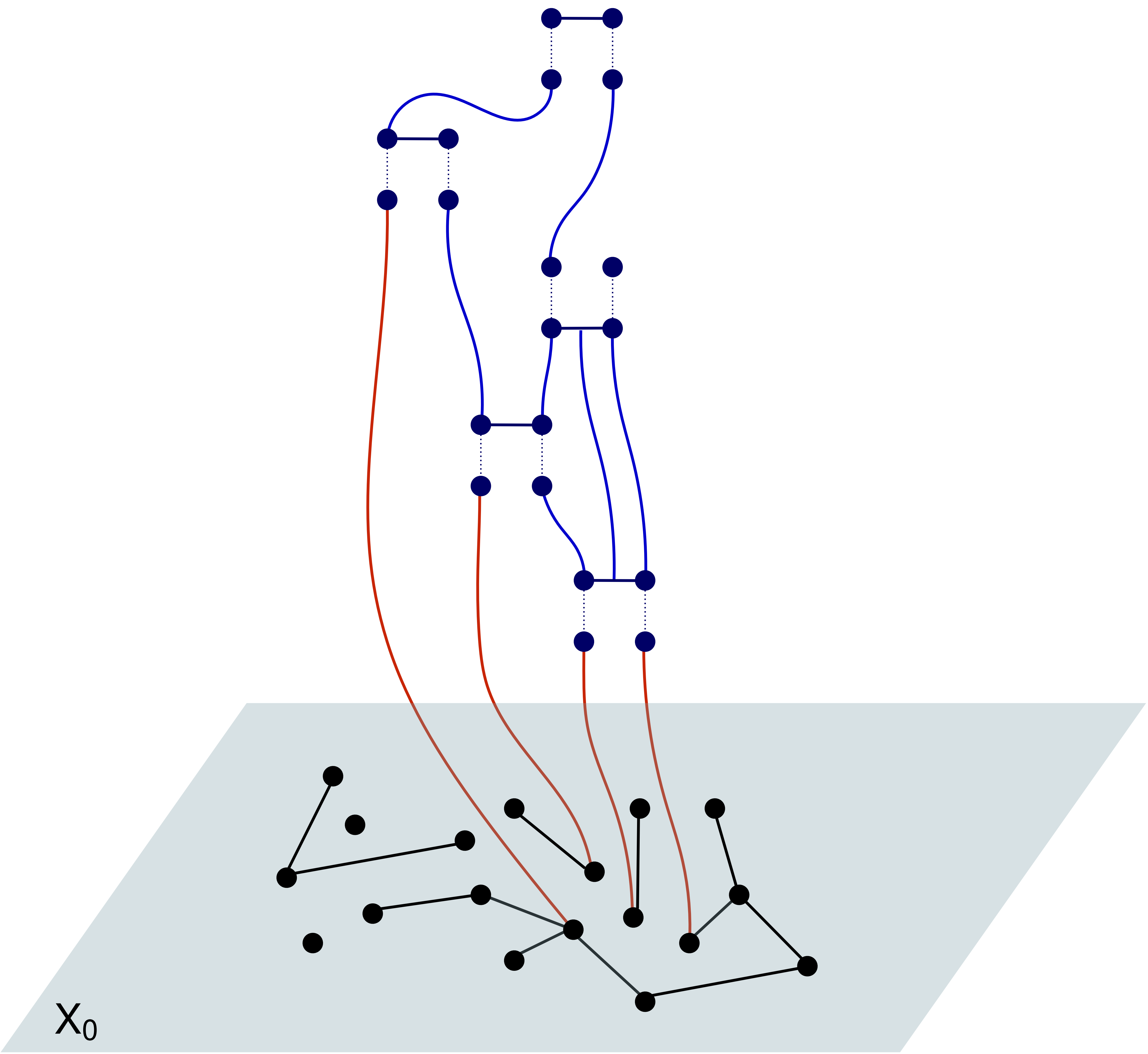




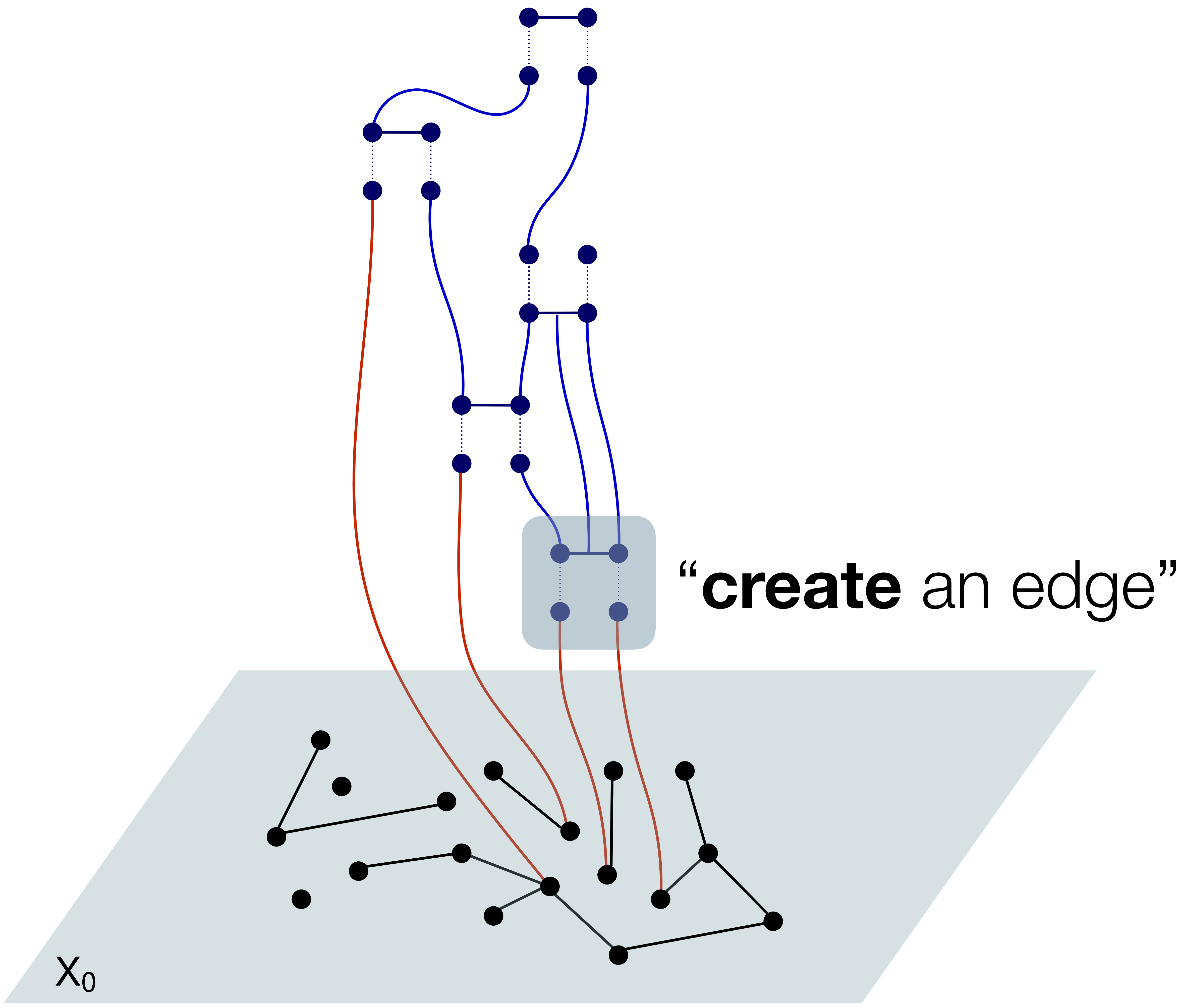


source: *The Kappa platform for rule-based modeling*, Boutillier, P., Maasha, M., Li, X., Medina-Abarca, H.F., Krivine, J., Feret, J., Cristescu, I., Forbes, A.G. and Fontana, W., 2018, *Bioinformatics*, *34*(13), pp.i583-i592.

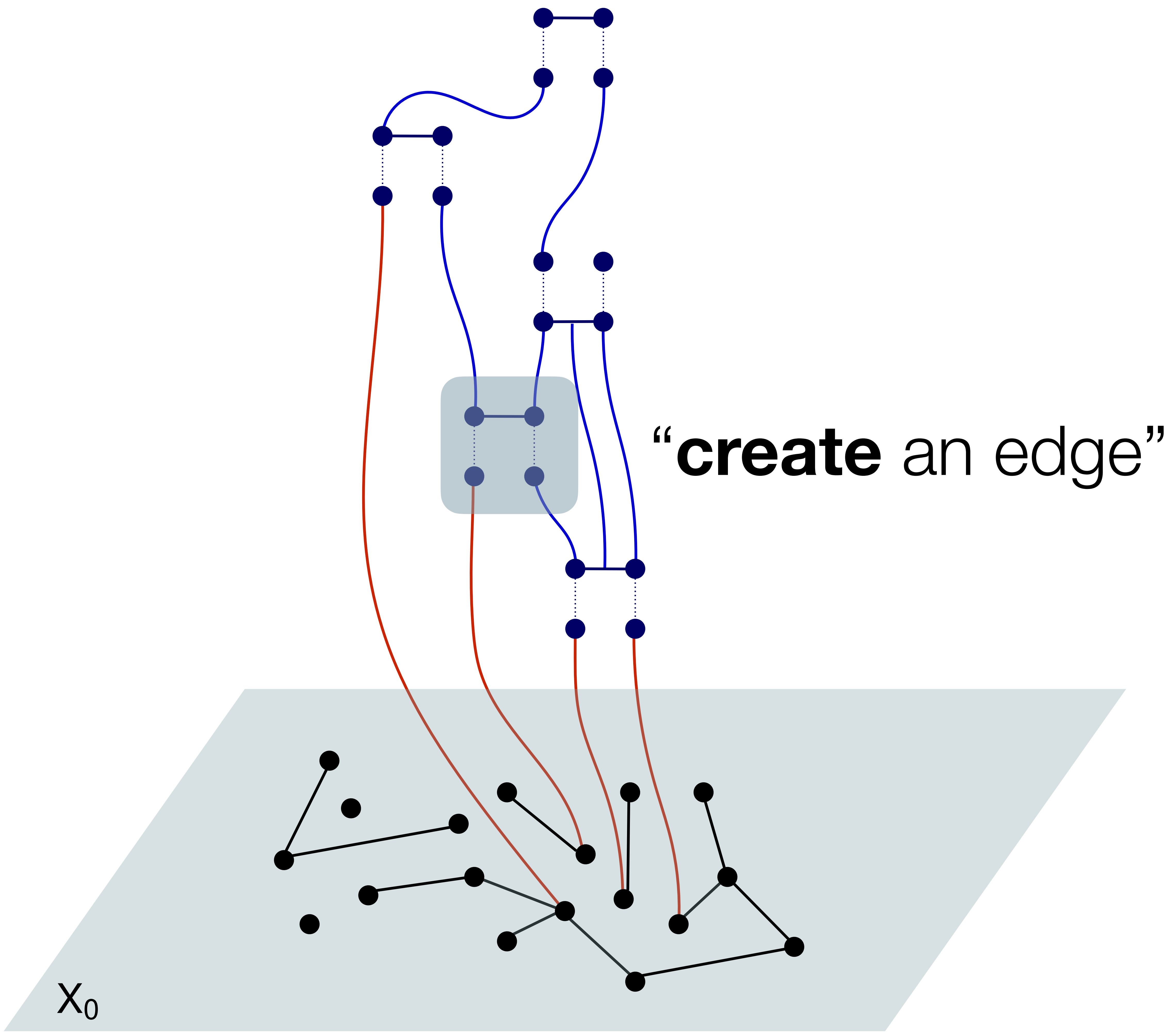

X_0



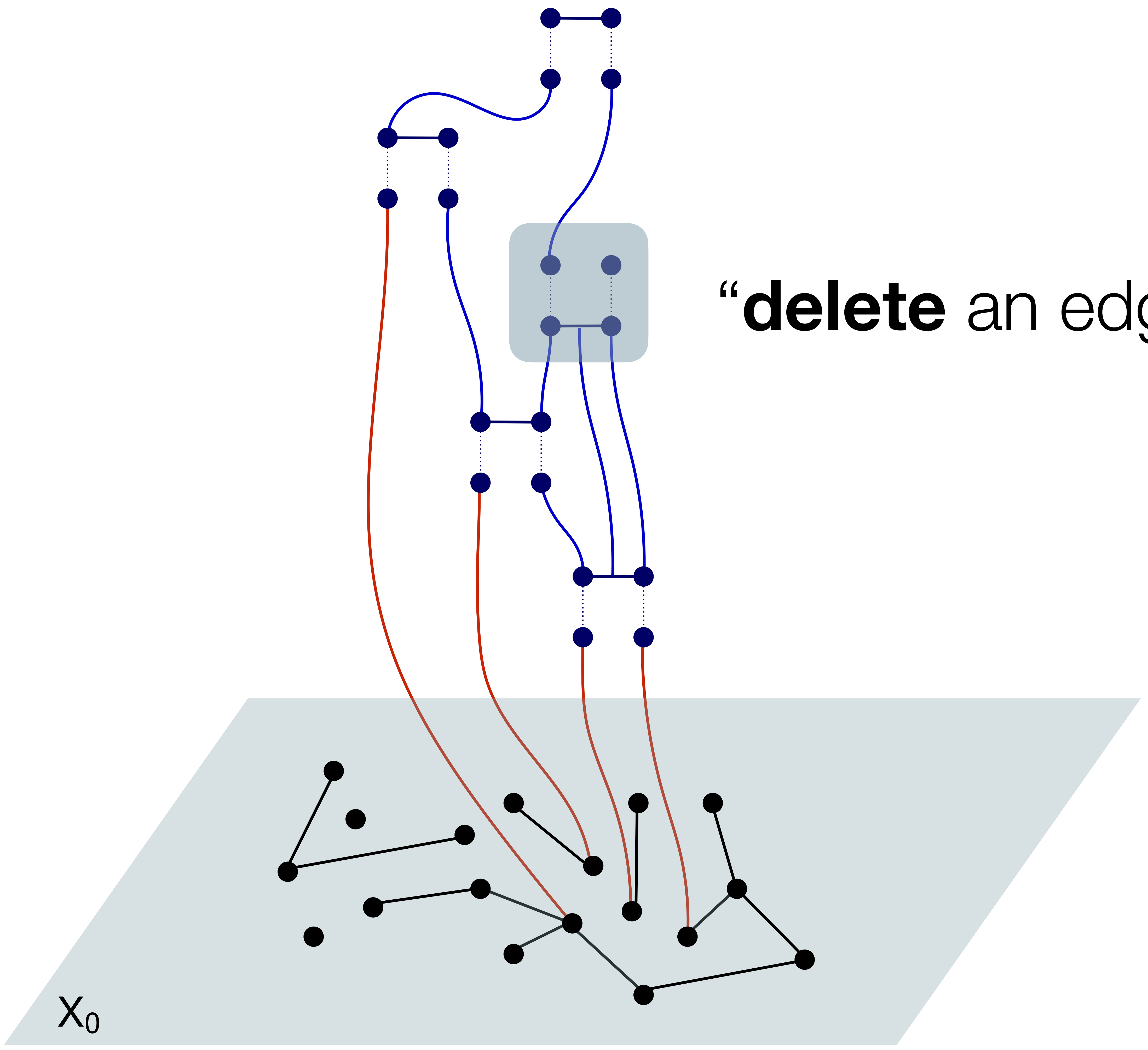
input graph



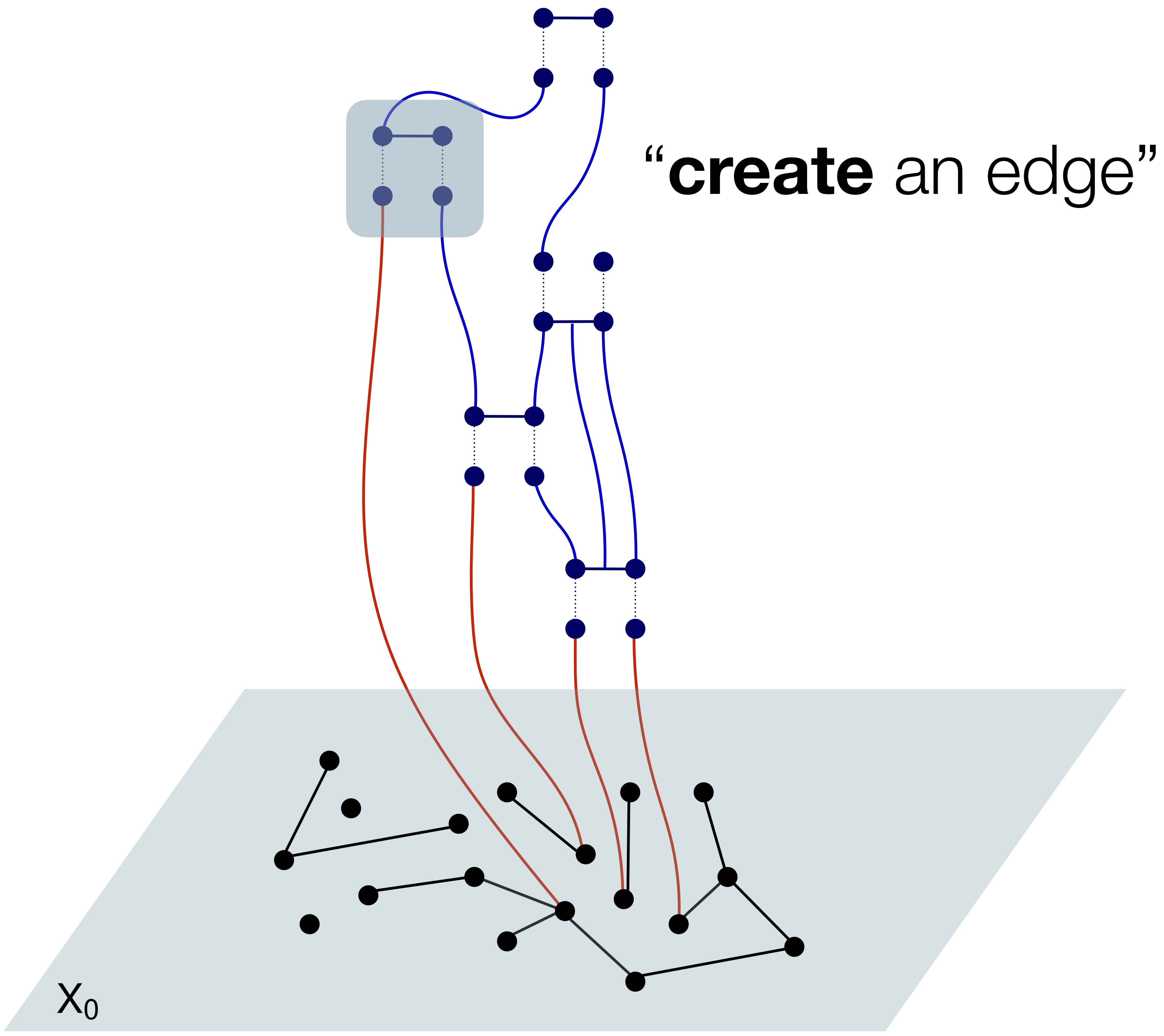
“**create** an edge”
X_0



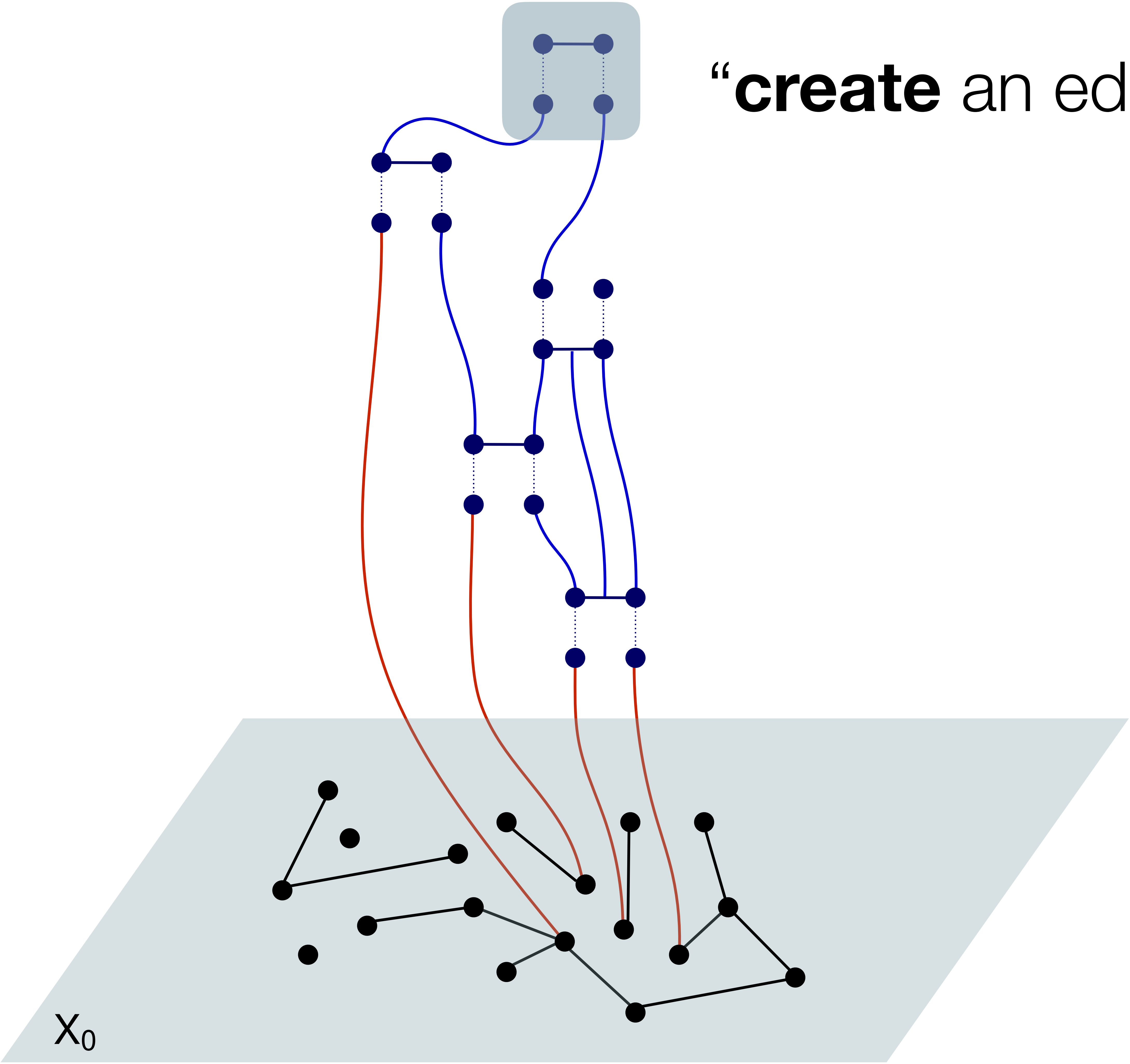
“**create** an edge”
X_0



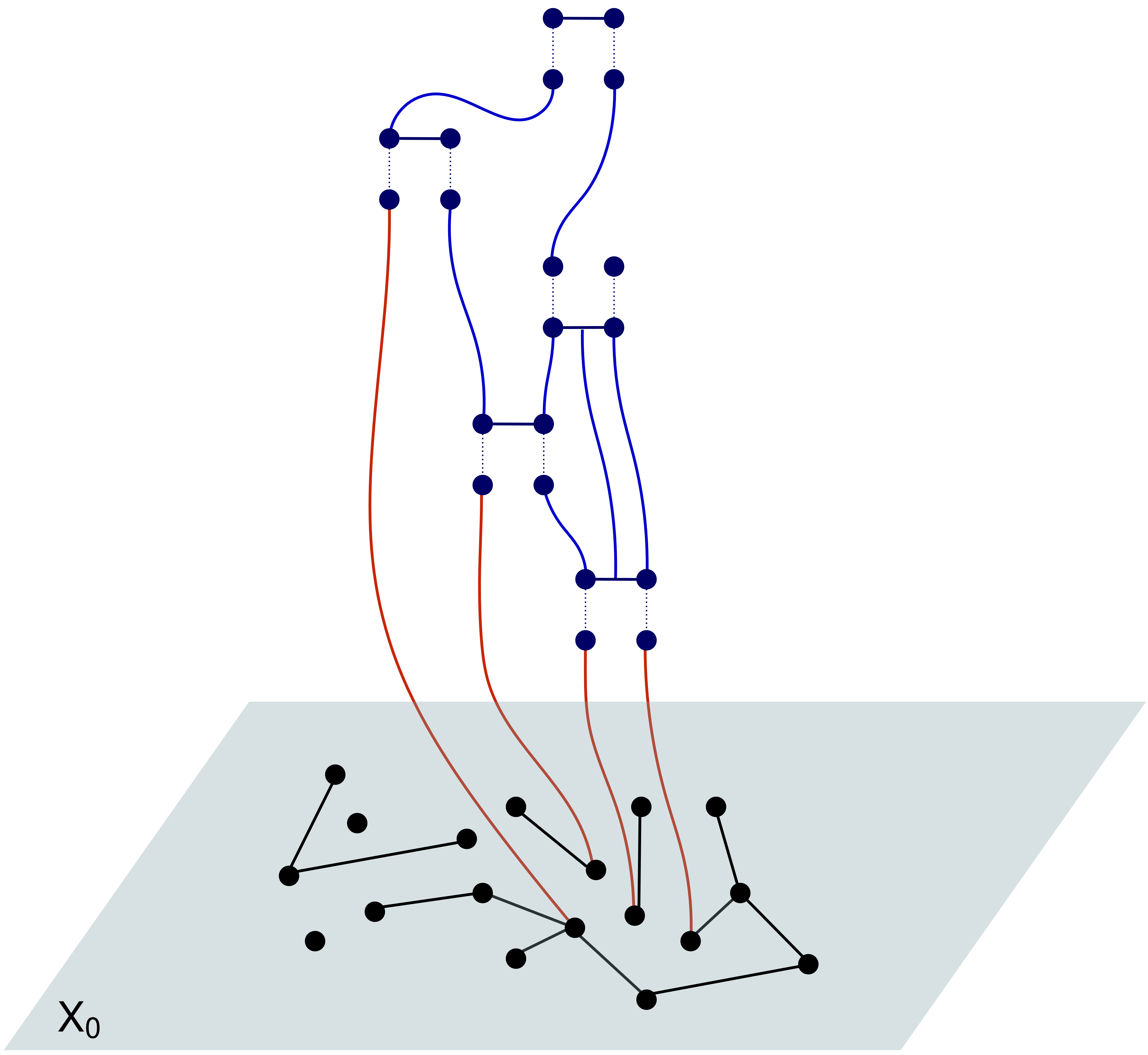
“**delete** an edge”

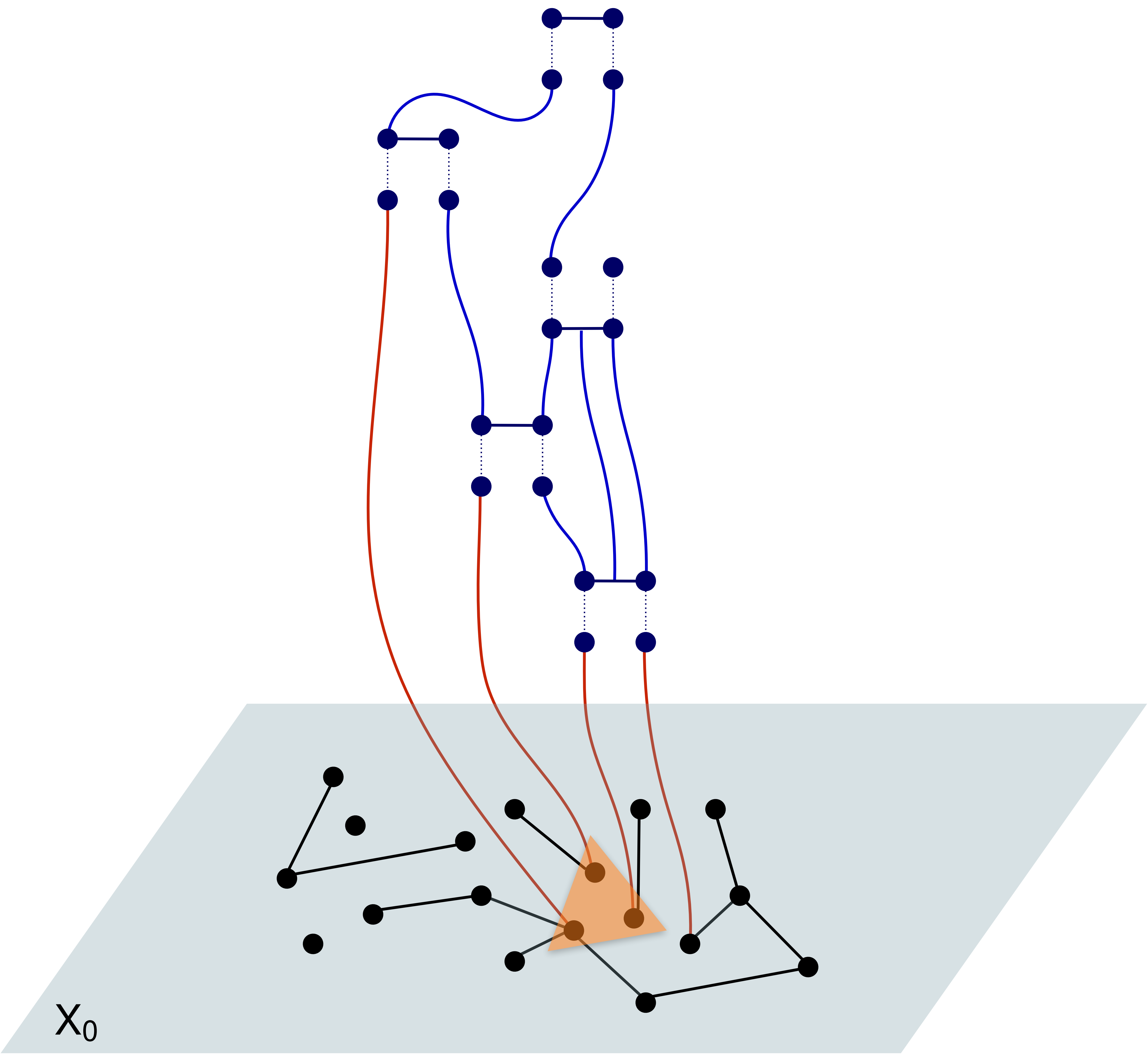


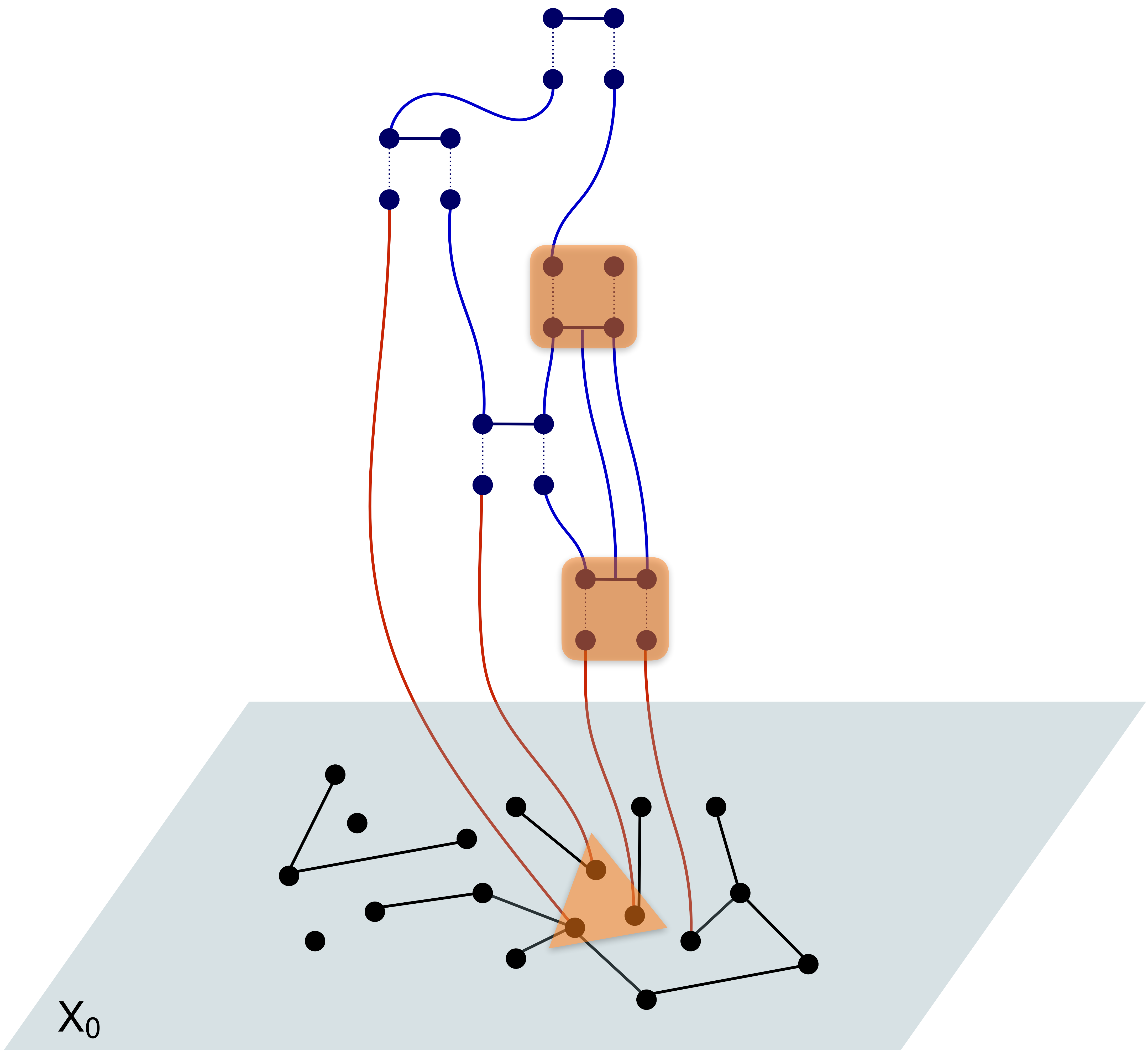
“**create** an edge”
X_0



“**create** an edge”

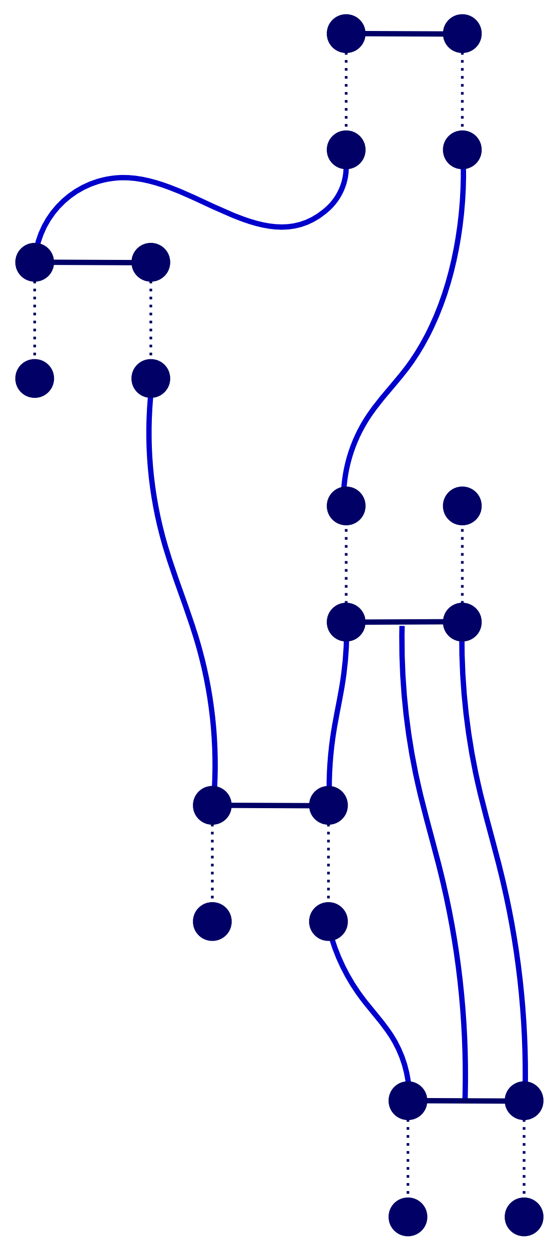

X$_0$


X0

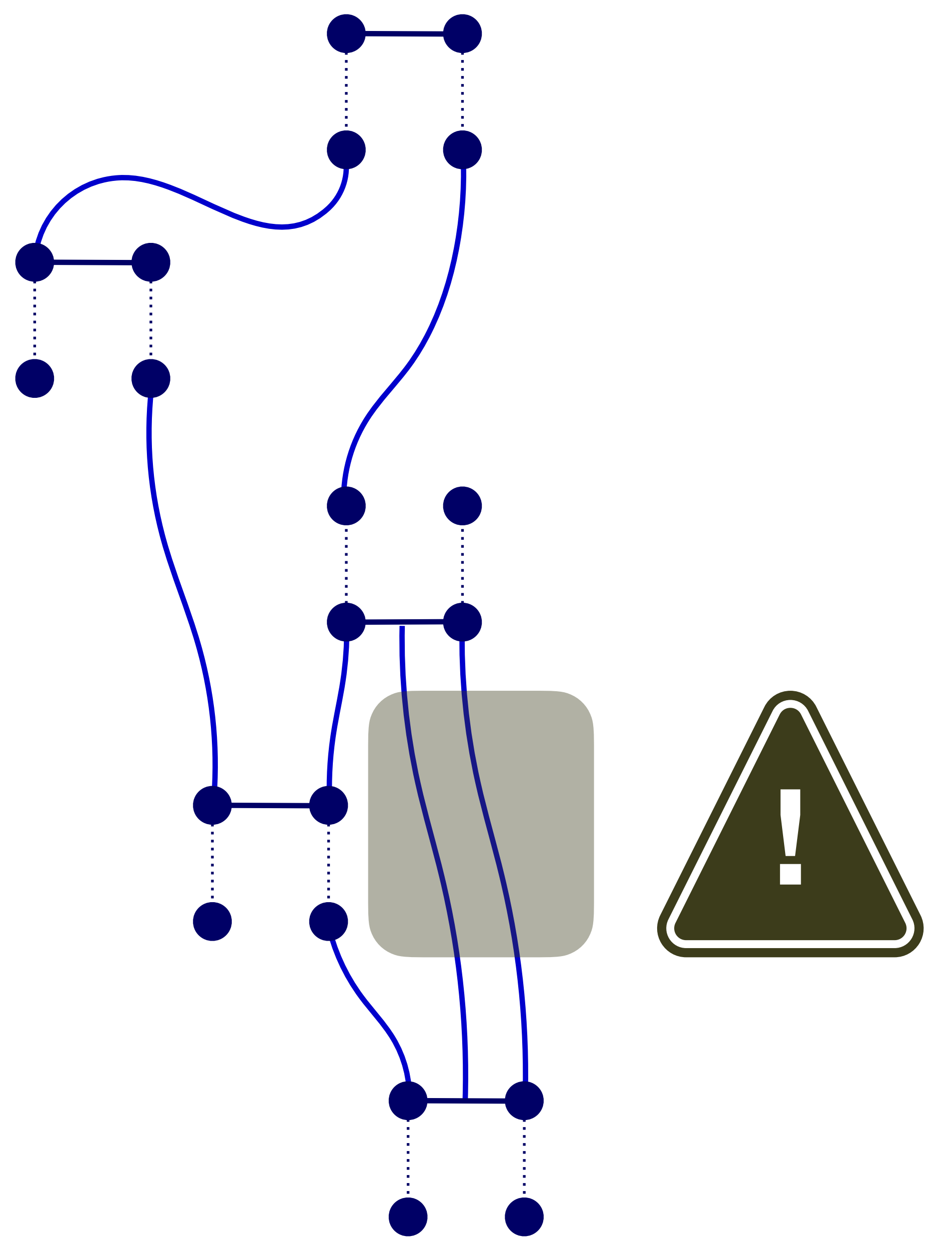


X_0

a **TRACELET**
(of length 5)



a **TRACELET**
(of length 5)



KEY CONCEPT:

Rule algebra formalism

$$\left(O \xleftarrow{r} I\right) \quad \rightsquigarrow \quad \delta\left(O \xleftarrow{r} I\right)$$

a **rule**

a **basis vector**
of a **vector space** $\mathcal{R}$

$$\left(O \xleftarrow{r} I\right) \quad \rightsquigarrow \quad \delta\left(O \xleftarrow{r} I\right)$$

a **rule**

a **basis vector** of a **vector space** $\mathcal{R}$

Definition: the **rule algebra product** $*_{\mathcal{R}} : \mathcal{R} \times \mathcal{R} \to \mathcal{R}$ is defined via

$$\delta(r_2) *_{\mathcal{R}} \delta(r_1) := \sum_{\mu \in M_{r_2}(r_1)} \delta\left(r_2 \overset{\mu}{\blacktriangleleft} r_1\right)$$

"sum over ways to compose the rules"

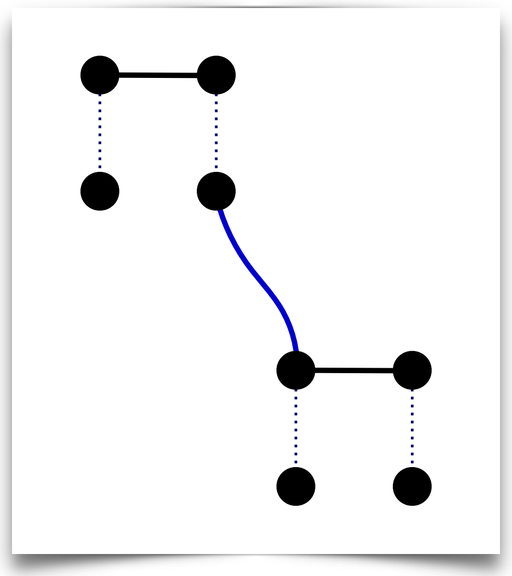
$$\left(O \xleftarrow{r} I\right) \rightsquigarrow \delta\left(O \xleftarrow{r} I\right)$$

a **rule** — a **basis vector** of a **vector space** $\mathcal{R}$

Definition: the **rule algebra product** $*_{\mathcal{R}} : \mathcal{R} \times \mathcal{R} \to \mathcal{R}$ is defined via

$$\delta(r_2) *_{\mathcal{R}} \delta(r_1) := \sum_{\mu \in M_{r_2}(r_1)} \delta\left(r_2 \overset{\mu}{\blacktriangleleft} r_1\right)$$

"sum over ways to compose the rules"



$$\begin{array}{ccccccc}
O_2 & \xleftarrow{r_2} & I_2 & \xleftarrow{\mu} & O_1 & \xleftarrow{r_1} & I_1 \\
\downarrow & & \searrow & & \swarrow & & \downarrow \\
O_{21} & \xleftarrow{r_2'} & & N_{21} & & \xleftarrow{r_1'} & I_{21}
\end{array}$$

$$r_2 \overset{\mu}{\blacktriangleleft} r_1 := r_2' \circ r_1'$$

Physics insight: the **rule algebra** formalism

Definition: the **rule algebra product** $*_{\mathcal{R}} : \mathcal{R} \times \mathcal{R} \to \mathcal{R}$ is defined via

$$\delta(\mathsf{r}_2) *_{\mathcal{R}} \delta(\mathsf{r}_1) := \sum_{\mu \in \mathsf{M}_{\mathsf{r}_2}(\mathsf{r}_1)} \delta\left(\mathsf{r}_2 \overset{\mu}{\blacktriangleleft} \mathsf{r}_1\right)$$

"sum over ways to compose the rules"

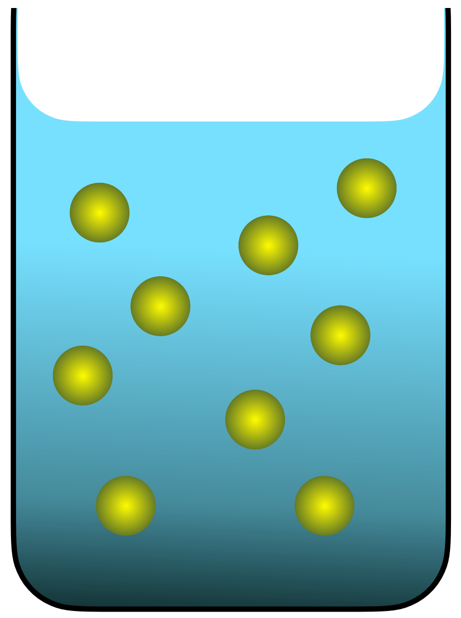
Theorem LiCS 2016, CSL 2018, GCM 2019, LMCS 2020, ICGT 2020

The **rule algebra** $(\mathcal{R}, *_{\mathcal{R}})$ is an **associative unital algebra**, with **unit element** $\delta(\varnothing \leftharpoonup \varnothing)$.

$\Rightarrow$ a new fundamental tool in **rewriting theory**, **combinatorics** and **concurrency theory**

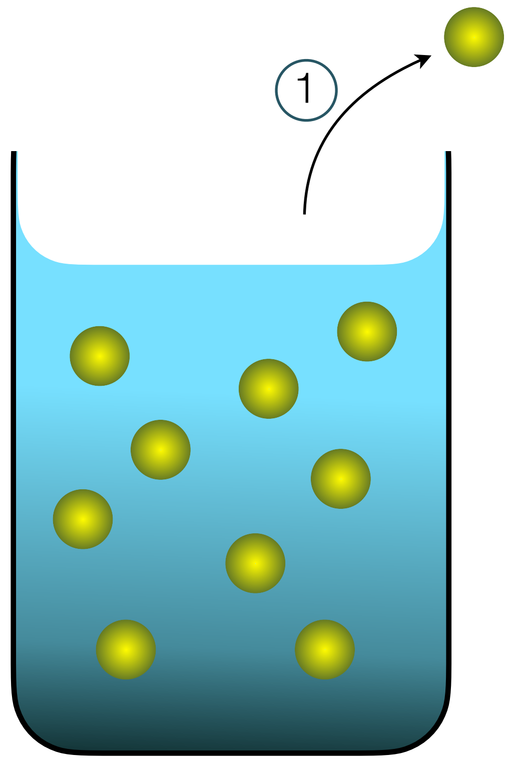
Mathematics of **chemical reactions**

Example: $2X \xleftharpoondown{\alpha} X \qquad (\alpha \in \mathbb{R}_{>0})$



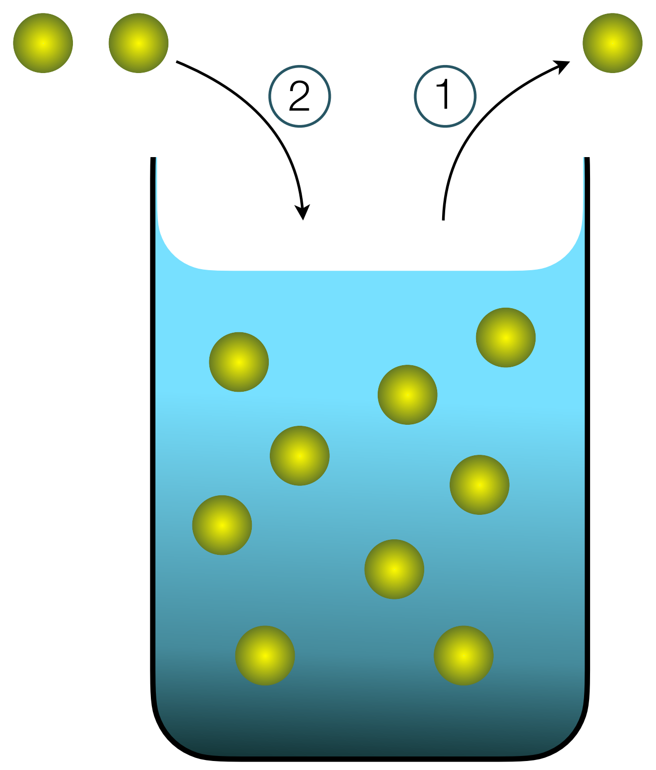
Mathematics of **chemical reactions**

Example: $2X \xleftarrow{\alpha} X \qquad (\alpha \in \mathbb{R}_{>0})$



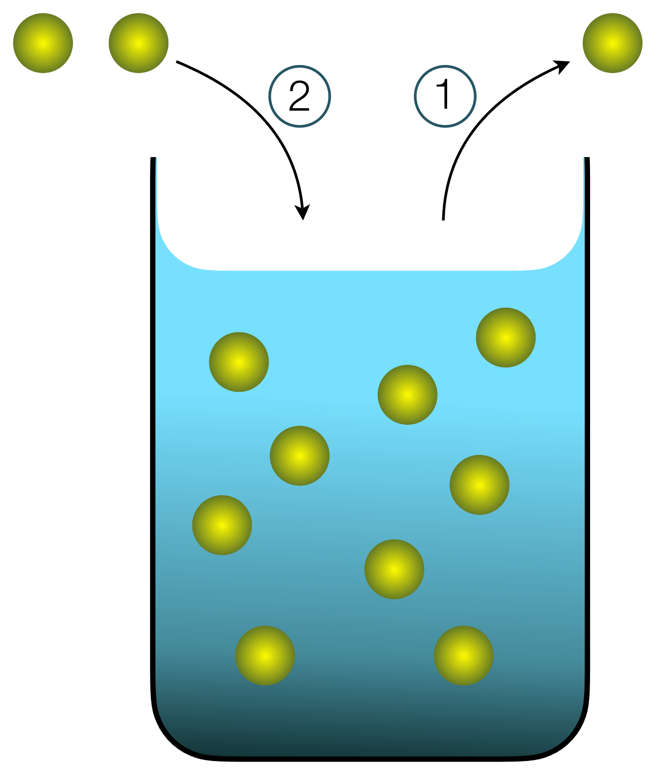
Mathematics of **chemical reactions**

Example: $2X \xleftarrow{\alpha} X \qquad (\alpha \in \mathbb{R}_{>0})$



Mathematics of **chemical reactions**

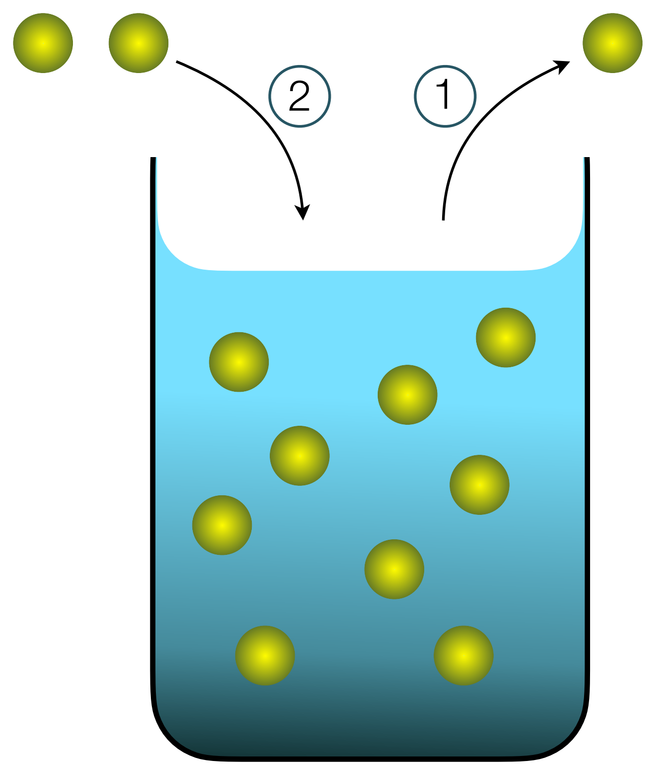
Example: $2X \xleftharpoondown{\alpha} X$ $(\alpha \in \mathbb{R}_{>0})$



$p_n(t) := \Pr(\#X = n \text{ at time } t) = ?$

Mathematics of **chemical reactions**

Example: $2X \xleftharpoondown{\alpha} X \qquad (\alpha \in \mathbb{R}_{>0})$

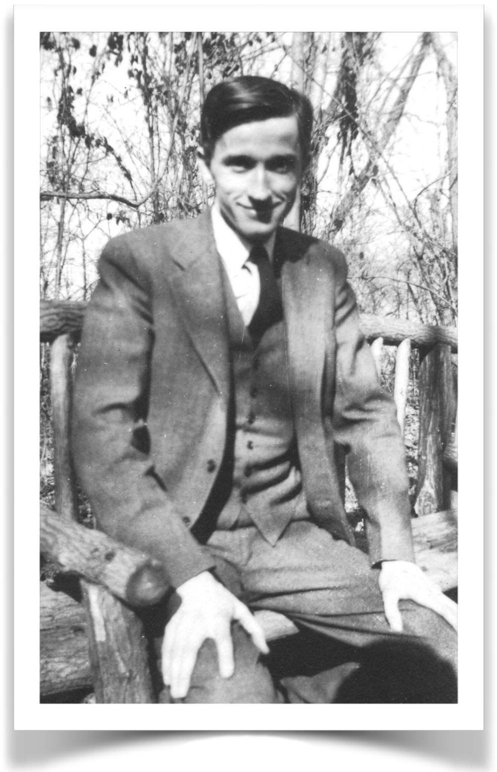


$p_n(t) := \Pr(\#X = n \text{ at time } t) = ?$

Delbrück (1940): $P(t;x) := \sum_{n\geq 0} p_n(t)\, x^n$

$$\partial_t P(t;x) = \left[\alpha\left(\hat{x}^2\partial_x - \hat{x}\partial_x\right)\right] P(t;x)$$

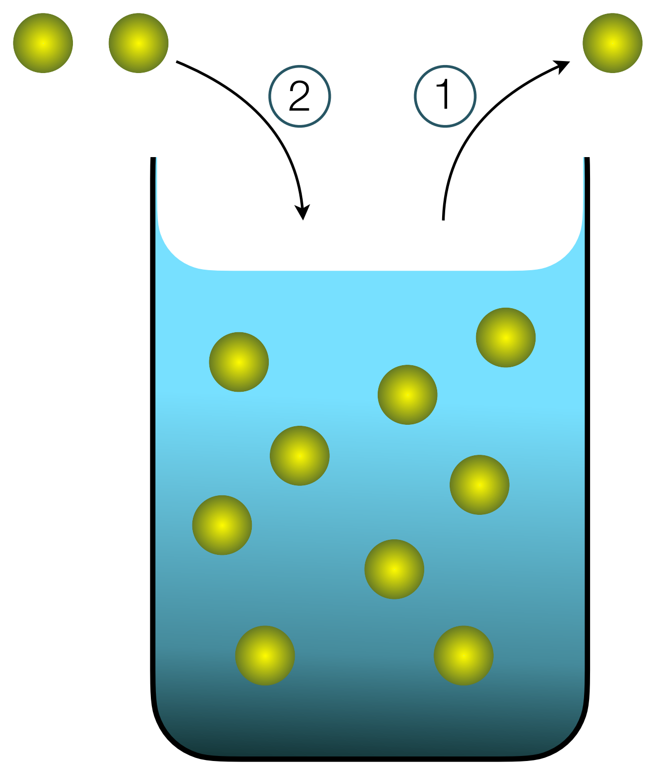
a **linear operator...**



Max Delbrück (1906-1981)
1969 **Nobel Prize** laureate
(medicine and physiology)

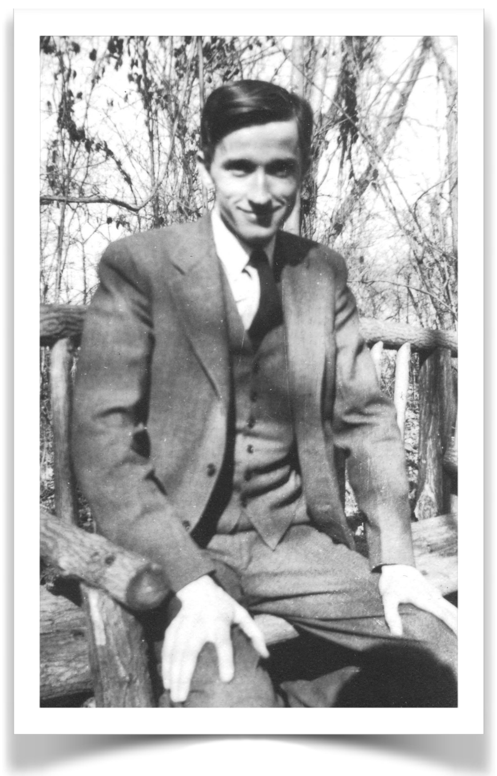
Mathematics of **chemical reactions**

Example: $2X \xleftarrow{\alpha} X \qquad (\alpha \in \mathbb{R}_{>0})$



$$p_n(t) \;:=\; \Pr(\#X = n \text{ at time } t) \;=\; ?$$

Delbrück (1940): $$P(t;x) \;:=\; \sum_{n\geq 0} p_n(t)\, x^n$$



Max Delbrück (1906-1981)
1969 **Nobel Prize** laureate
(medicine and physiology)

$$\partial_t P(t;x) = \left[\alpha\left(\hat{x}^2\partial_x - \hat{x}\partial_x\right)\right] P(t;x)$$

a **linear operator...**

$$\hat{x}(x^n) := x^{n+1}\,, \qquad \partial_x(x^n) := \begin{cases} 0 & \text{if } n = 0 \\ n \cdot x^{n-1} & \text{if } n > 0 \end{cases}$$

Rule algebra framework (Part II)

Observation: x^n — **basis vector** (of the vector space of polynomials in x)

Rule algebra framework (Part II)

Observation: x^n — **basis vector** (of the vector space of polynomials in x)

⇒ **analogous concept** for **rewriting theory**:

$|X\rangle$ — **basis vector** (of a vector space of **configurations** $\hat{\mathbf{C}}$,
e.g. **graphs**, **trees**, **molecules**, ….)

Rule algebra framework (Part II)

Observation: x^n — **basis vector** (of the vector space of polynomials in x)

⇒ **analogous concept** for **rewriting theory**:

$|X\rangle$ — **basis vector** (of a vector space of **configurations** $\hat{\mathbf{C}}$,
e.g. **graphs**, **trees**, **molecules**, ….)

Example: $|n\rangle := |\bullet \ldots \bullet\rangle$ (here: configuration = **iso-class** of graph)

n vertices

Rule algebra framework (Part II)

Observation: x^n — **basis vector** (of the vector space of polynomials in x)

⇒ **analogous concept** for **rewriting theory**:

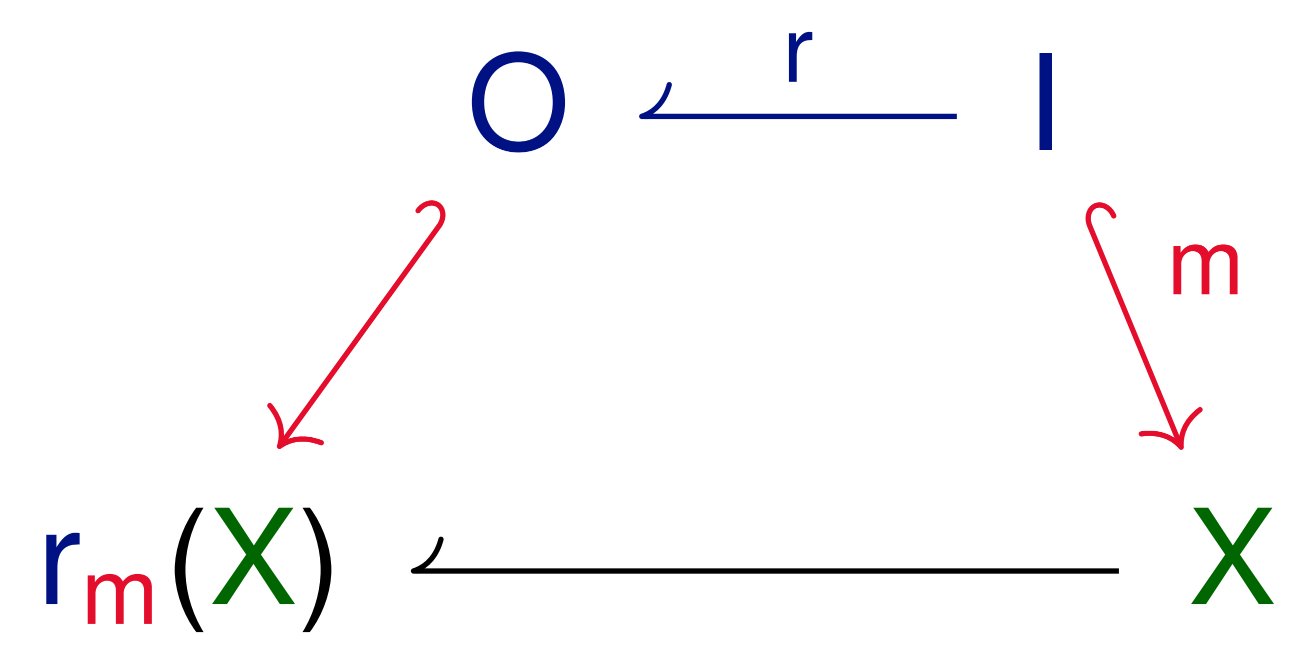
$|X\rangle$ — **basis vector** (of a vector space of **configurations** $\hat{\mathbf{C}}$,
e.g. **graphs**, **trees**, **molecules**, ….)

Example: $|n\rangle := |\underbrace{\bullet \ldots \bullet}_{\textbf{n}\text{ vertices}}\rangle$ (here: configuration = **iso-class** of graph)

Key step: from **rules** to **linear operators** on $\hat{\mathbf{C}}$

$$\rho(\delta(r))\,|X\rangle := \sum_{m \in M_r(X)} |r_m(X)\rangle$$

"sum over **all ways** to apply **r** to **X**"



Rule algebra framework (Part II)

$$\rho(\delta(r))\,|X\rangle := \sum_{m \in M_r(X)} |r_m(X)\rangle$$

Theorem LiCS 2016, CSL 2018, GCM 2019, LMCS 2020, ICGT 2020

$\rho : \mathcal{R} \to \mathrm{End}(\hat{\mathbf{C}})$ is a **representation** of the **rule algebra** $(\mathcal{R}, *_{\mathcal{R}})$, i.e.

$$\rho(\delta(r_2))\rho(\delta(r_1))\,|X\rangle = \rho(\delta(r_2) *_{\mathcal{R}} \delta(r_1))\,|X\rangle$$

Rule algebra framework (Part II)

$$\rho(\delta(r))\,|X\rangle := \sum_{m \in M_r(X)} |r_m(X)\rangle$$

Theorem — LiCS 2016, CSL 2018, GCM 2019, LMCS 2020, ICGT 2020

$\rho : \mathcal{R} \to \mathrm{End}(\hat{\mathbf{C}})$ is a **representation** of the **rule algebra** $(\mathcal{R}, *_{\mathcal{R}})$, i.e.

$$\rho(\delta(r_2))\rho(\delta(r_1))\,|X\rangle = \rho(\delta(r_2) *_{\mathcal{R}} \delta(r_1))\,|X\rangle$$

Example:

$$|n\rangle := |\underbrace{\bullet \ldots \bullet}_{n \text{ vertices}}\rangle \quad \leftrightarrow \quad x^n$$

$$\rho(\delta(\bullet \leftharpoonup \varnothing))\,|n\rangle = |n+1\rangle \quad \leftrightarrow \quad \hat{x}(x^n) = x^{n+1}$$

$$\rho(\delta(\varnothing \leftharpoonup \bullet))\,|n\rangle = \begin{cases} 0 & \text{if } n = 0 \\ n \cdot |n-1\rangle & \text{if } n > 0 \end{cases} \quad \leftrightarrow \quad \partial_x(x^n) = \begin{cases} 0 & \text{if } n = 0 \\ n \cdot x^{n-1} & \text{if } n > 0 \end{cases}$$

Rule algebra framework (Part II)

$$\rho(\delta(r))\,|X\rangle := \sum_{m\in M_r(X)} |r_m(X)\rangle$$

Theorem LiCS 2016, CSL 2018, GCM 2019, LMCS 2020, ICGT 2020

$\rho : \mathcal{R} \to \mathrm{End}(\hat{\mathbf{C}})$ is a **representation** of the **rule algebra** $(\mathcal{R}, *_{\mathcal{R}})$, i.e.

$$\rho(\delta(r_2))\,\rho(\delta(r_1))\,|X\rangle = \rho(\delta(r_2) *_{\mathcal{R}} \delta(r_1))\,|X\rangle$$

$$|n\rangle := |\underbrace{\bullet \ldots \bullet}_{\mathbf{n}\text{ vertices}}\rangle$$

Example: $\leftrightarrow \quad x^n$

$$\rho(\delta(\bullet \leftharpoonup \varnothing))\,|n\rangle = |n+1\rangle \quad \leftrightarrow \quad \hat{x}(x^n) = x^{n+1}$$

$$\rho(\delta(\varnothing \leftharpoonup \bullet))\,|n\rangle = \begin{cases} 0 & \text{if } n = 0 \\ n \cdot |n-1\rangle & \text{if } n > 0 \end{cases} \quad \leftrightarrow \quad \partial_x(x^n) = \begin{cases} 0 & \text{if } n = 0 \\ n \cdot x^{n-1} & \text{if } n > 0 \end{cases}$$

Application to the case of the reaction $2X \overset{\alpha}{\leftharpoonup} X \quad (\alpha \in \mathbb{R}_{>0})$

$$\alpha\left(\hat{x}^2\partial_x - \hat{x}\partial_x\right)$$

Rule algebra framework (Part II)

$$\rho(\delta(r))\,|X\rangle := \sum_{m\in M_r(X)} |r_m(X)\rangle$$

Theorem LiCS 2016, CSL 2018, GCM 2019, LMCS 2020, ICGT 2020

$\rho : \mathcal{R} \to \mathrm{End}(\hat{\mathbf{C}})$ is a **representation** of the **rule algebra** $(\mathcal{R}, *_{\mathcal{R}})$, i.e.

$$\rho(\delta(r_2))\rho(\delta(r_1))\,|X\rangle = \rho(\delta(r_2) *_{\mathcal{R}} \delta(r_1))\,|X\rangle$$

$$|n\rangle := |\underbrace{\bullet \ldots \bullet}_{n \text{ vertices}}\rangle \qquad \textbf{Example:} \quad \leftrightarrow \quad x^n$$

$$\rho(\delta(\bullet \leftharpoonup \varnothing))\,|n\rangle = |n+1\rangle \quad \leftrightarrow \quad \hat{x}(x^n) = x^{n+1}$$

$$\rho(\delta(\varnothing \leftharpoonup \bullet))\,|n\rangle = \begin{cases} 0 & \text{if } n = 0 \\ n \cdot |n-1\rangle & \text{if } n > 0 \end{cases} \quad \leftrightarrow \quad \partial_x(x^n) = \begin{cases} 0 & \text{if } n = 0 \\ n \cdot x^{n-1} & \text{if } n > 0 \end{cases}$$

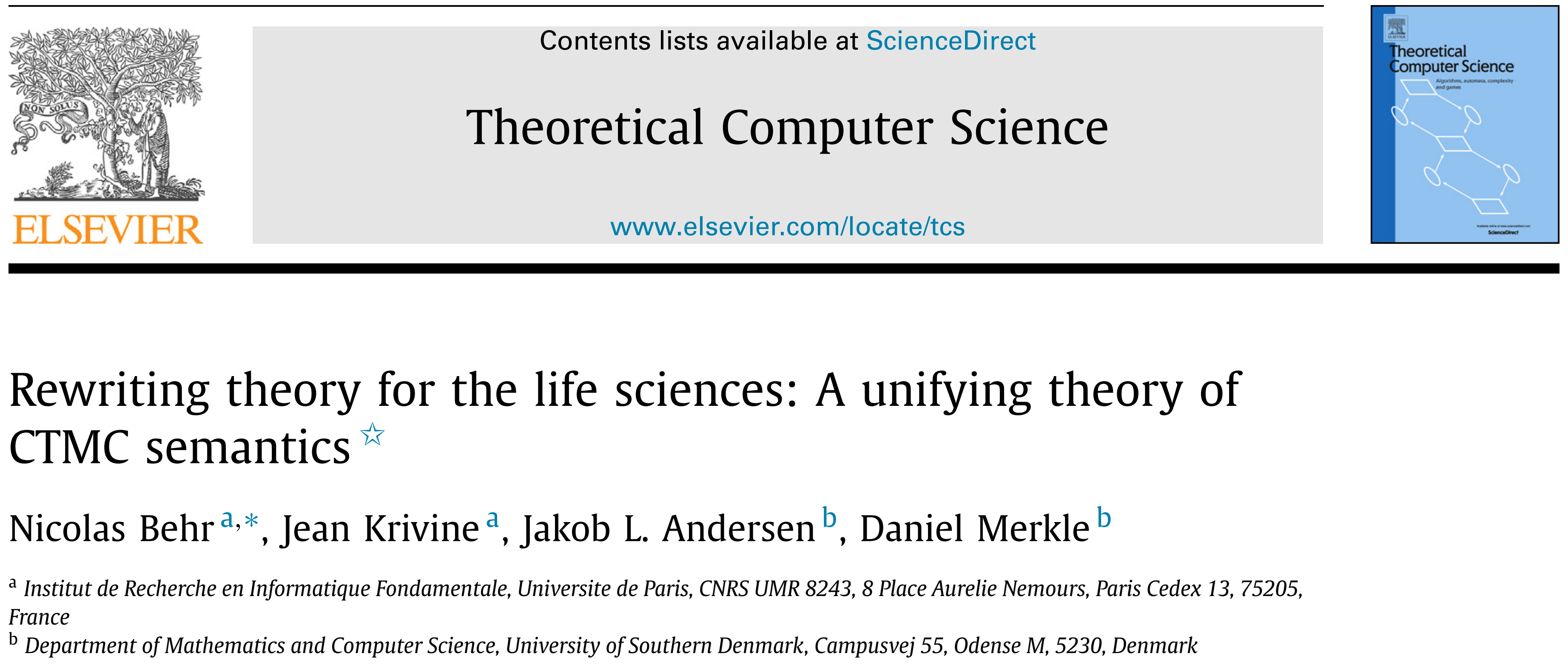
Application to the case of the reaction $2X \xleftharpoonup{\alpha} X$ $\quad (\alpha \in \mathbb{R}_{>0})$

$$\alpha\left(\rho(\delta(\bullet\,\bullet \leftharpoonup \bullet)) - \rho(\delta(\bullet \leftharpoonup \bullet))\right) \quad \leftrightarrow \quad \alpha\left(\hat{x}^2\partial_x - \hat{x}\partial_x\right)$$

$\Rightarrow$ Delbrück's evolution operator **explained via rewriting theory!**

set of **rules** and **input state** (distribution)

continuous-time Markov chains



Contents lists available at ScienceDirect

Theoretical Computer Science

www.elsevier.com/locate/tcs

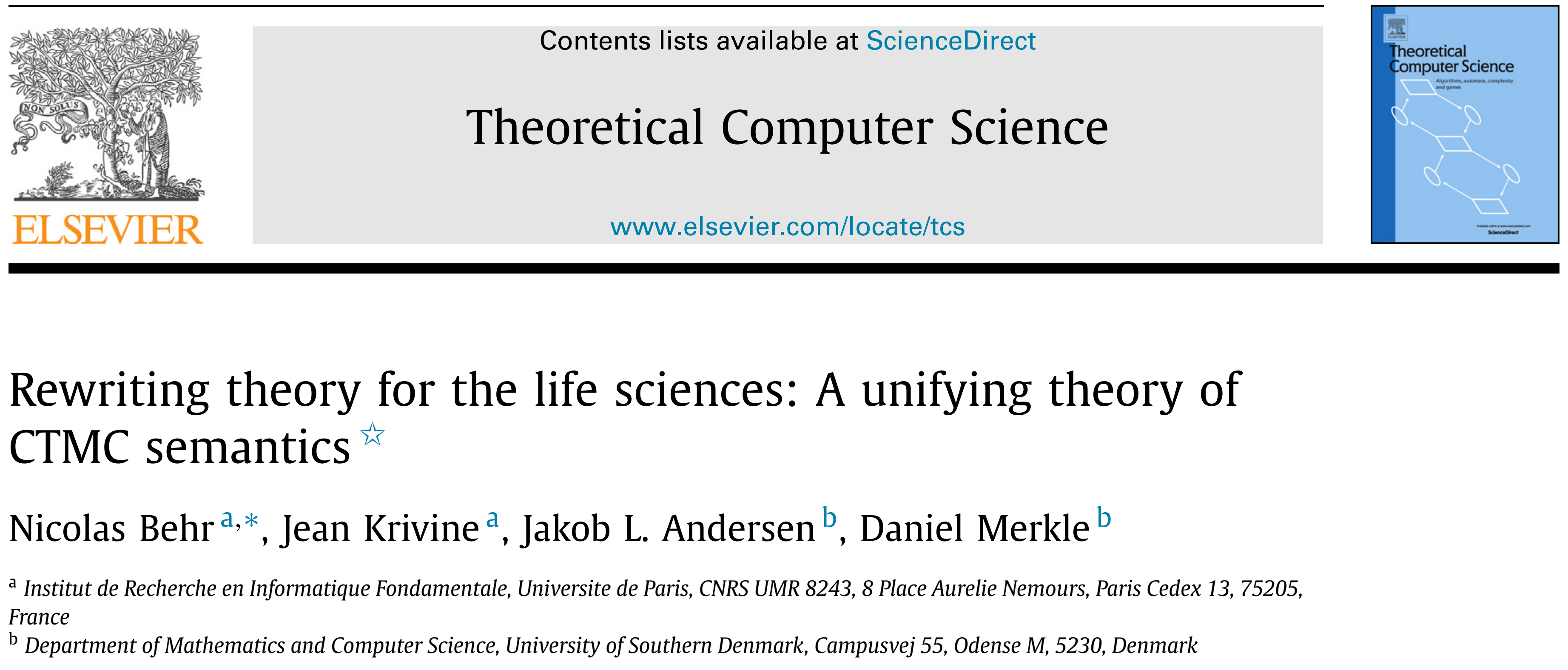
Rewriting theory for the life sciences: A unifying theory of CTMC semantics ☆

Nicolas Behr [a,*], Jean Krivine [a], Jakob L. Andersen [b], Daniel Merkle [b]

[a] *Institut de Recherche en Informatique Fondamentale, Universite de Paris, CNRS UMR 8243, 8 Place Aurelie Nemours, Paris Cedex 13, 75205, France*
[b] *Department of Mathematics and Computer Science, University of Southern Denmark, Campusvej 55, Odense M, 5230, Denmark*

set of **rules** and **input state** (distribution)

continuous-time Markov chains


Contents lists available at ScienceDirect

Theoretical Computer Science

www.elsevier.com/locate/tcs

Rewriting theory for the life sciences: A unifying theory of CTMC semantics ☆

Nicolas Behr[a,*], Jean Krivine[a], Jakob L. Andersen[b], Daniel Merkle[b]

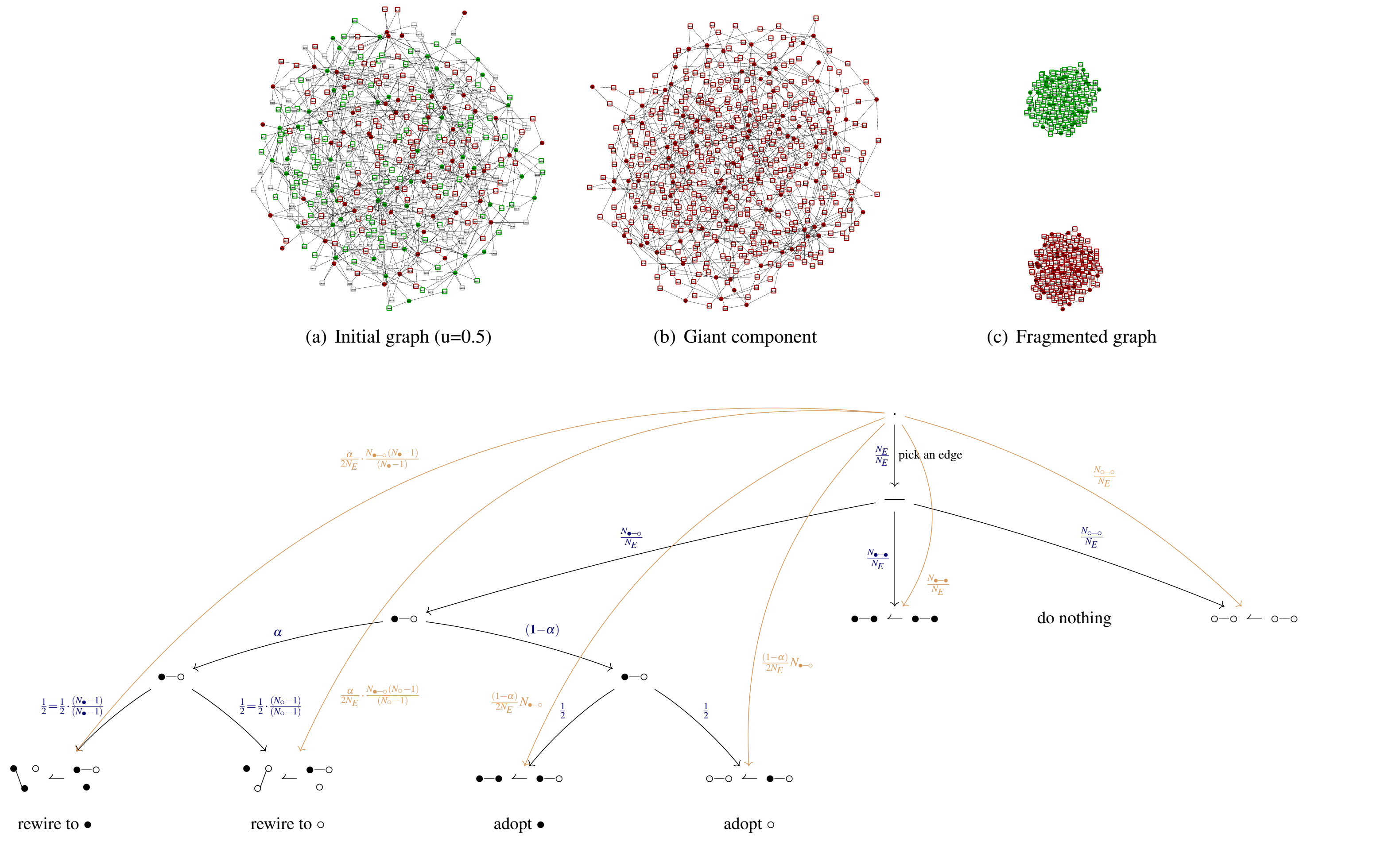
[a] Institut de Recherche en Informatique Fondamentale, Universite de Paris, CNRS UMR 8243, 8 Place Aurelie Nemours, Paris Cedex 13, 75205, France

[b] Department of Mathematics and Computer Science, University of Southern Denmark, Campusvej 55, Odense M, 5230, Denmark

set of **rules** and **input state** (distribution)

discrete-time Markov chains

Stochastic Graph Rewriting For Social Network Modeling



continuous-time Markov chains

Contents lists available at ScienceDirect

Theoretical Computer Science

www.elsevier.com/locate/tcs

Rewriting theory for the life sciences: A unifying theory of CTMC semantics ☆

Nicolas Behr [a,*], Jean Krivine [a], Jakob L. Andersen [b], Daniel Merkle [b]

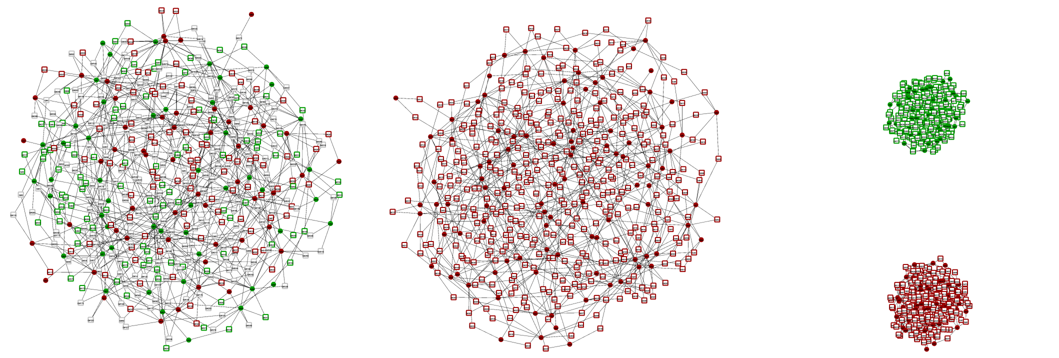
[a] Institut de Recherche en Informatique Fondamentale, Universite de Paris, CNRS UMR 8243, 8 Place Aurelie Nemours, Paris Cedex 13, 75205, France

[b] Department of Mathematics and Computer Science, University of Southern Denmark, Campusvej 55, Odense M, 5230, Denmark

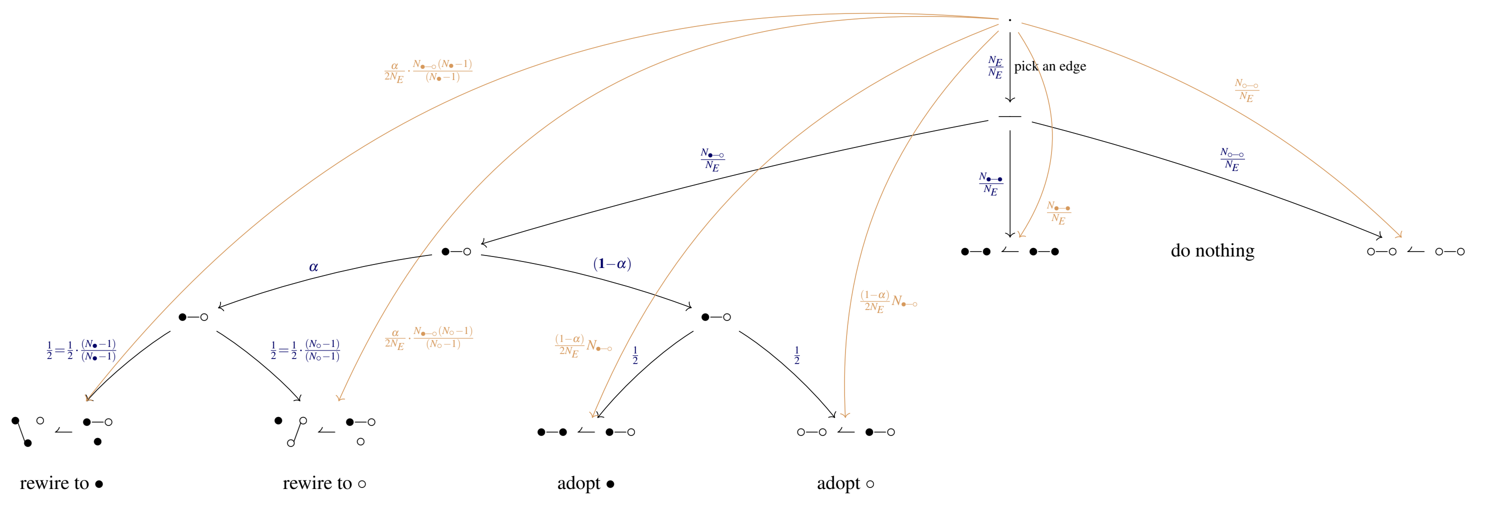
set of **rules** and **input state** (distribution)

discrete-time Markov chains

Stochastic Graph Rewriting For Social Network Modeling



(a) Initial graph (u=0.5) (b) Giant component (c) Fragmented graph



combinatorics

On Stochastic Rewriting and Combinatorics via Rule-Algebraic Methods*

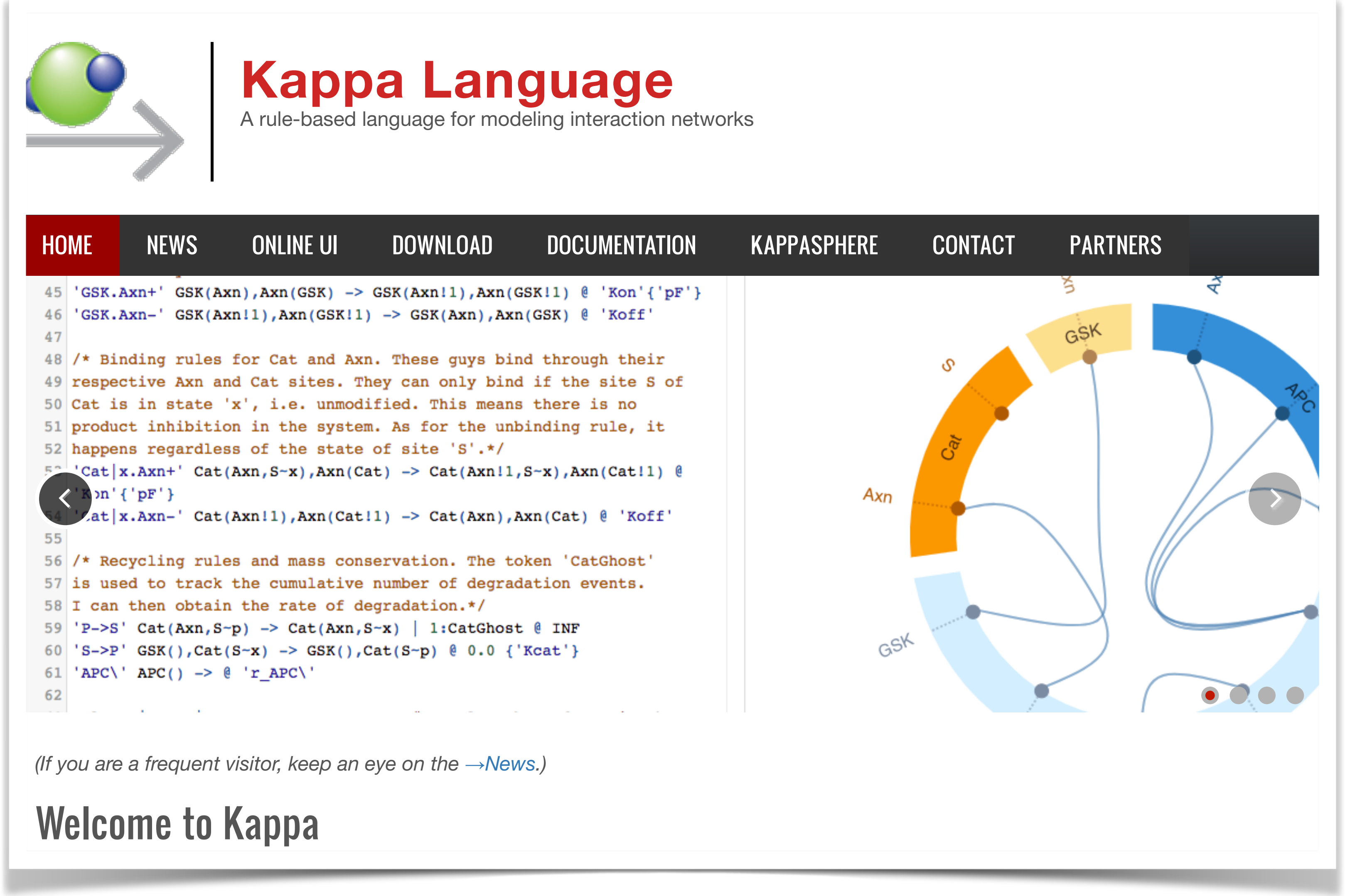
Nicolas Behr

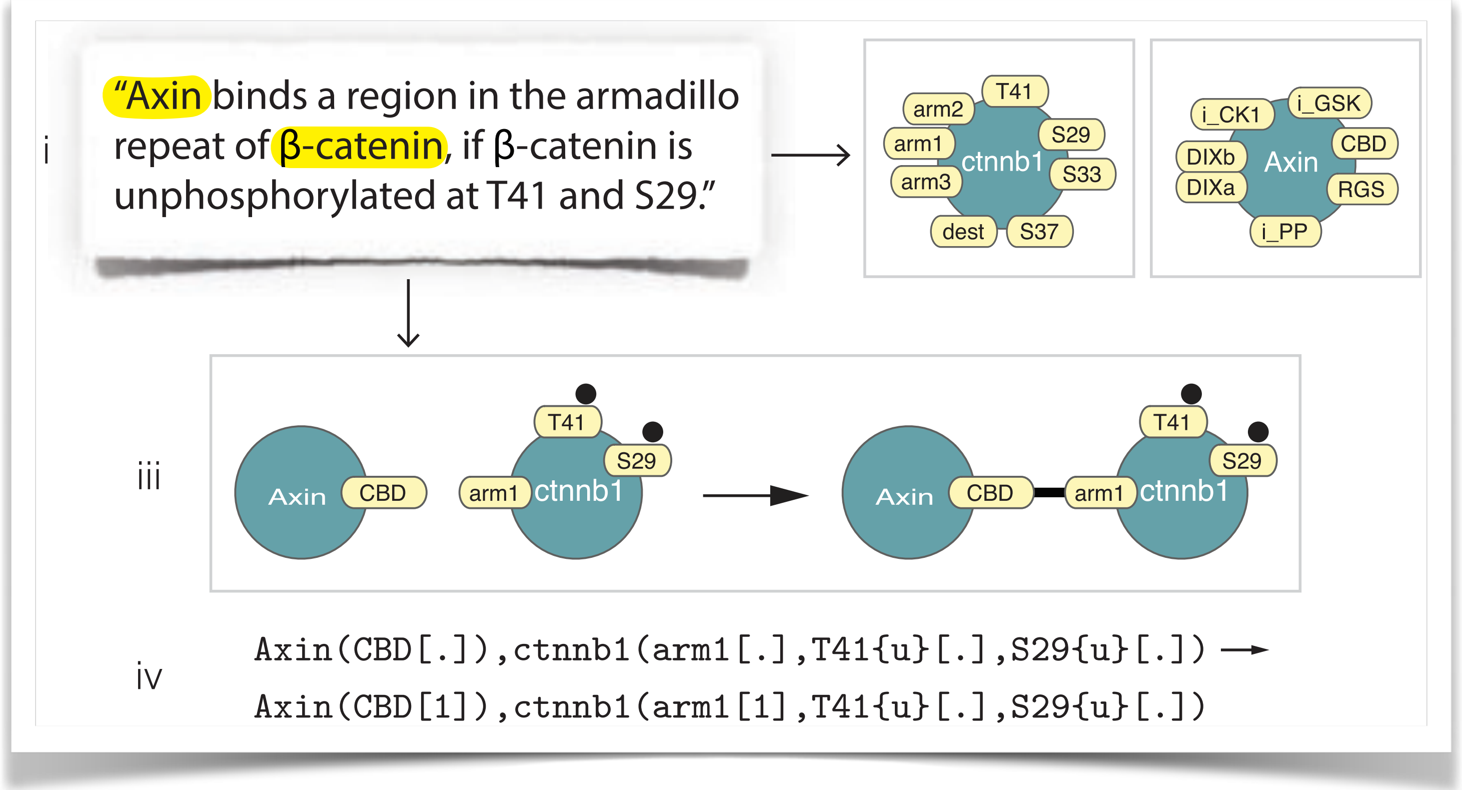
Université de Paris, CNRS, IRIF
F-75006, Paris, France

nicolas.behr@irif.fr

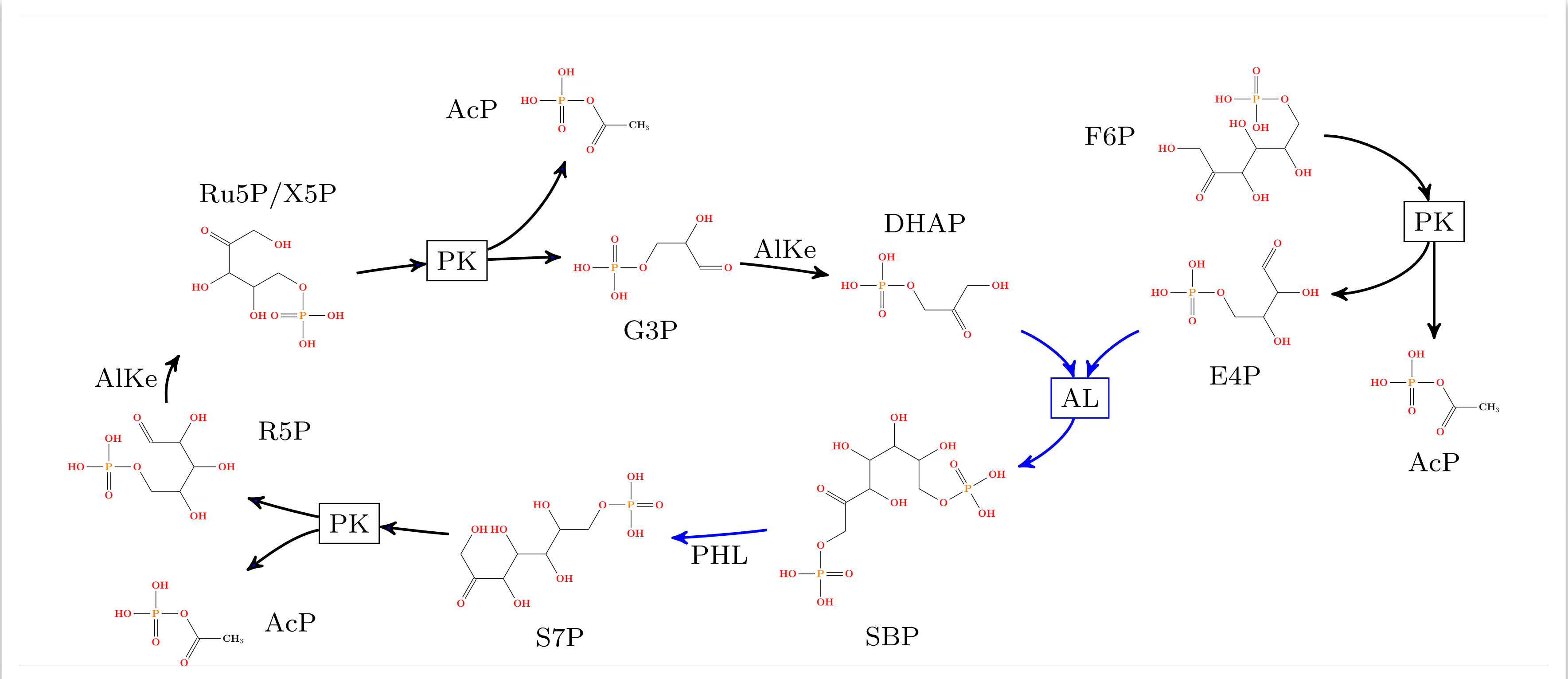
Rewriting in the life sciences: **bio-** and **chemo-informatics**

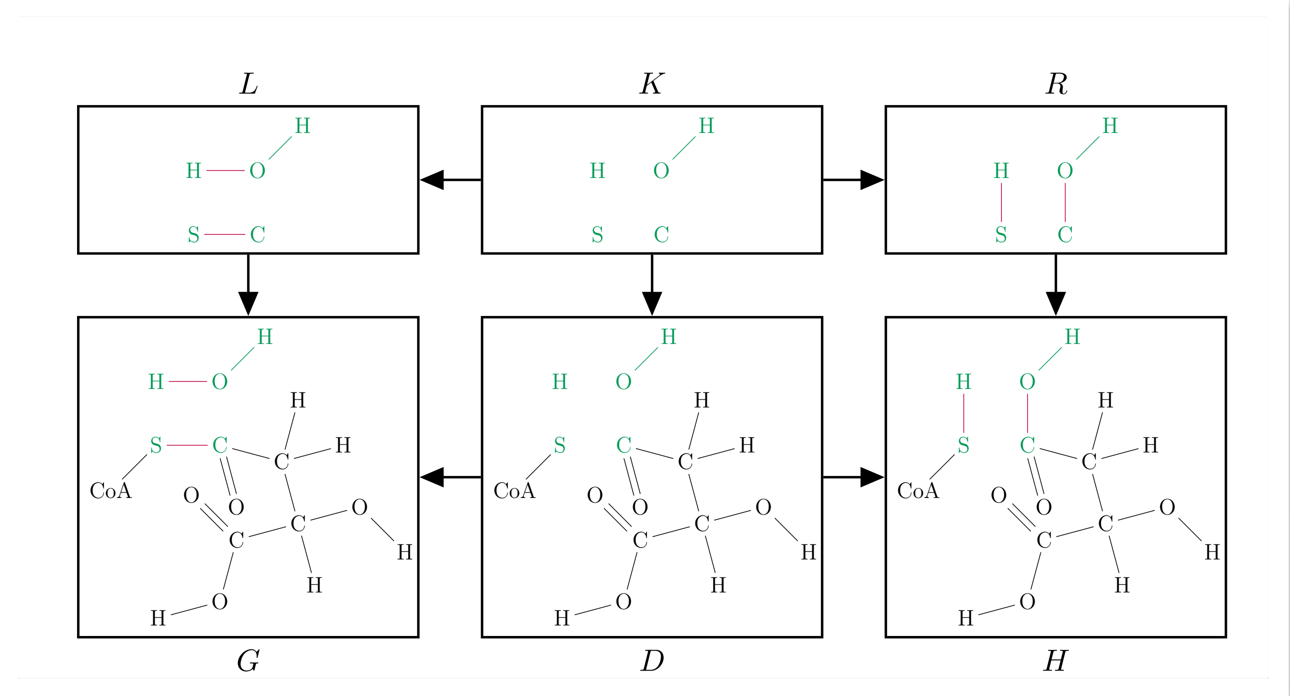
KAPPA





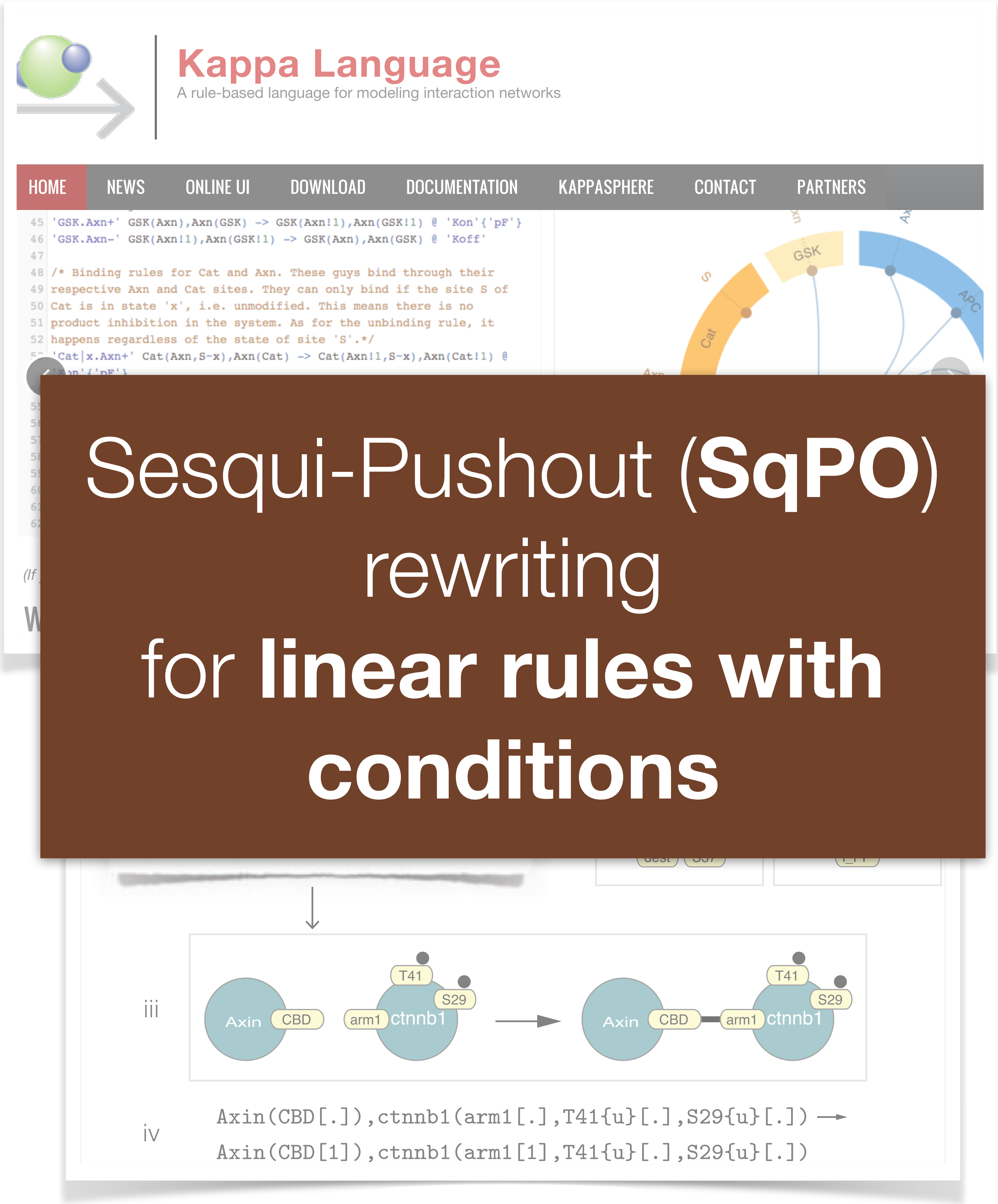
MØD





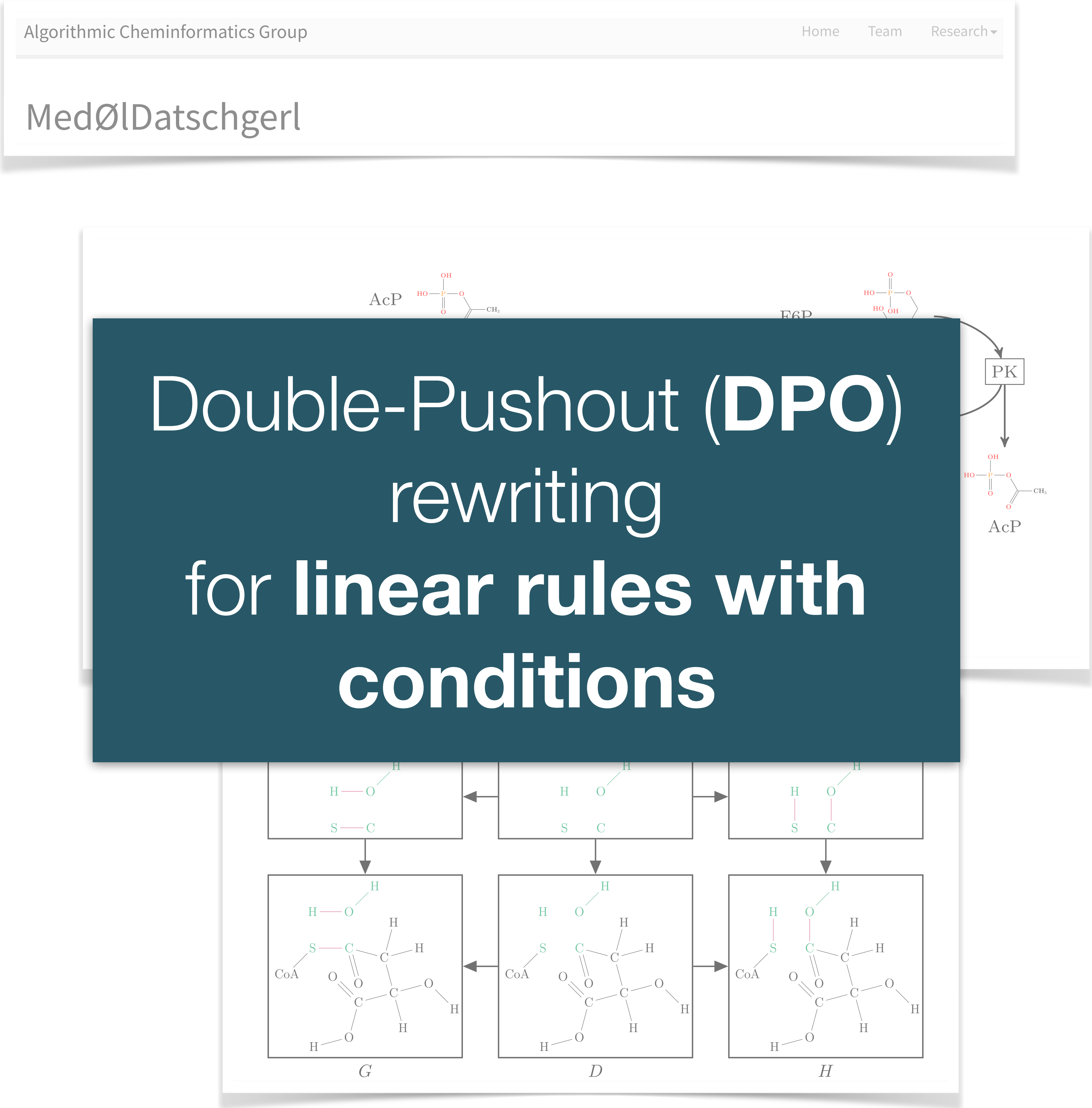
Rewriting in the life sciences: **bio-** and **chemo-informatics**

KAPPA



Sesqui-Pushout (**SqPO**) rewriting for **linear rules with conditions**

MØD



Double-Pushout (**DPO**) rewriting for **linear rules with conditions**

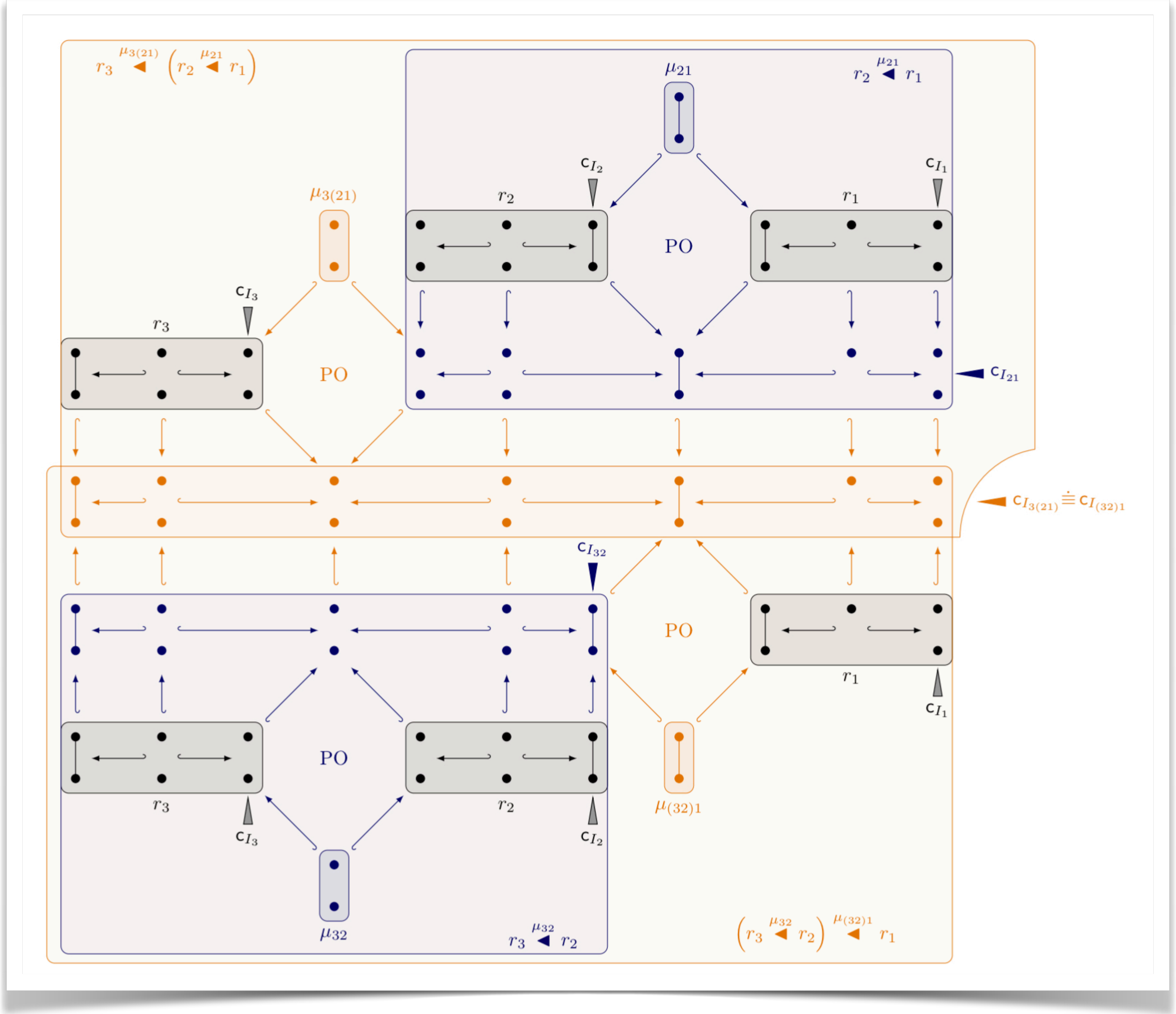
The foundation: **"compositional" rewriting theory for linear rules with conditions** (**DPO & SqPO**)

Compositionality of Rewriting Rules with Conditions

Nicolas Behr and Jean Krivine

IRIF, Université Paris-Diderot (Paris 07), F-75013 Paris, France

We extend the notion of compositional associative rewriting as recently studied in the rule algebra framework literature to the setting of rewriting rules with conditions. Our methodology is category-theoretical in nature, where the definition of rule composition operations is encoding the non-deterministic sequential concurrent application of rules in Double-Pushout (DPO) and Sesqui-Pushout (SqPO) rewriting with application conditions based upon $\mathcal{M}$-adhesive categories. We uncover an intricate interplay between the category-theoretical concepts of conditions on rules and morphisms, the compositionality and compatibility of certain shift and transport constructions for conditions, and thirdly the property of associativity of the composition of rules.



PAPERS ABOUT EDITORIAL POLICIES FOR AUTHORS FOR REVIEWERS

COMPOSITIONALITY

THE OPEN-ACCESS JOURNAL FOR THE MATHEMATICS OF COMPOSITION

Logical Methods in Computer Science
Volume 16, Issue 3, 2020, pp. 3:1–3:45
https://lmcs.episciences.org/

Submitted May 03, 2019
Published Jul. 10, 2020

COMBINATORIAL CONVERSION AND MOMENT BISIMULATION FOR STOCHASTIC REWRITING SYSTEMS

NICOLAS BEHR [a], VINCENT DANOS [b], AND ILIAS GARNIER [b]

[a] IRIF, Université Paris-Diderot, F-75205 Paris Cedex 13, France
e-mail address, Corresponding author: nicolas.behr@irif.fr

[b] Département d'Informatique de l'ENS, ENS, CNRS, PSL University Paris, France
e-mail address: {vincent.danos,ilias.garnier}@di.ens.fr

Abstract. We develop a novel method to analyze the dynamics of stochastic rewriting systems evolving over finitary adhesive, extensive categories. Our formalism is based on the so-called rule algebra framework [4, 7] and exhibits an intimate relationship between the combinatorics of the rewriting rules (as encoded in the rule algebra) and the dynamics which these rules generate on observables (as encoded in the stochastic mechanics formalism). We introduce the concept of combinatorial conversion, whereby under certain technical conditions the evolution equation for (the exponential generating function of) the statistical moments of observables can be expressed as the action of certain differential operators on formal power series. This permits us to formulate the novel concept of moment-bisimulation, whereby two dynamical systems are compared in terms of their evolution of sets of observables that are in bijection. In particular, we exhibit non-trivial examples of graphical rewriting systems that are moment-bisimilar to certain discrete rewriting systems (such as branching processes or the larger class of stochastic chemical reaction systems). Our results point towards applications of a vast number of existing well-established exact and approximate analysis techniques developed for chemical reaction systems to the far richer class of general stochastic rewriting systems.

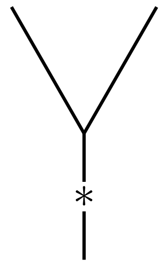
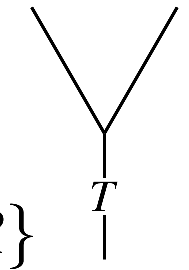
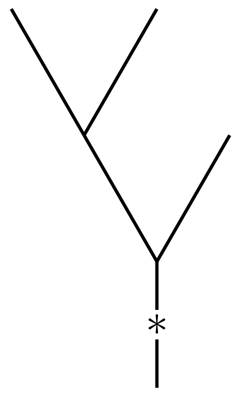
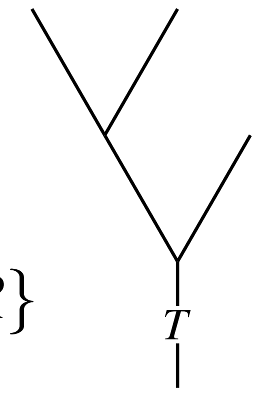
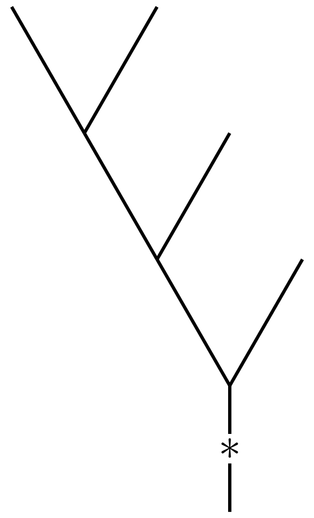
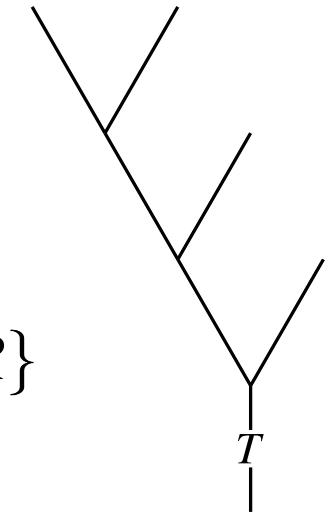
On Stochastic Rewriting and Combinatorics via Rule-Algebraic Methods*

Nicolas Behr
Université de Paris, CNRS, IRIF
F-75006, Paris, France
nicolas.behr@irif.fr

Building upon the rule-algebraic stochastic mechanics framework, we present new results on the relationship of stochastic rewriting systems described in terms of continuous-time Markov chains, their embedded discrete-time Markov chains and certain types of generating function expressions in combinatorics. We introduce a number of generating function techniques that permit a novel form of static analysis for rewriting systems based upon marginalizing distributions over the states of the rewriting systems via pattern-counting observables.

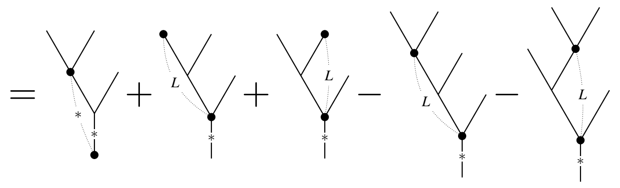
TERMGRAPH 2020

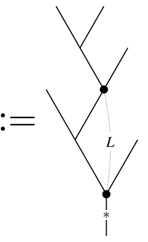
Pattern count distributions for planar rooted binary trees

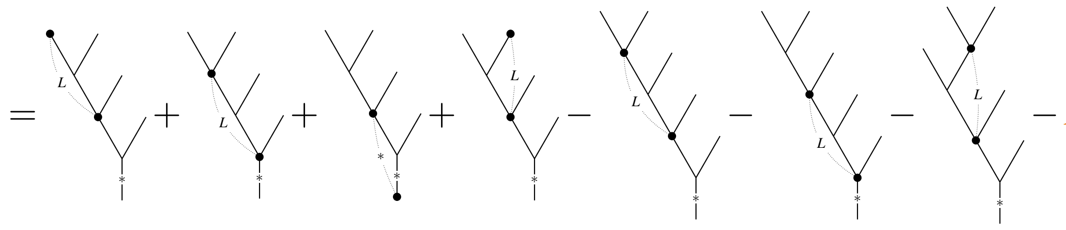
$\hat{O}_{P1} :=$  $\equiv \sum_{T\in\{I,L,R\}}$  , $\hat{O}_{P2} :=$  $\equiv \sum_{T\in\{I,L,R\}}$  , $\hat{O}_{P3} :=$  $\equiv \sum_{T\in\{I,L,R\}}$ 

$$\mathscr{G}(\lambda;\underline{\omega}) := \langle| e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle\,, \quad \underline{\omega}\cdot\underline{\hat{O}} := \varepsilon\hat{O}_E + \gamma\hat{O}_{P1} + \mu\hat{O}_{P2} + \nu\hat{O}_{P3}$$

$$\begin{aligned}
\tfrac{\partial}{\partial\lambda}\mathscr{G}(\lambda;\underline{\omega}) &= \langle| \left(e^{ad_{\underline{\omega}\cdot\underline{\hat{O}}}}(\hat{G})\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \overset{(*)}{=} \langle| \left(e^{ad_{\nu\hat{O}_{P3}}}\left(e^{ad_{\mu\hat{O}_{P2}}}\left(e^{ad_{\varepsilon\hat{O}_E+\gamma\hat{O}_{P1}}}(\hat{G})\right)\right)\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \left(e^{ad_{\nu\hat{O}_{P3}}}\left(e^{ad_{\mu\hat{O}_{P2}}}(\hat{G})\right)\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \left(e^{ad_{\nu\hat{O}_{P3}}}\left(\hat{G} + (e^{\mu}-1)[\hat{O}_{P2},\hat{G}]\right)\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \big(\hat{G} + (e^{\mu}-1)[\hat{O}_{P2},\hat{G}] \\
&\qquad + e^{\mu}(e^{\nu}-1)[\hat{O}_{P3},\hat{G}] + (e^{\nu}-1)(e^{\mu}-e^{-\nu})\hat{R}_{P3'}\big) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \big(2\hat{O}_E + 3(e^{\mu}-1)\hat{O}_{P1} + (4e^{\mu+\nu} - 6e^{\mu} + 2)\hat{O}_{P2} \\
&\qquad + (3e^{\mu} + e^{-\nu} - 3e^{\mu+\nu} - 1)\hat{O}_{P3}\big) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \big(2\tfrac{\partial}{\partial\varepsilon} + 3(e^{\mu}-1)\tfrac{\partial}{\partial\gamma} + (4e^{\mu+\nu} - 6e^{\mu} + 2)\tfrac{\partial}{\partial\mu} \\
&\qquad + (3e^{\mu} + e^{-\nu} - 3e^{\mu+\nu} - 1)\tfrac{\partial}{\partial\nu}\big) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle
\end{aligned}$$

$[\hat{O}_{P2},\hat{G}] =$ 

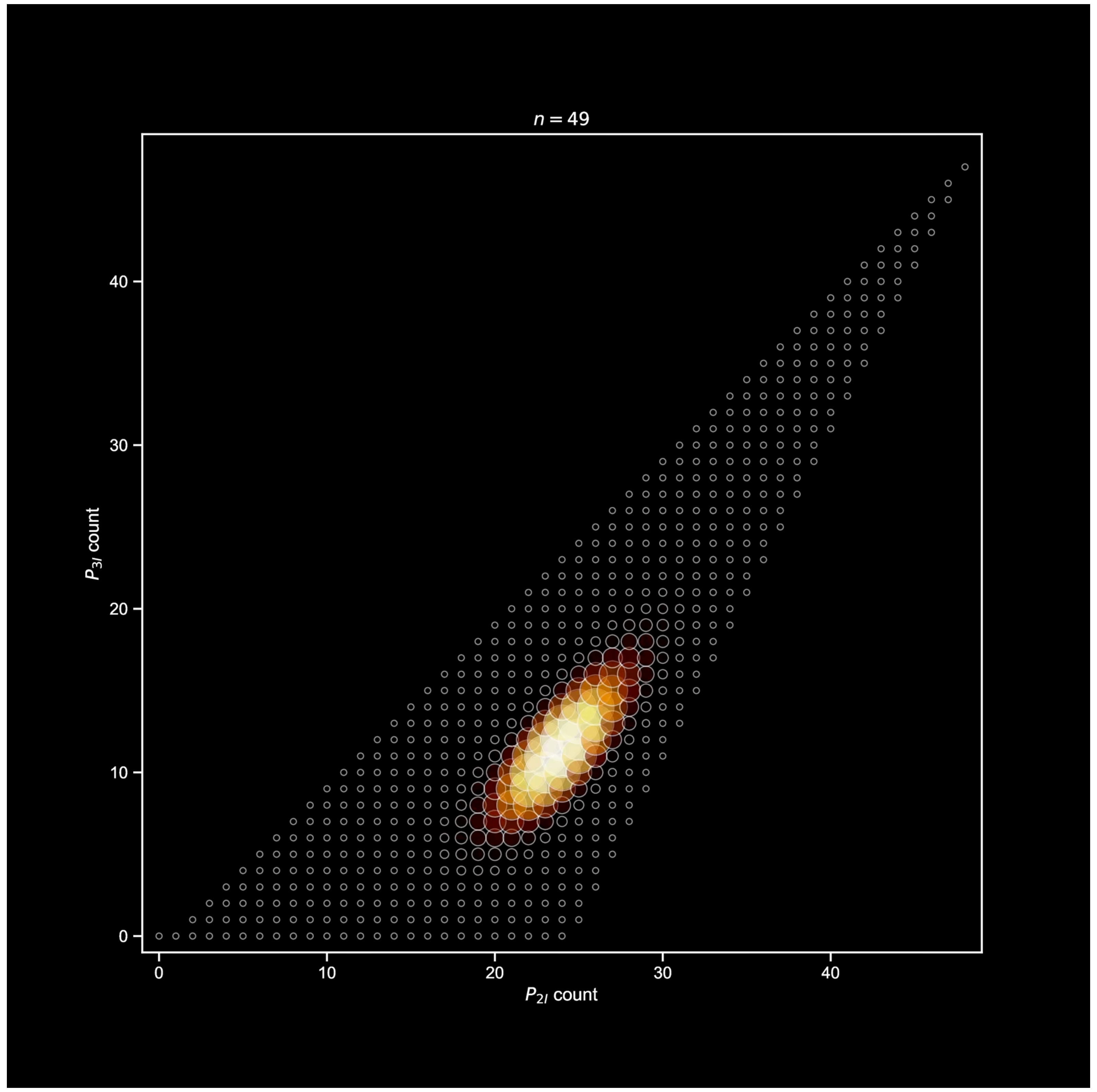
$\hat{R}_{P3'} :=$ 

$[\hat{O}_{P3},\hat{G}] =$  $- \hat{R}_{P3'}$

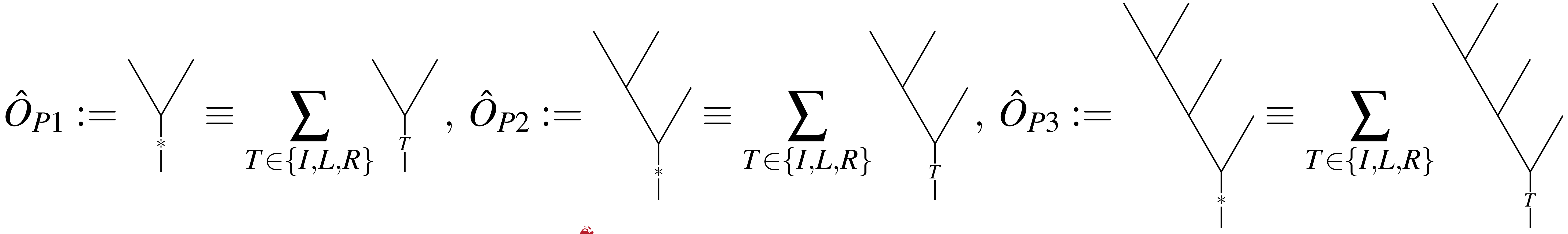
$$[\hat{O}_{P2},[\hat{O}_{P2},\hat{G}]] = [\hat{O}_{P2},\hat{G}]\,, \quad [\hat{O}_{P2},[\hat{O}_{P3},\hat{G}]] = [\hat{O}_{P3},\hat{G}] + \hat{R}_{P3}$$

$$[\hat{O}_{P3},[\hat{O}_{P3},\hat{G}]] = [\hat{O}_{P3},\hat{G}] + 2\hat{R}_{P3'}\,, \quad [\hat{O}_{P2},\hat{R}_{P3'}] = 0\,, \quad [\hat{O}_{P3},\hat{R}_{P3'}] = -\hat{R}_{P3'}$$

$$\langle|\,[\hat{O}_{P2},\hat{G}] = \langle|\,(3\hat{O}_{P1} - 2\hat{O}_{P2})\,, \quad \langle|\,[\hat{O}_{P3},\hat{G}] = \langle|\,(4\hat{O}_{P2} - 3\hat{O}_{P3})\,, \quad \langle|\,\hat{R}_{P3'} = \langle|\,\hat{O}_{P3}$$

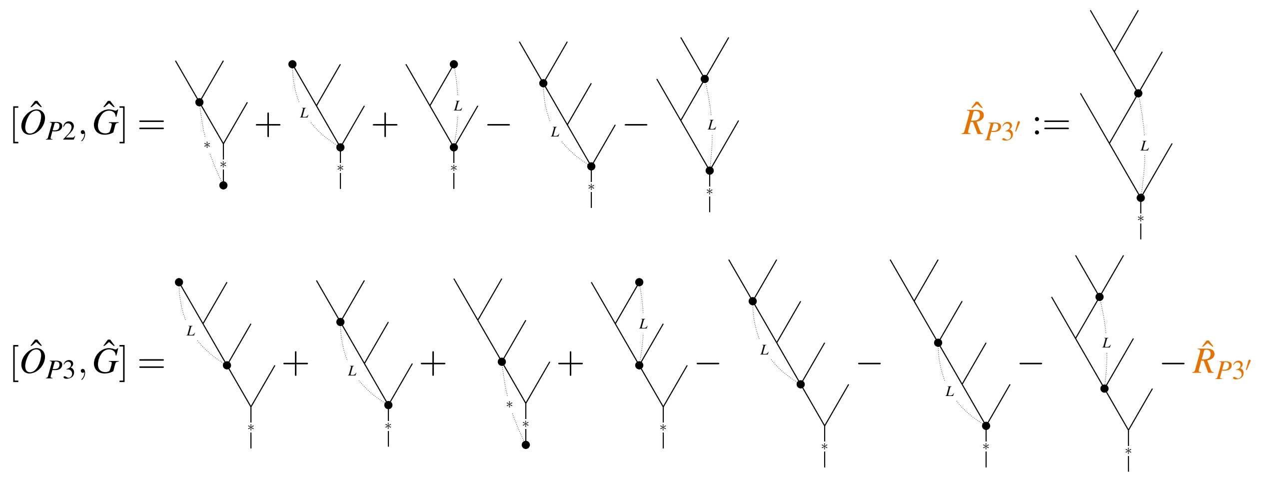


Pattern count distributions for **planar rooted binary trees**



$$\mathscr{G}(\lambda;\underline{\omega}) := \langle| e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle\,, \quad \underline{\omega}\cdot\underline{\hat{O}} := \varepsilon\hat{O}_E + \gamma\hat{O}_{P1} + \mu\hat{O}_{P2} + \nu\hat{O}_{P3}$$

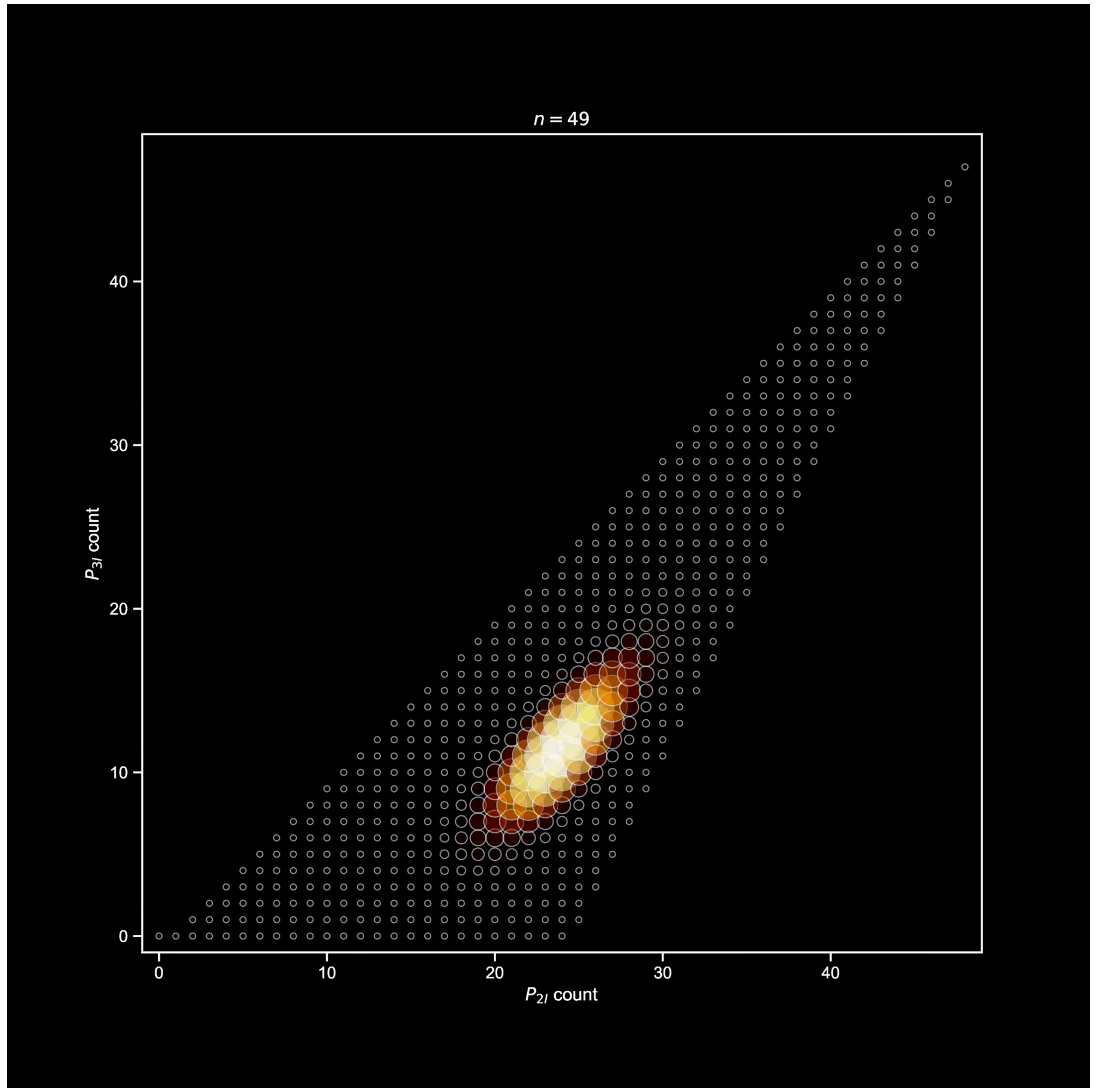
$$\begin{aligned}
\tfrac{\partial}{\partial\lambda}\mathscr{G}(\lambda;\underline{\omega}) &= \langle| \left(e^{ad_{\underline{\omega}\cdot\underline{\hat{O}}}}(\hat{G})\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \overset{(*)}{=} \langle| \left(e^{ad_{\nu\hat{O}_{P3}}}\left(e^{ad_{\mu\hat{O}_{P2}}}\left(e^{ad_{\varepsilon\hat{O}_E+\gamma\hat{O}_{P1}}}(\hat{G})\right)\right)\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \left(e^{ad_{\nu\hat{O}_{P3}}}\left(e^{ad_{\mu\hat{O}_{P2}}}(\hat{G})\right)\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \left(e^{ad_{\nu\hat{O}_{P3}}}\left(\hat{G} + (e^{\mu}-1)[\hat{O}_{P2},\hat{G}]\right)\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \big(\hat{G} + (e^{\mu}-1)[\hat{O}_{P2},\hat{G}] \\
&\qquad + e^{\mu}(e^{\nu}-1)[\hat{O}_{P3},\hat{G}] + (e^{\nu}-1)(e^{\mu}-e^{-\nu})\hat{R}_{P3'}\big) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \big(2\hat{O}_E + 3(e^{\mu}-1)\hat{O}_{P1} + (4e^{\mu+\nu} - 6e^{\mu} + 2)\hat{O}_{P2} \\
&\qquad + (3e^{\mu} + e^{-\nu} - 3e^{\mu+\nu} - 1)\hat{O}_{P3}\big) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle \\
&= e^{2\varepsilon+\gamma}\langle| \big(2\tfrac{\partial}{\partial\varepsilon} + 3(e^{\mu}-1)\tfrac{\partial}{\partial\gamma} + (4e^{\mu+\nu} - 6e^{\mu} + 2)\tfrac{\partial}{\partial\mu} \\
&\qquad + (3e^{\mu} + e^{-\nu} - 3e^{\mu+\nu} - 1)\tfrac{\partial}{\partial\nu}\big) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} ||\rangle
\end{aligned}$$



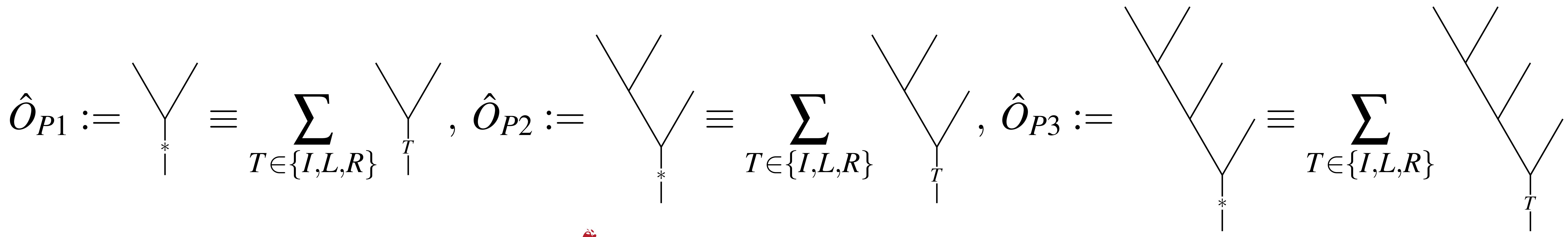
$$[\hat{O}_{P2},[\hat{O}_{P2},\hat{G}]] = [\hat{O}_{P2},\hat{G}]\,, \quad [\hat{O}_{P2},[\hat{O}_{P3},\hat{G}]] = [\hat{O}_{P3},\hat{G}] + \hat{R}_{P3}$$

$$[\hat{O}_{P3},[\hat{O}_{P3},\hat{G}]] = [\hat{O}_{P3},\hat{G}] + 2\hat{R}_{P3'}\,, \quad [\hat{O}_{P2},\hat{R}_{P3'}] = 0\,, \quad [\hat{O}_{P3},\hat{R}_{P3'}] = -\hat{R}_{P3'}$$

$$\langle|\,[\hat{O}_{P2},\hat{G}] = \langle|\,(3\hat{O}_{P1} - 2\hat{O}_{P2})\,, \quad \langle|\,[\hat{O}_{P3},\hat{G}] = \langle|\,(4\hat{O}_{P2} - 3\hat{O}_{P3})\,, \quad \langle|\,\hat{R}_{P3'} = \langle|\,\hat{O}_{P3}$$

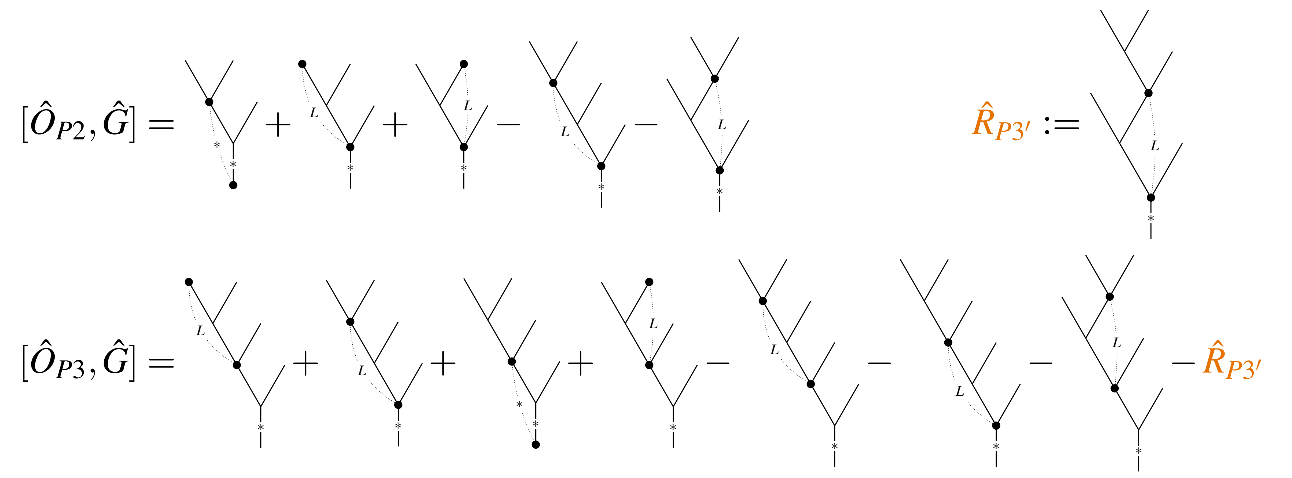


Pattern count distributions for planar rooted binary trees



$$\mathscr{G}(\lambda;\underline{\omega}) := \langle | e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} || \rangle\,, \quad \underline{\omega}\cdot\underline{\hat{O}} := \varepsilon\hat{O}_E + \gamma\hat{O}_{P1} + \mu\hat{O}_{P2} + \nu\hat{O}_{P3}$$

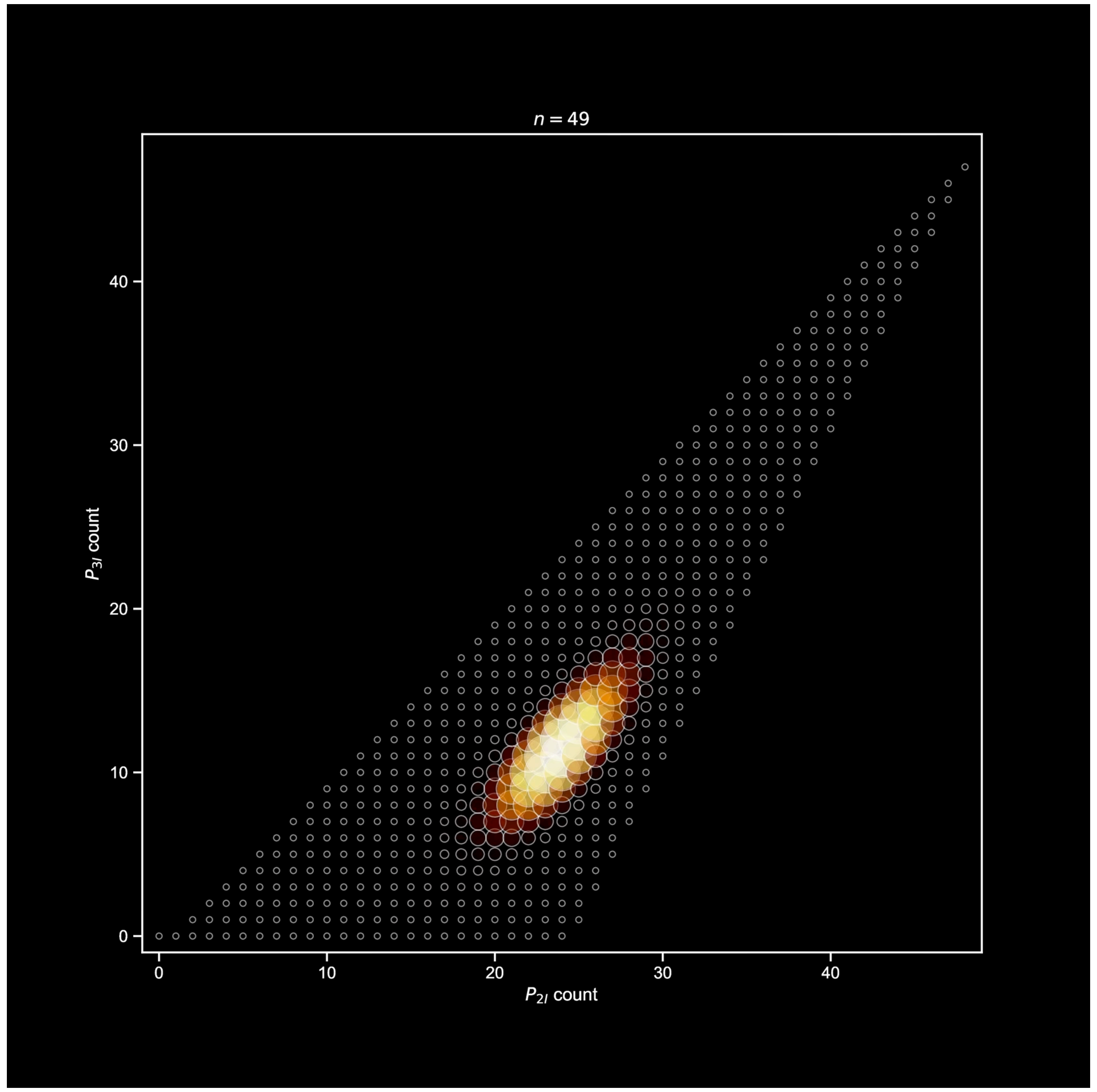
$$\begin{aligned}
\frac{\partial}{\partial\lambda}\mathscr{G}(\lambda;\underline{\omega}) &= \langle | \left(e^{ad_{\underline{\omega}\cdot\underline{\hat{O}}}}(\hat{G})\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} || \rangle \overset{(*)}{=} \langle | \left(e^{ad_{\nu\hat{O}_{P3}}}\left(e^{ad_{\mu\hat{O}_{P2}}}\left(e^{ad_{\varepsilon\hat{O}_E+\gamma\hat{O}_{P1}}}(\hat{G})\right)\right)\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} || \rangle \\
&= e^{2\varepsilon+\gamma} \langle | \left(e^{ad_{\nu\hat{O}_{P3}}}\left(e^{ad_{\mu\hat{O}_{P2}}}(\hat{G})\right)\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} || \rangle \\
&= e^{2\varepsilon+\gamma} \langle | \left(e^{ad_{\nu\hat{O}_{P3}}}\left(\hat{G} + (e^{\mu}-1)[\hat{O}_{P2},\hat{G}]\right)\right) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} || \rangle \\
&= e^{2\varepsilon+\gamma} \langle | \big(\hat{G} + (e^{\mu}-1)[\hat{O}_{P2},\hat{G}] \\
&\qquad + e^{\mu}(e^{\nu}-1)[\hat{O}_{P3},\hat{G}] + (e^{\nu}-1)(e^{\mu}-e^{-\nu})\hat{R}_{P3'}\big) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} || \rangle \\
&= e^{2\varepsilon+\gamma} \langle | \big(2\hat{O}_E + 3(e^{\mu}-1)\hat{O}_{P1} + (4e^{\mu+\nu} - 6e^{\mu} + 2)\hat{O}_{P2} \\
&\qquad + (3e^{\mu} + e^{-\nu} - 3e^{\mu+\nu} - 1)\hat{O}_{P3}\big) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} || \rangle \\
&= e^{2\varepsilon+\gamma} \langle | \big(2\tfrac{\partial}{\partial\varepsilon} + 3(e^{\mu}-1)\tfrac{\partial}{\partial\gamma} + (4e^{\mu+\nu} - 6e^{\mu} + 2)\tfrac{\partial}{\partial\mu} \\
&\qquad + (3e^{\mu} + e^{-\nu} - 3e^{\mu+\nu} - 1)\tfrac{\partial}{\partial\nu}\big) e^{\underline{\omega}\cdot\underline{\hat{O}}} e^{\lambda\hat{G}} || \rangle
\end{aligned}$$



$$[\hat{O}_{P2},[\hat{O}_{P2},\hat{G}]] = [\hat{O}_{P2},\hat{G}]\,, \quad [\hat{O}_{P2},[\hat{O}_{P3},\hat{G}]] = [\hat{O}_{P3},\hat{G}] + \hat{R}_{P3}$$

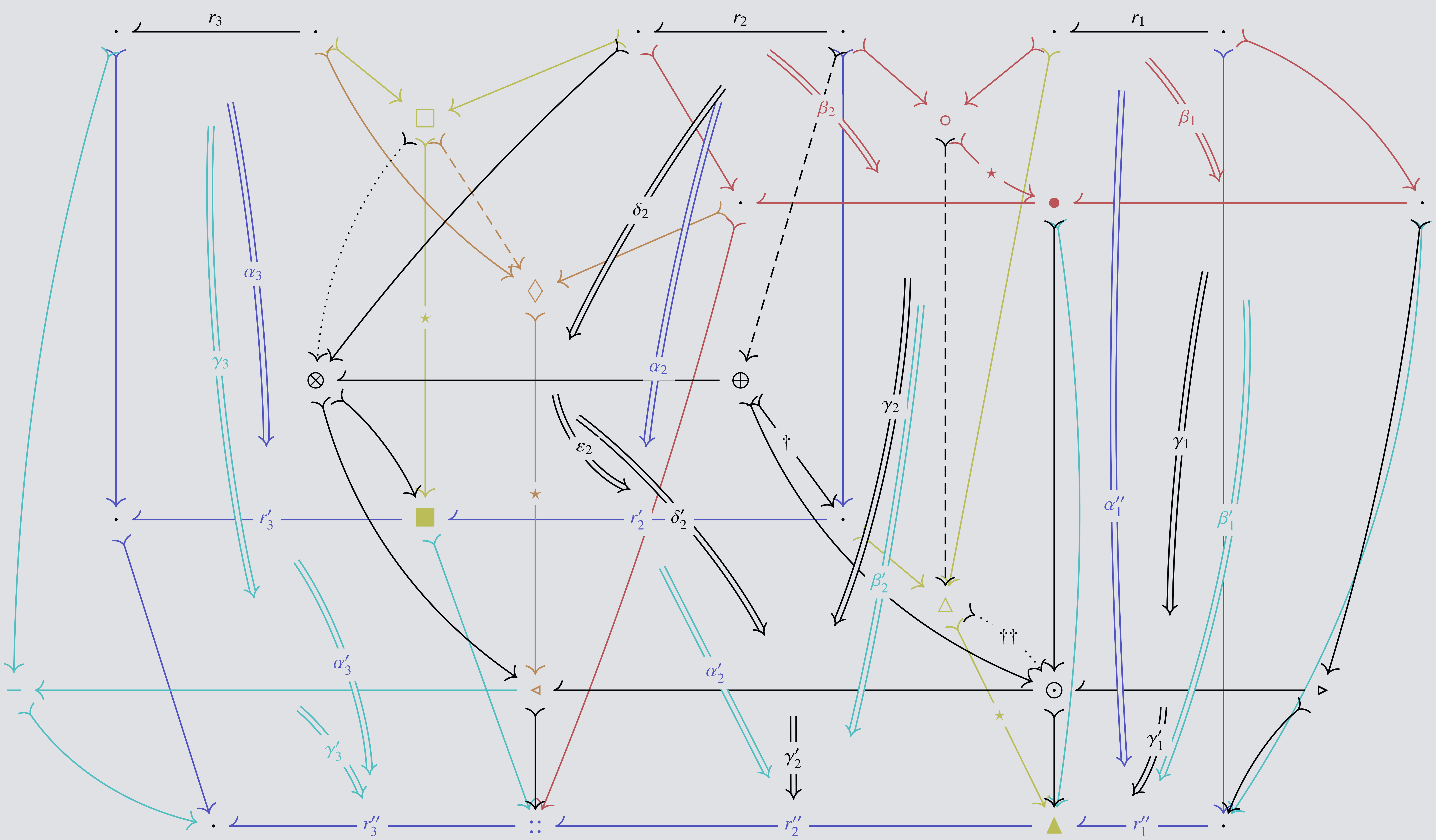
$$[\hat{O}_{P3},[\hat{O}_{P3},\hat{G}]] = [\hat{O}_{P3},\hat{G}] + 2\hat{R}_{P3'}\,, \quad [\hat{O}_{P2},\hat{R}_{P3'}] = 0\,, \quad [\hat{O}_{P3},\hat{R}_{P3'}] = -\hat{R}_{P3'}$$

$$\langle | [\hat{O}_{P2},\hat{G}] = \langle | (3\hat{O}_{P1} - 2\hat{O}_{P2})\,, \quad \langle | [\hat{O}_{P3},\hat{G}] = \langle | (4\hat{O}_{P2} - 3\hat{O}_{P3})\,, \quad \langle | \hat{R}_{P3'} = \langle | \hat{O}_{P3}$$



SOCS 2020

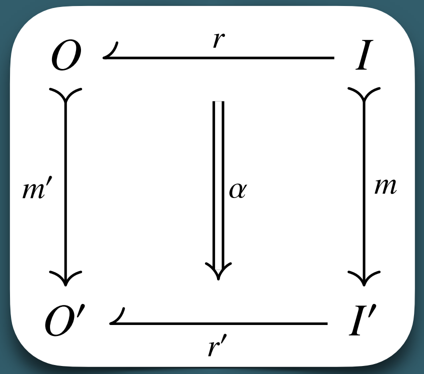
Invited talk @
"Species and operads in combinatorics and semantics"

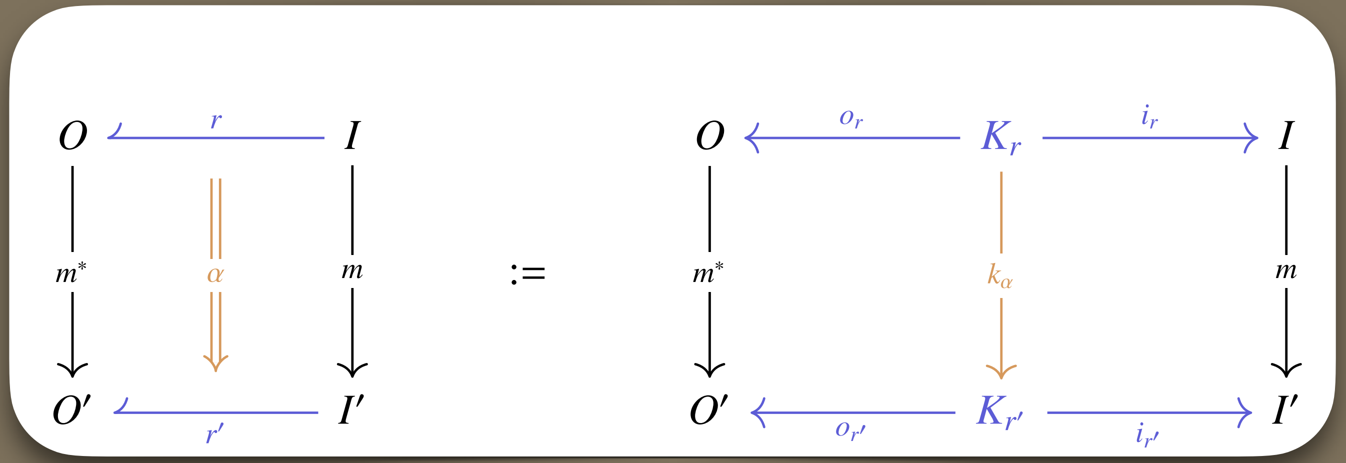


PART 2: FUNDAMENTALS OF COMPOSITIONAL REWRITING THEORY

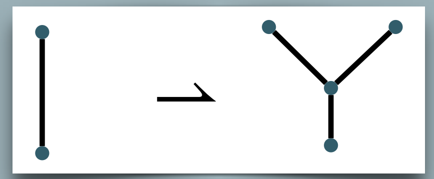
From fibrational and double-categorical concepts to applications

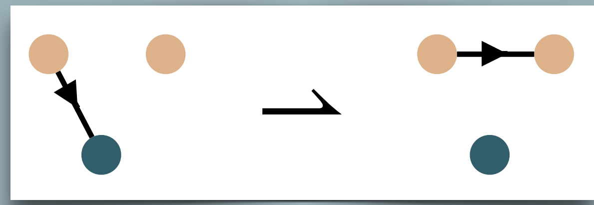
compositional rewriting double categories (crDCs)



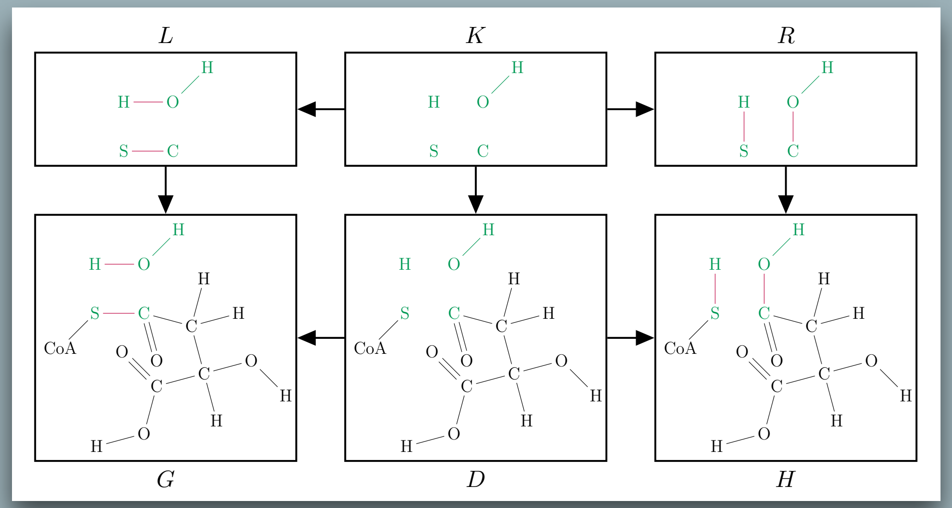


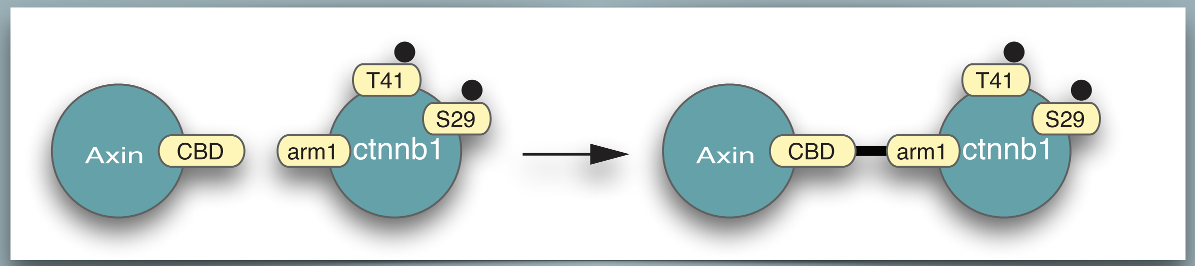
Explicit **rewriting semantics** (DPO, SqPO, …)





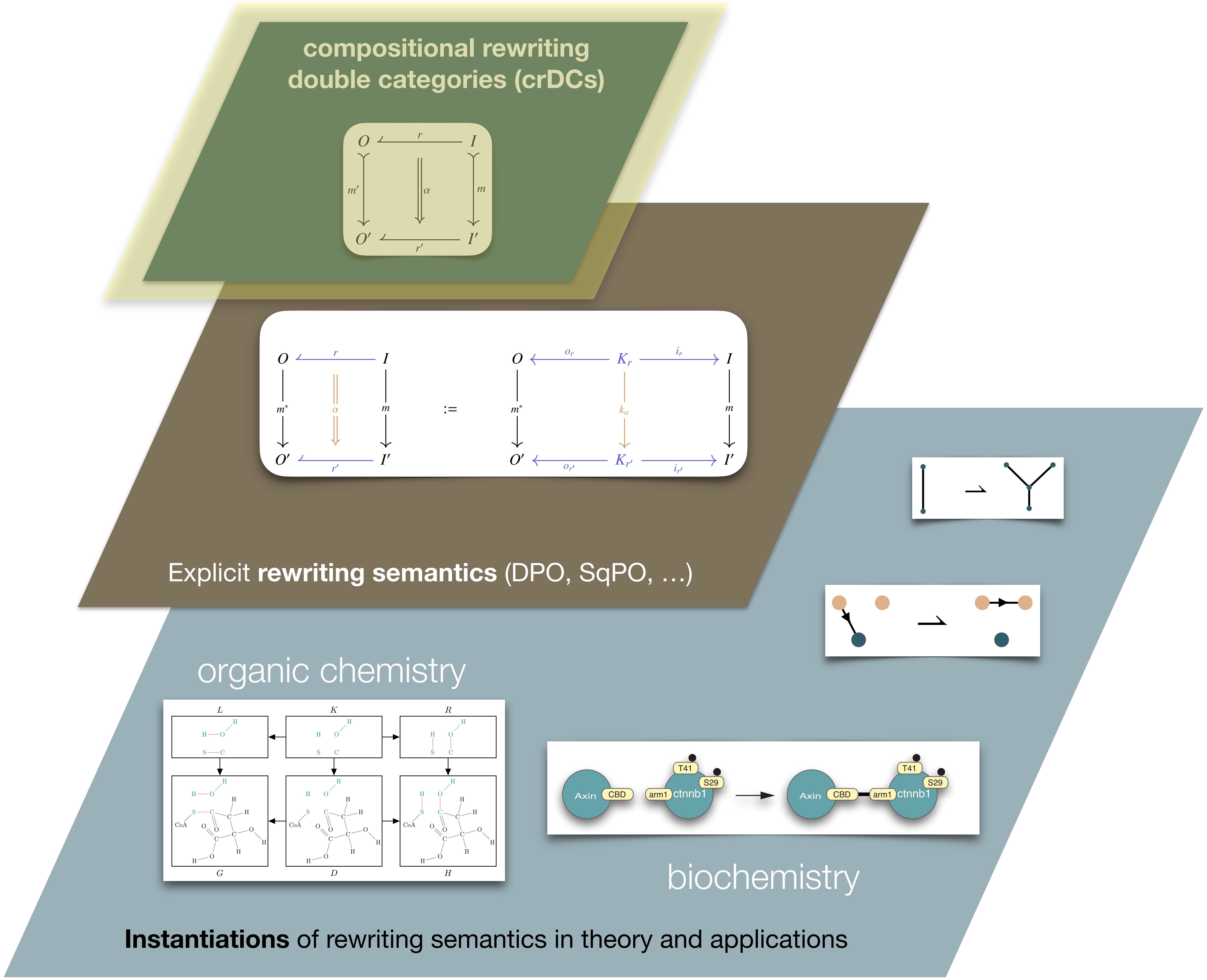
organic chemistry





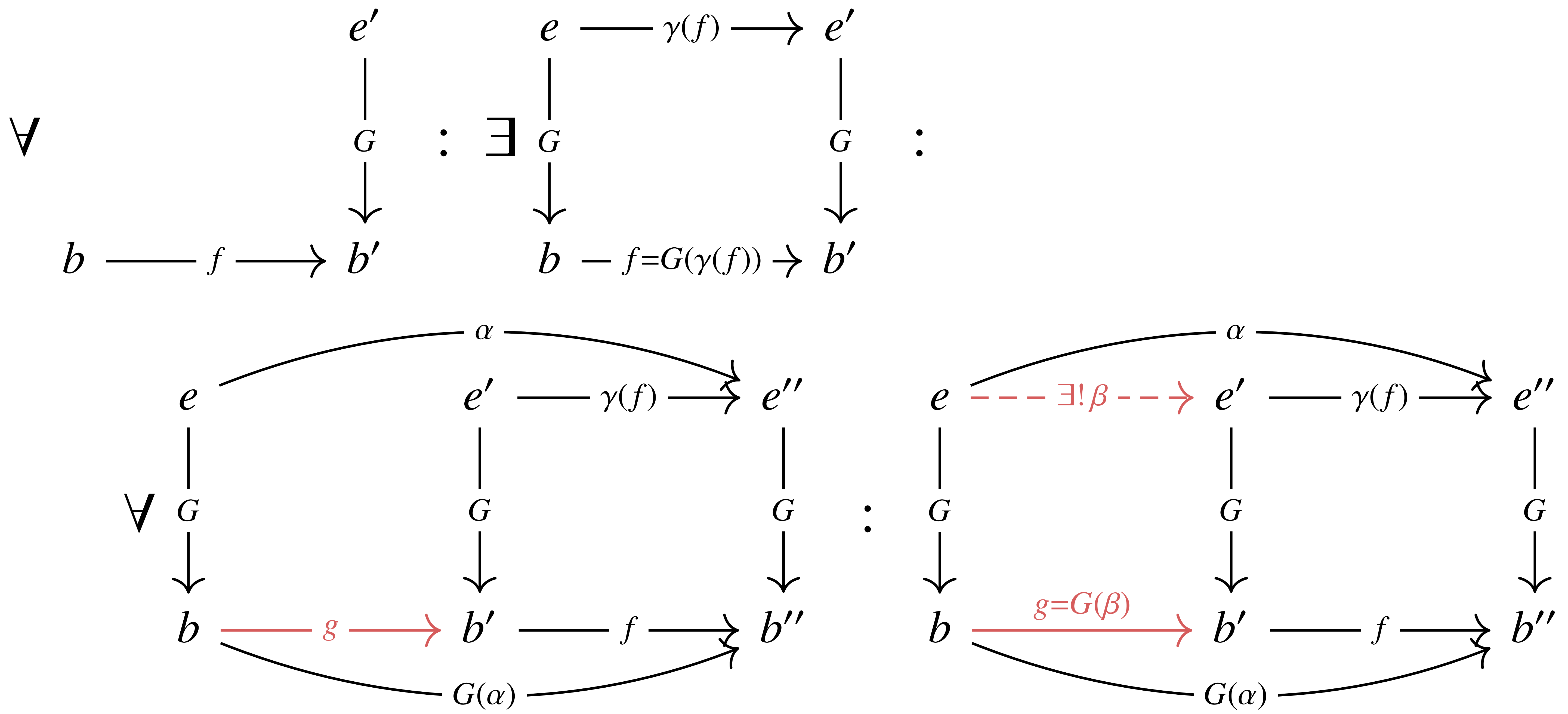
biochemistry

Instantiations of rewriting semantics in theory and applications


compositional rewriting
double categories (crDCs)
Explicit rewriting semantics (DPO, SqPO, ...)
organic chemistry
biochemistry
Axin
CBD
arm1
ctnnb1
T41
S29
Instantiations of rewriting semantics in theory and applications

Fibrational structures — traditional variants

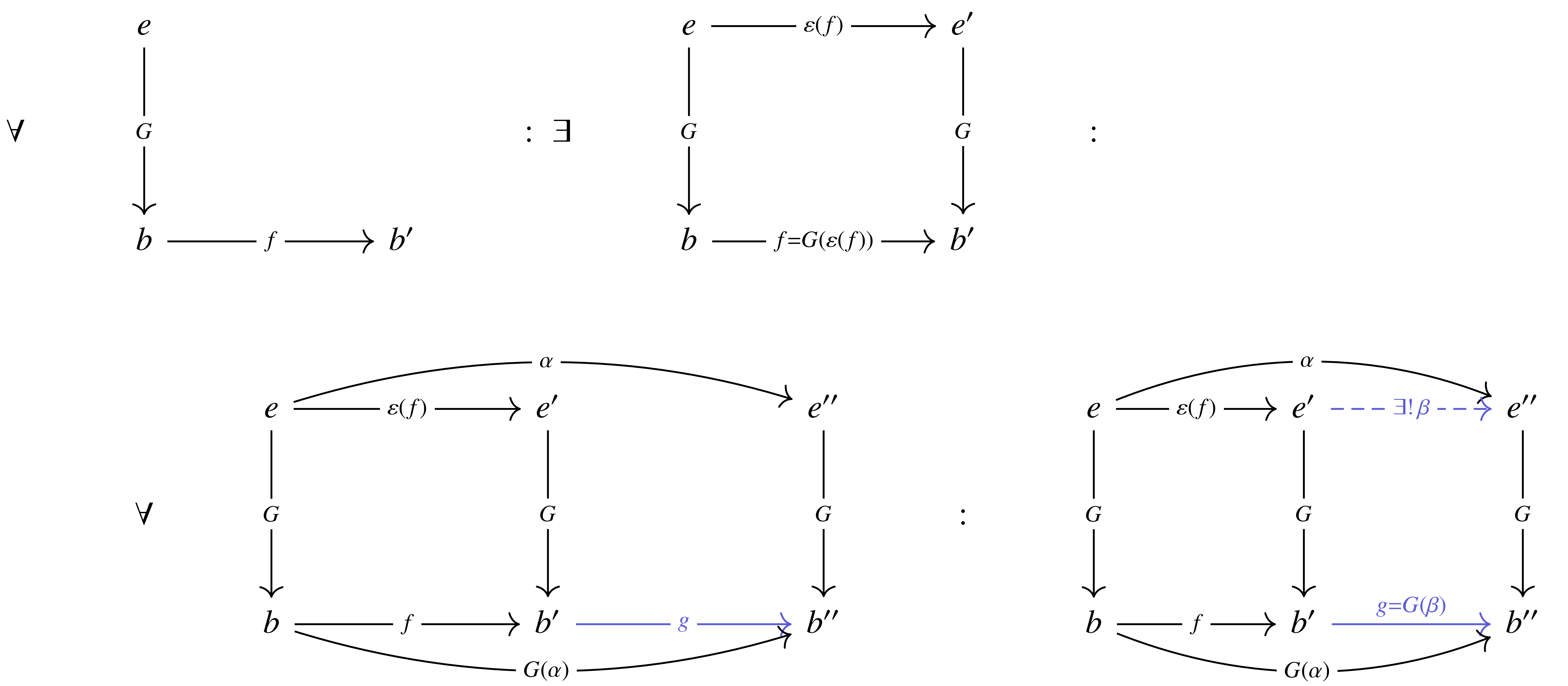
Definition 1. A functor $G : \mathbf{E} \to \mathbf{B}$ is a *Grothendieck fibration* if the following property holds:



(3)

Fibrational structures — traditional variants

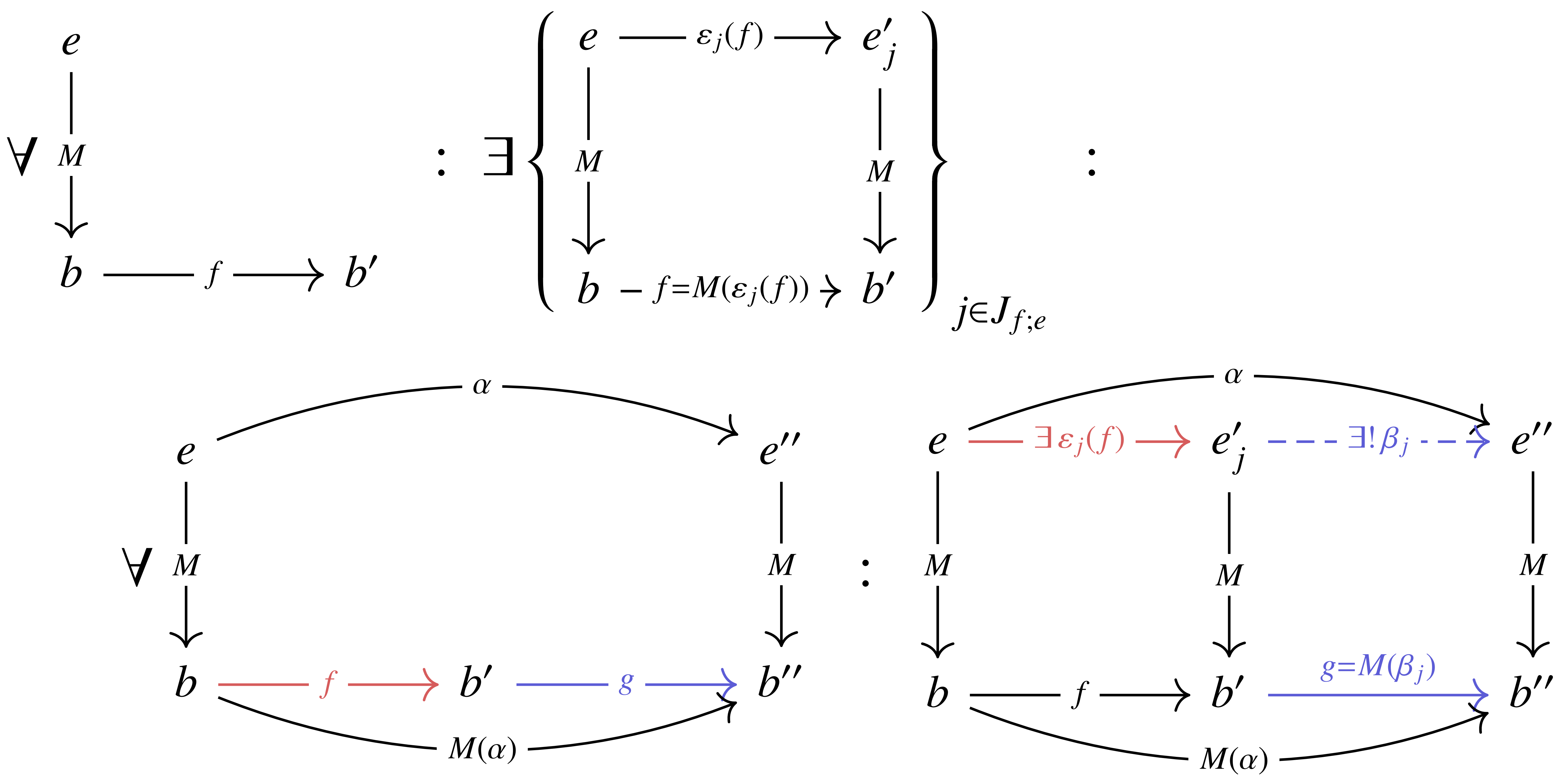
Definition 2. A functor $G : \mathbf{E} \to \mathbf{B}$ is a *Grothendieck opfibration* if the following property holds:



(4)

Fibrational structures — “multi” variants à la Diers

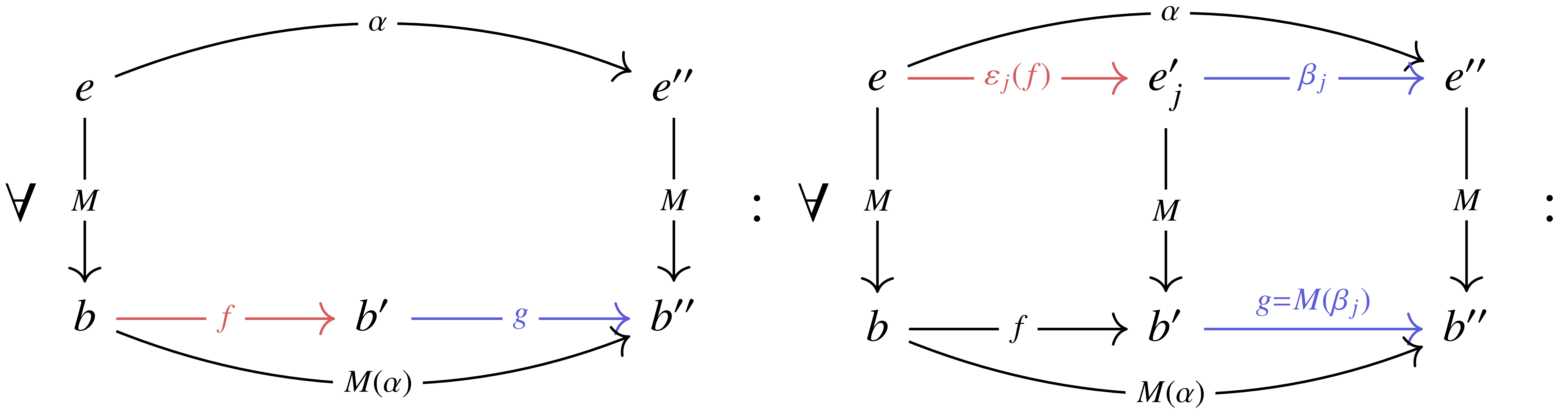
Definition 3. A functor $M : \mathbf{E} \to \mathbf{B}$ is a *multi-opfibration* if the following property holds:



$$\wedge\ \forall k \in J_{f;e} :\ (\exists e'_k - \beta_k \to e'' : \alpha = \beta_k \circ \varepsilon_k(f) \wedge M(\beta_k) = g)$$
$$\Rightarrow \exists!\ e'_j - \phi \to e'_k \in \mathsf{iso}(\mathbf{E}) : \varepsilon_k(f) = \phi \circ \varepsilon_j(f) \wedge M(\phi) = id_{b'} \qquad (5)$$

Fibrational structures — “multi” variants à la Diers

Corollary 1. *Let $M : \mathbf{E} \to \mathbf{B}$ be a multi-opfibration. Then the following* lifting property of isomorphisms *is satisfied:*

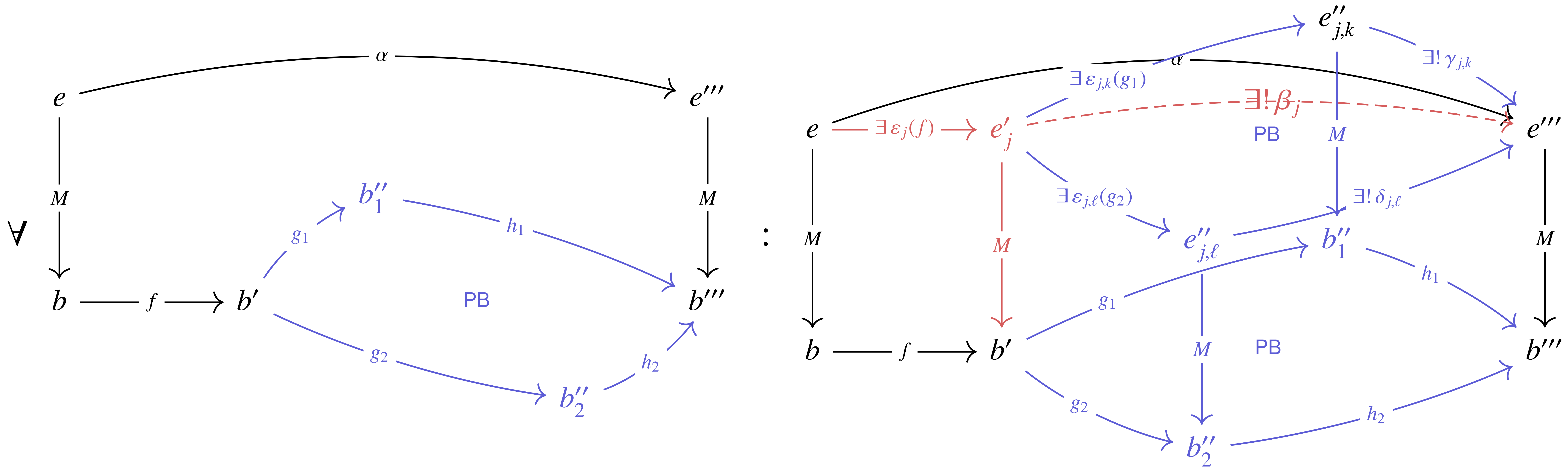


(6)

$$(g \in \mathsf{iso}(\mathbf{B}) \;\Rightarrow\; \beta_j \in \mathsf{iso}(\mathbf{E})) \wedge (f \in \mathsf{iso}(\mathbf{B}) \;\Rightarrow\; \varepsilon_j(f) \in \mathsf{iso}(\mathbf{E}))$$

Fibrational structures — “multi” variants à la Diers

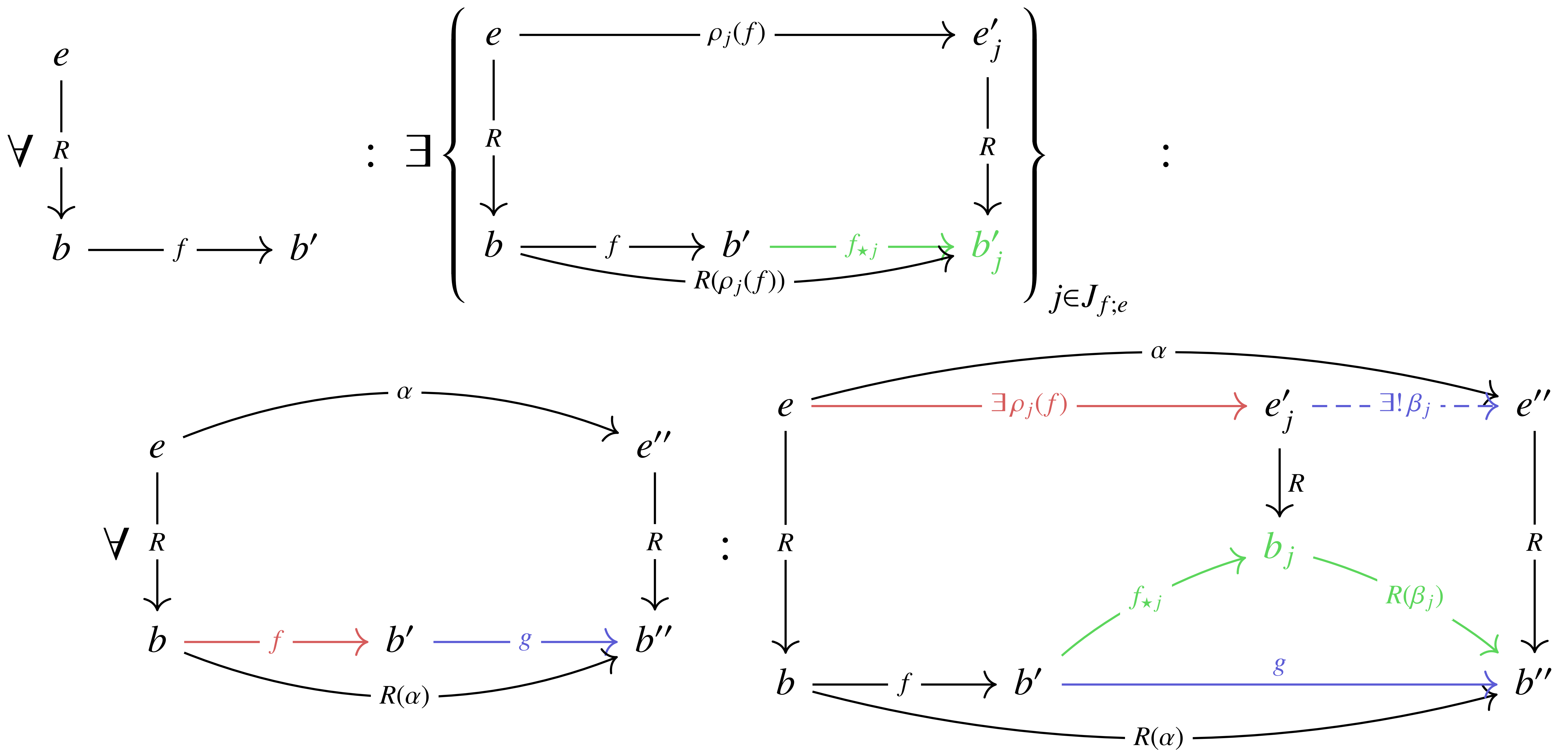
Lemma 2 (Pullback-splitting lemma for multi-opfibrations). *Let* $\mathbf{E}$ *be a category that has pullbacks, and let* $M : \mathbf{E} \to \mathbf{B}$ *be a multi-opfibration. Then the following property holds:*



(9)

Fibrational structures — "residual multi" variants

Definition 4. A functor $R : \mathbf{E} \to \mathbf{B}$ is a *residual multi-opfibration* if the following property holds:



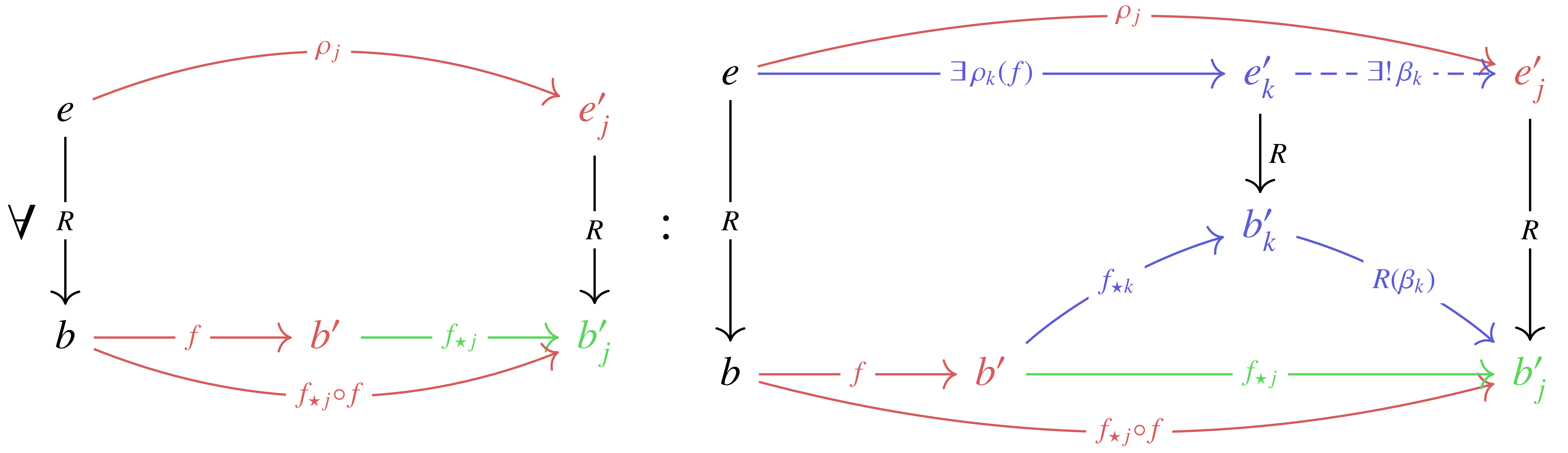
(11)

$$\wedge \quad \forall k \in J_{f;e} : (\exists\, e'_k - \beta_k \to e'' : \beta_k \circ \rho_k(f) = \alpha \wedge g = R(\beta_k) \circ f_{\star k})$$

$$\Rightarrow \exists!\, e'_j - \phi \to e'_k \in \mathsf{iso}(\mathbf{E}) : \rho_k(f) = \phi \circ \rho_j(f) \wedge \beta_j = \beta_k \circ \phi \wedge f_{\star k} = R(\phi) \circ f_{\star j}$$

Fibrational structures — “residual multi” variants

Corollary 2. *Let $R : \mathbf{E} \to \mathbf{B}$ be a residual multi-opfibration. Then residues have the following universal property:*

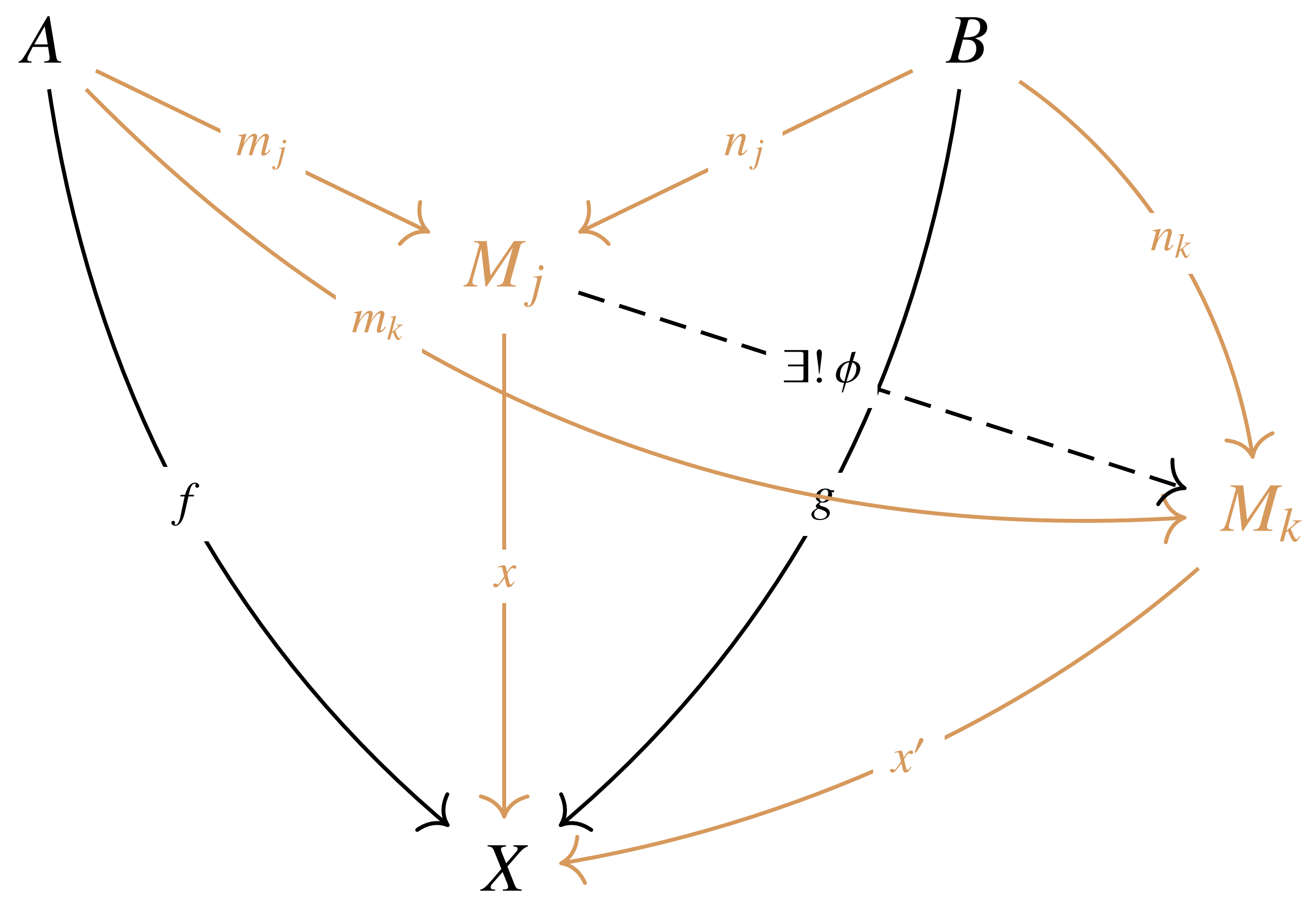


$$\Rightarrow \beta_k \in \mathsf{iso}(\mathbf{C}) \wedge R(\beta_k) \in \mathsf{iso}(\mathbf{B}) \quad (12)$$

In particular, this property entails that if a residue $f_{\star k}$ factorizes a residue $f_{\star j}$ as $f_{\star j} = R(\beta_k) \circ f_{\star k}$ for some $\beta_k \in \mathbf{E}$, then the residues $f_{\star j}$ and $f_{\star_k}$ (both of the same morphism $f \in \mathbb{B}$) are related by an isomorphism $R(\beta_k) \in \mathsf{iso}(\mathbf{B})$, as are their liftings $\rho_j(f) = \beta_k \circ \rho_k(f)$ via $\beta_k \in \mathsf{iso}(\mathbf{E})$.

Multi-sums (à la Diers)

Definition 11. Let $\mathbf{C}$ be a category. A *multi-sum* $\sum(A, B)$ of two objects A and B of $\mathbf{C}$ is a family of cospans $\{A - m_j \to M_j \leftarrow n_j - B\}_{j \in J}$ such that for every cospan $A - f \to X \leftarrow g - B$, there exists a $j \in J$ and morphism $M_j - x \to X$ such that $f = x \circ m_j$ and $g = x \circ n_j$, and with the following *(multi-) universal property*: for every $j, k \in J$ such that the corresponding multi-sum elements factor the cospan $A - f \to X \leftarrow g - B$, there exists a unique isomorphism $M_j - \phi \to M_k$ such that $x = x' \circ \phi$:

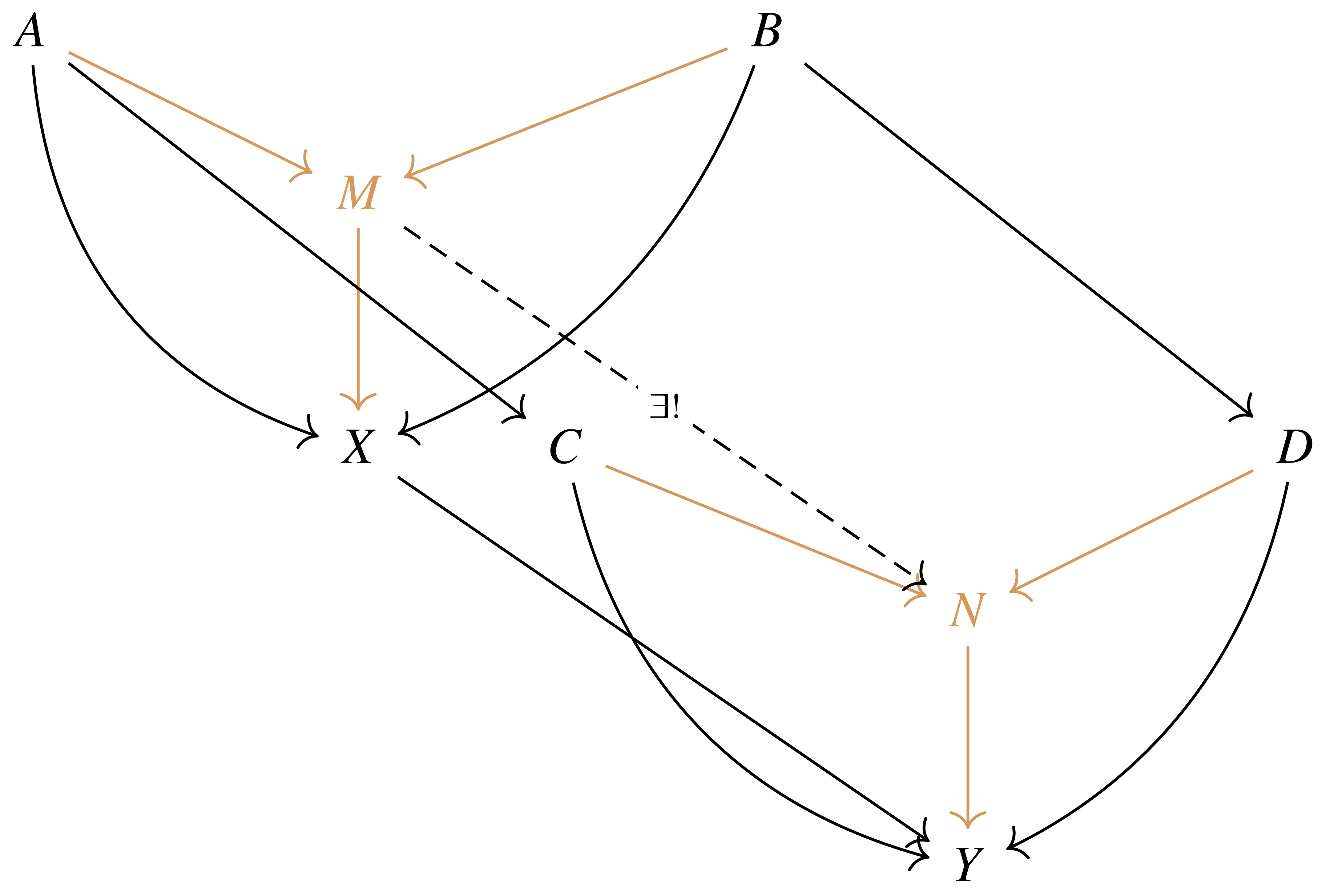


(40)

We say that $\mathbf{C}$ *has multi-sums* if every pair of objects has a multi-sum.

Multi-sums (à la Diers)

Lemma 6 (Multi-sum extension). *Let* **C** *be a category that has multi-sums and that has pullbacks. Then for every commutative diagram such as in* (41) *below, where* $A \to M \leftarrow B$ *and* $C \to N \leftarrow D$ *are multi-sum elements, there exists a universal arrow* $M \to N$ *that makes the diagram commute.*



(41)

Preliminaries: some notational conventions for double categories

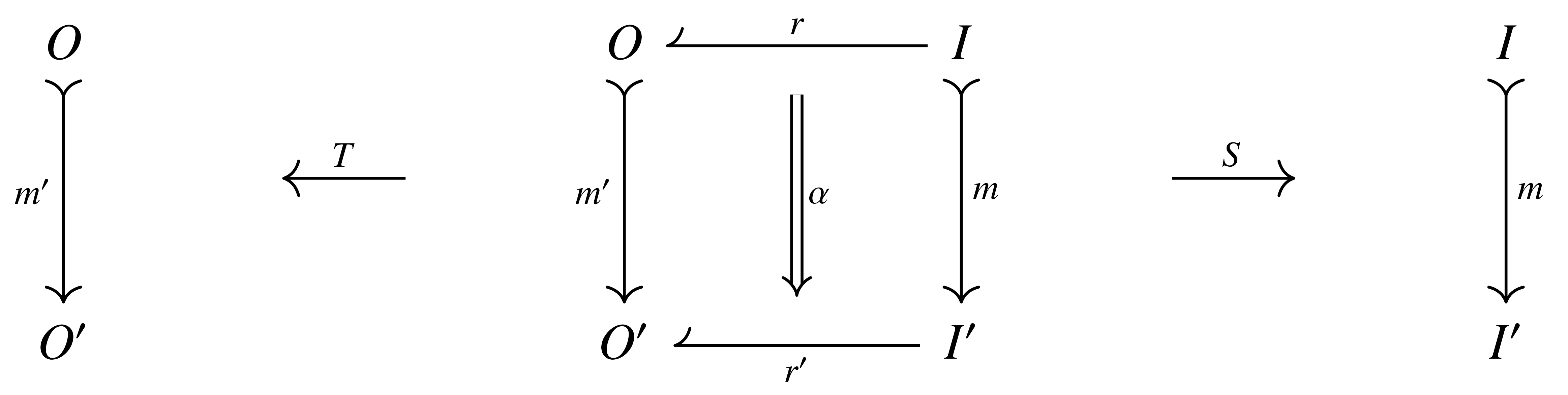


Figure 2: Convention for source and target functors for double categories.

Definition 12 (Cf. e.g. [50, 49, 51]). A *double category (DC)* $\mathbb{D}$ is a weakly internal category in the 2-category $\mathcal{CAT}$ of all categories [52][16].

In particular, this entails that a double category consists of a category $\mathbb{D}_0$ of *objects* and *vertical morphisms*, and a category $\mathbb{D}_1$ of *horizontal morphisms* and *squares* of $\mathbb{D}$, equipped with functors $S, T : \mathbb{D}_1 \to \mathbb{D}_0$, referred to as *source* and *target* functors, respectively (cf. Figure 2), and with a functor $U : \mathbb{D}_0 \to \mathbb{D}_1$ which maps every object A of $\mathbb{D}_0$ to a *horizontal unit* U_A (depicted in Figure 3(d) as identity horizontal morphisms), and every morphism f of $\mathbb{D}_0$ to a *horizontal unit square* U_f (depicted in Figure 3(d) as squares annotated with the symbol $id_{\ldots}$ for better readability). We denote vertical morphisms by $\rightarrowtail$ and horizontal morphisms by $\leftharpoondown$, respectively. We denote by $\diamond_v$ the *vertical composition* of squares as in Figure 3(a) (i.e., the associative composition operation of $\mathbb{D}_1$). $\mathbb{D}$ moreover carries a weakly associative *horizontal composition* of squares (cf. Figure 3(b)) $\diamond_h : \mathbb{D}_1 \times_{\mathbb{D}_0} \mathbb{D}_1 \to \mathbb{D}_1$. Finally, for technical convenience, we assume without loss of generality[17] that both types of compositions are strictly unitary (cf. Figures 3(c) and 3(d)).

Preliminaries: some notational conventions for double categories

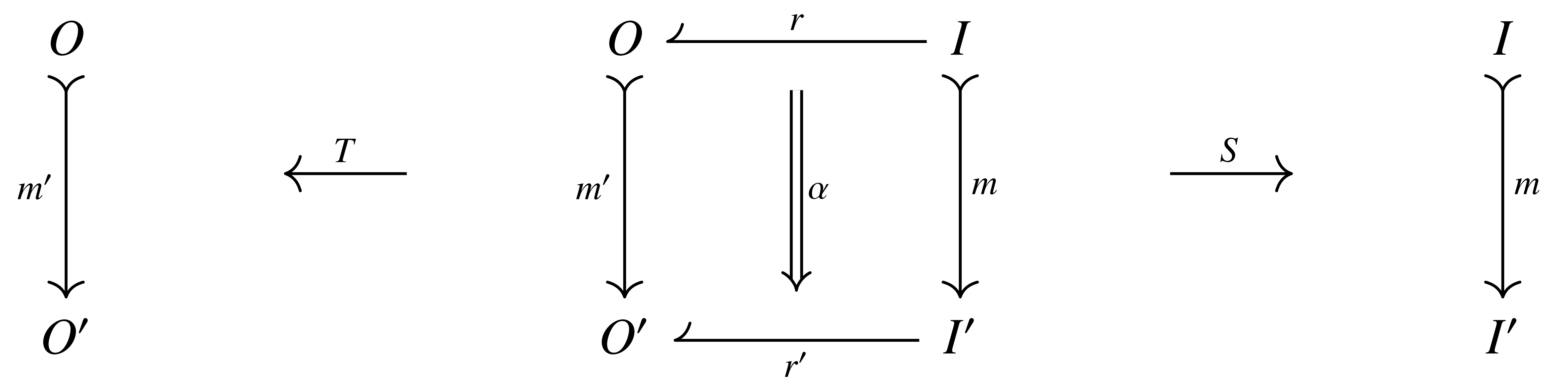
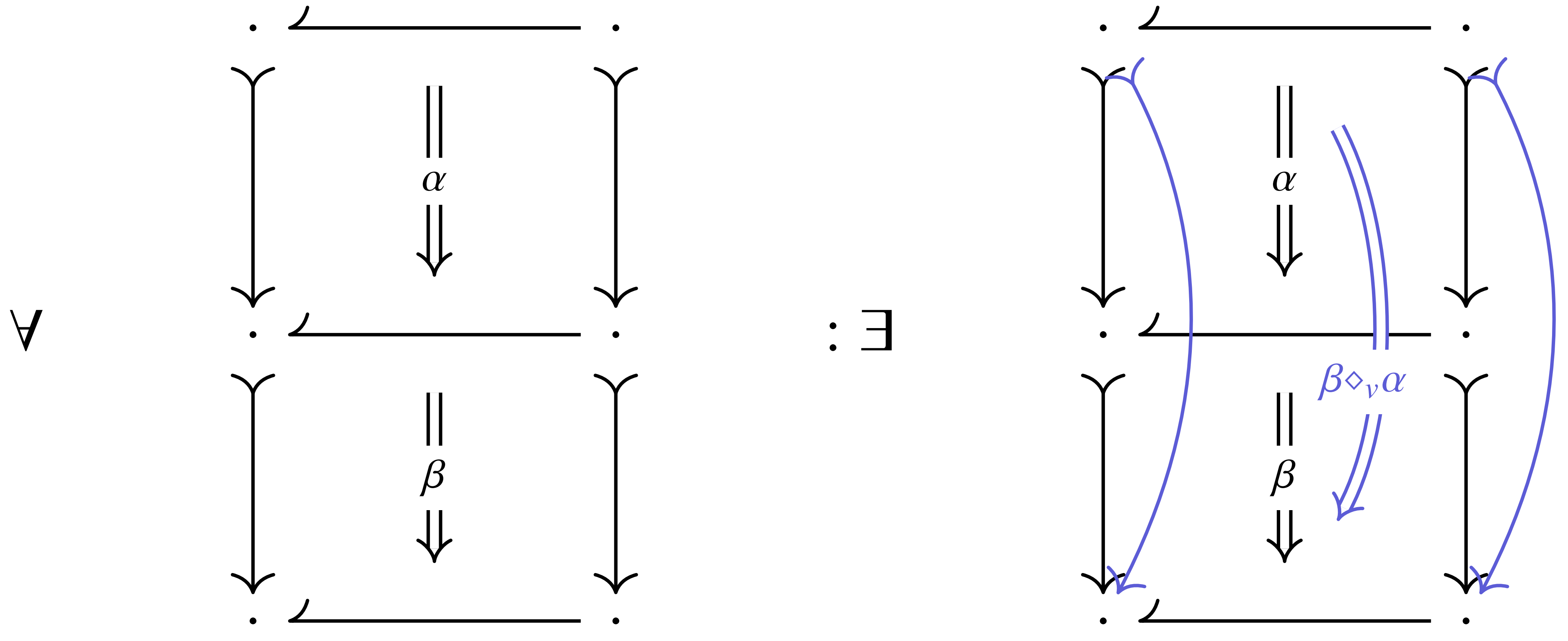
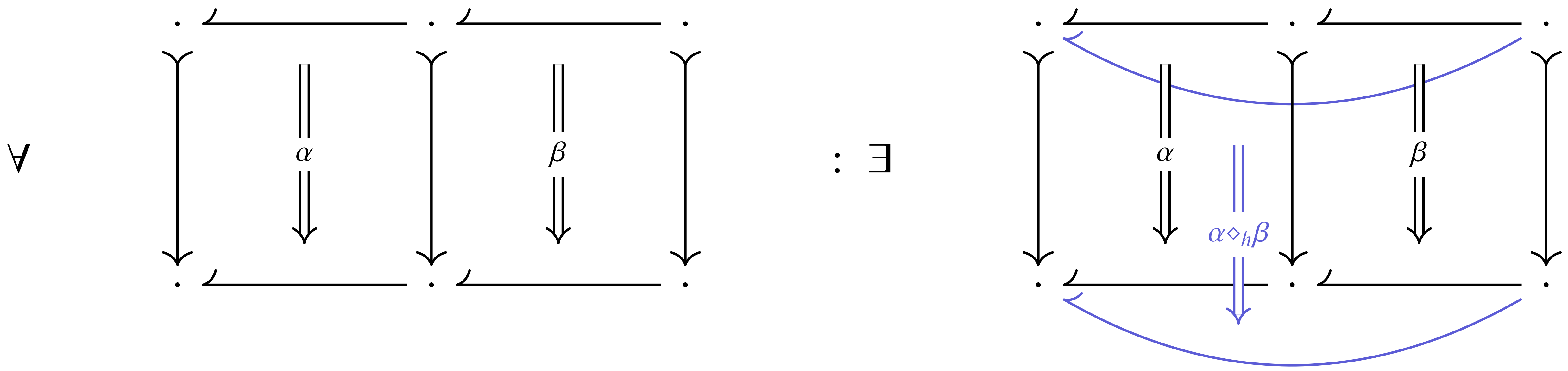


Figure 2: Convention for source and target functors for double categories.



(a) Vertical composition $\diamond_v$.



(b) Horizontal composition $\diamond_h$.

KEY CONCEPT:

compositional rewriting double categories (crDCs)

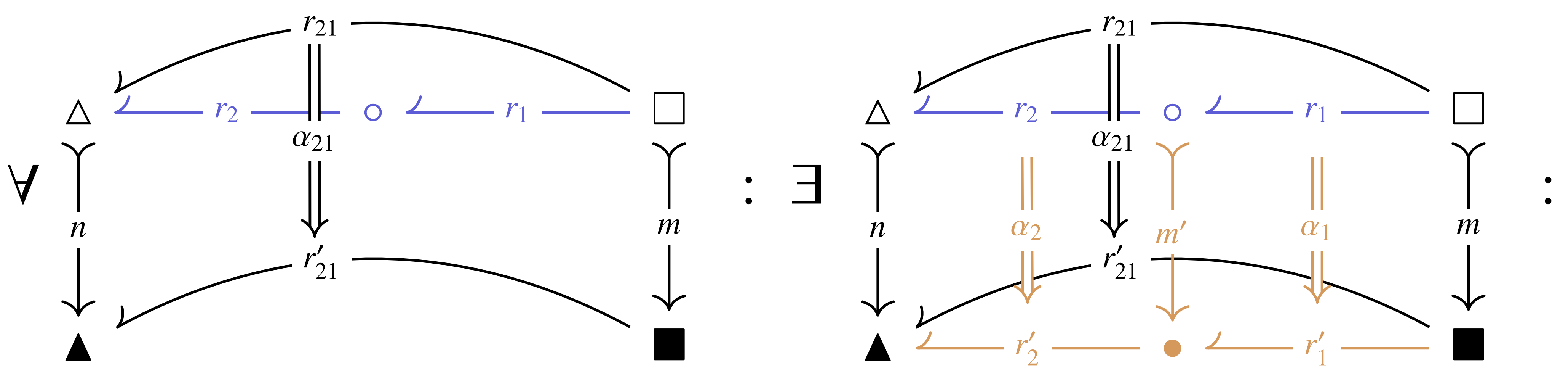
Compositional rewriting double categories (crDCs)

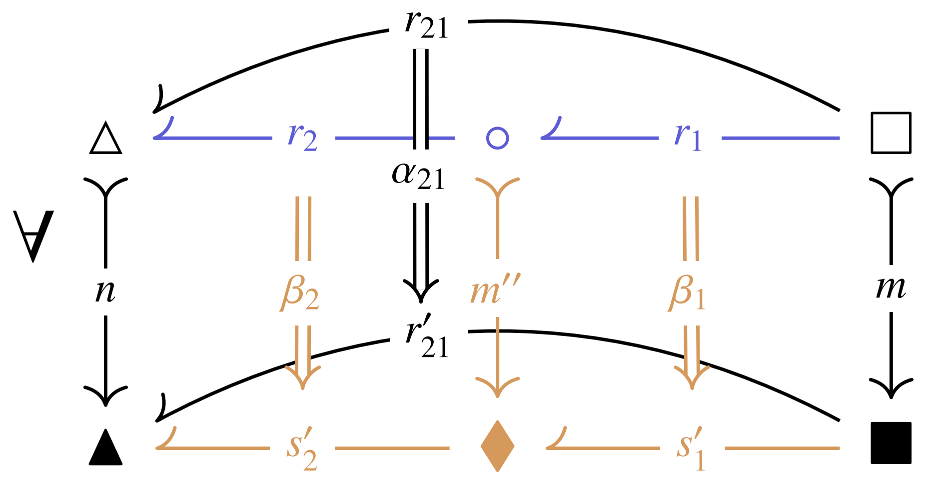
Definition 13. A double category (DC) $\mathbb{D}$ is a *compositional rewriting DC (crDC)* if it has the following properties:

(i) $\mathbb{D}_0$ has multi-sums.

(ii) *$\mathbb{D}_0$ and $\mathbb{D}_1$ have pullbacks*. (This entails in particular that for $i \in \{1, 2\}$, *$\mathbb{D}_i$ morphisms are stable under pullback*, and *pullbacks in $\mathbb{D}_i$ are effective*, i.e., for any span of $\mathbb{D}_i$ morphisms extending a pullback diagram in $\mathbb{D}_i$, the unique mediating morphism is in $\mathbb{D}_i$.)

(iii) Squares in $\mathbb{D}$ have the following *horizontal decomposition property*:





$$: \ \exists! \bullet \xrightarrow{\varphi} \blacklozenge \in \mathsf{iso}(\mathbb{D}_0) \ : \ m'' = \varphi \circ m' \tag{43}$$

(iv) The source functor $S : \mathbb{D}_1 \to \mathbb{D}_0$ is a multi-opfibration.

(v) The target functor $T : \mathbb{D}_1 \to \mathbb{D}_0$ is a residual multi-opfibration.

Compositional rewriting double categories (crDCs)

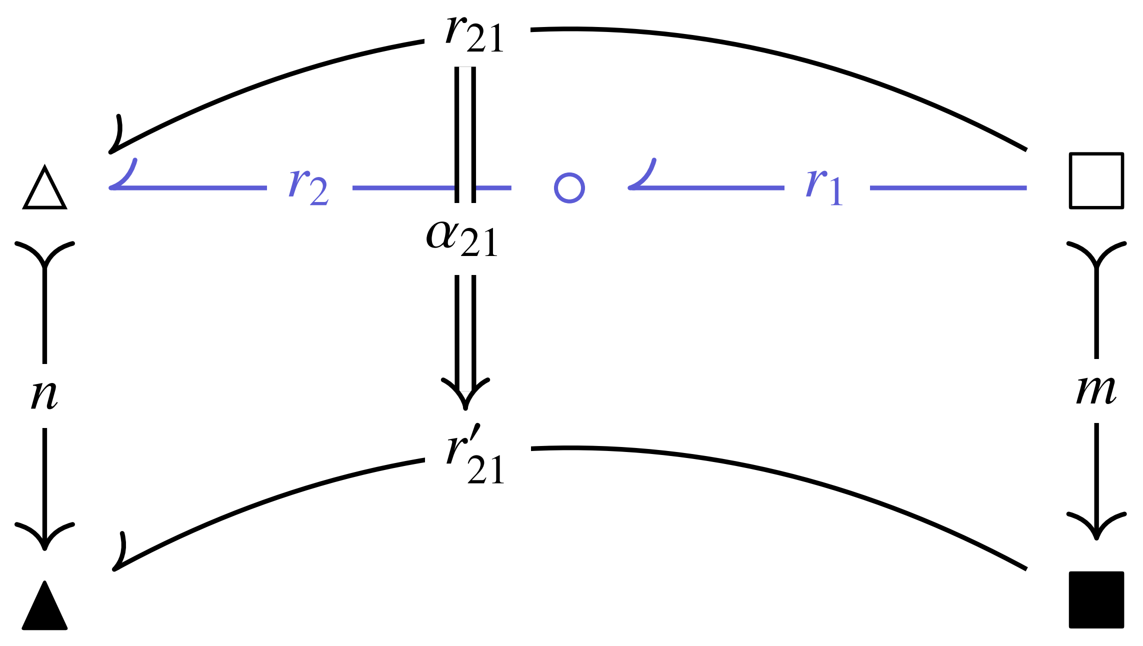
Definition 13. A double category (DC) $\mathbb{D}$ is a *compositional rewriting DC (crDC)* if it has the following properties:

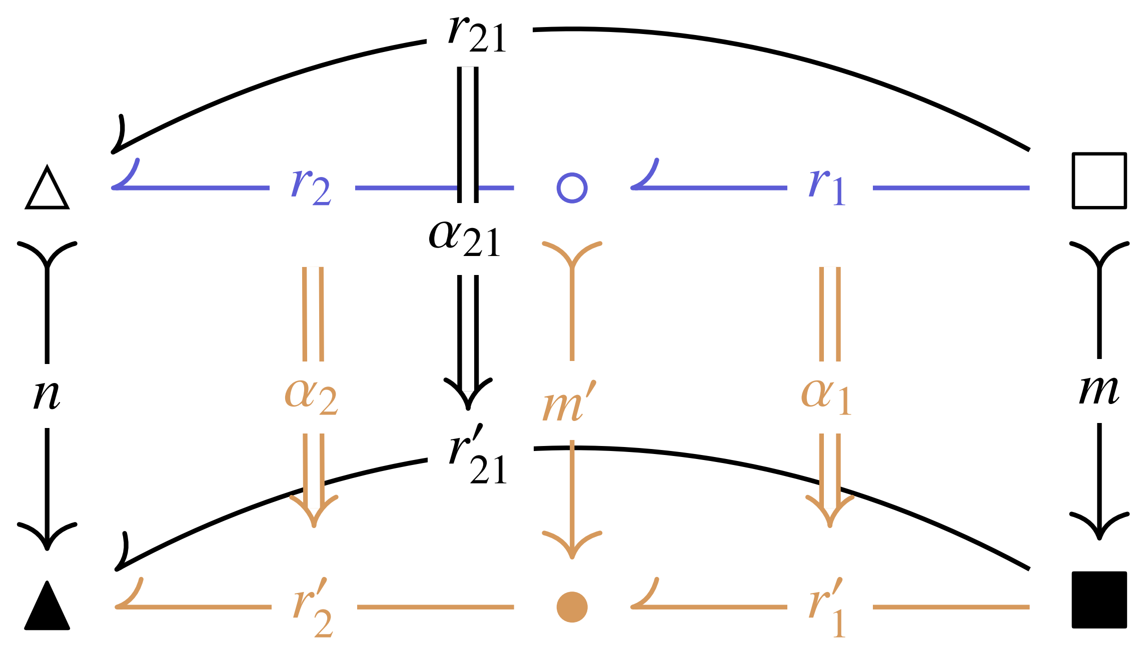
(i) $\mathbb{D}_0$ has multi-sums.

(ii) $\mathbb{D}_0$ *and* $\mathbb{D}_1$ *have pullbacks*. (This entails in particular that for $i \in \{1, 2\}$, $\mathbb{D}_i$ *morphisms are stable under pullback*, and *pullbacks in* $\mathbb{D}_i$ *are effective*, i.e., for any span of $\mathbb{D}_i$ morphisms extending a pullback diagram in $\mathbb{D}_i$, the unique mediating morphism is in $\mathbb{D}_i$.)

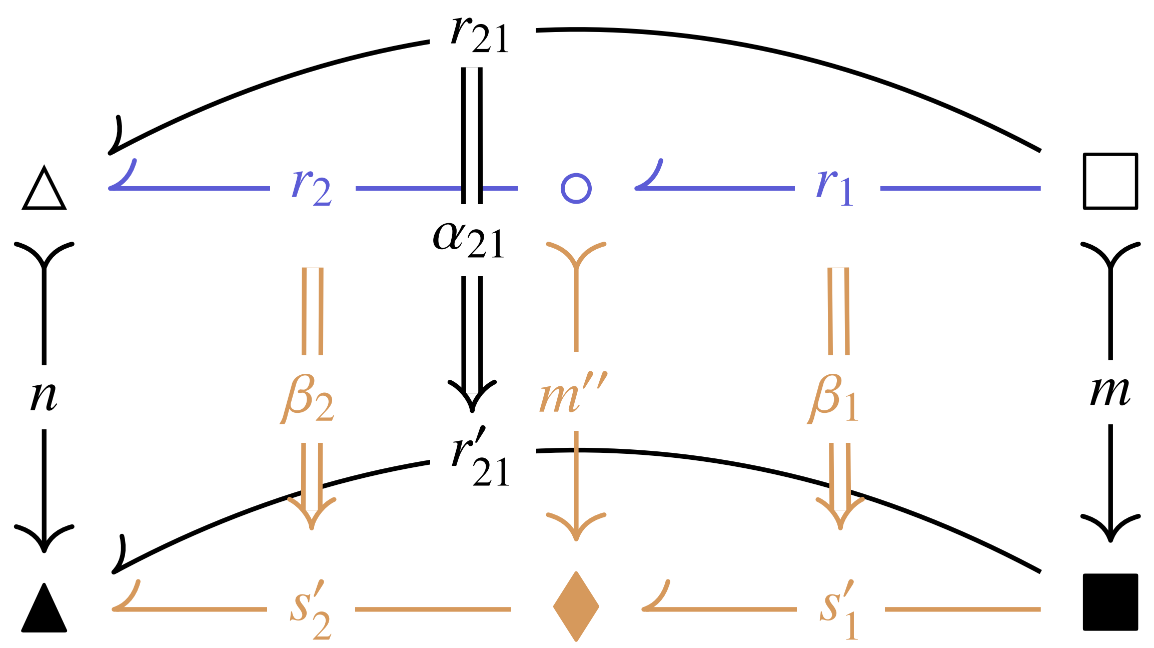
Compositional rewriting double categories (crDCs)

(iii) Squares in $\mathbb{D}$ have the following *horizontal decomposition property*:

$\forall$ 

$:\ \exists$ 

$:$

$\forall$ 

$:\ \exists! \bullet \xrightarrow{\varphi} \blacklozenge \in \mathrm{iso}(\mathbb{D}_0)\ :\ m'' = \varphi \circ m'$ (43)

Compositional rewriting double categories (crDCs)

(iv) The source functor $S : \mathbb{D}_1 \to \mathbb{D}_0$ is a multi-opfibration.

(v) The target functor $T : \mathbb{D}_1 \to \mathbb{D}_0$ is a residual multi-opfibration.

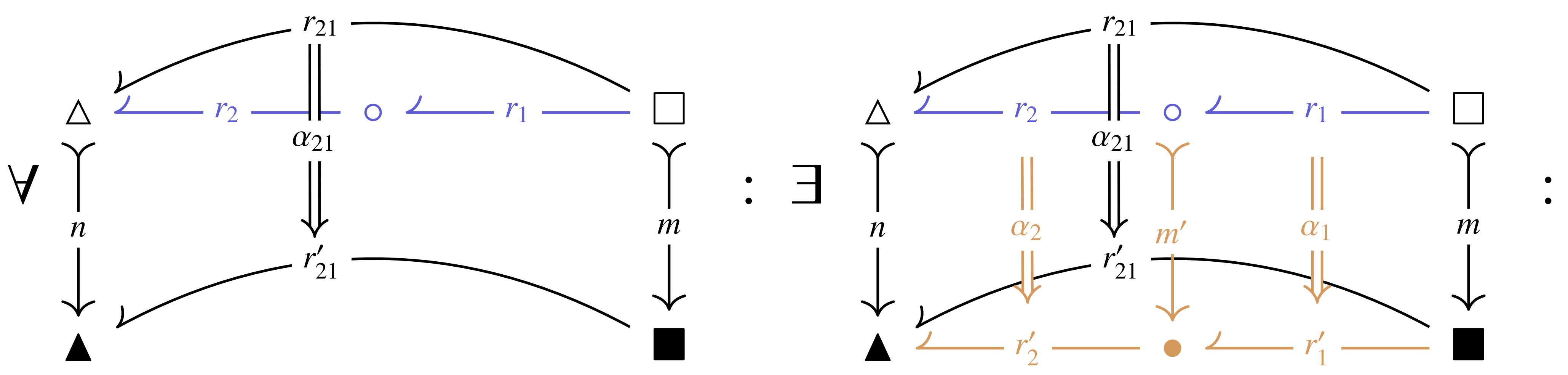
Compositional rewriting double categories (crDCs)

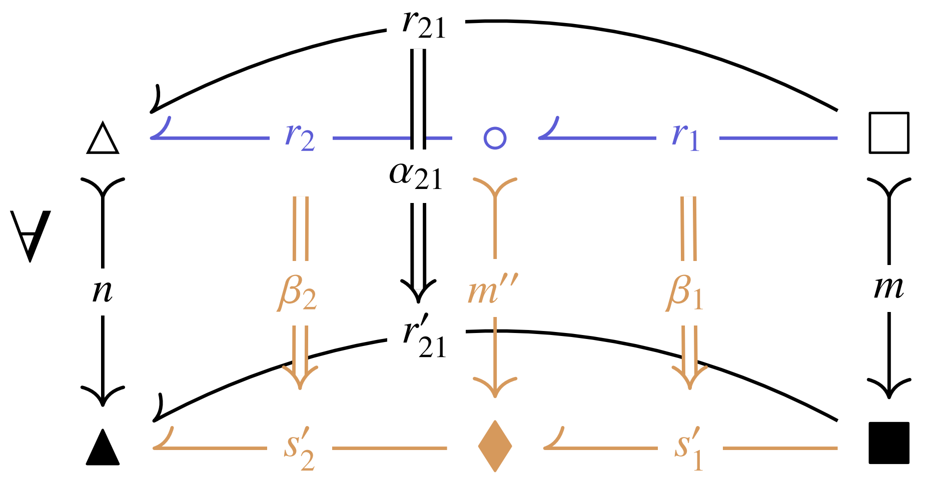
Definition 13. A double category (DC) $\mathbb{D}$ is a *compositional rewriting DC (crDC)* if it has the following properties:

(i) $\mathbb{D}_0$ has multi-sums.

(ii) *$\mathbb{D}_0$ and $\mathbb{D}_1$ have pullbacks*. (This entails in particular that for $i \in \{1, 2\}$, *$\mathbb{D}_i$ morphisms are stable under pullback*, and *pullbacks in $\mathbb{D}_i$ are effective*, i.e., for any span of $\mathbb{D}_i$ morphisms extending a pullback diagram in $\mathbb{D}_i$, the unique mediating morphism is in $\mathbb{D}_i$.)

(iii) Squares in $\mathbb{D}$ have the following *horizontal decomposition property*:





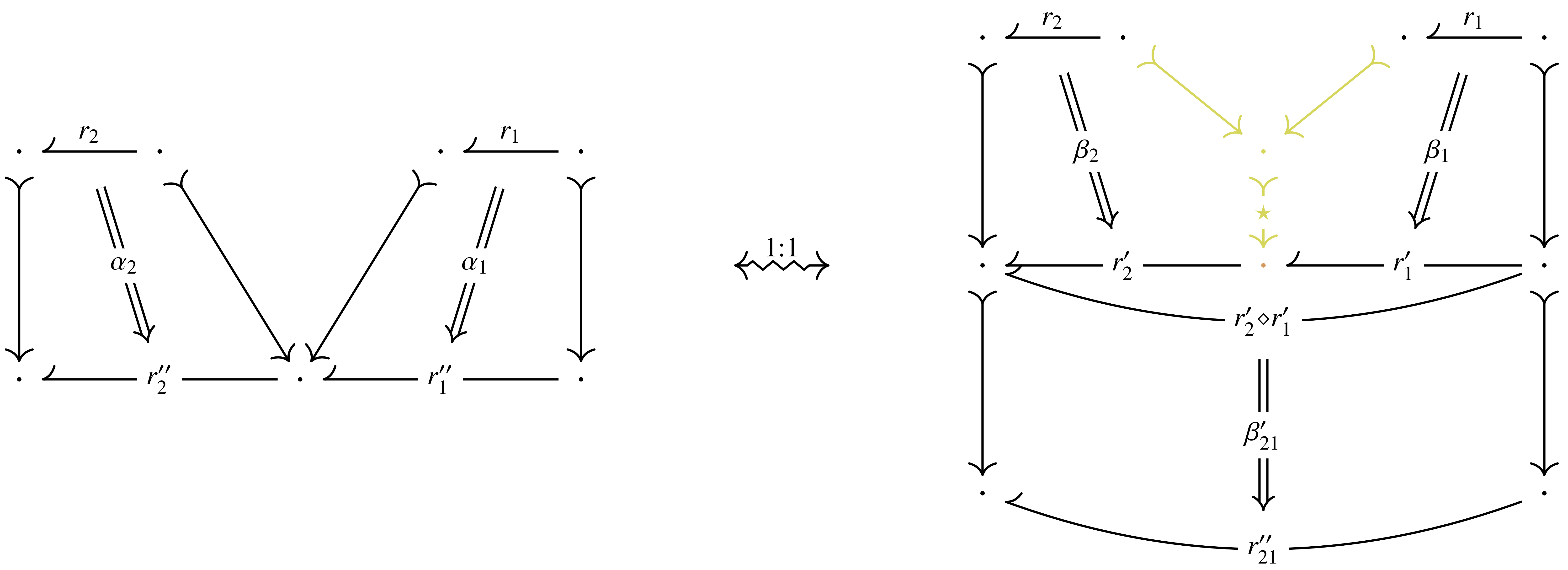
$$: \ \exists!\bullet \xrightarrow{\varphi} \blacklozenge \in \mathsf{iso}(\mathbb{D}_0) \ : \ m'' = \varphi \circ m' \tag{43}$$

(iv) The source functor $S : \mathbb{D}_1 \to \mathbb{D}_0$ is a multi-opfibration.

(v) The target functor $T : \mathbb{D}_1 \to \mathbb{D}_0$ is a residual multi-opfibration.

crDCs satisfy a (*universal!*) **Concurrency Theorem**

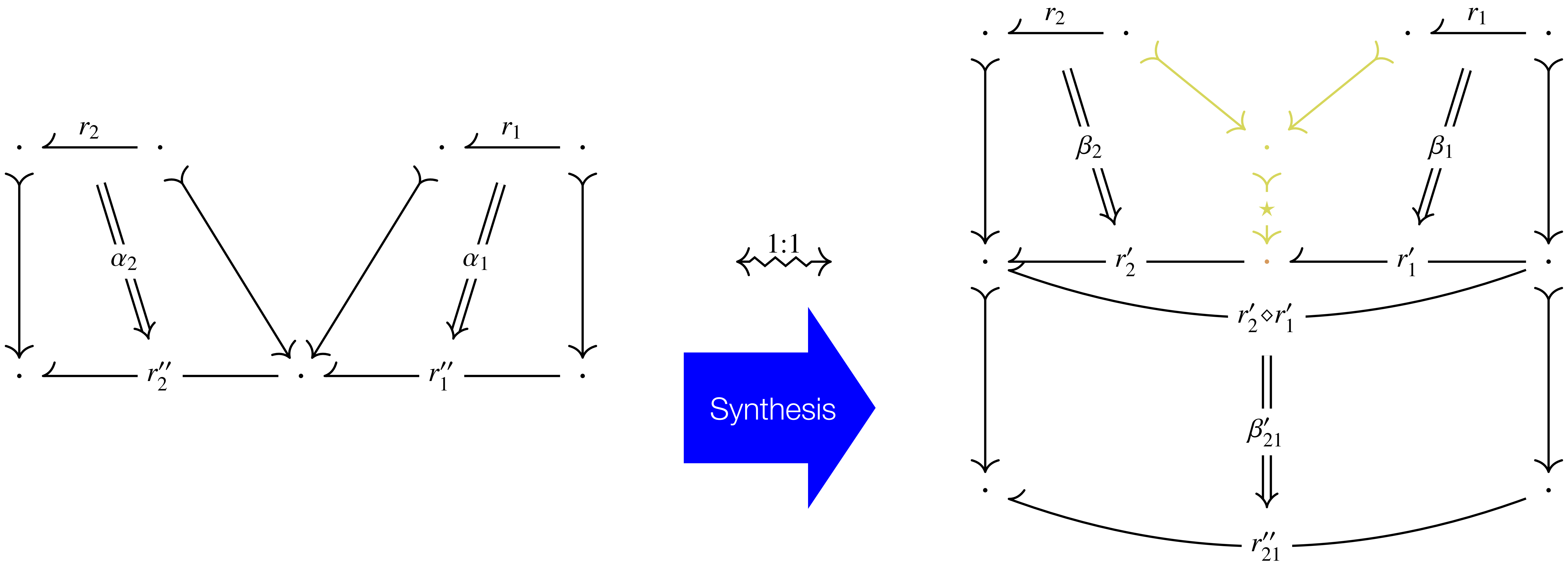
Theorem 8. *Let $\mathbb{D}$ be a compositional rewriting double category. Then the following statements hold (where the morphism marked $\star$ in the diagram on the right is a residue, and the cospan into its domain a multi-sum element.):*



(44)

crDCs satisfy a (*universal!*) **Concurrency Theorem**

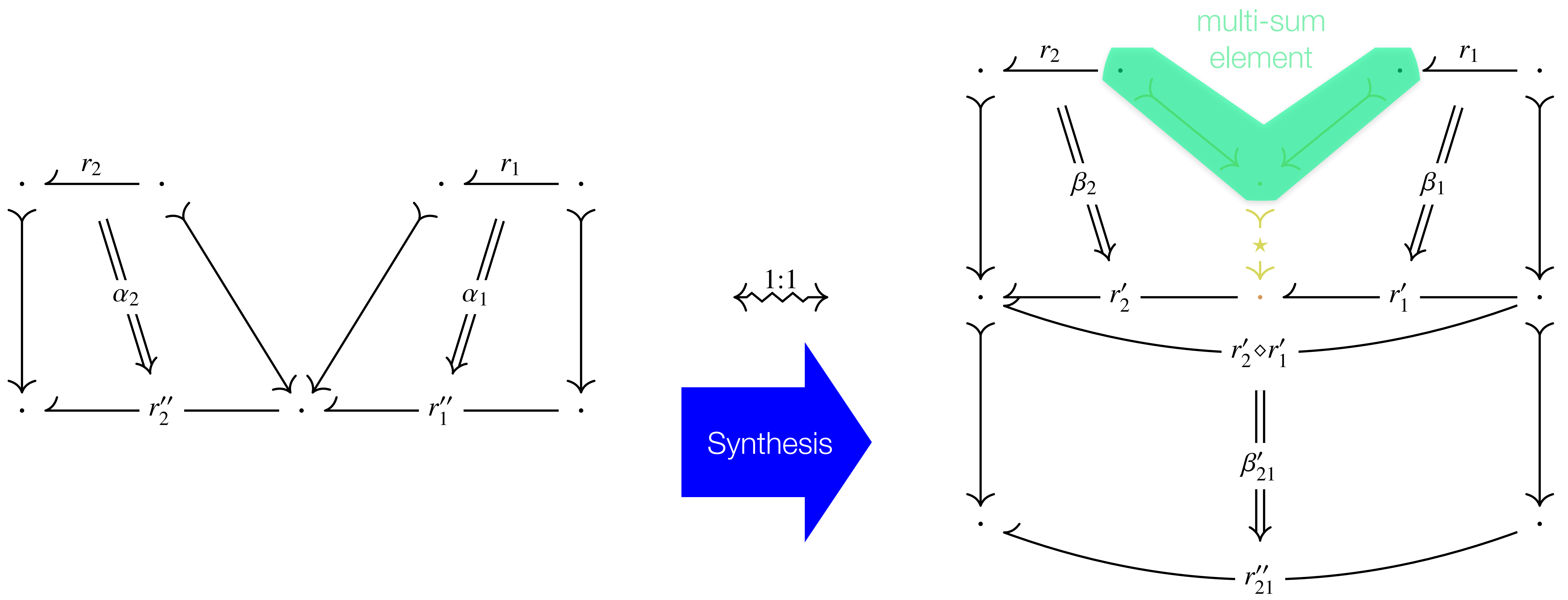
Theorem 8. *Let $\mathbb{D}$ be a compositional rewriting double category. Then the following statements hold (where the morphism marked $\star$ in the diagram on the right is a residue, and the cospan into its domain a multi-sum element.):*



$$(44)$$

crDCs satisfy a (*universal!*) **Concurrency Theorem**

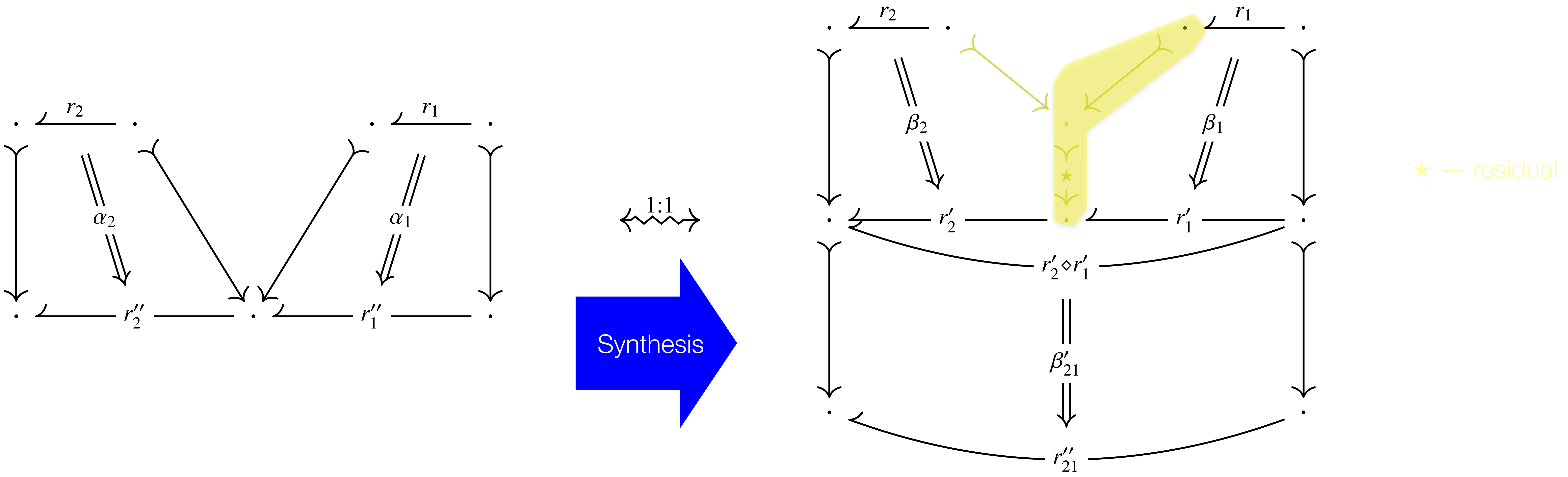
Theorem 8. *Let $\mathbb{D}$ be a compositional rewriting double category. Then the following statements hold (where the morphism marked $\star$ in the diagram on the right is a residue, and the cospan into its domain a multi-sum element.):*



(44)

crDCs satisfy a (*universal!*) **Concurrency Theorem**

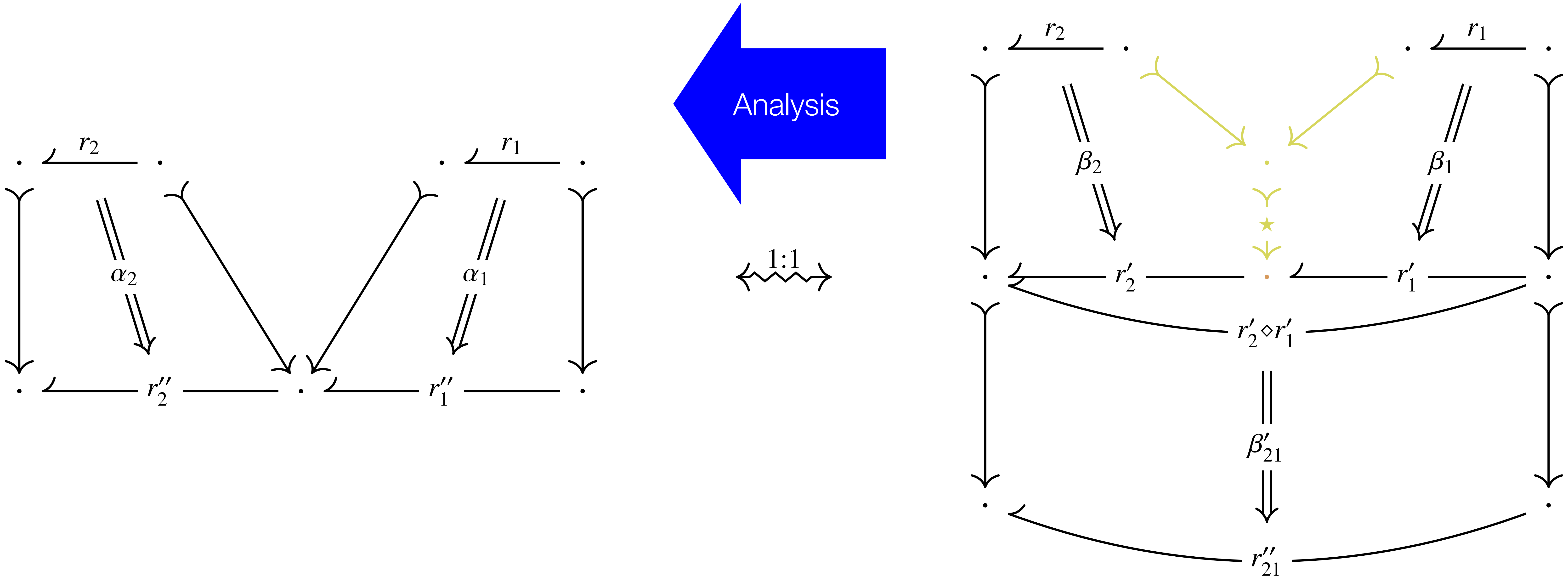
Theorem 8. *Let $\mathbb{D}$ be a compositional rewriting double category. Then the following statements hold (where the morphism marked $\star$ in the diagram on the right is a residue, and the cospan into its domain a multi-sum element.):*



(44)

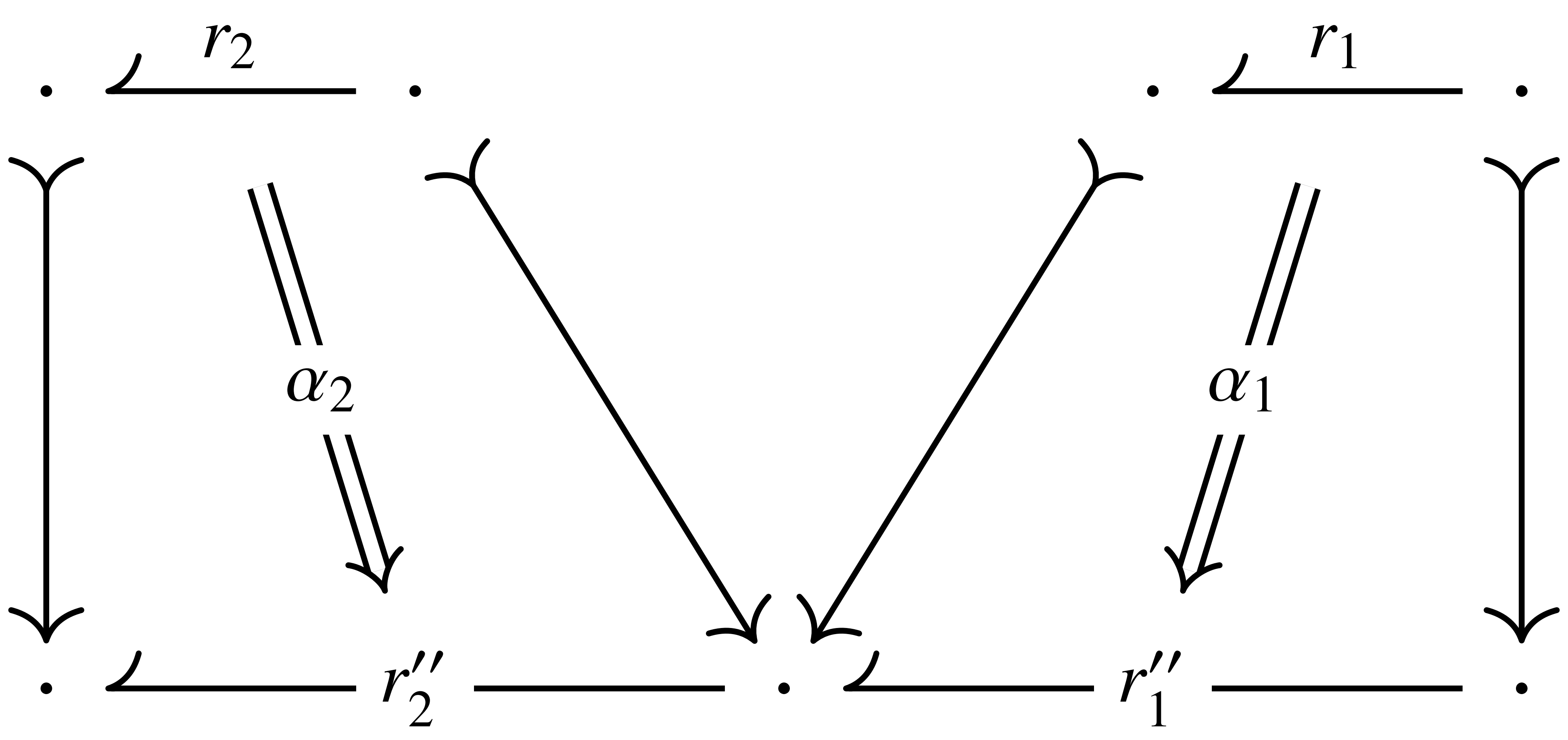
crDCs satisfy a (*universal!*) **Concurrency Theorem**

Theorem 8. *Let $\mathbb{D}$ be a compositional rewriting double category. Then the following statements hold (where the morphism marked $\star$ in the diagram on the right is a residue, and the cospan into its domain a multi-sum element.):*



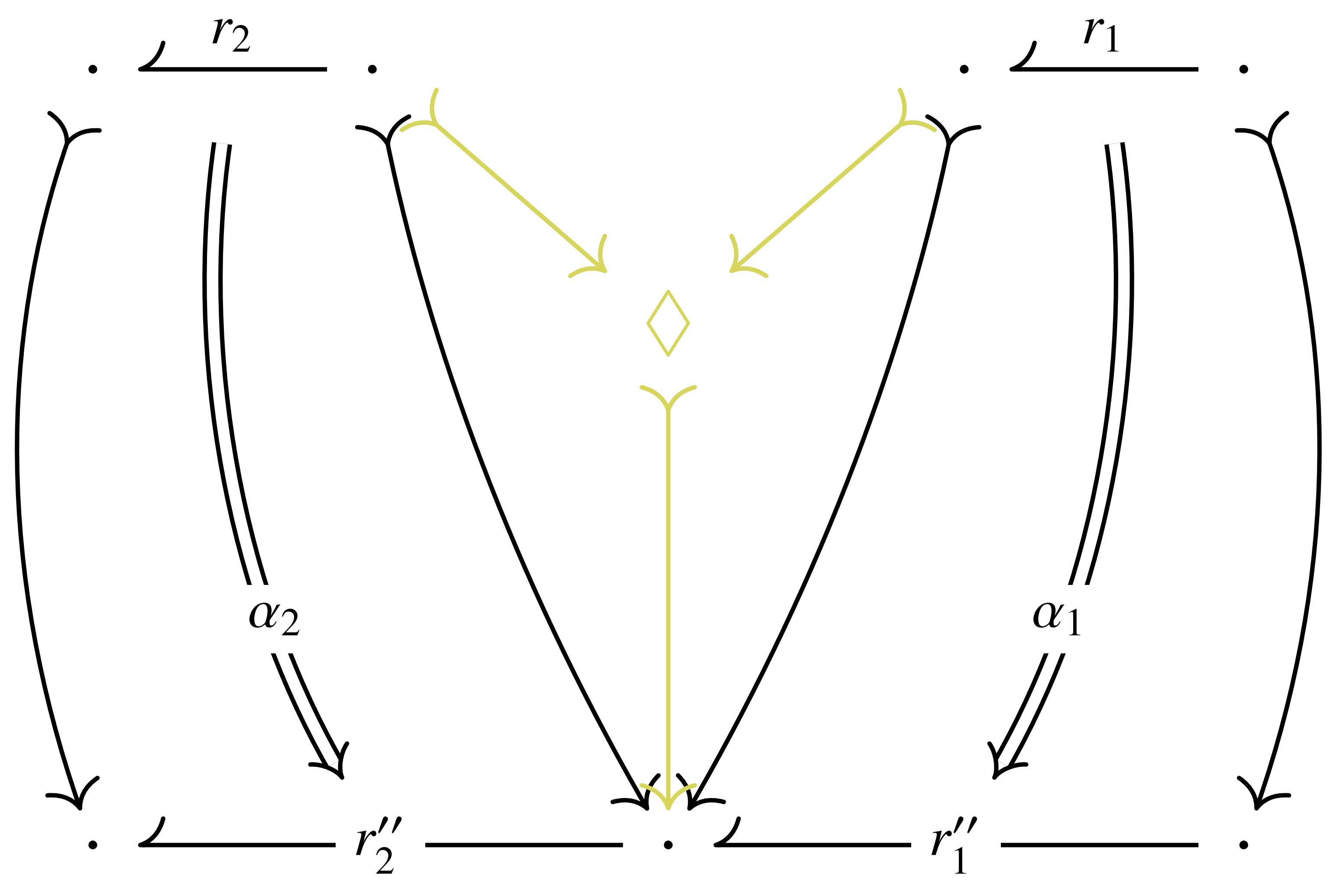
(44)

crDCs satisfy a (*universal!*) **Concurrency Theorem — PROOF**



PROOF. **Synthesis part:** Construct the diagram in (45) from the premise as follows:

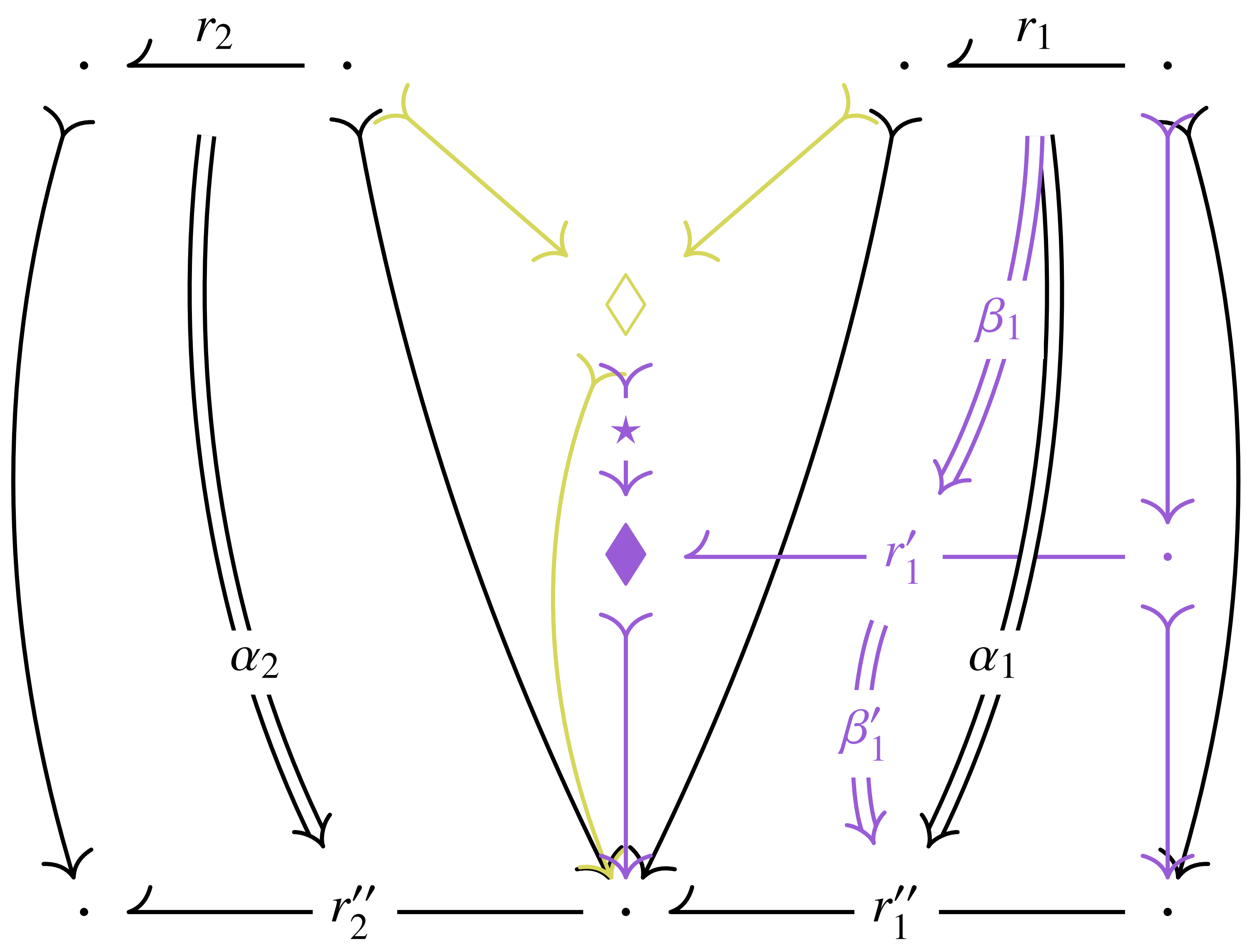
crDCs satisfy a (*universal!*) **Concurrency Theorem — PROOF**



Proof. **Synthesis part:** Construct the diagram in (45) from the premise as follows:

- Via the universal property of multi-sums, there exists a cospan of $\mathbb{D}_0$-morphisms into an object $\Diamond$ and a mediating $\mathcal{M}$-morphism $\Diamond \rightarrowtail \cdot$.

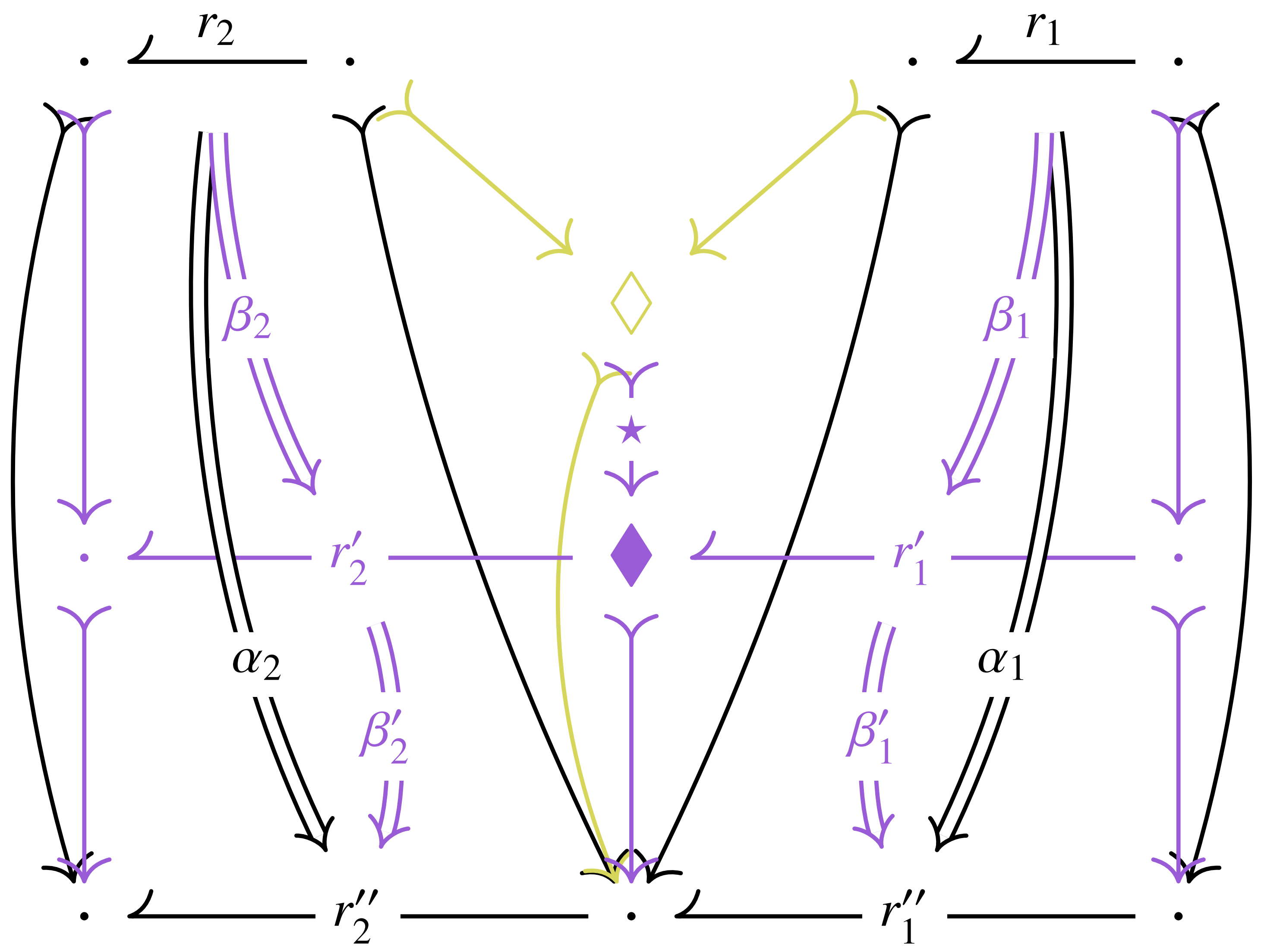
crDCs satisfy a (*universal!*) **Concurrency Theorem — PROOF**



PROOF. **Synthesis part:** Construct the diagram in (45) from the premise as follows:

- Via the universal property of multi-sums, there exists a cospan of $\mathbb{D}_0$-morphisms into an object $\lozenge$ and a mediating $\mathcal{M}$-morphism $\lozenge \rightarrowtail \cdot$.
- Since the target functor $T : \mathbb{D}_1 \to \mathbb{D}_0$ is a residual multi-opfibration, there exists a residue $\lozenge \rightarrowtail \blacklozenge$ (marked $\star$) and an $\mathbb{D}_0$-morphism $\blacklozenge \rightarrowtail \cdot$ such that $\alpha_1 = \beta'_1 \diamond_v \beta_1$.

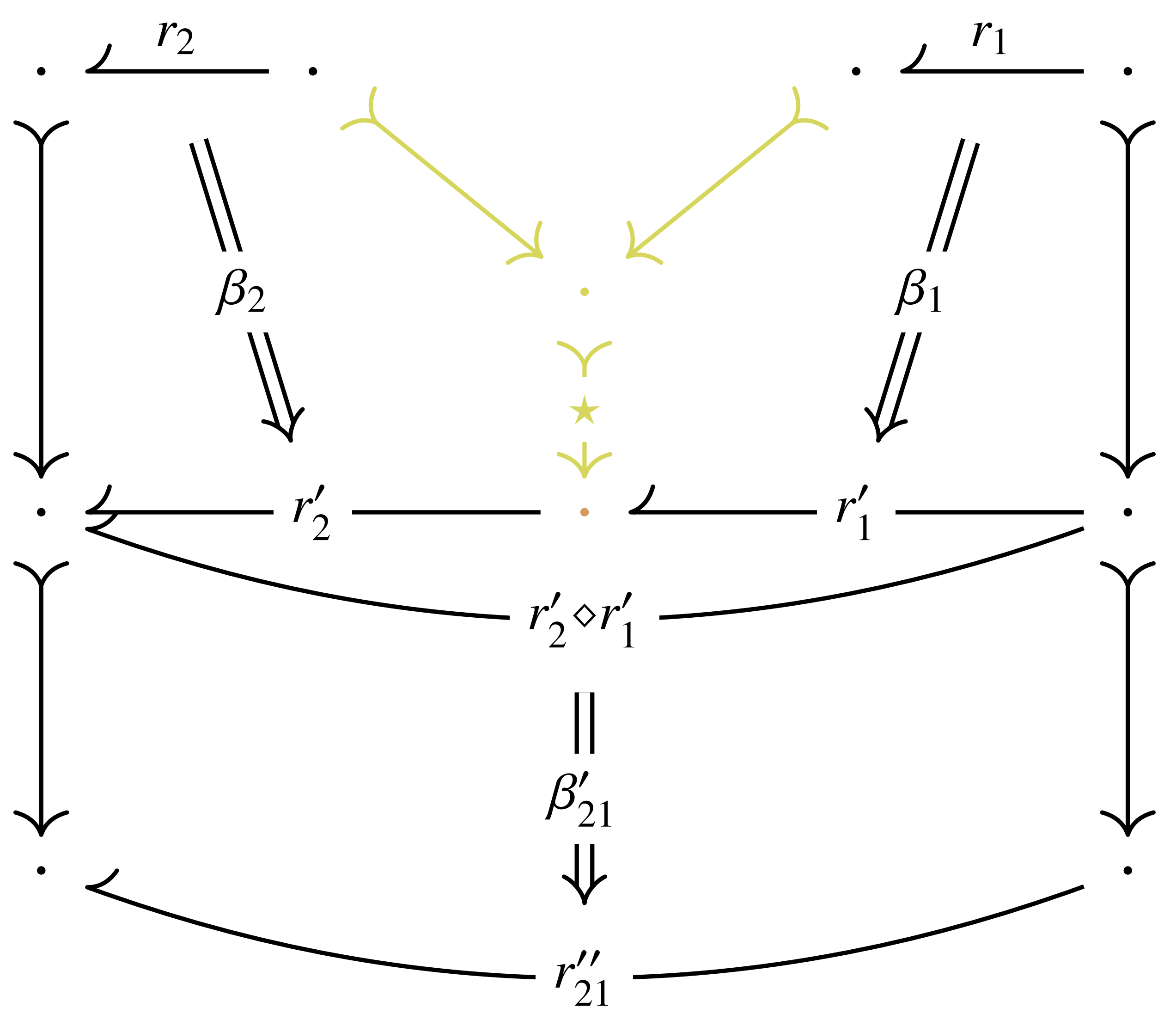
crDCs satisfy a (*universal!*) **Concurrency Theorem — PROOF**



PROOF. **Synthesis part:** Construct the diagram in (45) from the premise as follows:

- Via the universal property of multi-sums, there exists a cospan of $\mathbb{D}_0$-morphisms into an object $\lozenge$ and a mediating $\mathcal{M}$-morphism $\lozenge \rightarrowtail \cdot$.
- Since the target functor $T : \mathbb{D}_1 \to \mathbb{D}_0$ is a residual multi-opfibration, there exists a residue $\lozenge \rightarrowtail \blacklozenge$ (marked $\star$) and an $\mathbb{D}_0$-morphism $\blacklozenge \rightarrowtail \cdot$ such that $\alpha_1 = \beta'_1 \diamond_v \beta_1$.
- Since the source functor $S : \mathbb{D}_1 \to \mathbb{D}_0$ is a multi-opfibration, there exist direct derivations β_2 and β'_2 such that $\alpha_2 = \beta'_2 \diamond_v \beta_2$. Thus the claim follows by letting $\beta_{21} := \beta'_2 \diamond_h \beta'_1$.

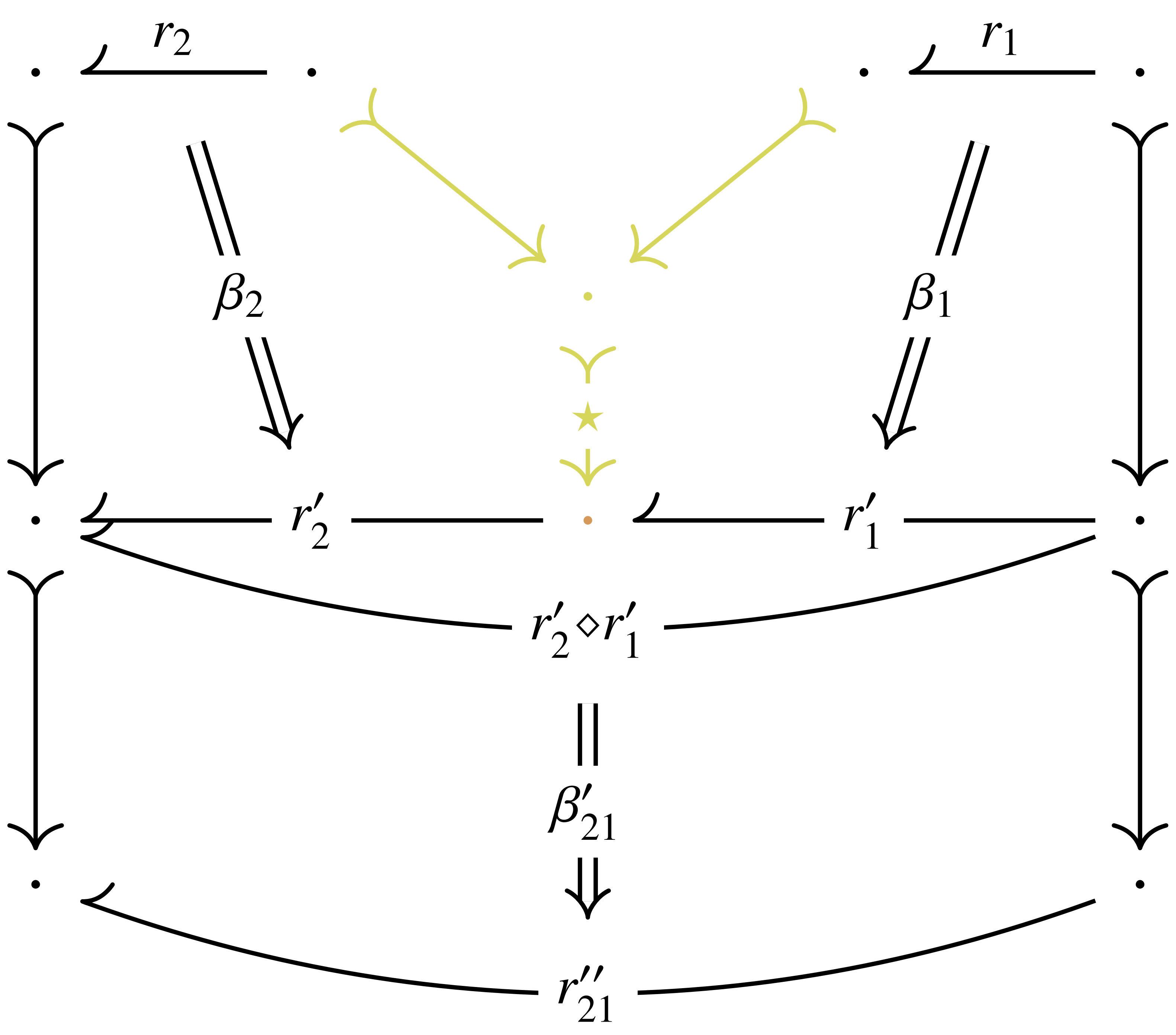
crDCs satisfy a (*universal!*) **Concurrency Theorem — PROOF**



PROOF. **Synthesis part:** Construct the diagram in (45) from the premise as follows:

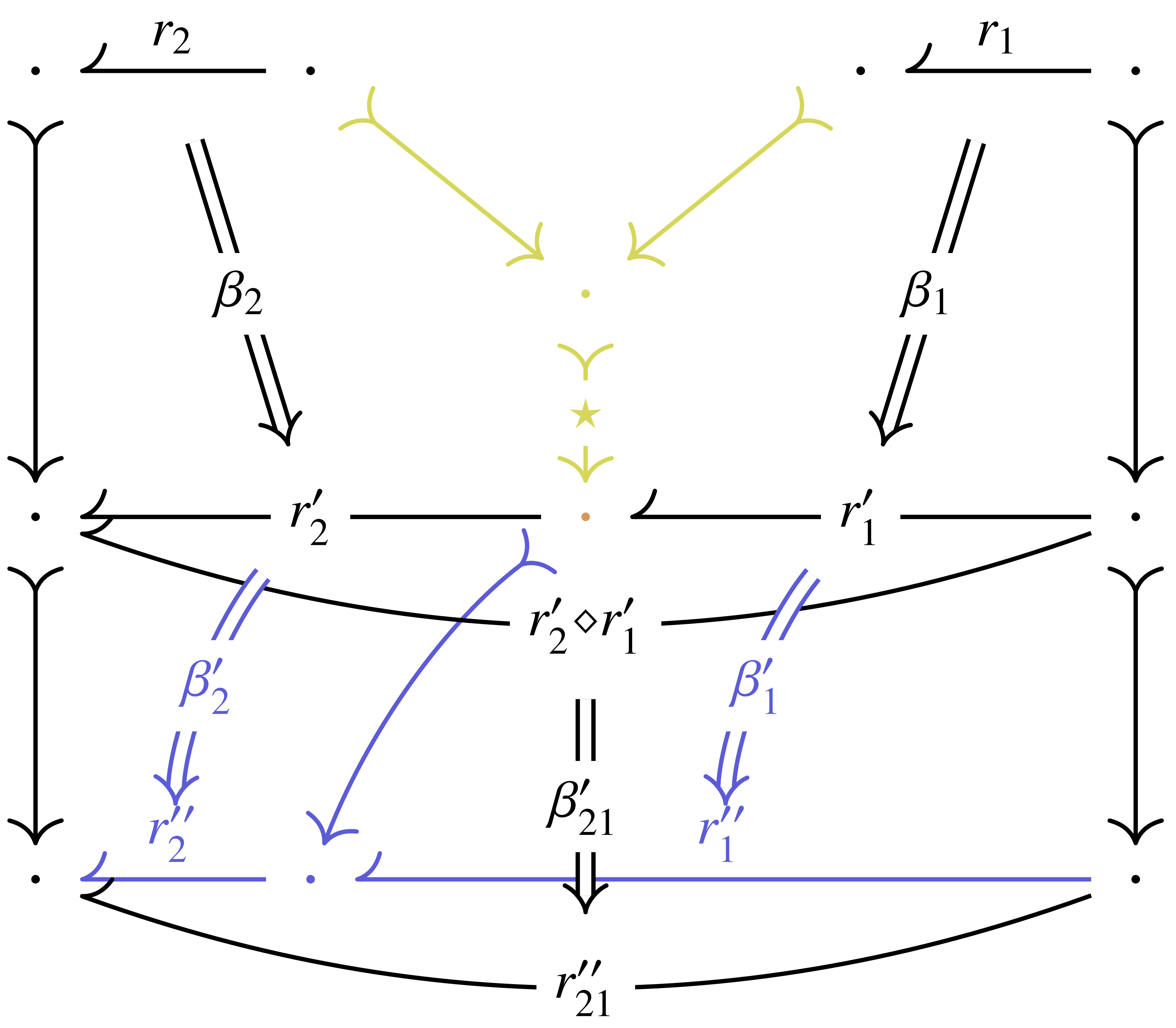
- Via the universal property of multi-sums, there exists a cospan of $\mathbb{D}_0$-morphisms into an object $\Diamond$ and a mediating $\mathcal{M}$-morphism $\Diamond \rightarrowtail \cdot$.
- Since the target functor $T : \mathbb{D}_1 \to \mathbb{D}_0$ is a residual multi-opfibration, there exists a residue $\Diamond \rightarrowtail \blacklozenge$ (marked $\star$) and an $\mathbb{D}_0$-morphism $\blacklozenge \rightarrowtail \cdot$ such that $\alpha_1 = \beta'_1 \diamond_v \beta_1$.
- Since the source functor $S : \mathbb{D}_1 \to \mathbb{D}_0$ is a multi-opfibration, there exist direct derivations β_2 and β'_2 such that $\alpha_2 = \beta'_2 \diamond_v \beta_2$. Thus the claim follows by letting $\beta_{21} := \beta'_2 \diamond_h \beta'_1$.

crDCs satisfy a (*universal!*) **Concurrency Theorem — PROOF**



Analysis part: Construct the diagram in (46) as follows:

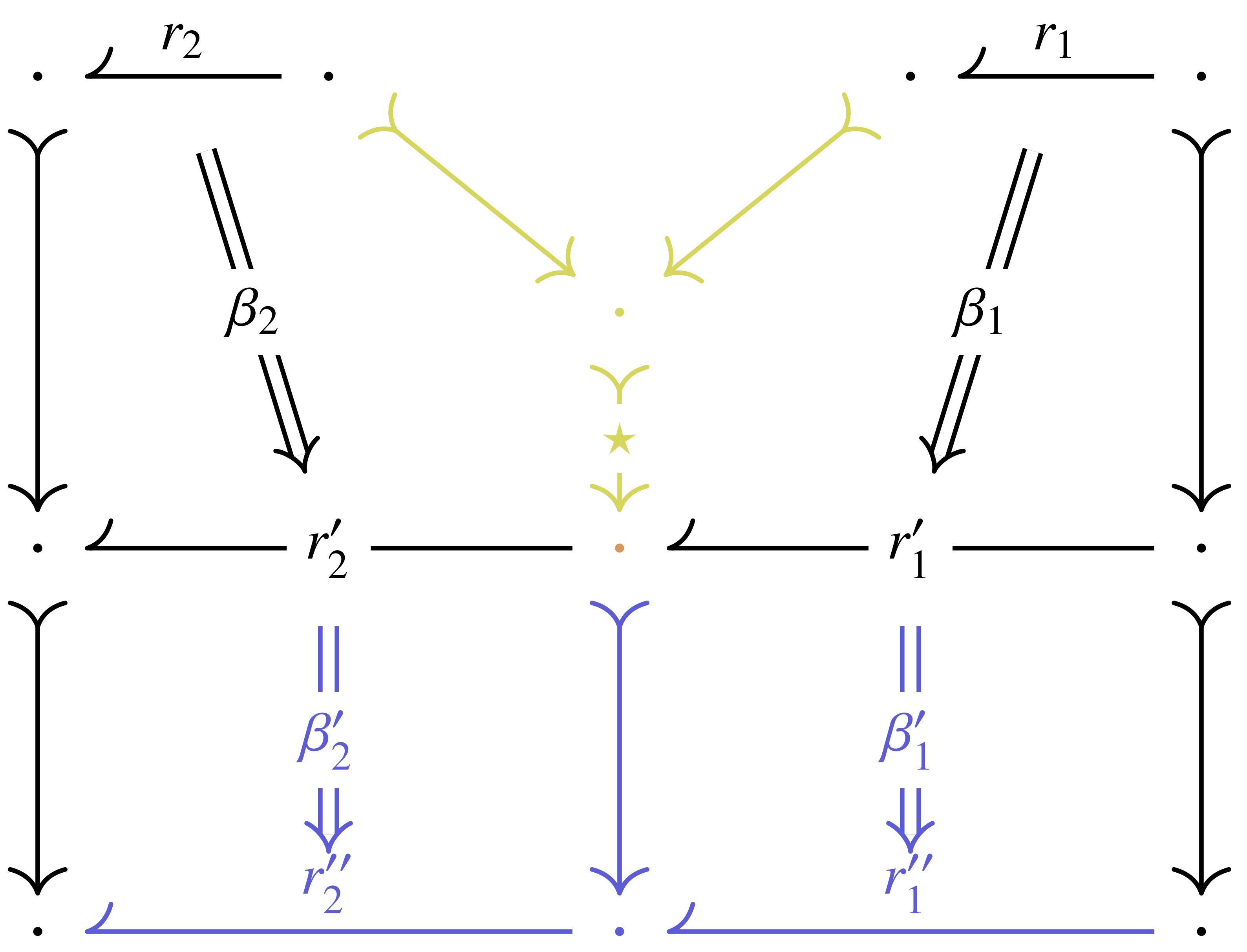
crDCs satisfy a (*universal!*) **Concurrency Theorem — PROOF**



Analysis part: Construct the diagram in (46) as follows:

- By the horizontal decomposition property of squares in $\mathbb{D}$, there exist squares β'_2 and β'_1 such that $\beta_{21} = \beta'_2 \diamond_h \beta'_1$.

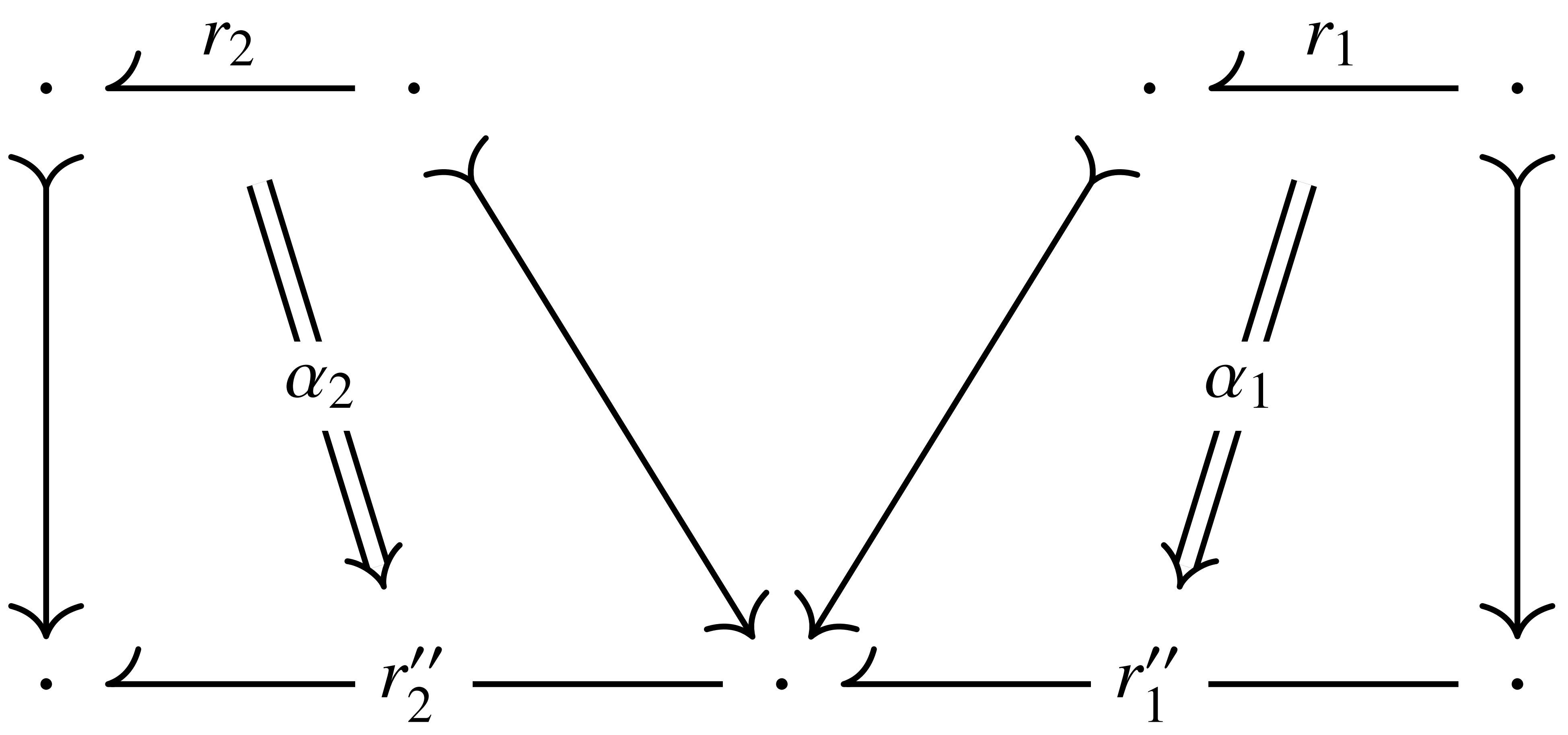
crDCs satisfy a (*universal!*) **Concurrency Theorem — PROOF**



Analysis part: Construct the diagram in (46) as follows:

- By the horizontal decomposition property of squares in $\mathbb{D}$, there exist squares β'_2 and β'_1 such that $\beta_{21} = \beta'_2 \diamond_h \beta'_1$.
- The claim follows be letting $\alpha_i := \beta'_i \diamond_v \beta_i$ for $i = 1, 2$.

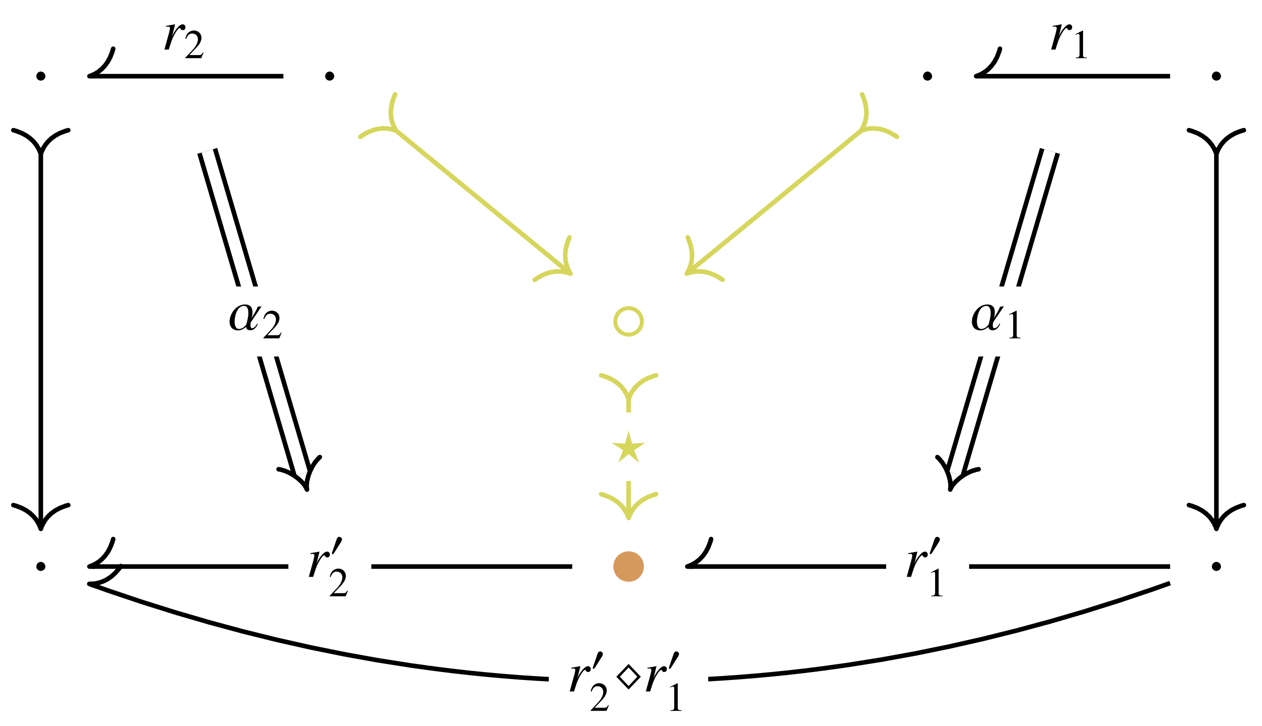
crDCs satisfy a (*universal!*) **Concurrency Theorem — PROOF**



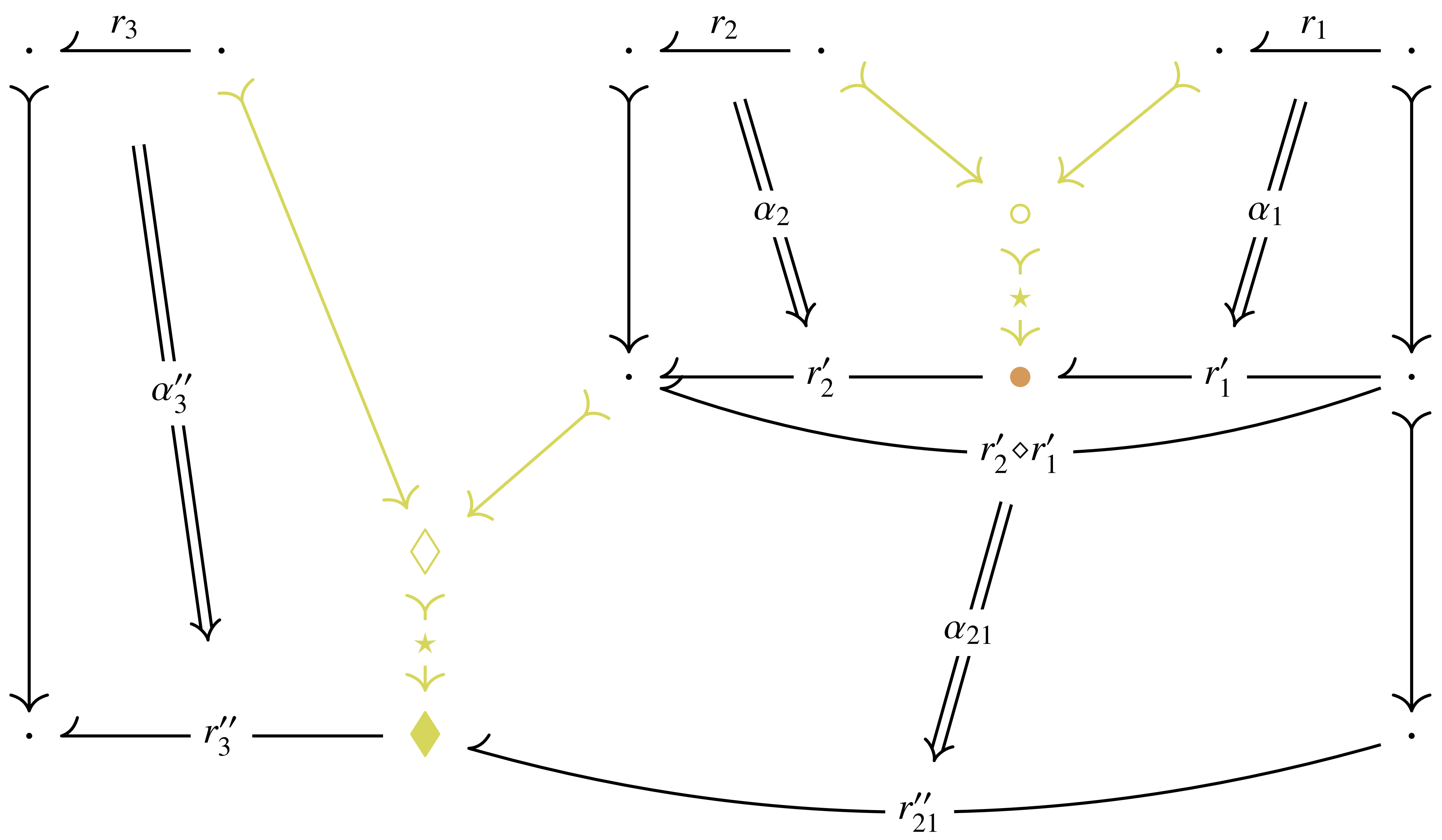
Analysis part: Construct the diagram in (46) as follows:

- By the horizontal decomposition property of squares in $\mathbb{D}$, there exist squares β'_2 and β'_1 such that $\beta_{21} = \beta'_2 \diamond_h \beta'_1$.
- The claim follows be letting $\alpha_i := \beta'_i \diamond_v \beta_i$ for $i = 1, 2$.

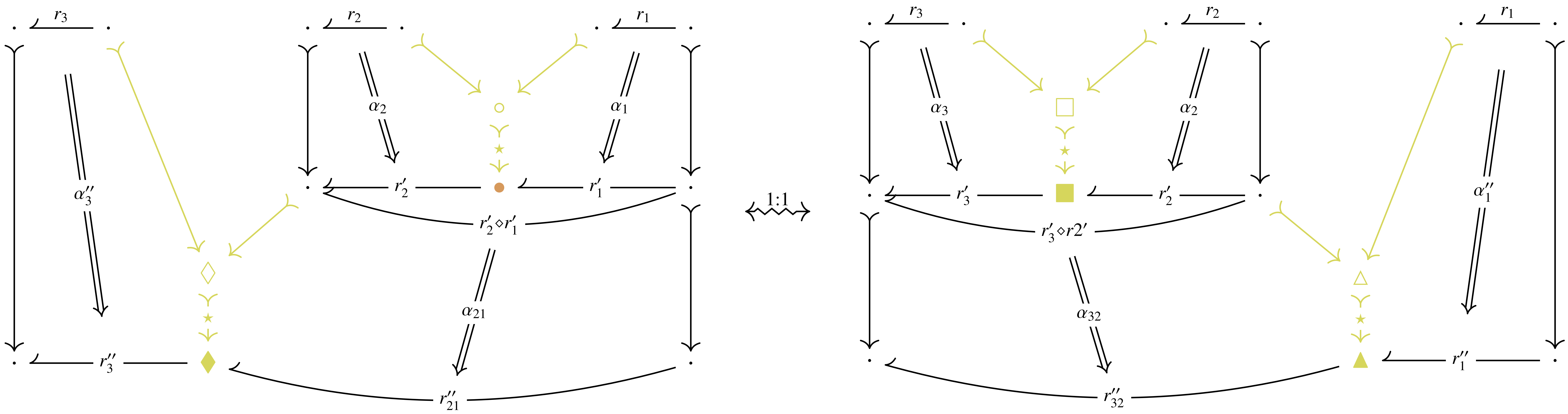
crDCs satisfy a (*universal!*) **Associativity Theorem** (= Thm. 9 in FCRT)



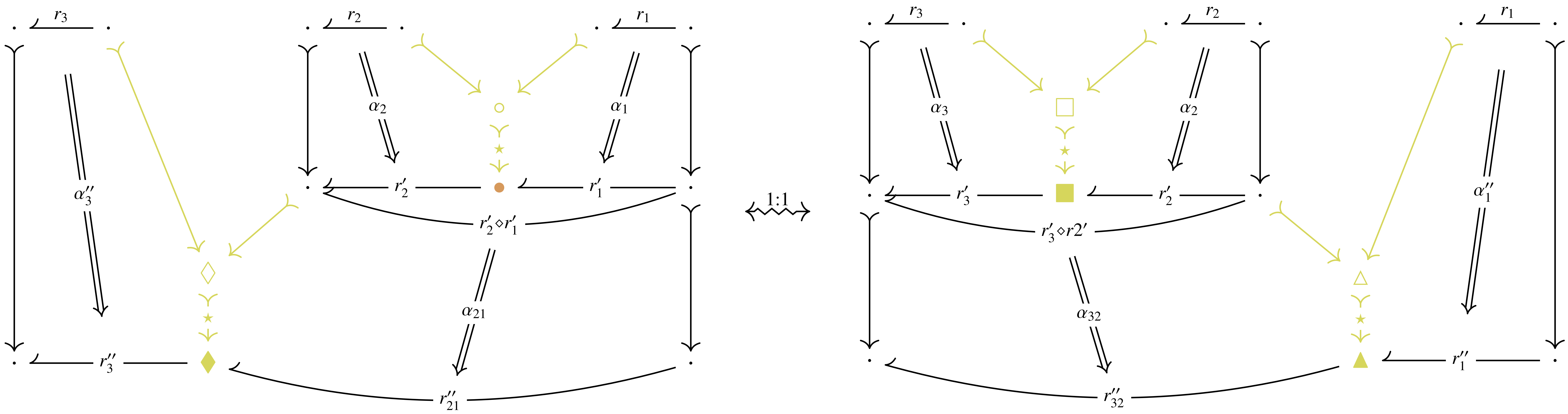
crDCs satisfy a (*universal!*) **Associativity Theorem** (= Thm. 9 in FCRT)



crDCs satisfy a (*universal!*) **Associativity Theorem** (= Thm. 9 in FCRT)



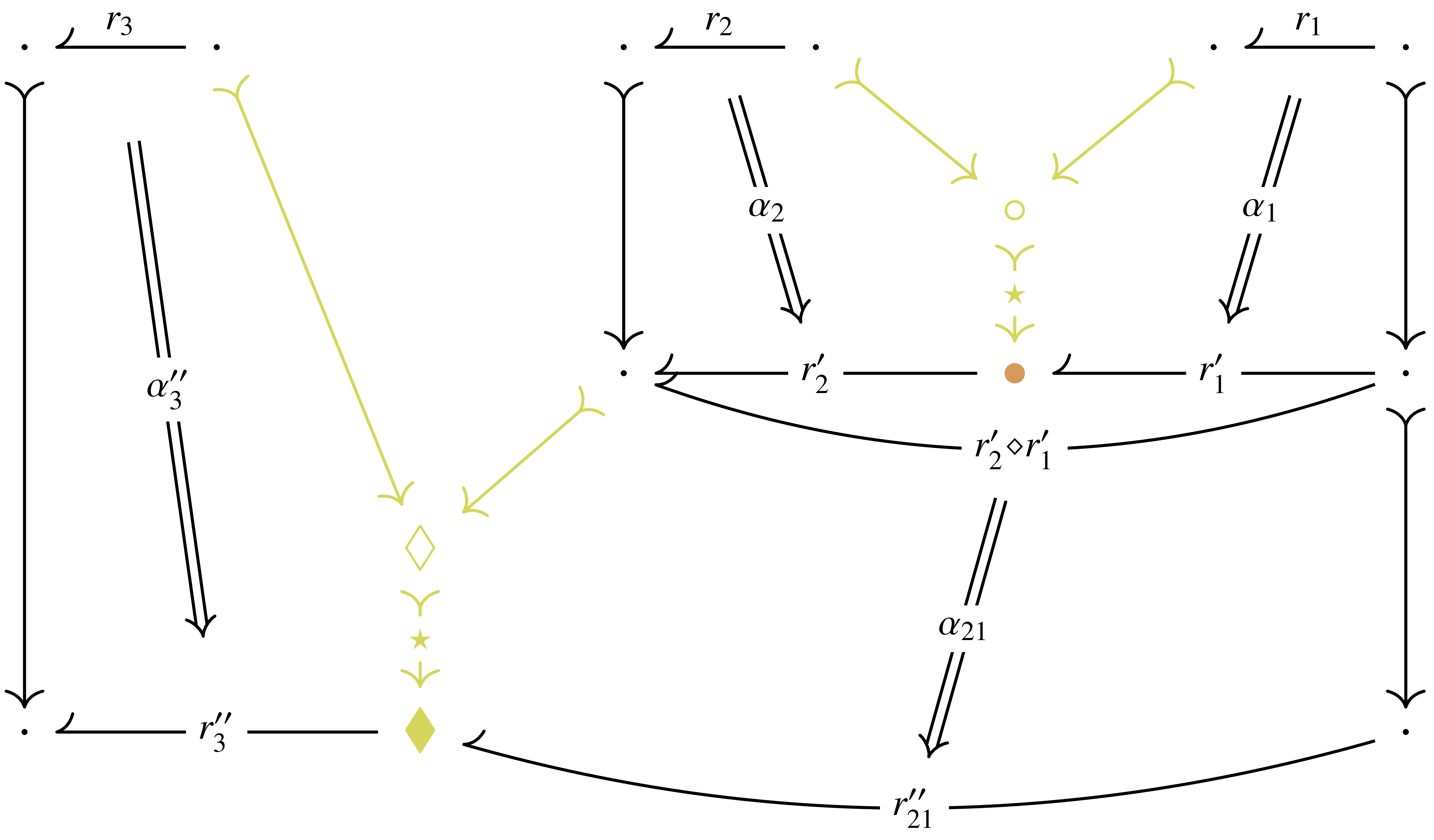
crDCs satisfy a (*universal!*) **Associativity Theorem** (= Thm. 9 in FCRT)



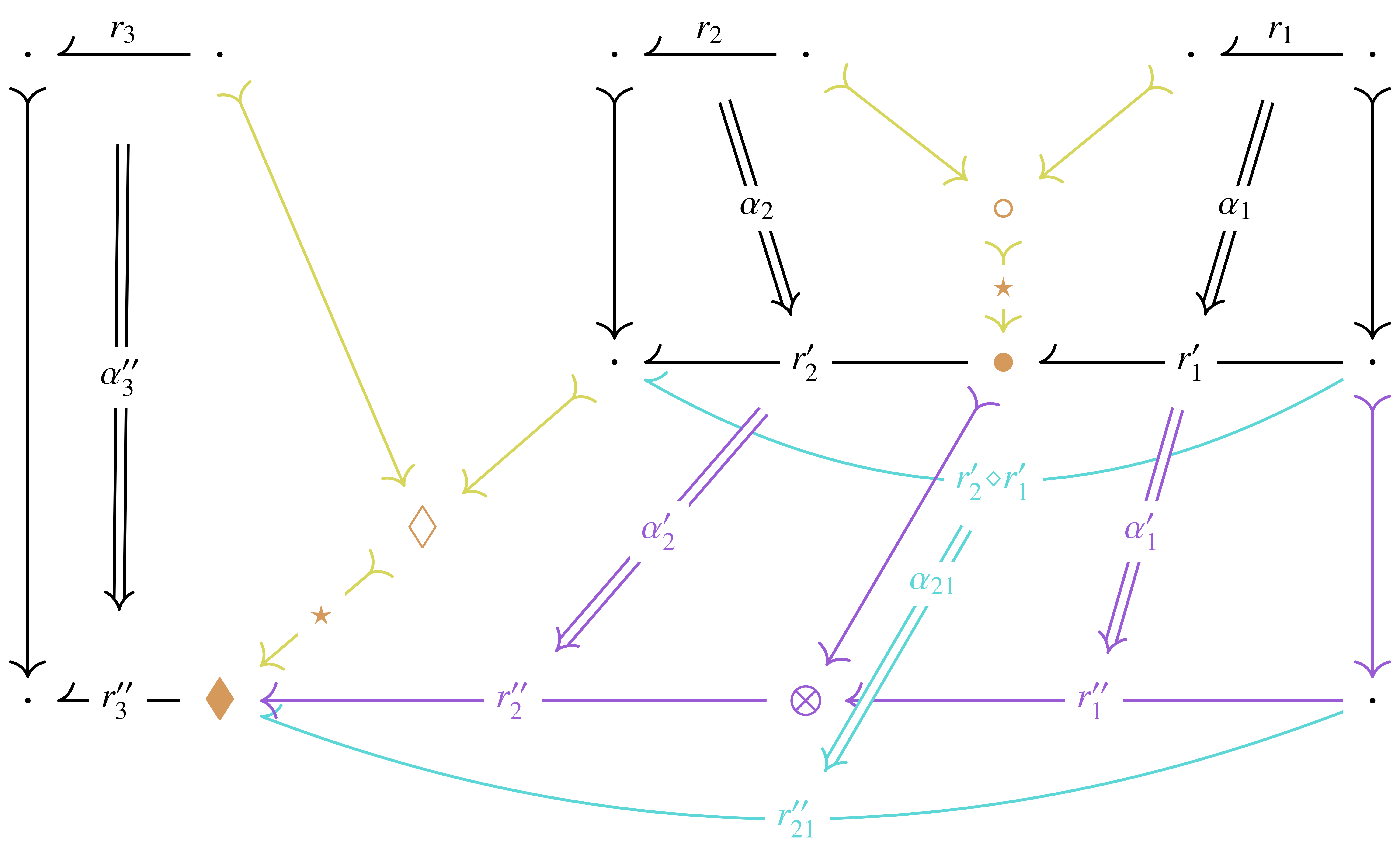
Moreover, the equivalence is such that in addition

$$r_3'' \diamond_h r_{21}'' \cong r_{32}'' \diamond_h r_1'' \,. \tag{49}$$

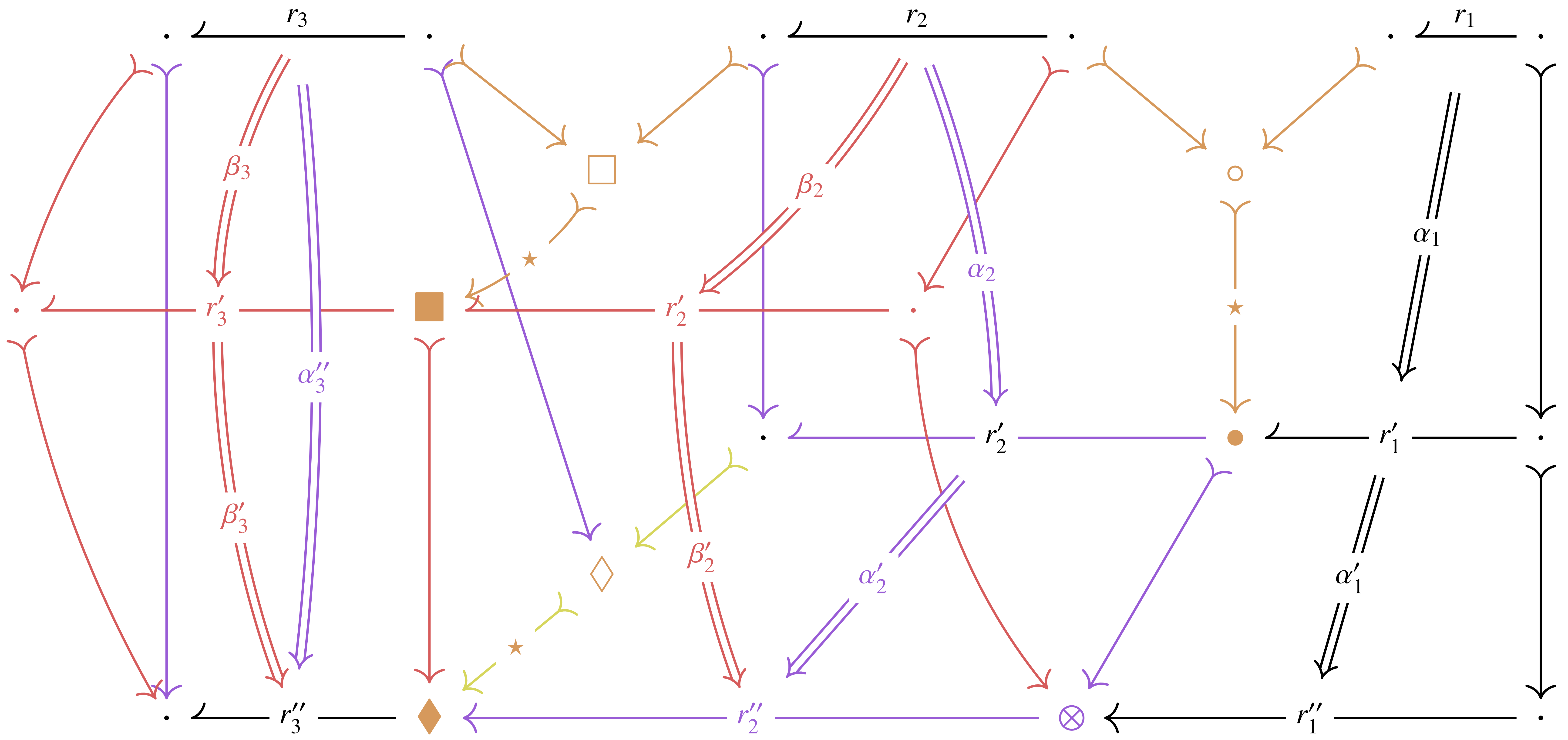
crDCs satisfy a (*universal!*) **Associativity Theorem** — PROOF SKETCH



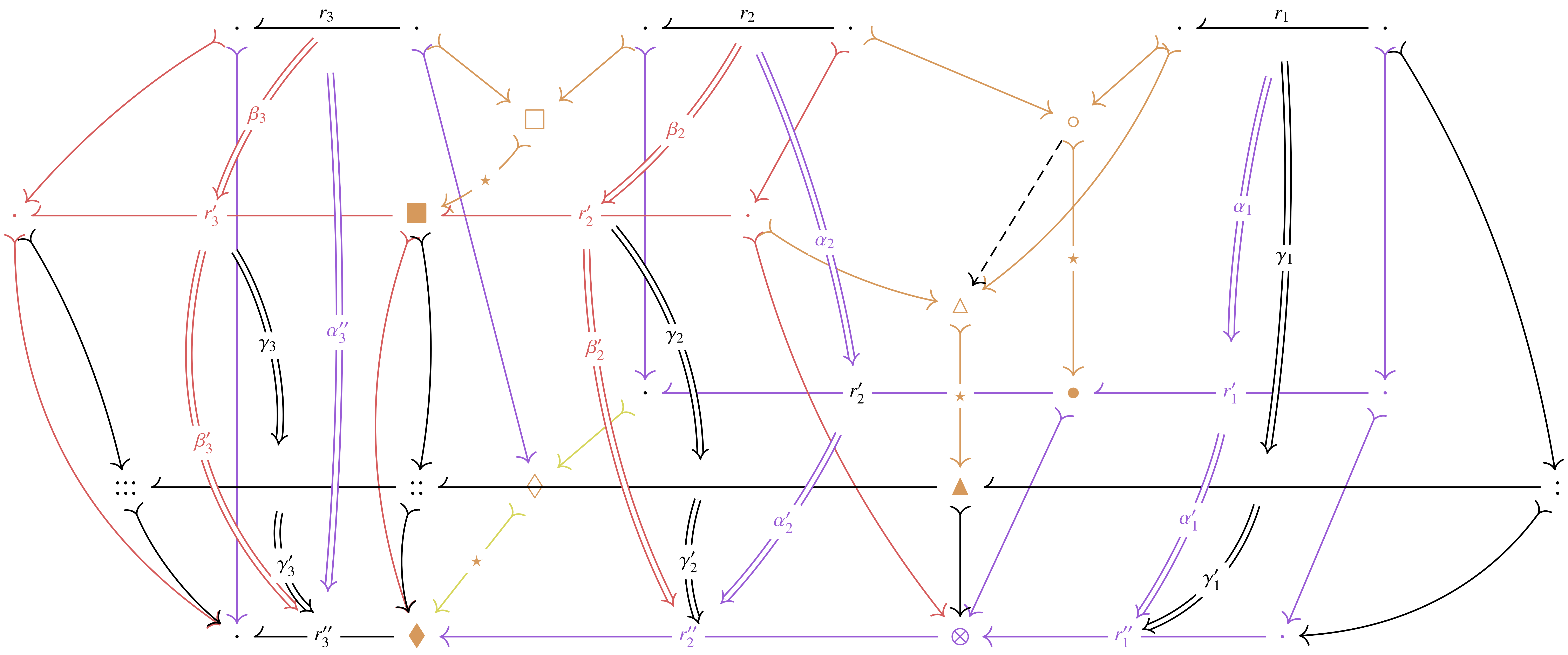
crDCs satisfy a (*universal!*) **Associativity Theorem** — PROOF SKETCH



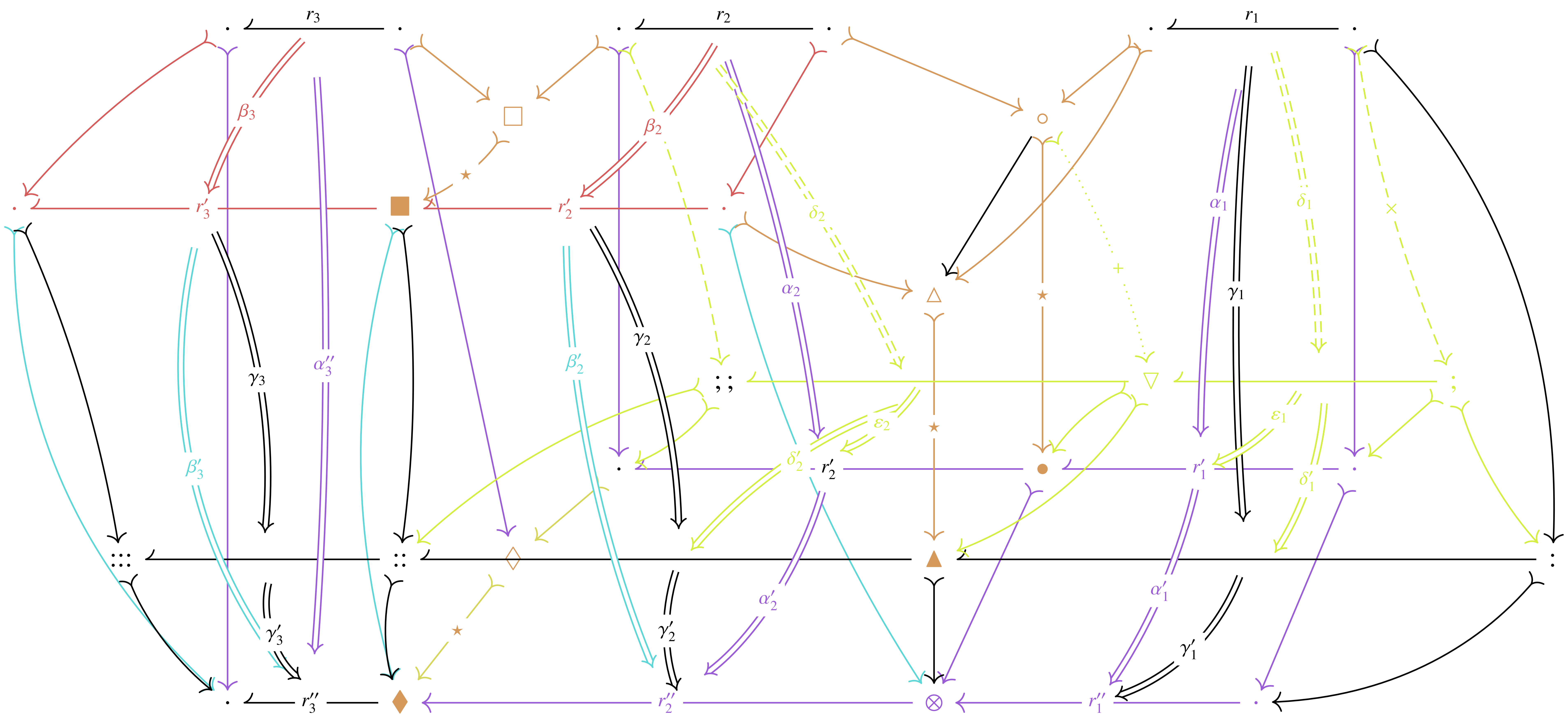
crDCs satisfy a (*universal!*) **Associativity Theorem** — PROOF SKETCH

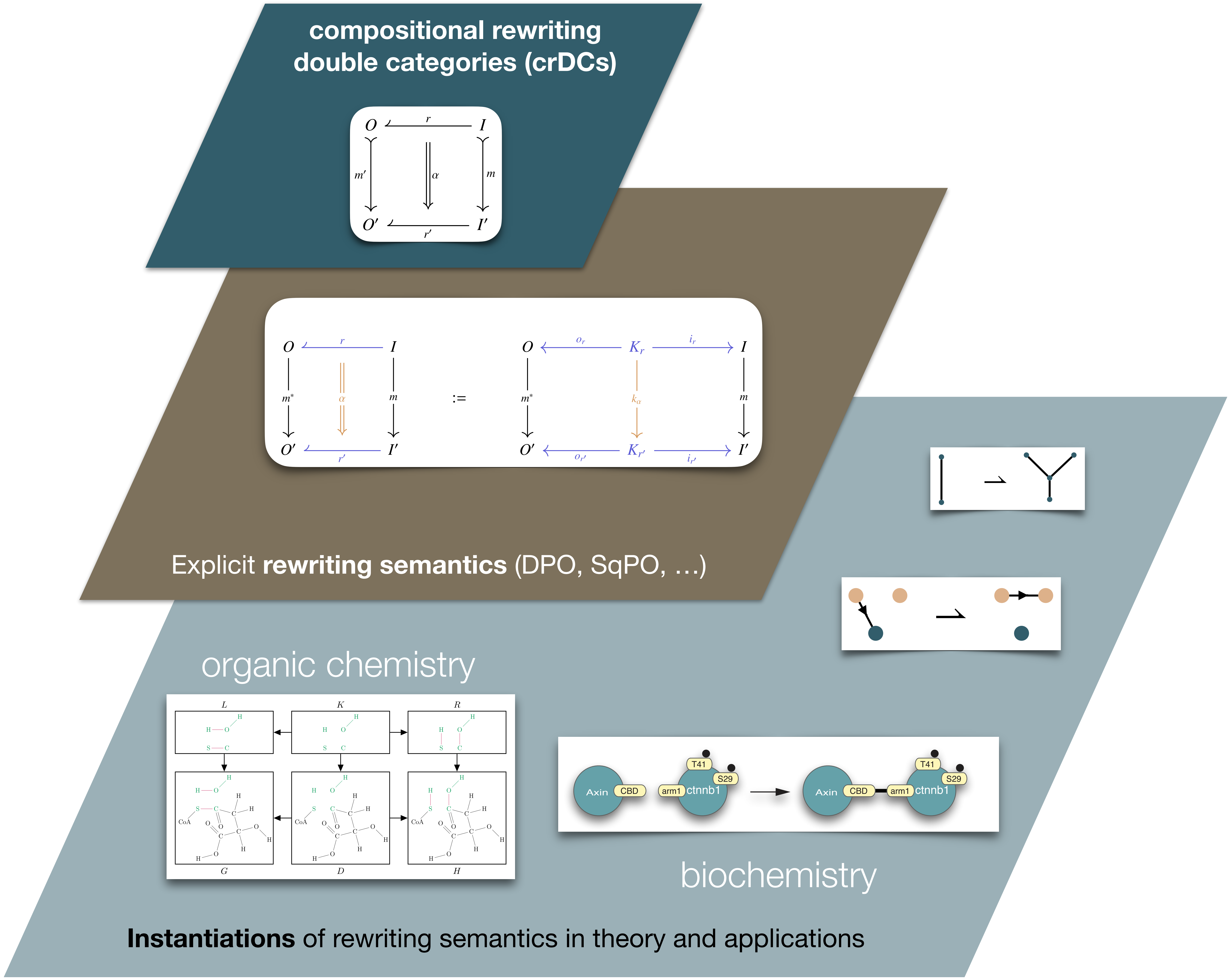


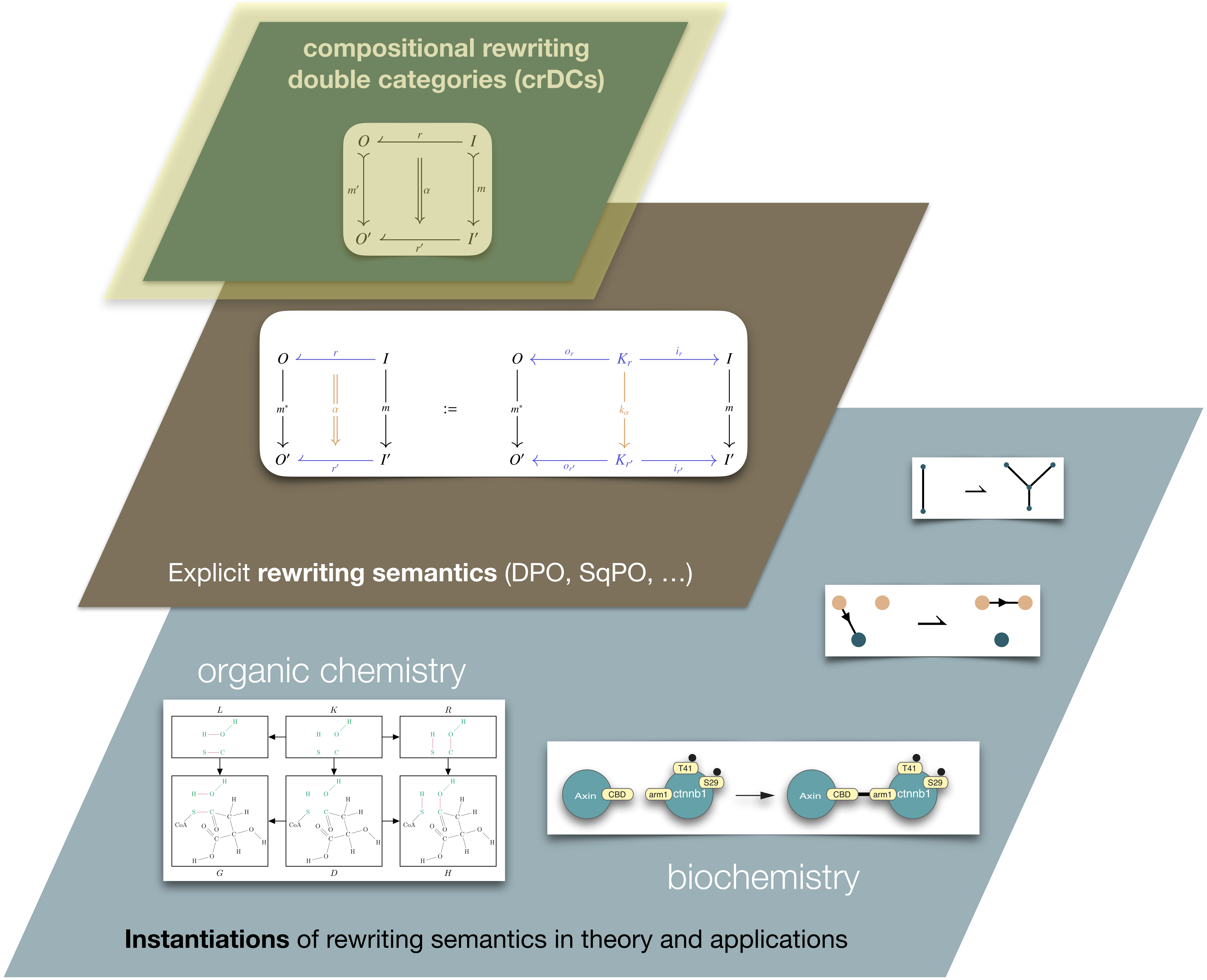
crDCs satisfy a (*universal!*) **Associativity Theorem** — PROOF SKETCH



crDCs satisfy a (*universal!*) **Associativity Theorem** — PROOF SKETCH




compositional rewriting
double categories (crDCs)
O r I
m′ α m
O′ r′ I′
O r I m* α m O′ r′ I′ := O o_r K_r i_r I m* k_α m O′ $o_{r'}$ $K_{r'}$ $i_{r'}$ I′
Explicit **rewriting semantics** (DPO, SqPO, …)
organic chemistry
L K R
G D H
CoA
Axin CBD arm1 ctnnb1 T41 S29
biochemistry
Instantiations of rewriting semantics in theory and applications

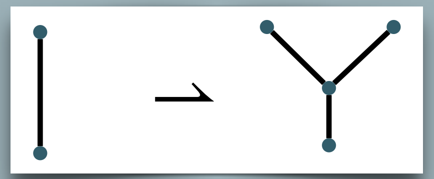

compositional rewriting
double categories (crDCs)
O
r
I
m′
α
m
O′
r′
I′
O
r
I
m*
α
m
O′
r′
I′
:=
O
o_r
K_r
i_r
I
m*
k_α
m
O′
o_r′
K_r′
i_r′
I′
Explicit **rewriting semantics** (DPO, SqPO, …)
organic chemistry
L
K
R
G
D
H
Axin
CBD
arm1
ctnnb1
T41
S29
biochemistry
Instantiations of rewriting semantics in theory and applications

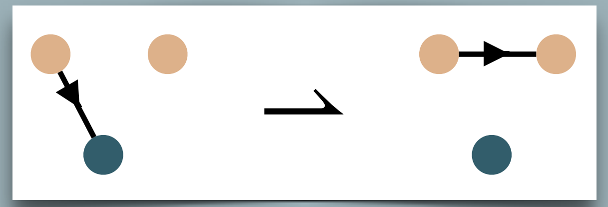
compositional rewriting double categories (crDCs)

$$
\begin{array}{ccc}
O & \xleftarrow{\;r\;} & I \\
{\scriptstyle m'}\downarrow & \Downarrow{\scriptstyle \alpha} & \downarrow{\scriptstyle m} \\
O' & \xleftarrow[\;r'\;]{} & I'
\end{array}
$$

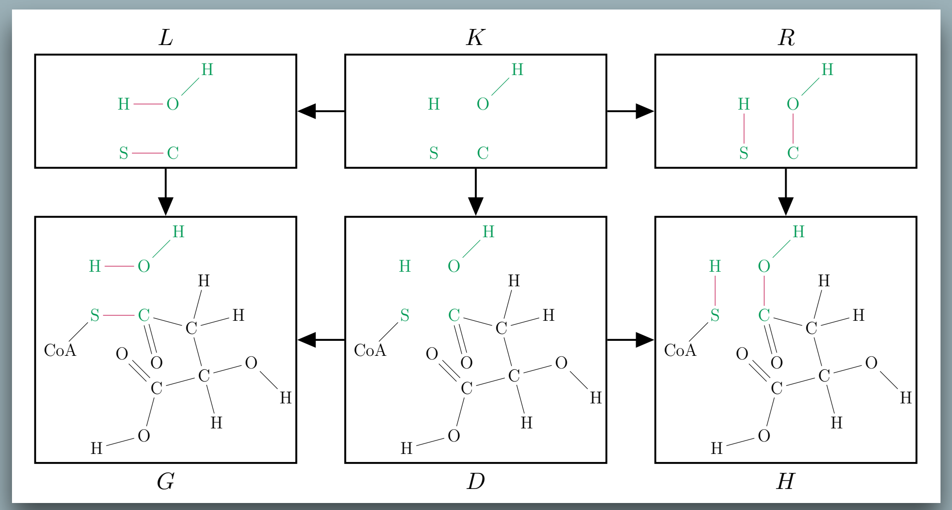
$$
\begin{array}{ccc}
O & \xleftarrow{\;r\;} & I \\
{\scriptstyle m^*}\downarrow & \Downarrow{\scriptstyle \alpha} & \downarrow{\scriptstyle m} \\
O' & \xleftarrow[\;r'\;]{} & I'
\end{array}
\quad := \quad
\begin{array}{ccccc}
O & \xleftarrow{\;o_r\;} & K_r & \xrightarrow{\;i_r\;} & I \\
{\scriptstyle m^*}\downarrow & & \downarrow{\scriptstyle k_\alpha} & & \downarrow{\scriptstyle m} \\
O' & \xleftarrow[\;o_{r'}\;]{} & K_{r'} & \xrightarrow[\;i_{r'}\;]{} & I'
\end{array}
$$

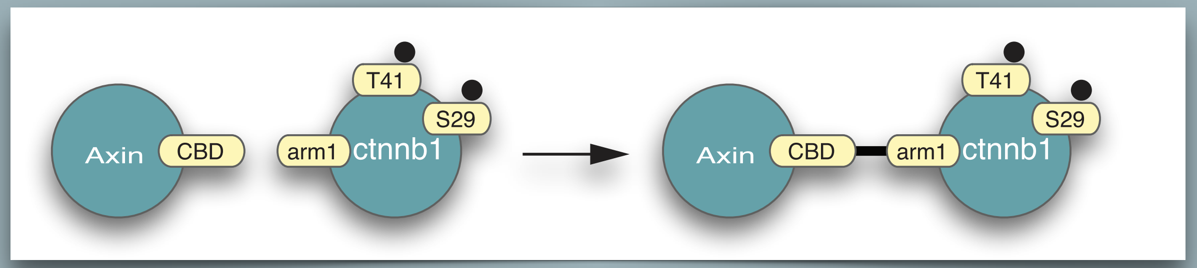
Explicit **rewriting semantics** (DPO, SqPO, …)





organic chemistry

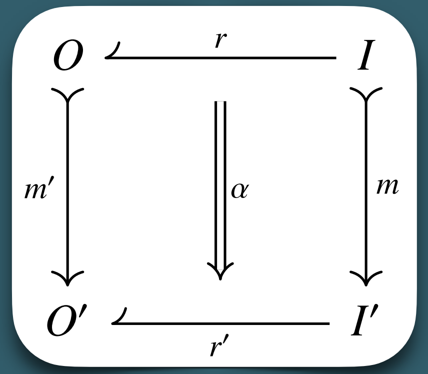


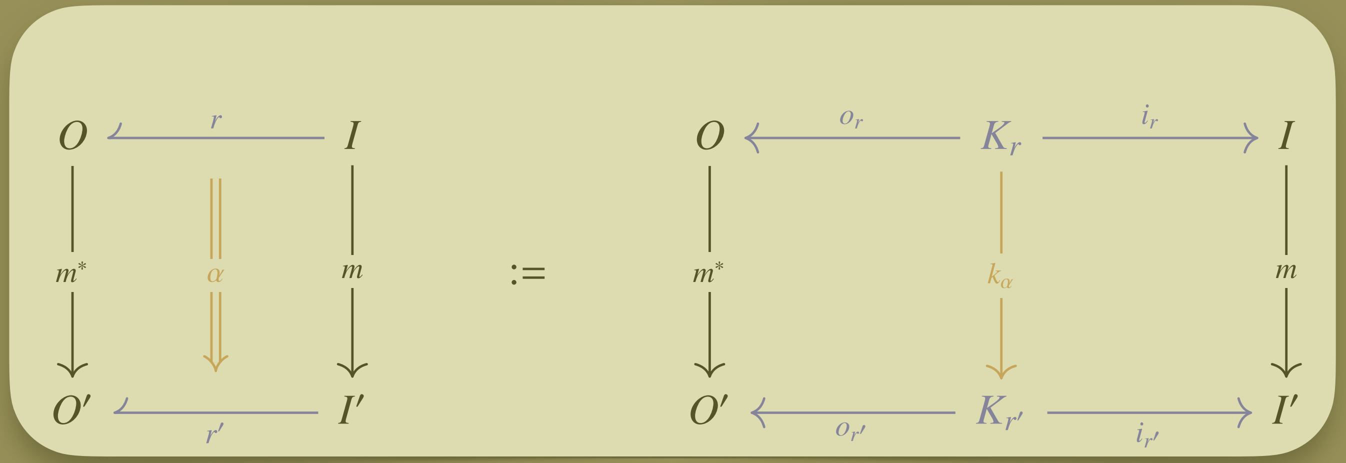


biochemistry

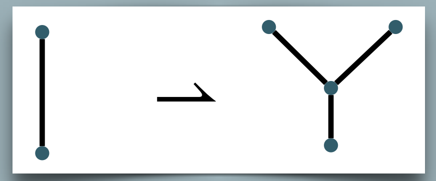
Instantiations of rewriting semantics in theory and applications

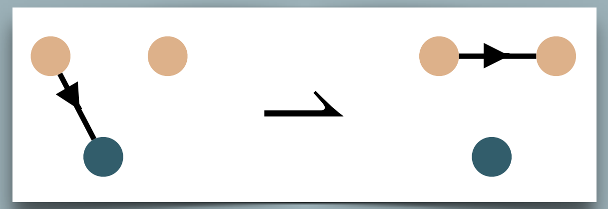
compositional rewriting double categories (crDCs)



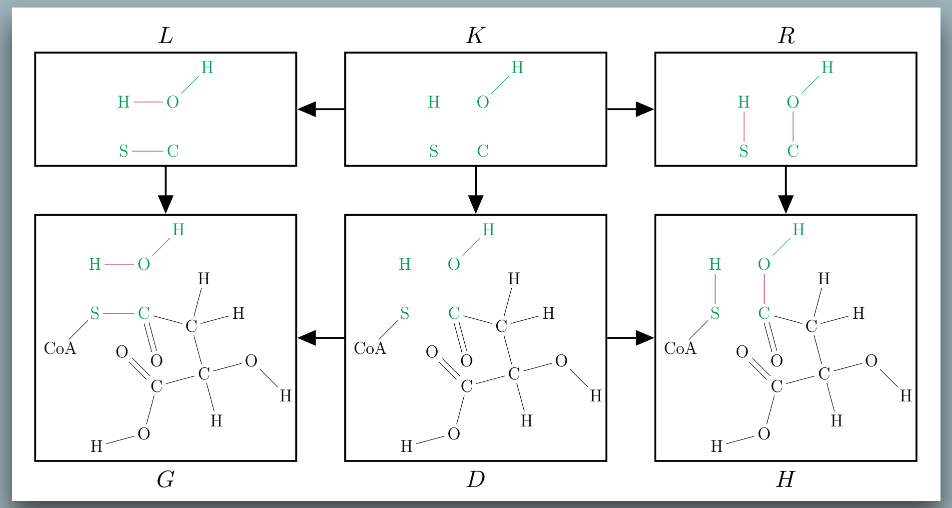


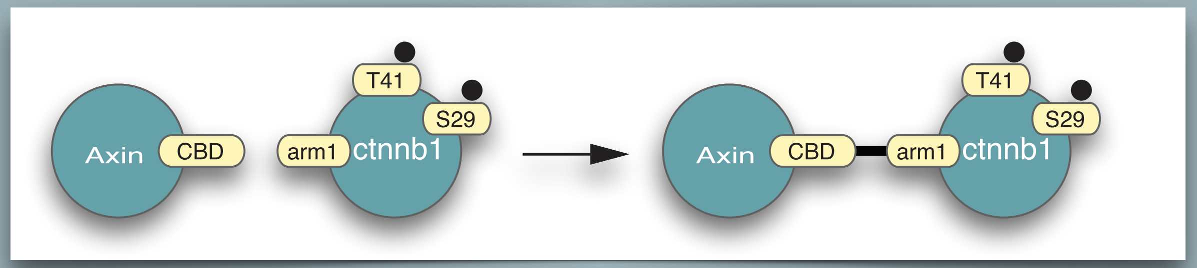
Explicit **rewriting semantics** (DPO, SqPO, …)





organic chemistry





biochemistry

Instantiations of rewriting semantics in theory and applications

Stable system of monics

Definition 5 ([35], Sec. 3.1). For a category $\mathbf{C}$, a stable system of monics $\mathcal{M}$ is a class of monomorphisms of $\mathbf{C}$ that

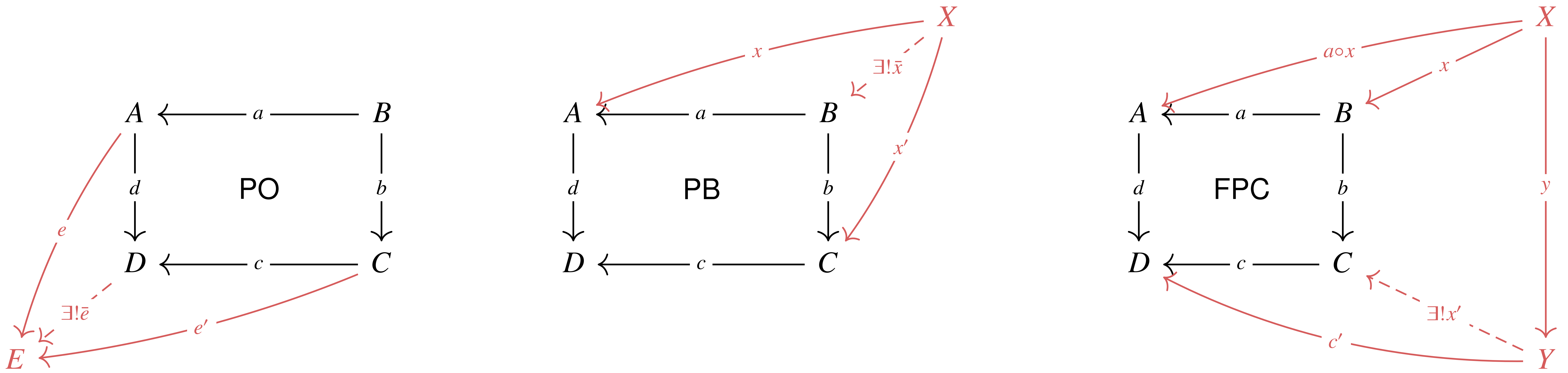
(i) *includes all isomorphisms*,

(ii) is *stable under composition*, and

(iii) is *stable under pullback* (i.e., if (f', m') is a pullback of (m, f) with $m \in \mathcal{M}$, then $m' \in \mathcal{M}$).

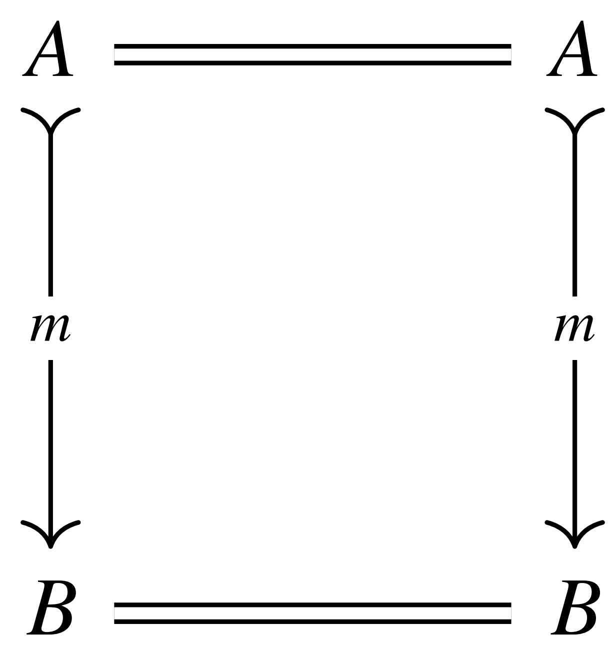
Throughout this paper, we will reserve the notation $\rightarrowtail$ for monics in $\mathcal{M}$, and $\hookrightarrow$ for generic monics.

Some **universal constructions**

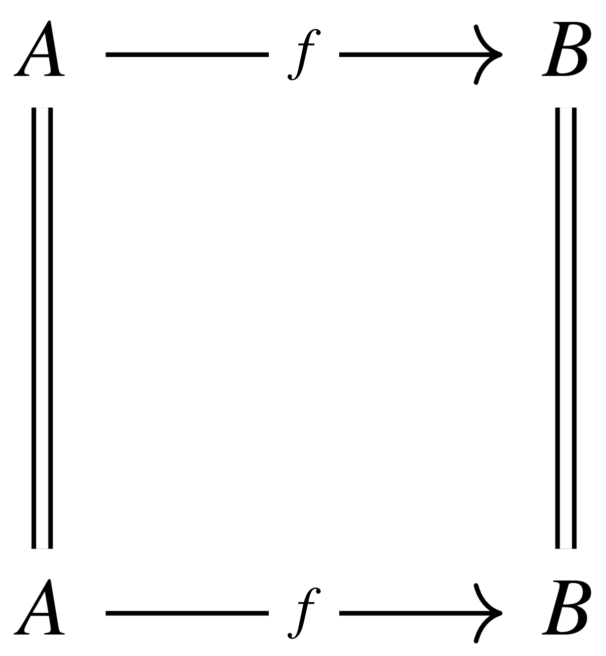


Some **universal constructions**

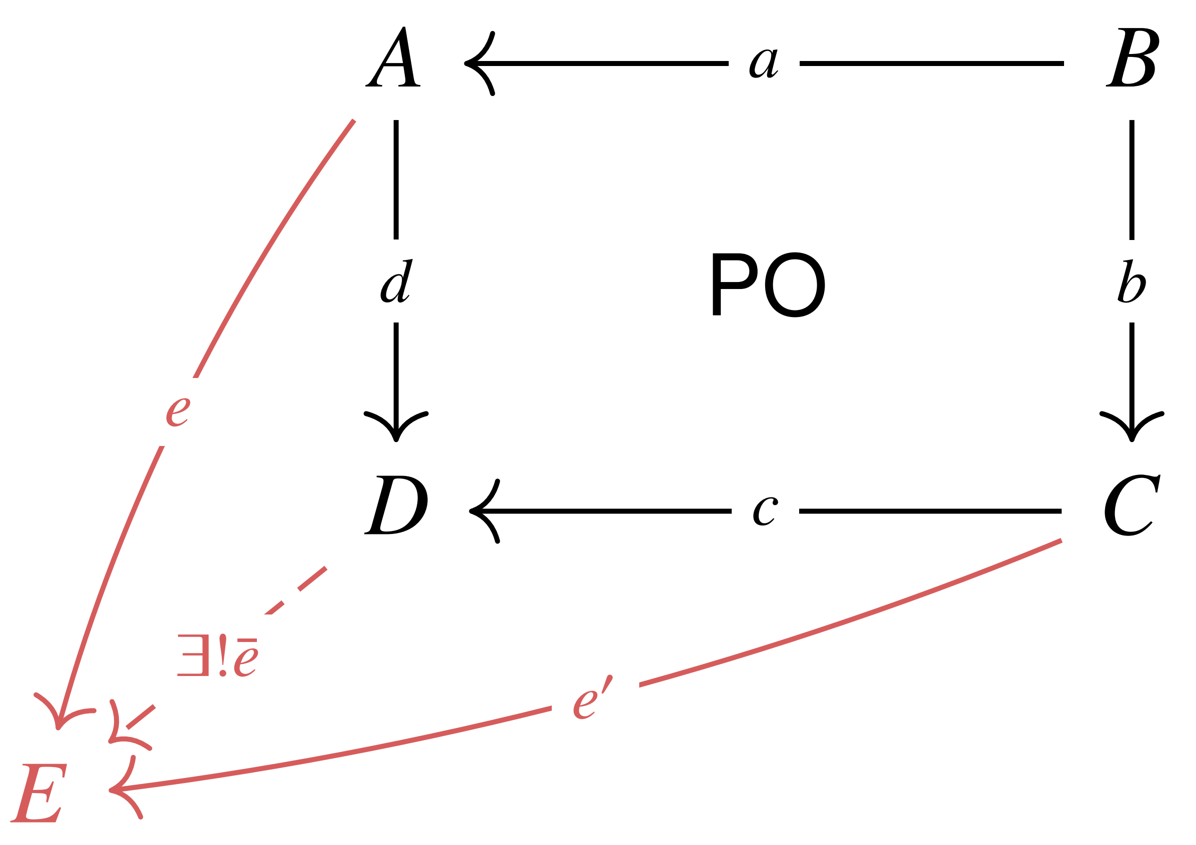
$(id_m) :=$

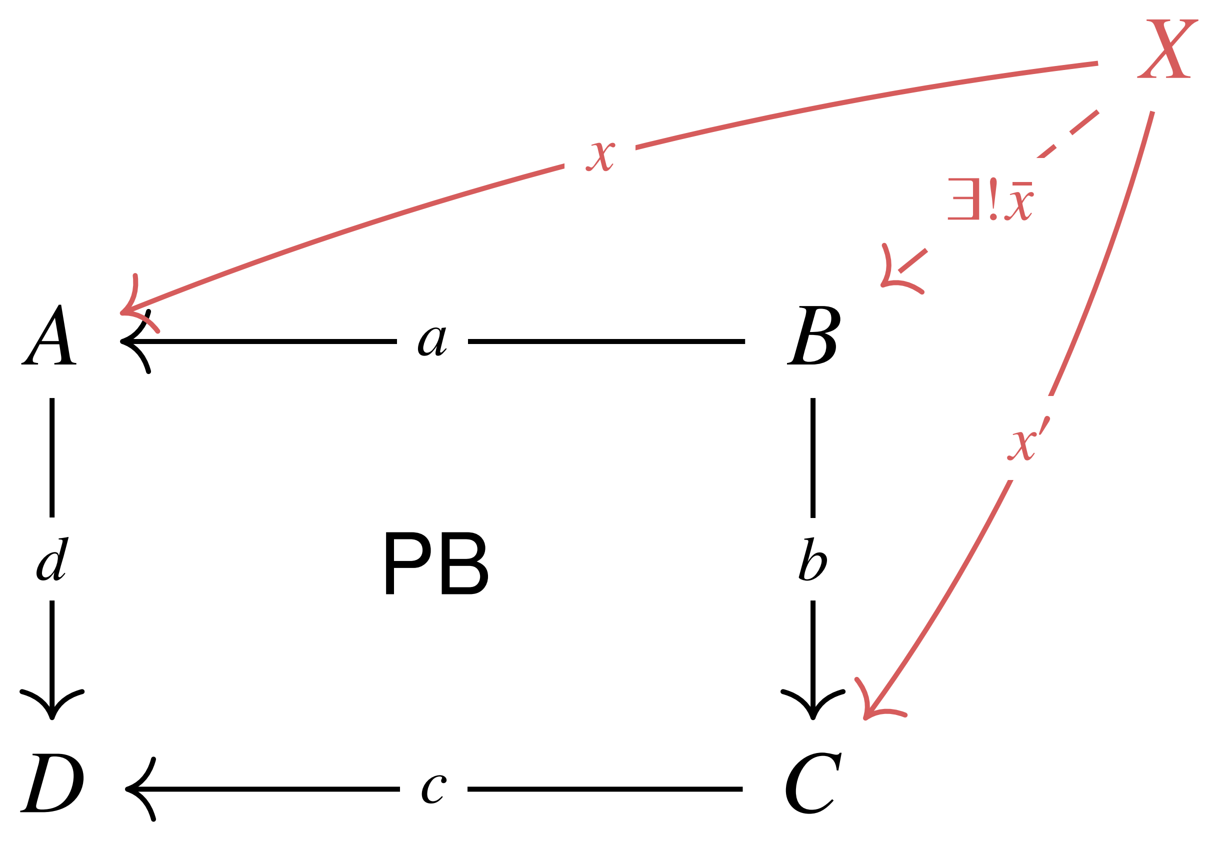


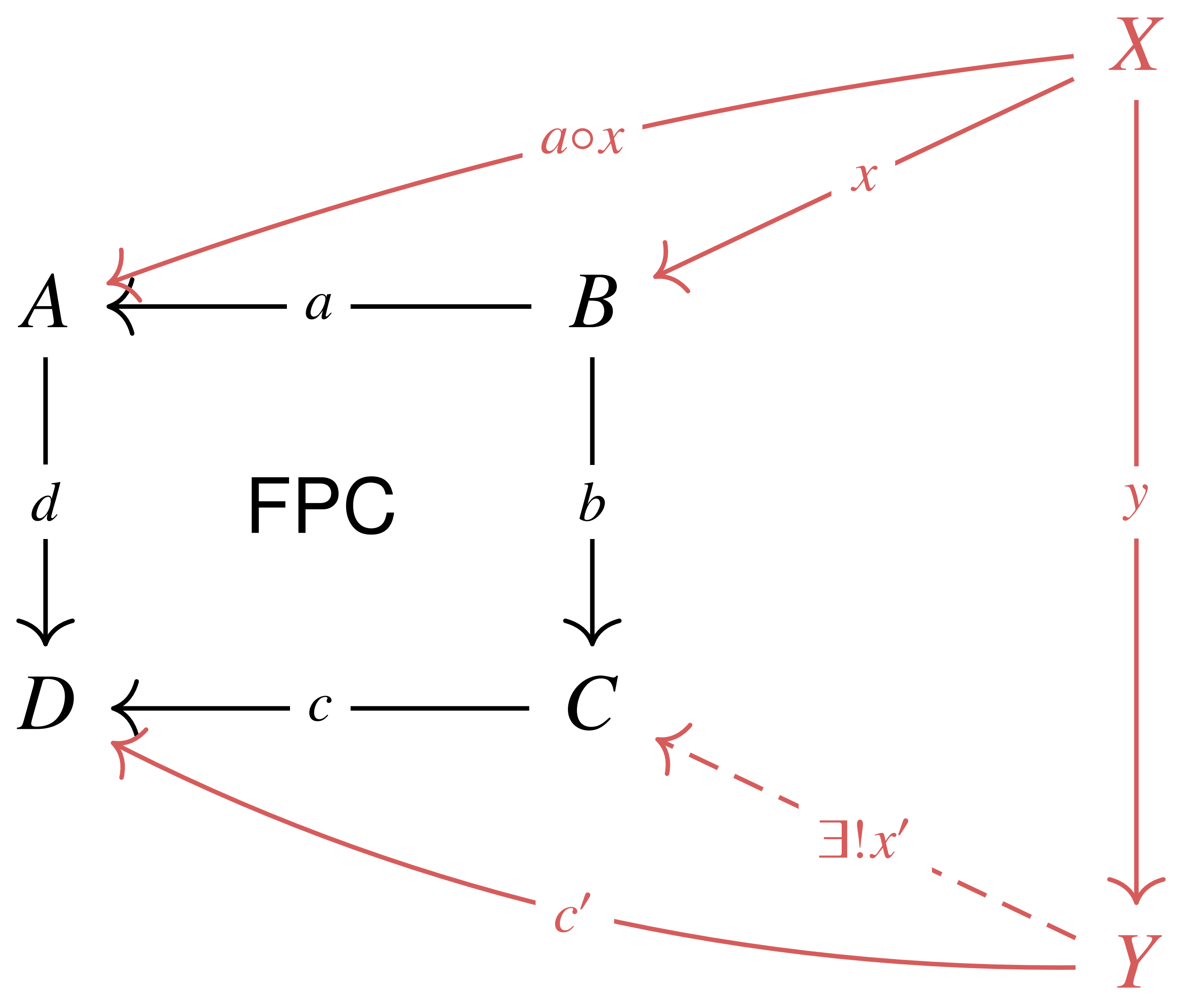
$id_f :=$



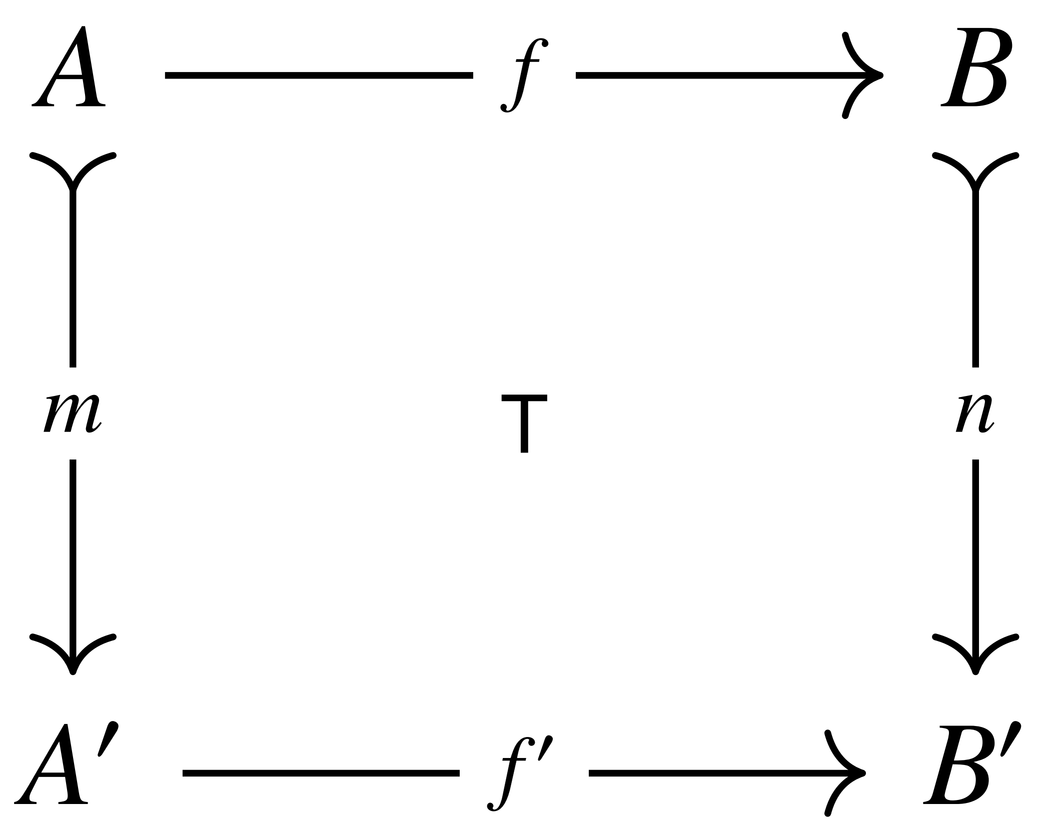
(simultaneously **PBs**, **POs** and **FPCs**)







“Vertical” and “horizontal” categories of **PBs**, **POs** and **FPCs**

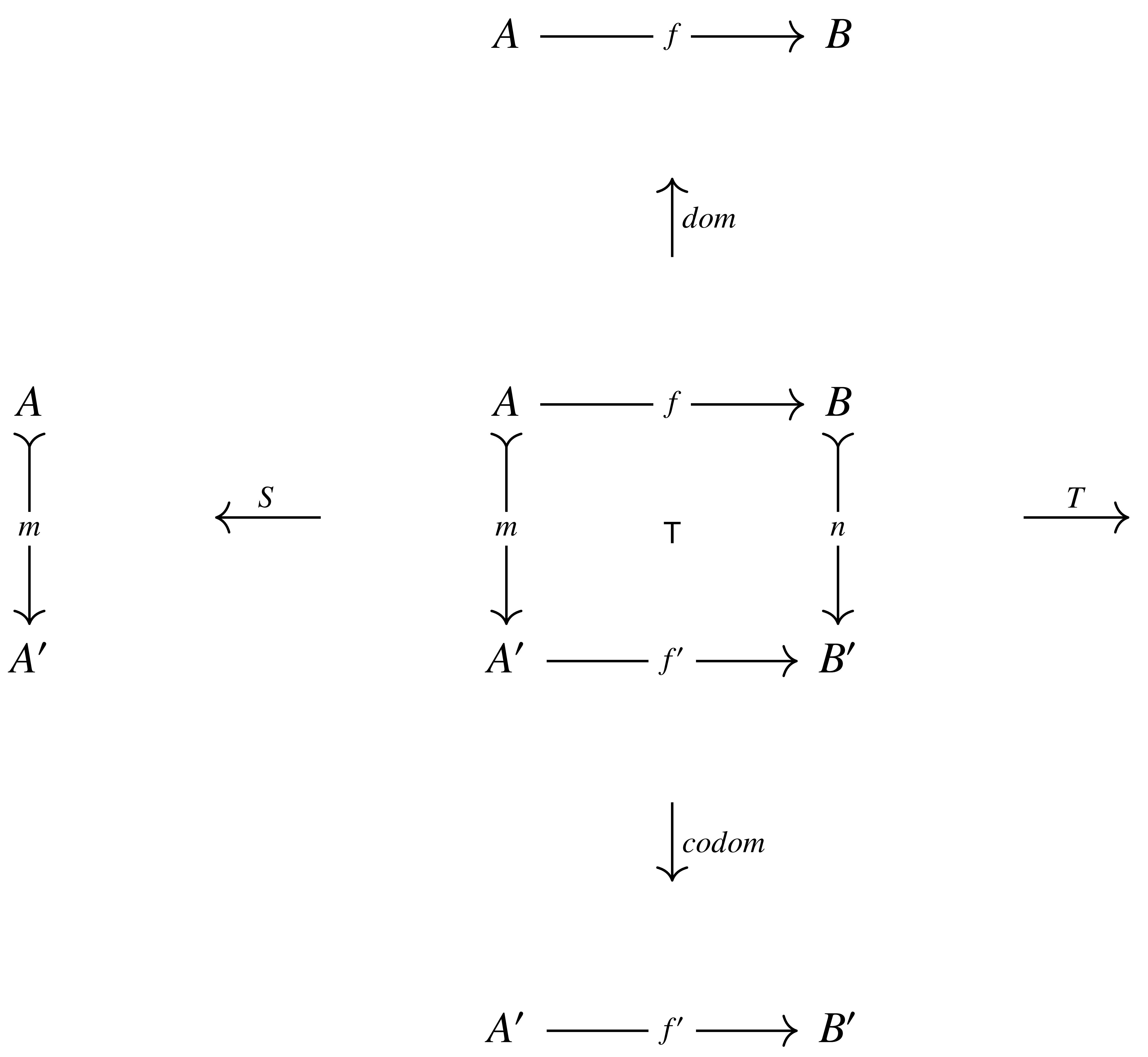


Definition 7. Let $\mathbf{C}$ be a category with a stable system of monics $\mathcal{M}$ that has pullbacks along $\mathcal{M}$-morphisms. Let T be a type of commutative squares, for which we consider PB (pullbacks), PO (pushouts), or FPC (final pullback complements). Then we define the following categories:

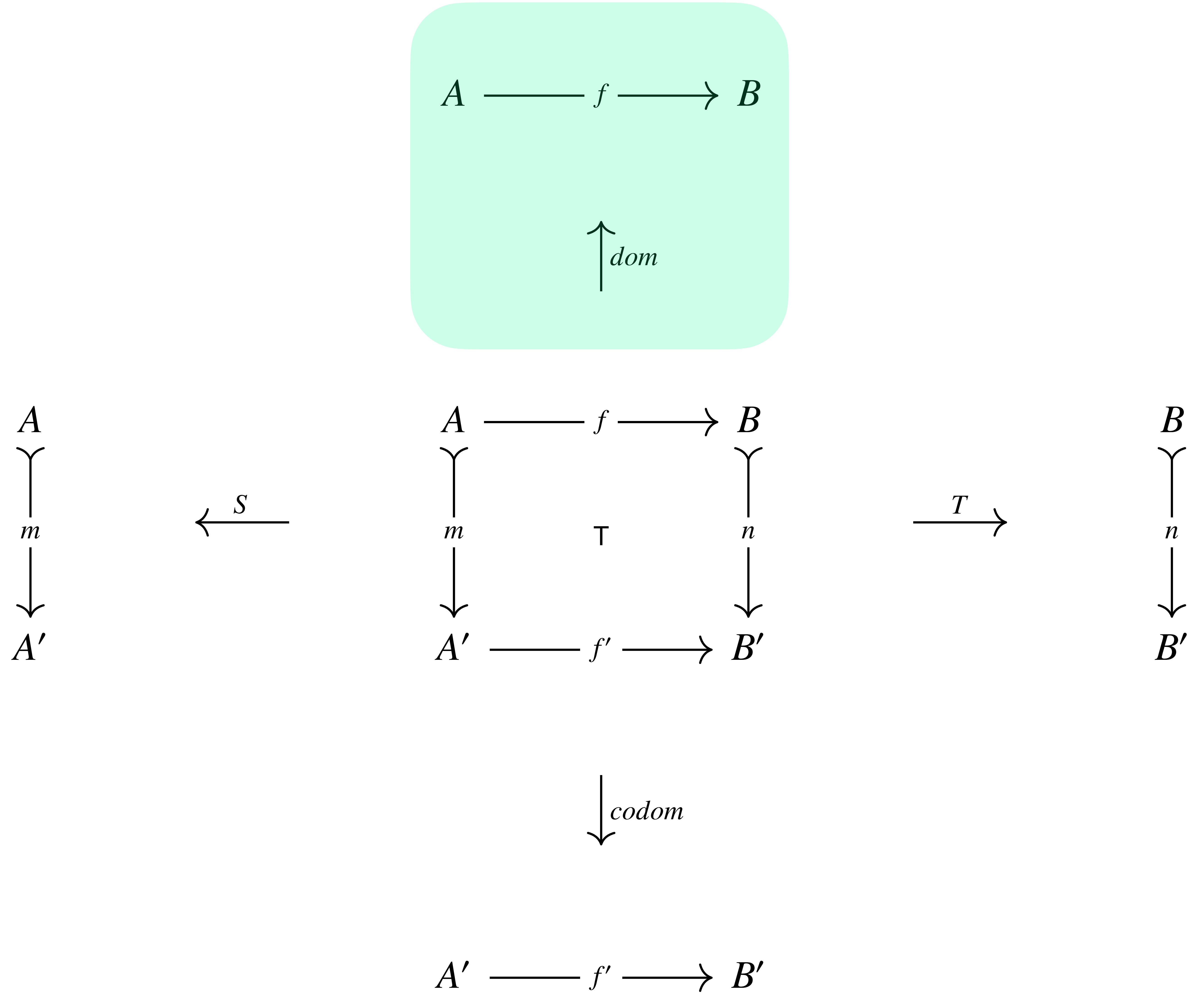
(i) $\mathsf{T}_h(\mathbf{C}, \mathcal{M})$ has as objects the morphisms of $\mathcal{M}$, and as morphisms commutative squares of type T along arbitrary morphisms of $\mathbf{C}$, and a morphism composition induced by *horizontal pasting* of squares of type T.

(ii) $\mathsf{T}_v(\mathbf{C}, \mathcal{M})$ has as objects the morphisms of $\mathbf{C}$, and as morphisms commutative squares of type T along $\mathcal{M}$-morphisms, and a morphism composition induced by *vertical pasting* of squares of type T.

Boundary functors



Boundary functors



Fibrational properties of the **domain functors** (suggested by *R. Garner*)

Theorem 1. *Let* $\mathbf{C}$ *be a category with a stable system of monics* $\mathcal{M}$*, and with the following additional properties:*

1. $\mathbf{C}$ *has pullbacks.*
2. $\mathbf{C}$ *has pushouts and final pullback complements (FPCs) along* $\mathcal{M}$*-morphisms.*
3. *Pushouts along* $\mathcal{M}$*-morphisms are* stable under pullbacks.
4. Pushouts along $\mathcal{M}$-morphisms are pullbacks.

Then the domain functor $dom : \mathsf{PB}_h(\mathbf{C}, \mathcal{M}) \to \mathbf{C}$ *from the category of pullback squares along* $\mathcal{M}$*-morphisms and under horizontal composition to the underlying category* $\mathbf{C}$ *satisfies the following properties:*[8]

(i) $dom : \mathsf{PB}_h(\mathbf{C}, \mathcal{M}) \to \mathbf{C}$ *is a Grothendieck fibration, with the Cartesian liftings given by FPCs.*

(ii) $dom : \mathsf{PB}_h(\mathbf{C}, \mathcal{M}) \to \mathbf{C}$ *is a Grothendieck opfibration, with the op-Cartesian liftings given by pushouts.*

Fibrational properties of the **domain functors** (suggested by *R. Garner*)

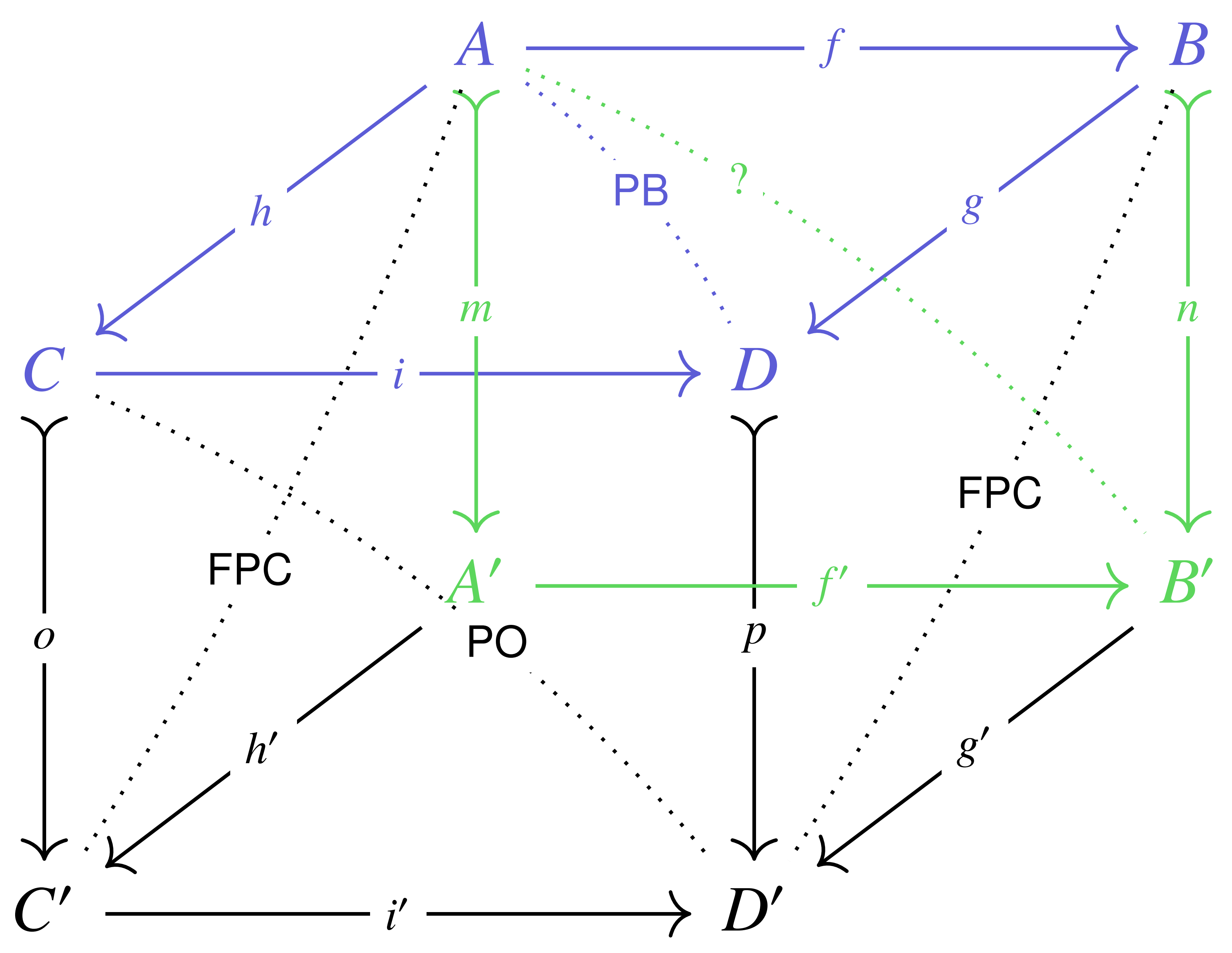
(iii) *dom* : $\mathsf{PB}_h(\mathbf{C}, \mathcal{M}) \to \mathbf{C}$ satisfies a Beck-Chevalley condition (BCC): *adopting the notation $m - (f, f') \to n$ for morphisms in $\mathsf{PB}_h(\mathbf{C}, \mathcal{M})$ (cf. Figure 1), consider a commutative square in $\mathsf{PB}_h(\mathbf{C}, \mathcal{M})$ that is mapped by dom into a pullback square in $\mathbf{C}$:*

$$
\begin{array}{ccc}
m & \xrightarrow{(f,f')} & n \\
{\scriptstyle (h.h')}\downarrow & & \downarrow{\scriptstyle (g,g')} \\
o & \xrightarrow[(i,i')]{} & p
\end{array}
\quad \overset{}{\underset{dom}{\longmapsto}} \quad
\begin{array}{ccc}
A & \xrightarrow{f} & B \\
{\scriptstyle h}\downarrow & \mathsf{PB} & \downarrow{\scriptstyle g} \\
C & \xrightarrow[i]{} & D
\end{array}
\tag{20}
$$

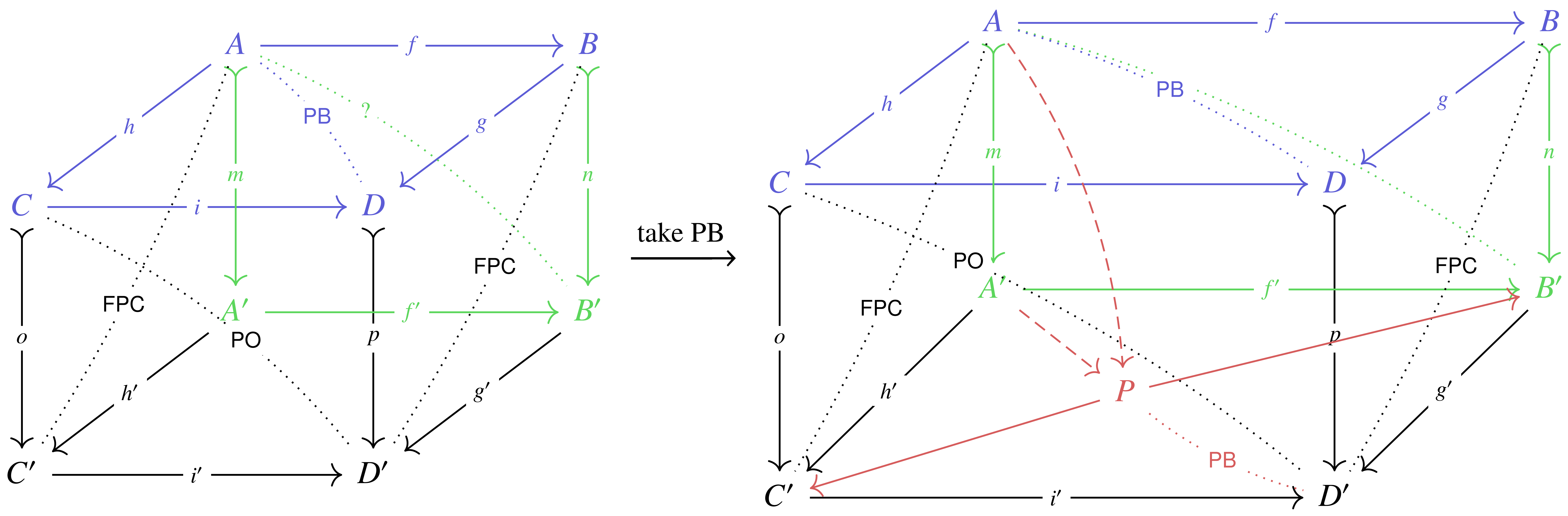
Then the following two equivalent conditions hold:

- (BCC-1): *(f, f') is op-Cartesian if (i, i') is op-Cartesian and (g, g') and (h, h') are Cartesian.*
- (BCC-2): *(g, g') is Cartesian if (h, h') is Cartesian and (f, f') and (i, i') are op-Cartesian.*

Fibrational properties of the **domain functors** (suggested by *R. Garner*)



Fibrational properties of the **domain functors** (suggested by *R. Garner*)



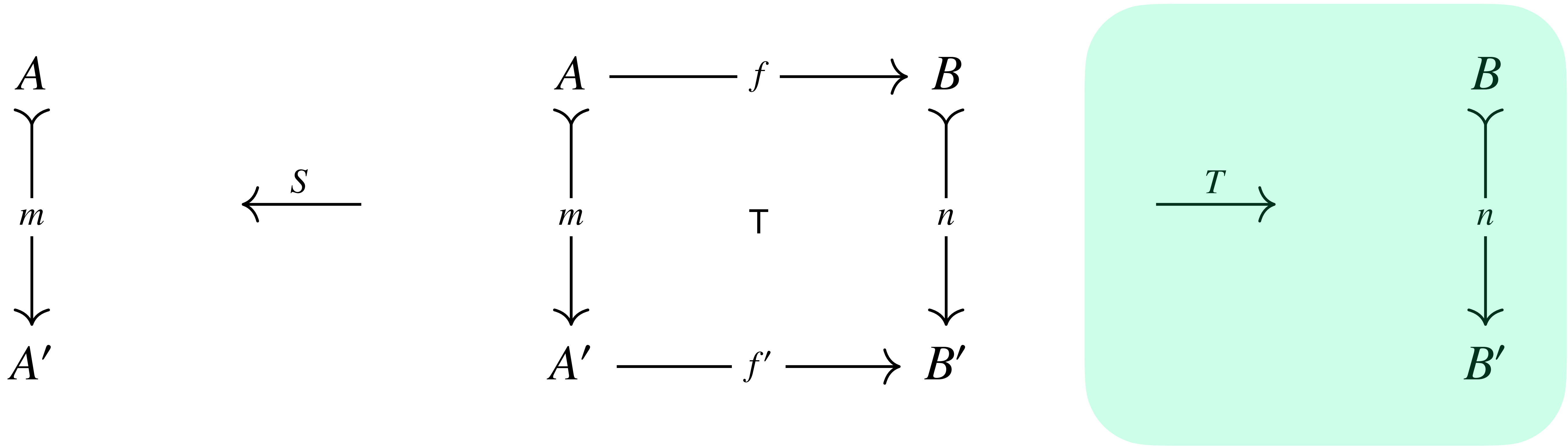
Fibrational properties of the **domain functors** (suggested by *R. Garner*)

Corollary 3. *Let* $\mathbf{C}$ *be a category with a stable system of monics* $\mathcal{M}$.

(i) If $\mathbf{C}$ *has pushouts along* $\mathcal{M}$*-morphisms, the functor dom* $: \mathsf{PO}_h(\mathbf{C}, \mathcal{M}) \to \mathbf{C}$ *is a Grothendieck opfibration.*

(ii) If $\mathbf{C}$ *has FPCs along* $\mathcal{M}$*-morphisms, the functor dom* $: \mathsf{FPC}_h(\mathbf{C}, \mathcal{M}) \to \mathbf{C}$ *is a Grothendieck fibration.*

Fibrational properties of the **target functors**



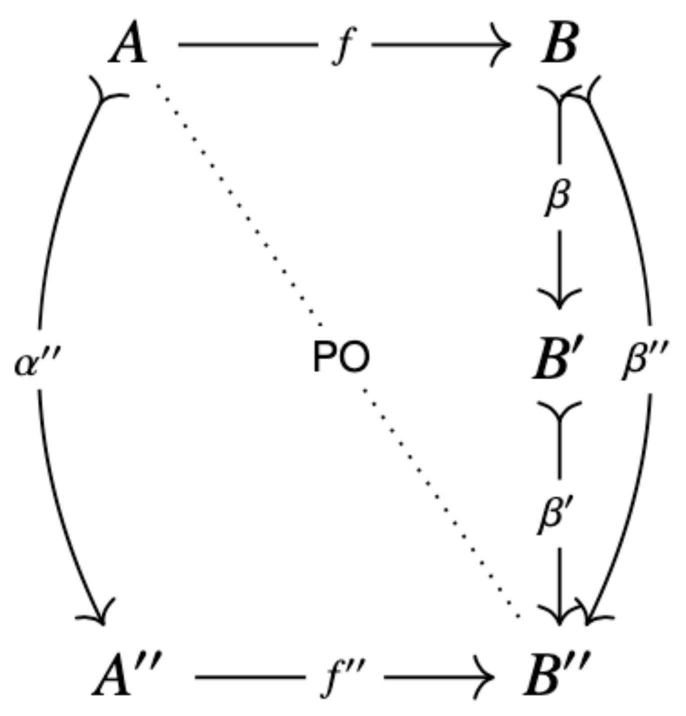
- $T : \mathsf{PB}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ carries no fibrational structures.
- $T : \mathsf{FPC}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ carries a Grothendieck opfibration structure.
- $T : \mathsf{PO}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ carries a multi-opfibration structure.

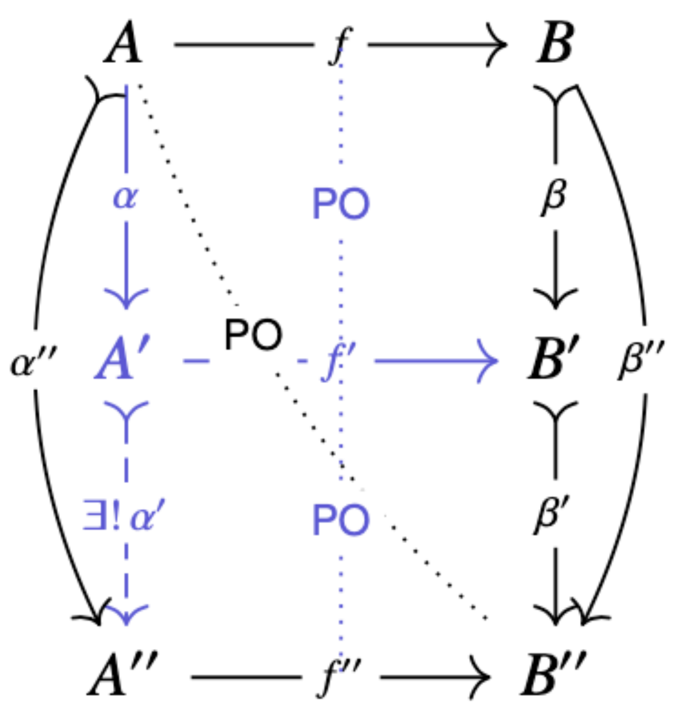
Multi-initial pushout complements

Definition 8. Let $\mathbf{C}$ be a category with a stable system of monics $\mathcal{M}$. For all composable sequences of morphisms of the form $A - f \to B \rightarrowtail \beta \to B'$ (i.e., with $\beta \in \mathcal{M}$), we define the following class:

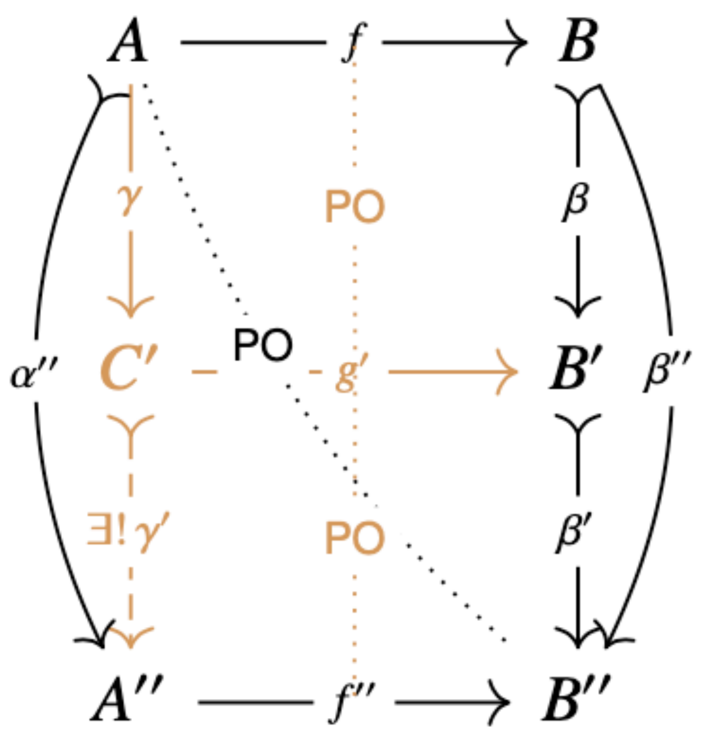
$$\mathcal{P}(f,\beta) := \{(A \rightarrowtail \alpha \to A', A' - f' \to B') \in \mathsf{mor}(\mathbf{C})^2 \mid \alpha \in \mathcal{M} \wedge (f',\beta) = \mathsf{PO}(\alpha, f)\}\,, \tag{26}$$

More explicitly, the class $\mathcal{P}(f,\beta)$ consists of all composable sequences of morphisms $A \rightarrowtail \alpha \to A' - f' \to B'$ such that there exists a pushout square in $\mathbf{C}$ whose boundary is given (α, f') and (f,β). Then we refer to $\mathcal{P}(f,\beta)$ as the ($\mathcal{M}$-) *multi-initial pushout complement (mIPC)* of (f,β) if the class satisfies the following *universal property*:

$\forall$ 

$: \exists(\alpha, f') \in \mathcal{P}(f,\beta) :$ 

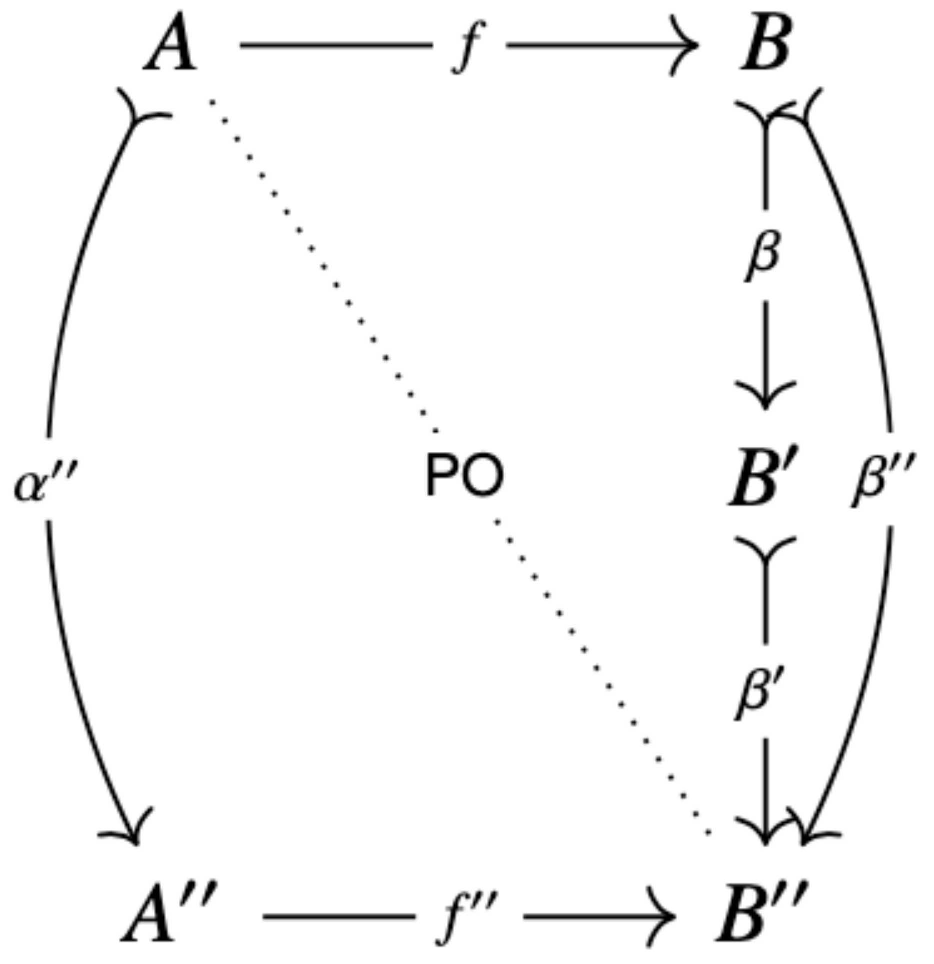
$:$

$\forall(\gamma, g') \in \mathcal{P}(f,\beta) :$ 

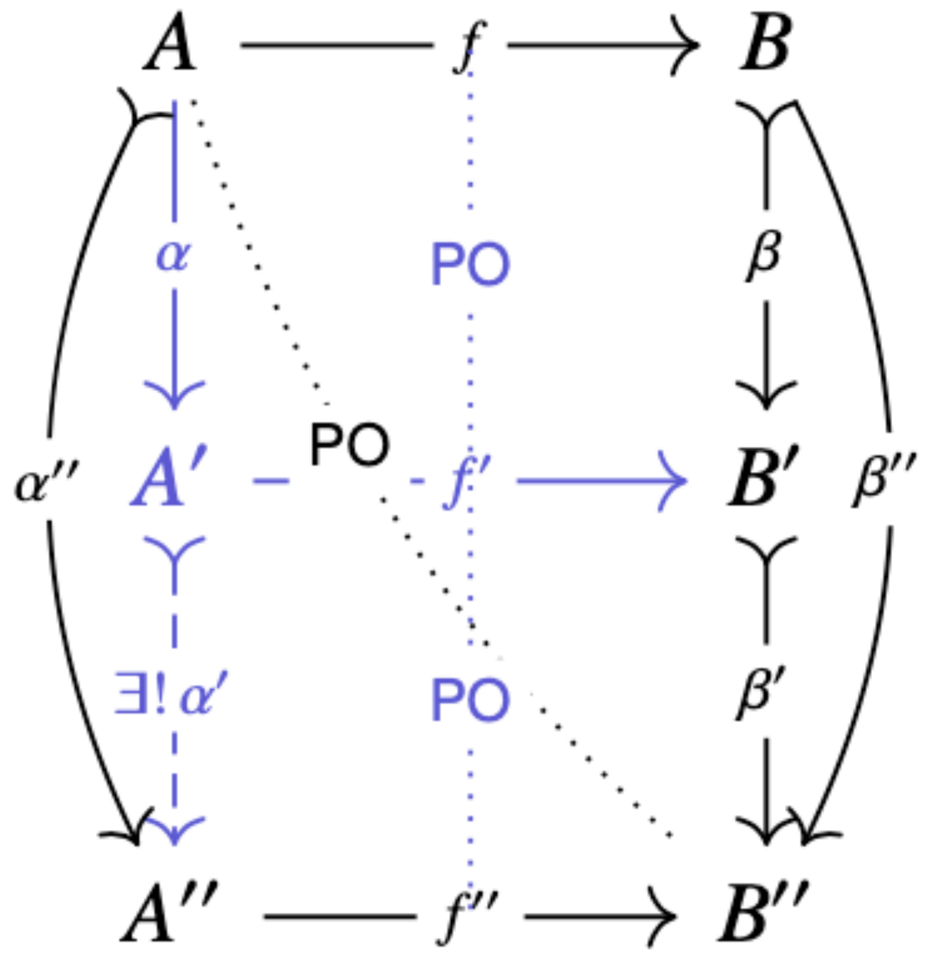
$: \exists A' - \varphi \to C' \in \mathsf{iso}(\mathbf{C}) : \gamma = \varphi \circ \alpha \wedge \alpha' = \gamma' \circ \varphi$

Multi-pushout complements

$\forall$

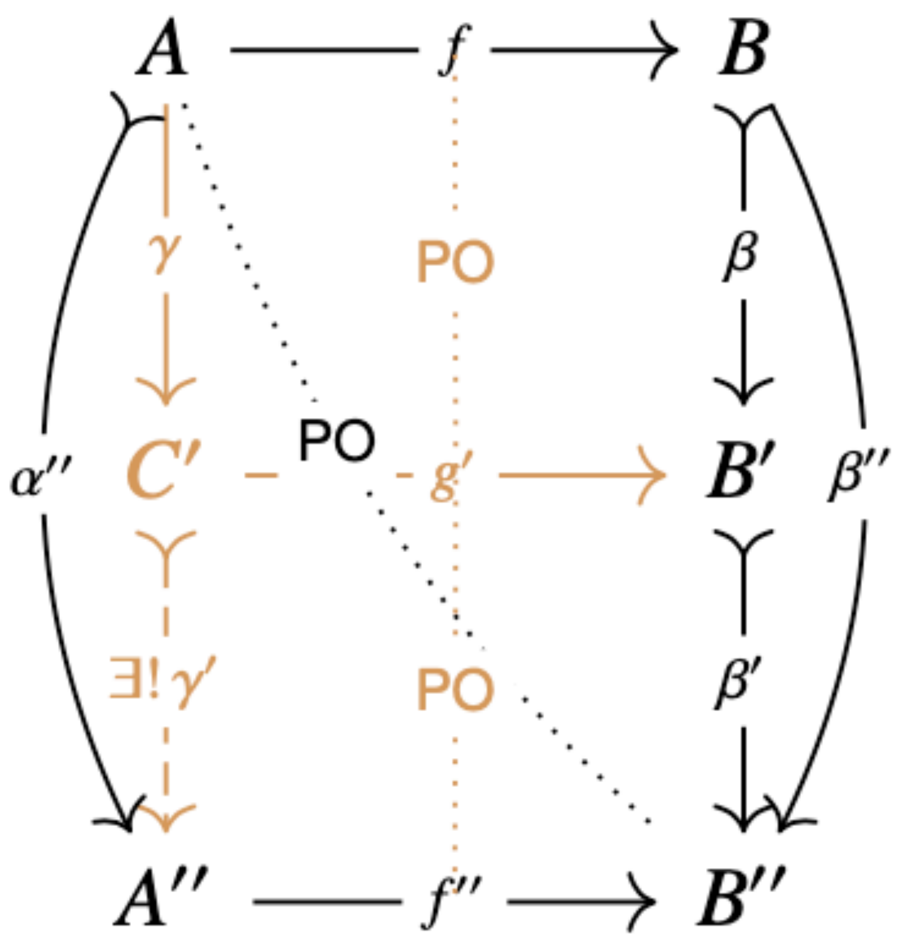


$: \exists(\alpha, f') \in \mathcal{P}(f,\beta) :$



$:$

$\forall(\gamma, g') \in \mathcal{P}(f,\beta) :$



$: \exists A' - \varphi \rightarrow C' \in \mathrm{iso}(\mathbf{C}) : \gamma = \varphi \circ \alpha \wedge \alpha' = \gamma' \circ \varphi$

On the **existence** of **multi-initial pushout complements**

Proposition 1. *Let* $\mathbf{C}$ *be a category with a stable system of monics* $\mathcal{M}$*. Then if* $\mathbf{C}$

(i) has pullbacks along $\mathcal{M}$*-morphisms, and*

(ii) pushouts along $\mathcal{M}$*-morphisms are stable under* $\mathcal{M}$*-pullbacks.*

Then $\mathbf{C}$ *has multi-initial pushout complements (mIPCs) along* $\mathcal{M}$*-morphisms.*

On the **existence** of **multi-initial pushout complements**

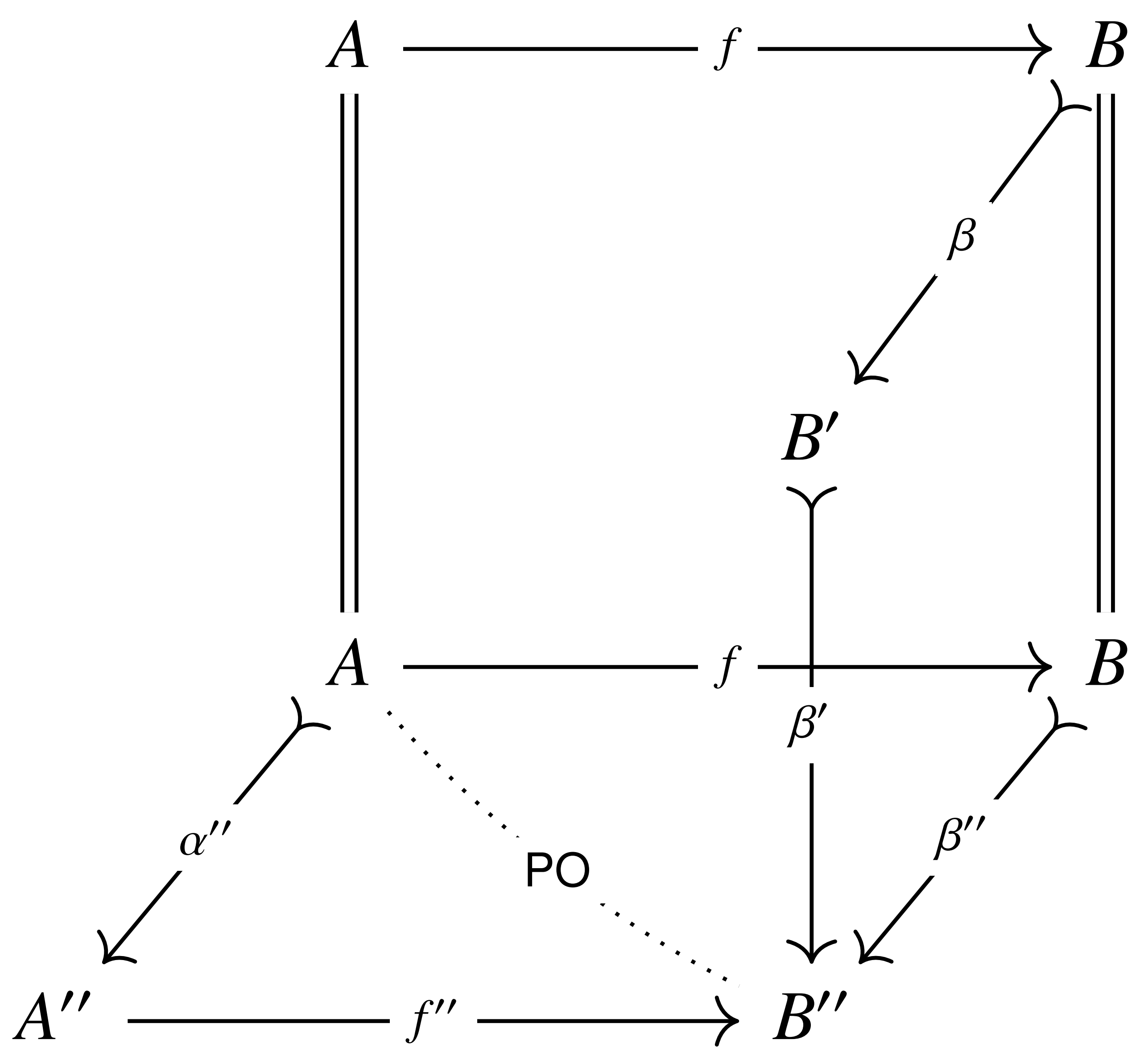
Proposition 1. *Let* **C** *be a category with a stable system of monics* $\mathcal{M}$*. Then if* **C**

(i) has pullbacks along $\mathcal{M}$*-morphisms, and*

(ii) pushouts along $\mathcal{M}$*-morphisms are stable under* $\mathcal{M}$*-pullbacks.*

Then **C** *has multi-initial pushout complements (mIPCs) along* $\mathcal{M}$*-morphisms.*

Proof. Let us construct the diagrams below:



On the **existence** of **multi-initial pushout complements**

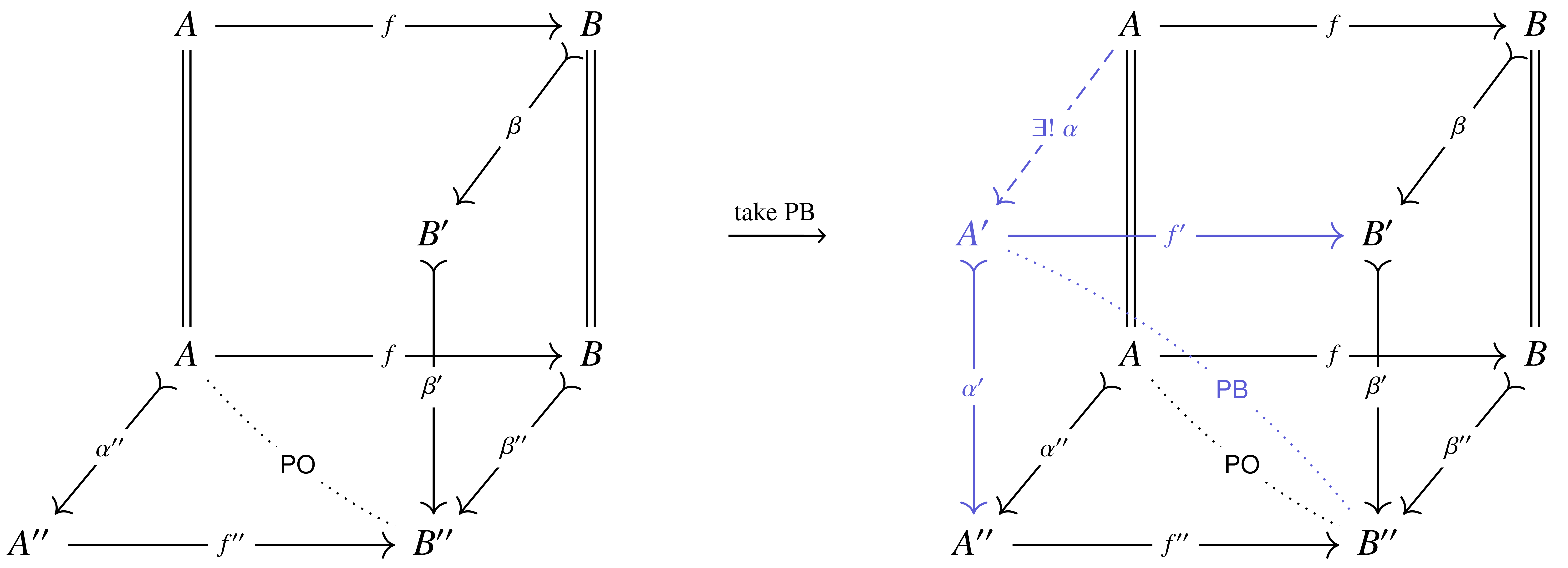
Proposition 1. *Let* **C** *be a category with a stable system of monics* $\mathcal{M}$*. Then if* **C**

(i) has pullbacks along $\mathcal{M}$-morphisms, and

(ii) pushouts along $\mathcal{M}$-morphisms are stable under $\mathcal{M}$-pullbacks.

Then **C** *has multi-initial pushout complements (mIPCs) along $\mathcal{M}$-morphisms.*

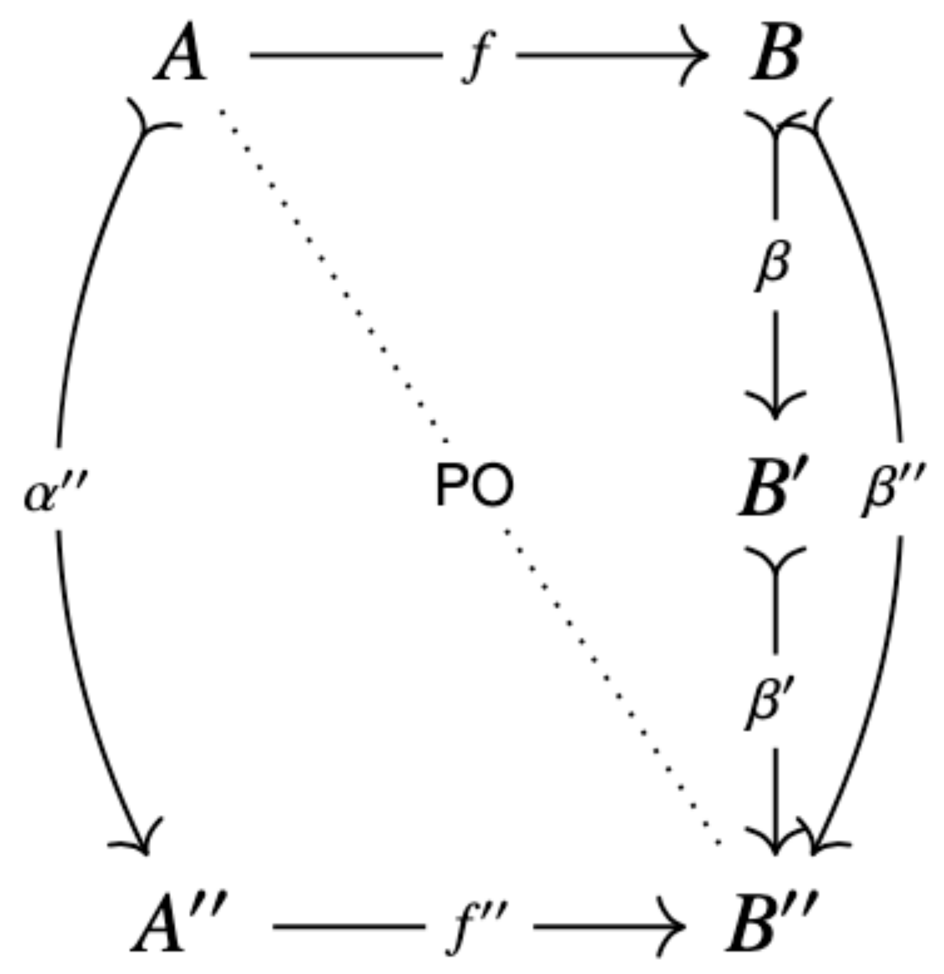
Proof. Let us construct the diagrams below:



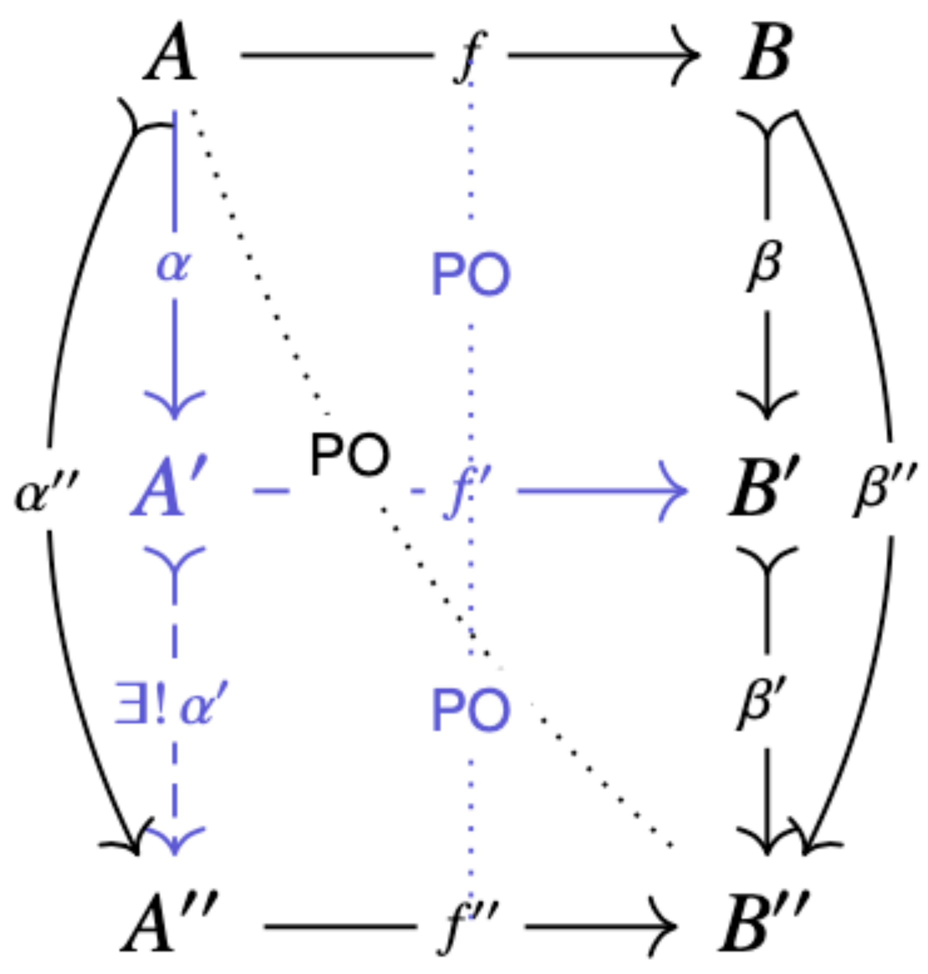
(28)

Multi-pushout complements

$\forall$

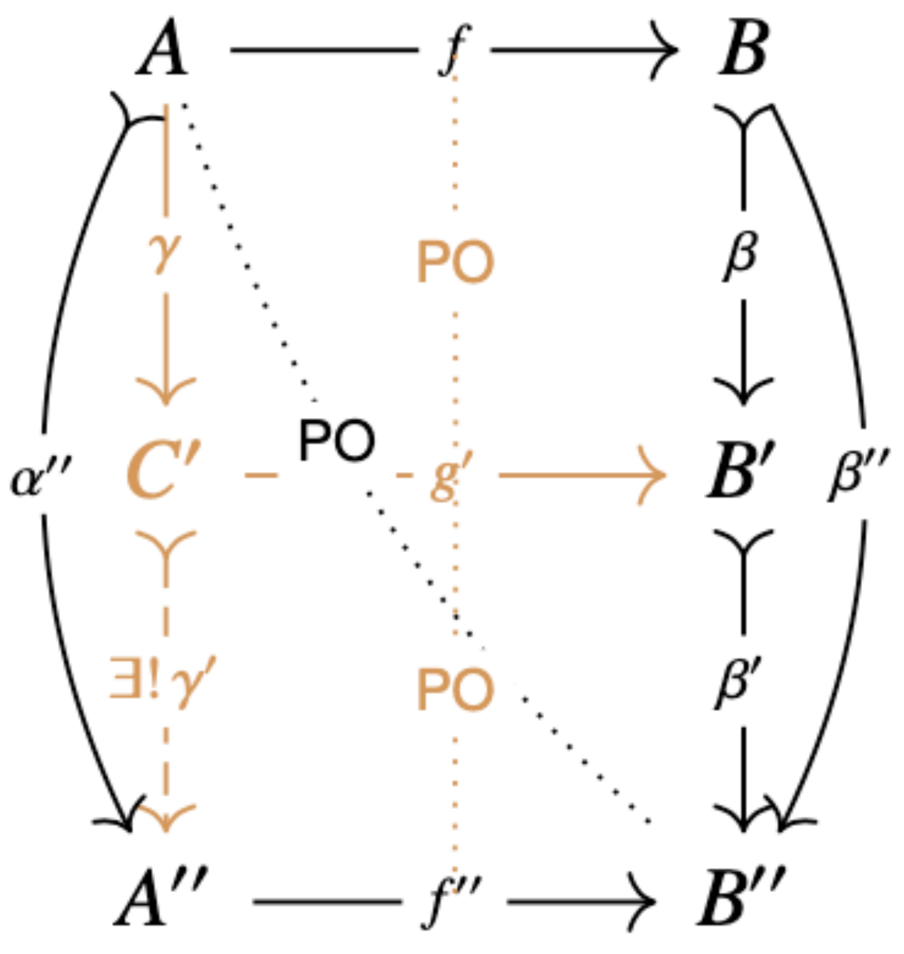


$: \exists(\alpha, f') \in \mathcal{P}(f,\beta) :$



$:$

$\forall(\gamma, g') \in \mathcal{P}(f,\beta) :$



$: \exists A' - \varphi \rightarrow C' \in \mathrm{iso}(\mathbf{C}) : \gamma = \varphi \circ \alpha \wedge \alpha' = \gamma' \circ \varphi$

Fibrational structures — “multi” variants à la Diers

Definition 3. A functor $M : \mathbf{E} \to \mathbf{B}$ is a *multi-opfibration* if the following property holds:

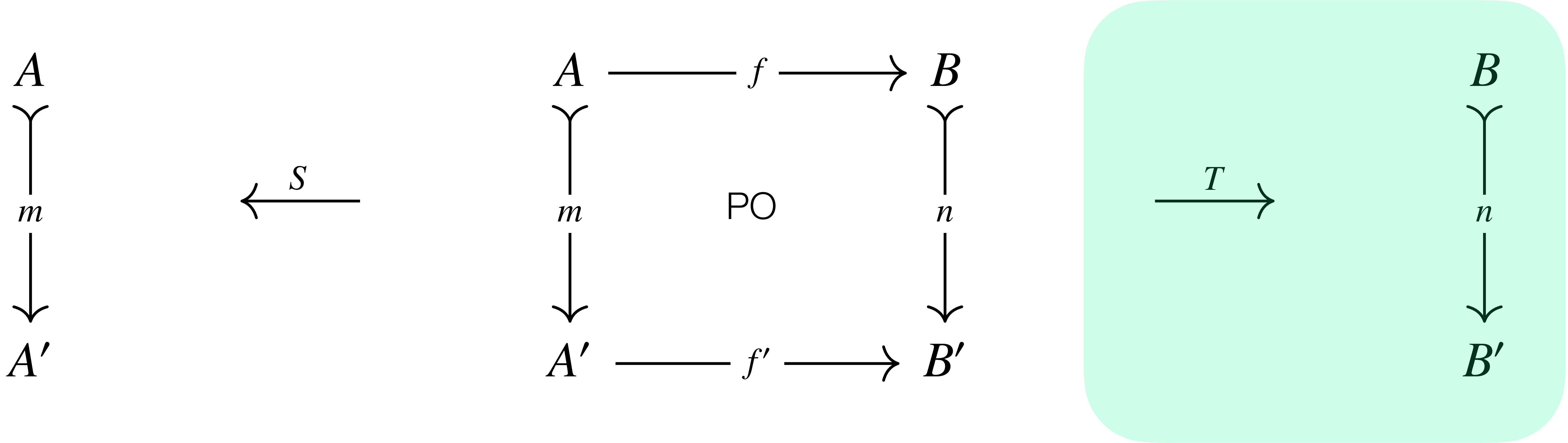
$$
\forall \begin{array}{c} e \\ \downarrow{\scriptstyle M} \\ b \xrightarrow{\;f\;} b' \end{array} \;:\; \exists \left\{ \begin{array}{ccc} e & \xrightarrow{\varepsilon_j(f)} & e'_j \\ \downarrow{\scriptstyle M} & & \downarrow{\scriptstyle M} \\ b & \xrightarrow{f=M(\varepsilon_j(f))} & b' \end{array} \right\}_{j \in J_{f;e}} \;:
$$

$$
\forall \begin{array}{ccccc} e & & \xrightarrow{\quad\alpha\quad} & & e'' \\ \downarrow{\scriptstyle M} & & & & \downarrow{\scriptstyle M} \\ b & \xrightarrow{f} & b' & \xrightarrow{g} & b'' \\ & & \underset{M(\alpha)}{\longrightarrow} & & \end{array} \;:\; \begin{array}{ccccc} & & \xrightarrow{\quad\alpha\quad} & & \\ e & \xrightarrow{\exists \varepsilon_j(f)} & e'_j & \overset{\exists! \beta_j}{\dashrightarrow} & e'' \\ \downarrow{\scriptstyle M} & & \downarrow{\scriptstyle M} & & \downarrow{\scriptstyle M} \\ b & \xrightarrow{f} & b' & \xrightarrow{g=M(\beta_j)} & b'' \\ & & \underset{M(\alpha)}{\longrightarrow} & & \end{array} \tag{5}
$$

$$
\wedge\; \forall k \in J_{f;e} :\; \left(\exists e'_k - \beta_k \to e'' : \alpha = \beta_k \circ \varepsilon_k(f) \wedge M(\beta_k) = g\right)
$$

$$
\Rightarrow \exists!\; e'_j - \phi \to e'_k \in \mathsf{iso}(\mathbf{E}) : \varepsilon_k(f) = \phi \circ \varepsilon_j(f) \wedge M(\phi) = id_{b'}
$$

$T : \mathrm{PO}_v(C, M) \to C|_M$ is a **multi-opfibration**



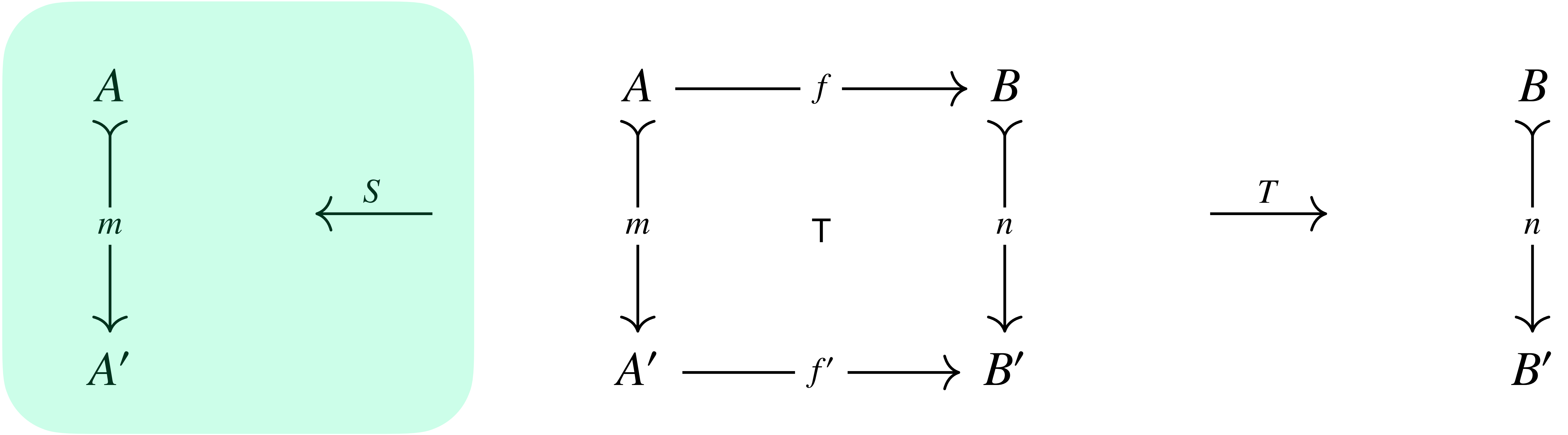
Theorem 4. *Let* $\mathbf{C}$ *be a category with a stable system of monics* $\mathcal{M}$*. Suppose that*

(i) $\mathbf{C}$ *has has pullbacks along* $\mathcal{M}$*-morphisms, and*

(ii) pushouts along $\mathcal{M}$*-morphisms are stable under* $\mathcal{M}$*-pullbacks in* $\mathbf{C}$*.*

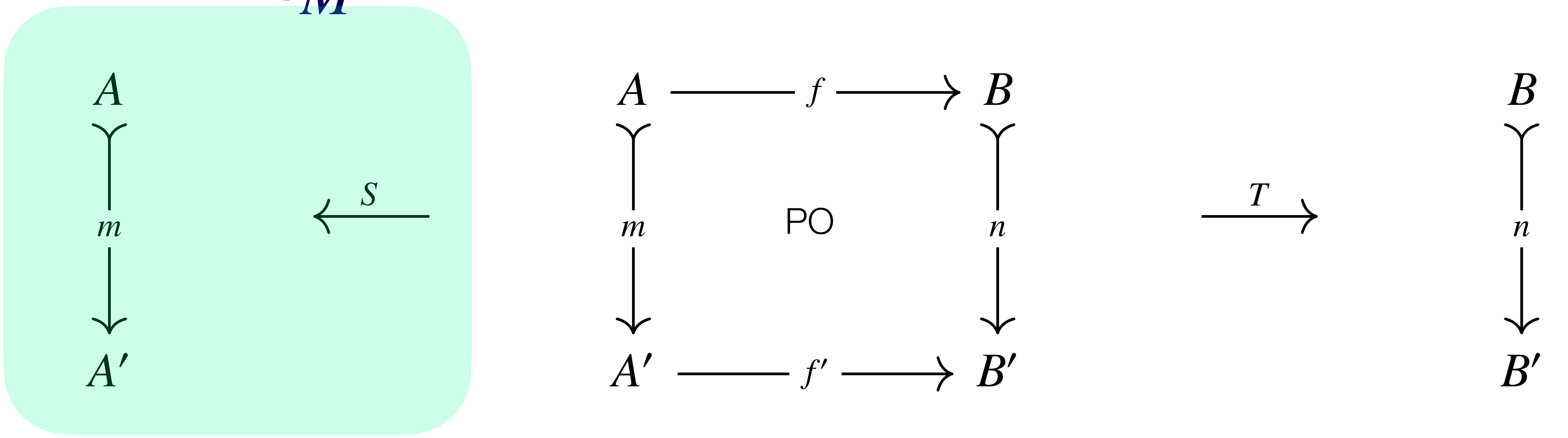
Then the target functor $T : \mathrm{PO}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ *is a multi-opfibration.*

Fibrational properties of the **source functors**



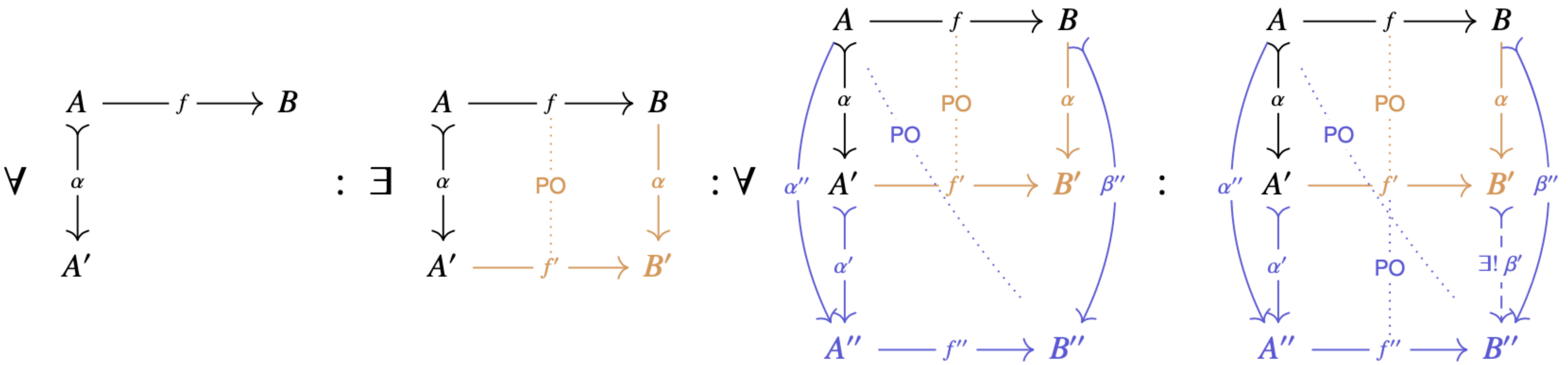
- $S : \mathsf{PB}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ carries no fibrational structures.
- $S : \mathsf{PO}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ carries a Grothendieck opfibration structure.
- $S : \mathsf{FPC}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ carries a residual multi-opfibration structure.

$S : \mathsf{PO}_v(C, M) \to C|_M$ is a **Grothendieck opfibration**



Theorem 5. *Let* **C** *be a category with a stable system of monics* $\mathcal{M}$*, that has pushouts along* $\mathcal{M}$*-morphisms, and such that* $\mathcal{M}$*-morphisms are stable under pushout. Then the source functor* $S : \mathsf{PO}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ *is a Grothendieck opfibration, with the op-Cartesian liftings provided by pushouts.*

Proof. It suffices to instantiate the definition of Grothendieck opfibration to the case at hand:



(29)

Factorization structures

Definition 9 ([34], Def. 14.1). For a category **C**, let E and M be classes of morphisms. By convention, in commutative diagrams, let morphisms in E be depicted as $\twoheadrightarrow$, and morphisms in M by $\rightarrowtail$. Then (E, M) is called a *factorization structure for morphisms* in **C**, and **C** is called *(E, M)-structured* iff

(i) both E and M are *closed under composition with isomorphisms*,

(ii) **C** *has (E, M)-factorizations of morphisms* (i.e., for every morphism f in **C**, there exist $m \in M$ and $e \in E$ such that $f = m \circ e$),

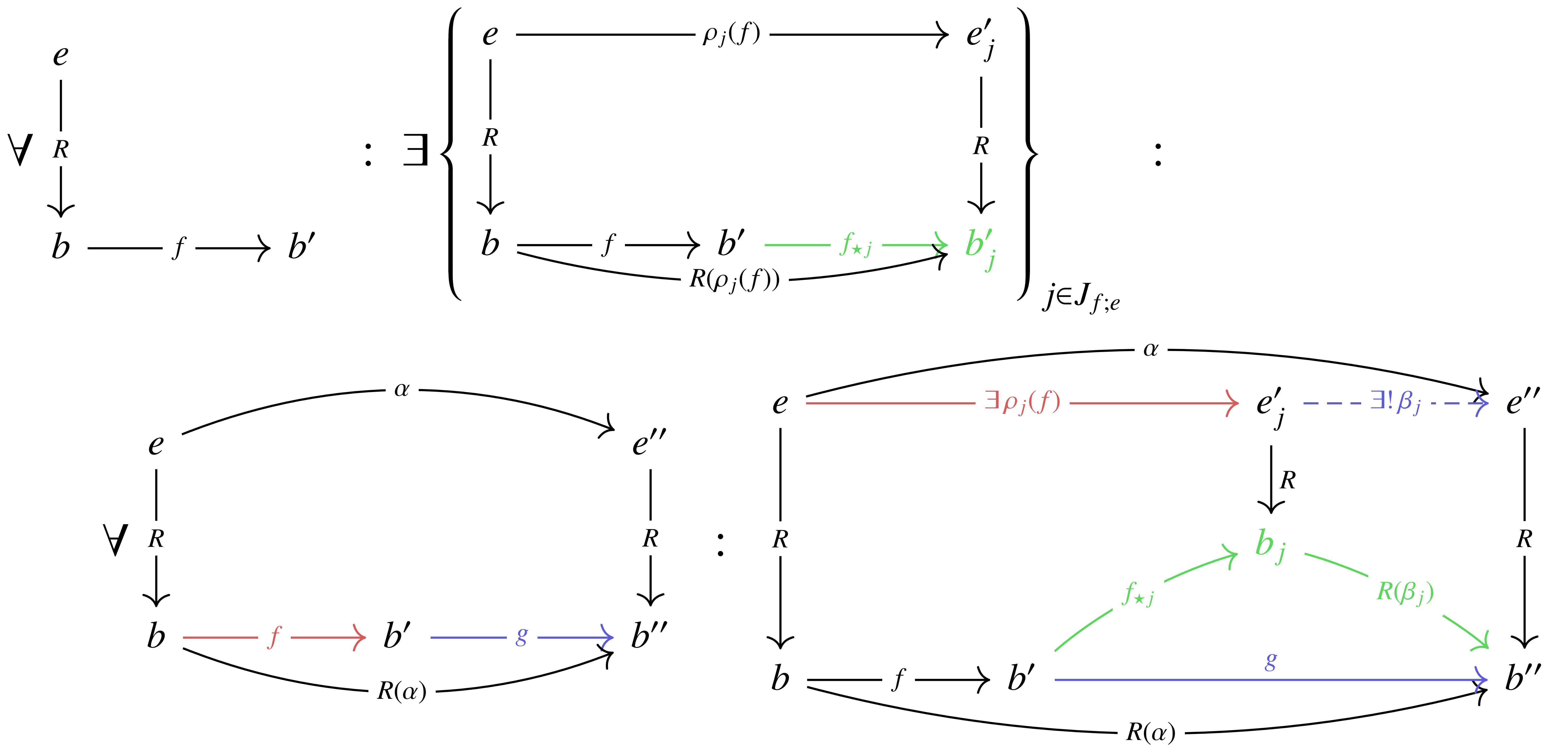
(iii) **C** *has the unique (E, M)-diagonalization property*:

$$\forall \begin{array}{ccc} A & \overset{e}{\twoheadrightarrow} & B \\ {\scriptstyle f}\downarrow & & \downarrow{\scriptstyle g} \\ C & \underset{m}{\rightarrowtail} & D \end{array} \; : \; \begin{array}{ccc} A & \overset{e}{\twoheadrightarrow} & B \\ {\scriptstyle f}\downarrow & \swarrow{\scriptstyle \exists! d} & \downarrow{\scriptstyle g} \\ C & \underset{m}{\rightarrowtail} & D \end{array} \tag{30}$$

In words: for all commutative squares as in (30) above, where $e \in E$ and $m \in M$, there exists a unique morphism d (referred to as the *diagonal*) such that $f = d \circ e$ and $g = m \circ d$.

Fibrational structures — “residual multi” variants

Definition 4. A functor $R : \mathbf{E} \to \mathbf{B}$ is a *residual multi-opfibration* if the following property holds:



(11)

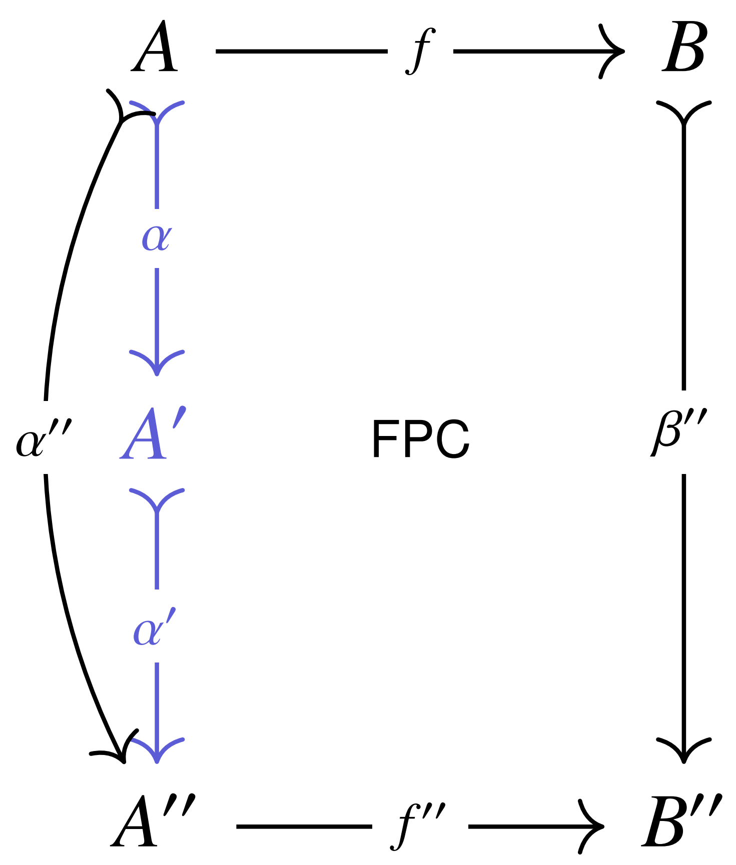
$$\wedge \quad \forall k \in J_{f;e} : (\exists\, e'_k - \beta_k \to e'' : \beta_k \circ \rho_k(f) = \alpha \wedge g = R(\beta_k) \circ f_{\star k})$$
$$\Rightarrow \exists!\, e'_j - \phi \to e'_k \in \mathsf{iso}(\mathbf{E}) : \rho_k(f) = \phi \circ \rho_j(f) \wedge \beta_j = \beta_k \circ \phi \wedge f_{\star k} = R(\phi) \circ f_{\star j}$$

$S : \mathsf{FPC}_v(C, M) \to C|_M$ is a **residual multi-opfibration**

Theorem 7. *Let* $\mathbf{C}$ *be a category with a stable system of monics* $\mathcal{M}$*, that is* $(\mathcal{E}, \mathcal{M})$*-structured, that has pullbacks, pushouts and FPCs along* $\mathcal{M}$*-morphisms, such that* $\mathcal{M}$*-morphisms are stable under pushout, and such that pushouts along* $\mathcal{M}$*-morphisms are stable under* $\mathcal{M}$*-pullbacks. Then* $S : \mathsf{FPC}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ *is a residual multi-opfibration.*

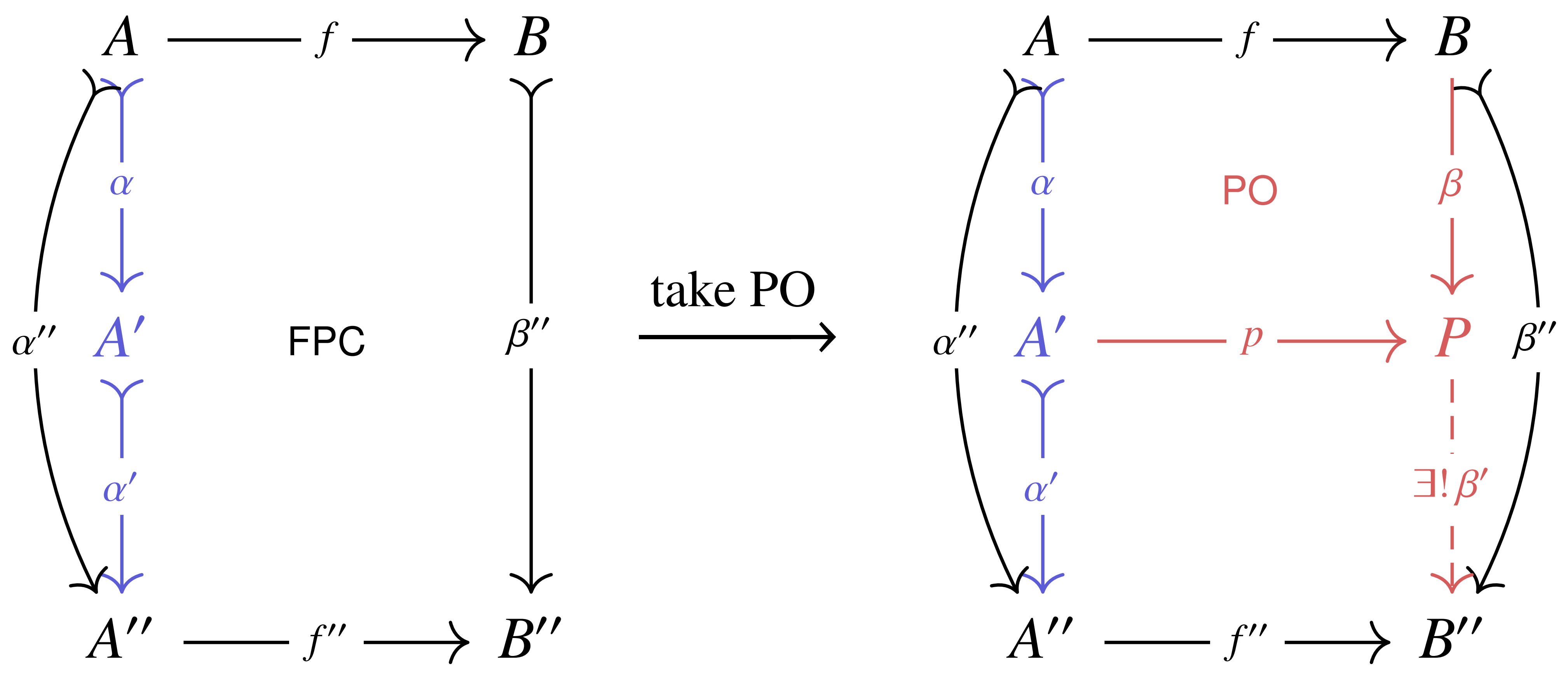
$S : \mathsf{FPC}_v(C, M) \to C|_M$ is a **residual multi-opfibration**

Theorem 7. *Let* $\mathbf{C}$ *be a category with a stable system of monics* $\mathcal{M}$*, that is* $(\mathcal{E}, \mathcal{M})$*-structured, that has pullbacks, pushouts and FPCs along* $\mathcal{M}$*-morphisms, such that* $\mathcal{M}$*-morphisms are stable under pushout, and such that pushouts along* $\mathcal{M}$*-morphisms are stable under* $\mathcal{M}$*-pullbacks. Then* $S : \mathsf{FPC}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ *is a residual multi-opfibration.*



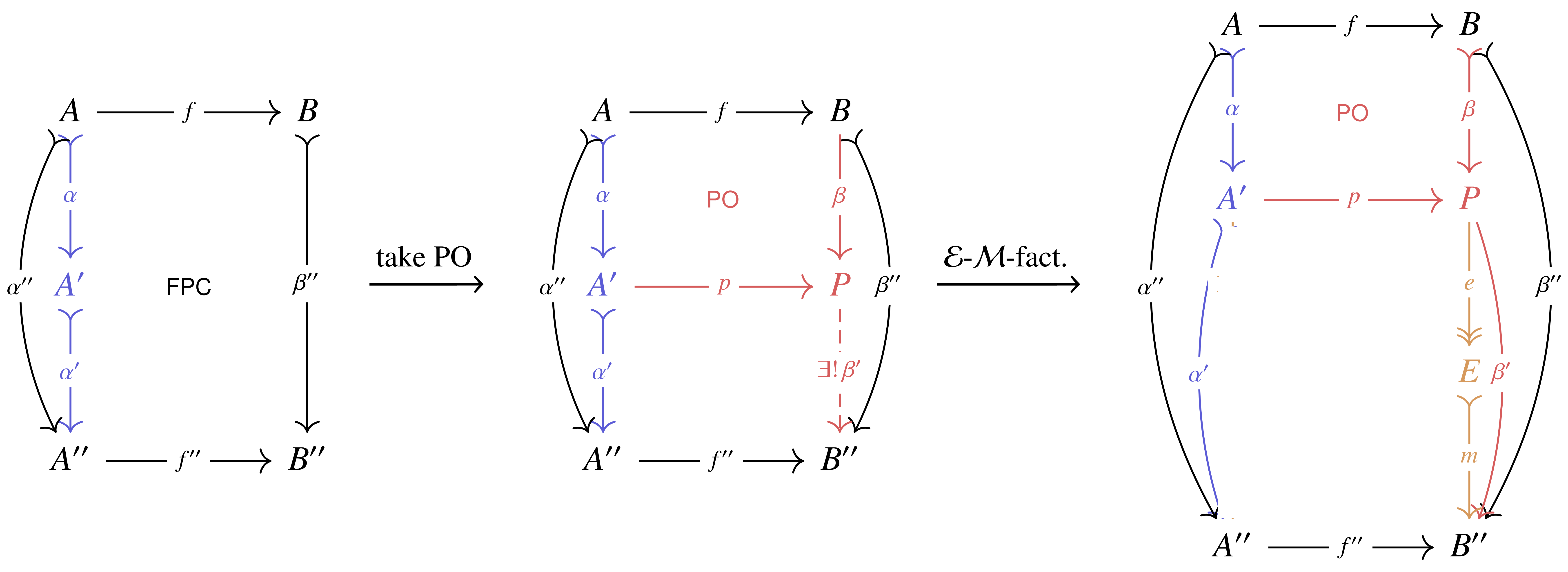
$S : \mathsf{FPC}_v(C, M) \to C|_M$ is a **residual multi-opfibration**

Theorem 7. *Let* $\mathbf{C}$ *be a category with a stable system of monics* $\mathcal{M}$*, that is* $(\mathcal{E}, \mathcal{M})$*-structured, that has pullbacks, pushouts and FPCs along* $\mathcal{M}$*-morphisms, such that* $\mathcal{M}$*-morphisms are stable under pushout, and such that pushouts along* $\mathcal{M}$*-morphisms are stable under* $\mathcal{M}$*-pullbacks. Then* $S : \mathsf{FPC}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ *is a residual multi-opfibration.*



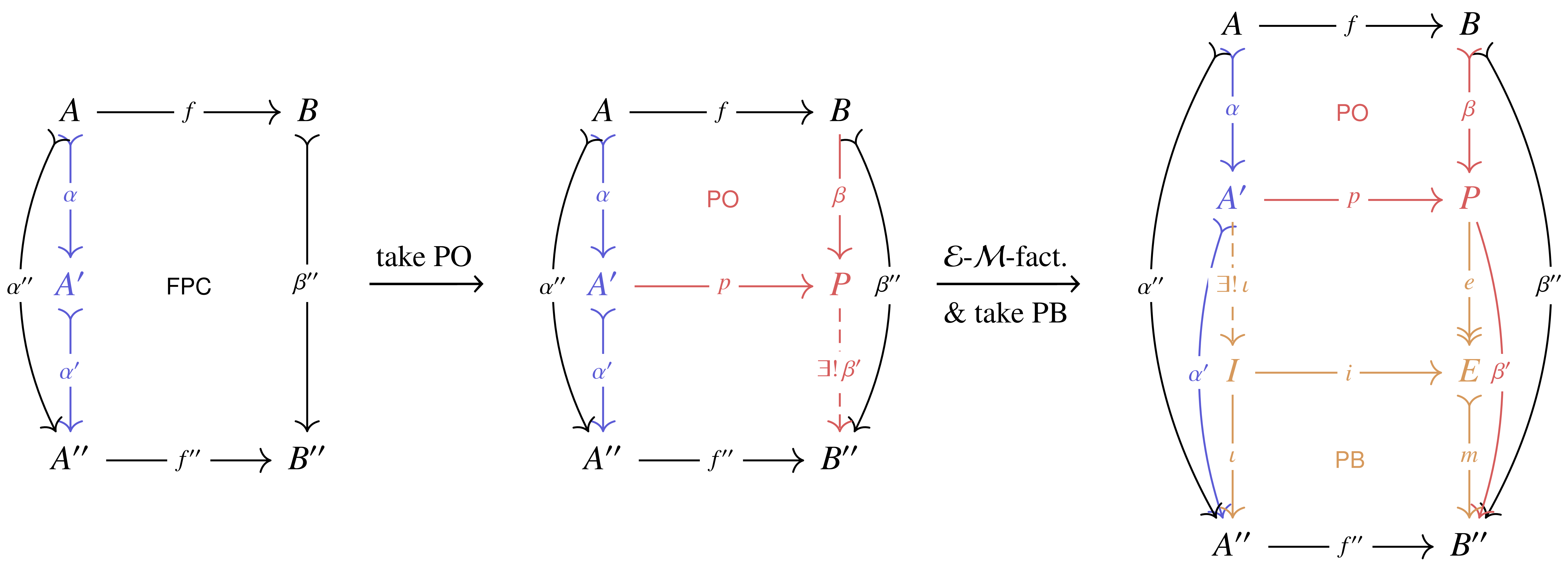
$S : \mathsf{FPC}_v(C, M) \to C|_M$ is a **residual multi-opfibration**

Theorem 7. *Let* $\mathbf{C}$ *be a category with a stable system of monics* $\mathcal{M}$*, that is* $(\mathcal{E}, \mathcal{M})$*-structured, that has pullbacks, pushouts and FPCs along* $\mathcal{M}$*-morphisms, such that* $\mathcal{M}$*-morphisms are stable under pushout, and such that pushouts along* $\mathcal{M}$*-morphisms are stable under* $\mathcal{M}$*-pullbacks. Then* $S : \mathsf{FPC}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ *is a residual multi-opfibration.*



$S : \mathsf{FPC}_v(C, M) \to C|_M$ is a **residual multi-opfibration**

Theorem 7. *Let* $\mathbf{C}$ *be a category with a stable system of monics* $\mathcal{M}$*, that is* $(\mathcal{E}, \mathcal{M})$*-structured, that has pullbacks, pushouts and FPCs along* $\mathcal{M}$*-morphisms, such that* $\mathcal{M}$*-morphisms are stable under pushout, and such that pushouts along* $\mathcal{M}$*-morphisms are stable under* $\mathcal{M}$*-pullbacks. Then* $S : \mathsf{FPC}_v(\mathbf{C}, \mathcal{M}) \to \mathbf{C}|_{\mathcal{M}}$ *is a residual multi-opfibration.*



KEY CONCEPT:

Examples of *compositional* categorical rewriting semantics

Examples of **categorical rewriting semantics**

Definition 23. Let $\mathbf{C}$ be a category with a stable system of monics $\mathcal{M}$.

(i) A *rule*, denoted $O \leftharpoonup r - I$, is a span $r = (O \leftarrow o_r - K_r - i_r \rightarrow I)$ in $\mathbf{C}$. We refer to a rule as

- *output-linear* if o_r is in $\mathcal{M}$,
- *input-linear* if i_r is in $\mathcal{M}$, and
- *linear* if both o_r and i_r are in $\mathcal{M}$.

We will also refer to arbitrary spans as *generic* rules.

Examples of **categorical rewriting semantics**

(ii) In *Double-Pushout (DPO) semantics*, a *direct derivation* is defined as a commutative diagram as in (75) below, where the vertical morphisms are in $\mathcal{M}$, and where the square marked $(\dagger_\alpha)$ is a pushout, while the square marked $(*_\alpha)$ is an element of an $\mathcal{M}$-multi-IPC (and thus in particular also a pushout). A category $\mathbf{C}$ is thus suitable for DPO-semantics if it has multi-initial pushout complements (mIPCs) along $\mathcal{M}$-morphisms, if it has pushouts along $\mathcal{M}$-morphisms, and if $\mathcal{M}$-morphisms are stable under pushout.

(iii) In *Sesqui-Pushout (SqPO) semantics*, a *direct derivation* is defined as a commutative diagram as in (75) below, where the vertical morphisms are in $\mathcal{M}$, and where the square marked $(\dagger_\alpha)$ is a pushout, while the square marked $(*_\alpha)$ is a final pullback complement (FPC). A category $\mathbf{C}$ is thus suitable for SqPO-semantics if it has FPCs along $\mathcal{M}$-morphisms, if it has pushouts along $\mathcal{M}$-morphisms, and if $\mathcal{M}$-morphisms are stable under pushout.

$$\begin{array}{ccc} O & \xleftarrow{\;r\;} & I \\ {\scriptstyle m^*}\downarrow & \overset{\alpha}{\Downarrow} & \downarrow{\scriptstyle m} \\ O' & \xleftarrow{\;r'\;} & I' \end{array} \quad := \quad \begin{array}{ccccc} O & \xleftarrow{\;o_r\;} & K_r & \xrightarrow{\;i_r\;} & I \\ {\scriptstyle m^*}\downarrow & (\dagger_\alpha) & \downarrow{\scriptstyle k_\alpha} & (*_\alpha) & \downarrow{\scriptstyle m} \\ O' & \xleftarrow{\;o_{r'}\;} & K_{r'} & \xrightarrow{\;i_{r'}\;} & I' \end{array} \tag{75}$$

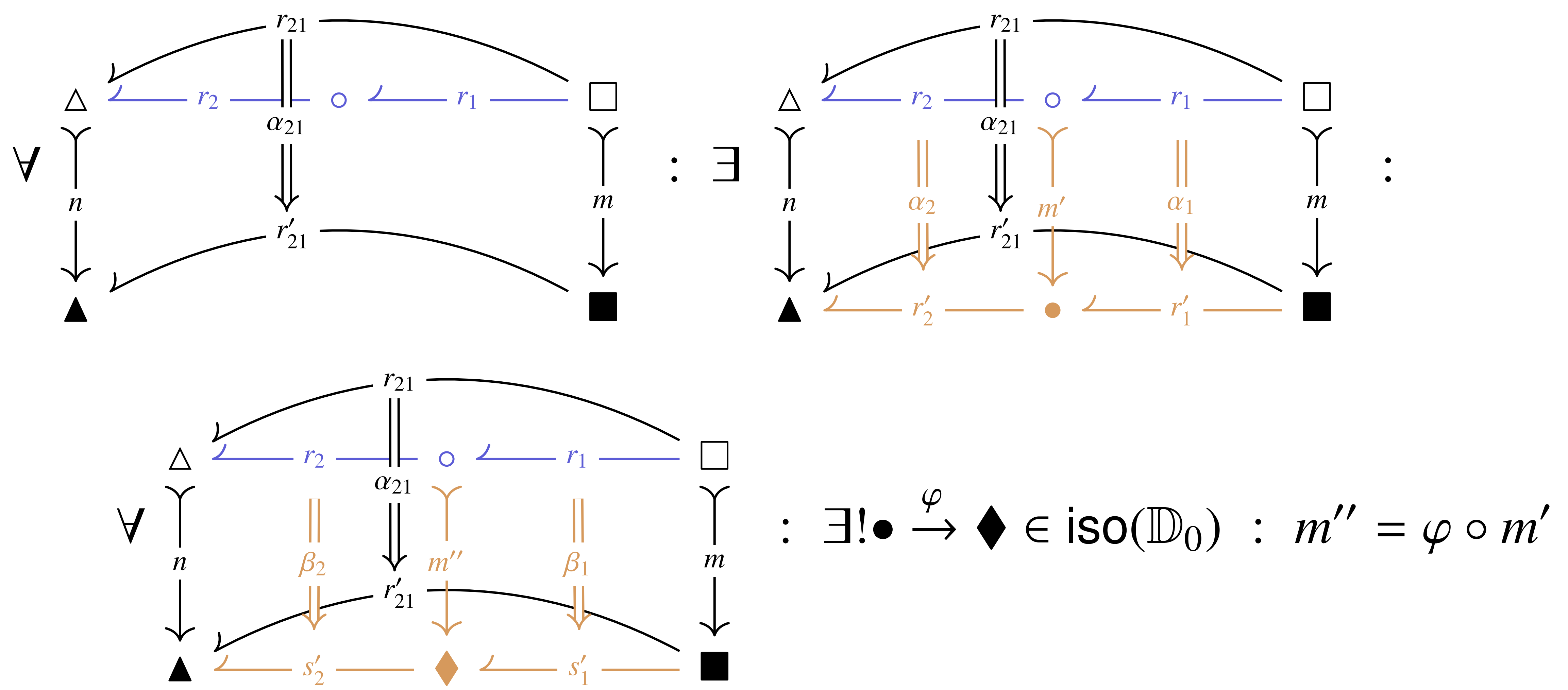
Compositional rewriting double categories (crDCs)

Definition 13. A double category (DC) $\mathbb{D}$ is a *compositional rewriting DC (crDC)* if it has the following properties:

(i) $\mathbb{D}_0$ has multi-sums.

(ii) *$\mathbb{D}_0$ and $\mathbb{D}_1$ have pullbacks*. (This entails in particular that for $i \in \{1, 2\}$, *$\mathbb{D}_i$ morphisms are stable under pullback*, and *pullbacks in $\mathbb{D}_i$ are effective*, i.e., for any span of $\mathbb{D}_i$ morphisms extending a pullback diagram in $\mathbb{D}_i$, the unique mediating morphism is in $\mathbb{D}_i$.)

(iii) Squares in $\mathbb{D}$ have the following *horizontal decomposition property*:



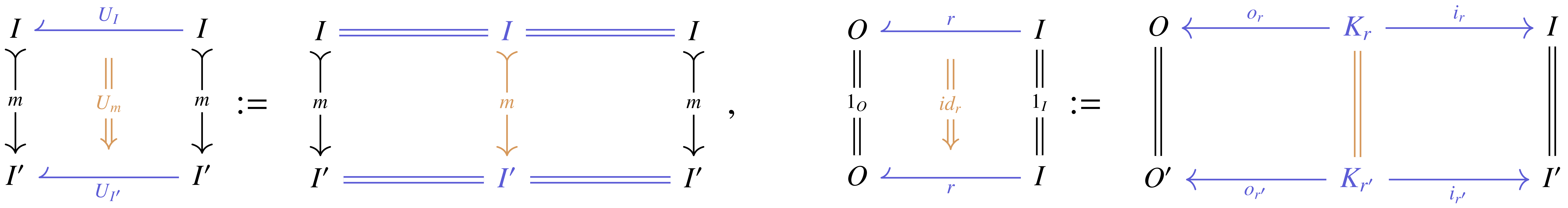
(43)

(iv) The source functor $S : \mathbb{D}_1 \to \mathbb{D}_0$ is a multi-opfibration.

(v) The target functor $T : \mathbb{D}_1 \to \mathbb{D}_0$ is a residual multi-opfibration.

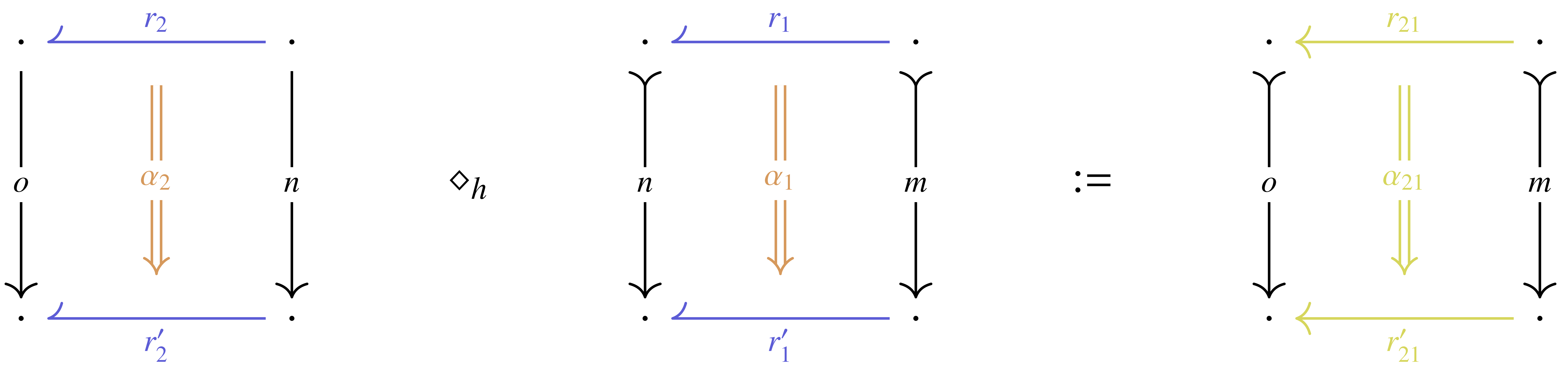
Existence of **horizontal** and **vertical units**

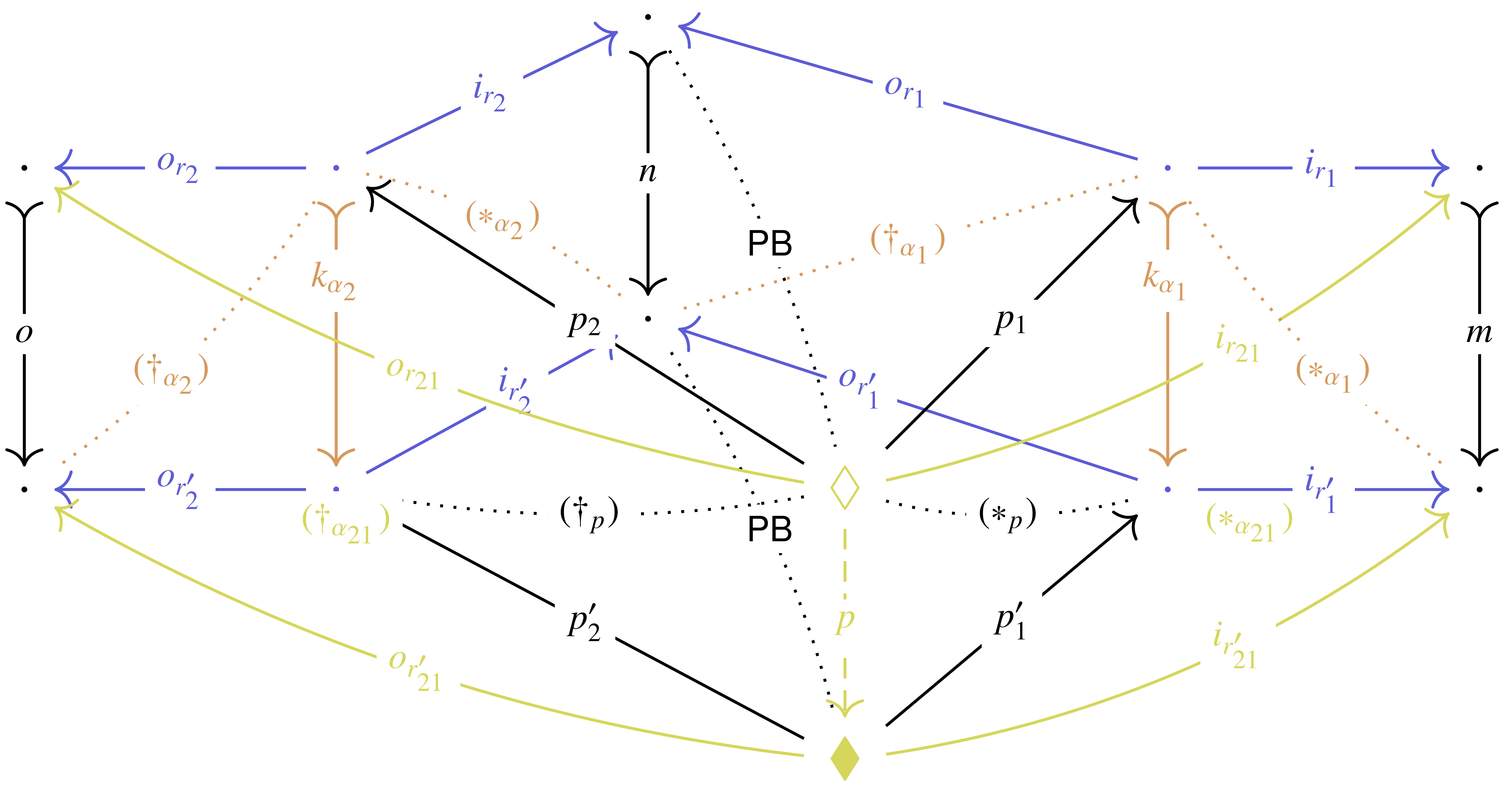
Corollary 7. *For all eight semantics of Definition 23, the resulting definitions of* $\mathbb{D}_0$ *and* $\mathbb{D}_1$ *have horizontal and vertical units in the following form:*



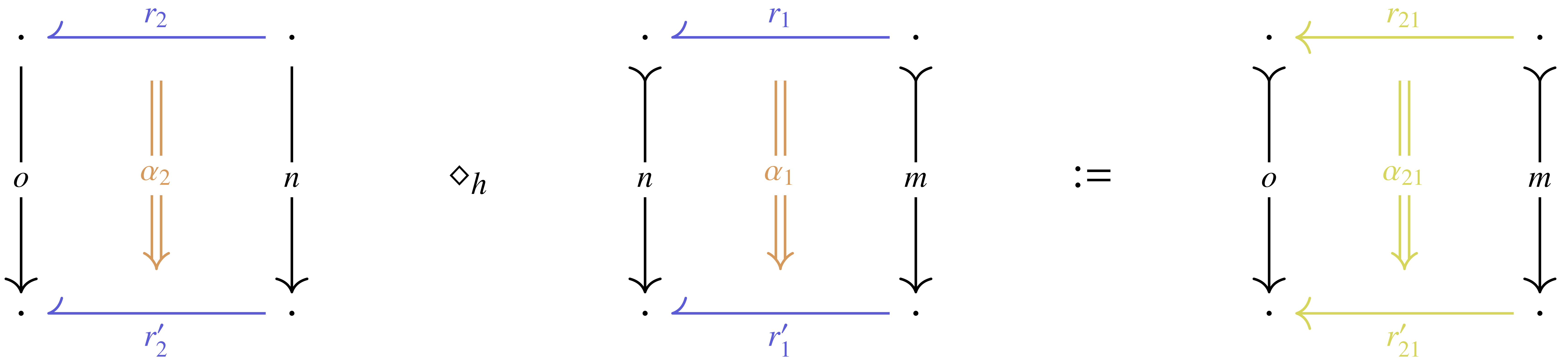
(77)

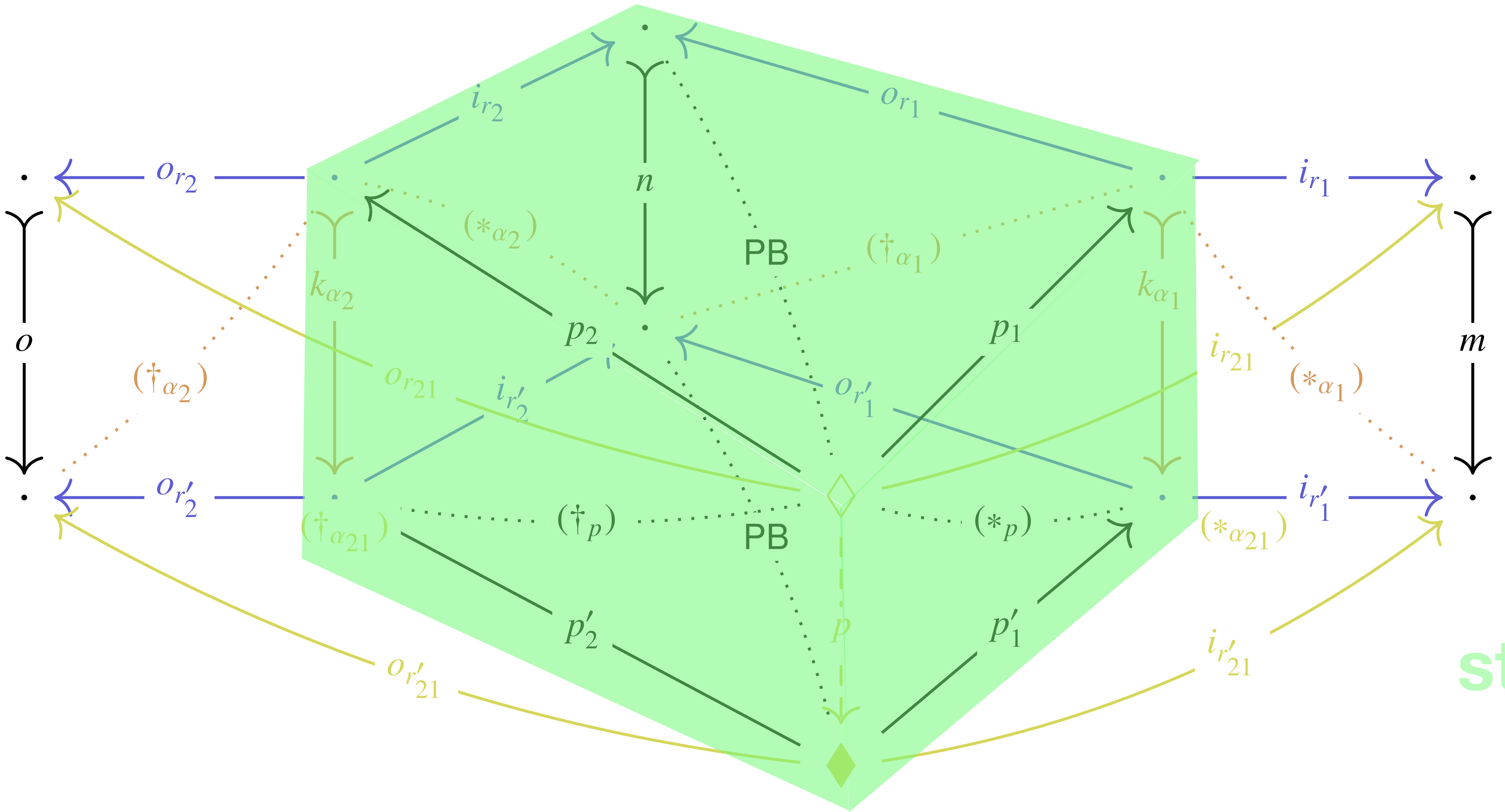
Horizontal composition





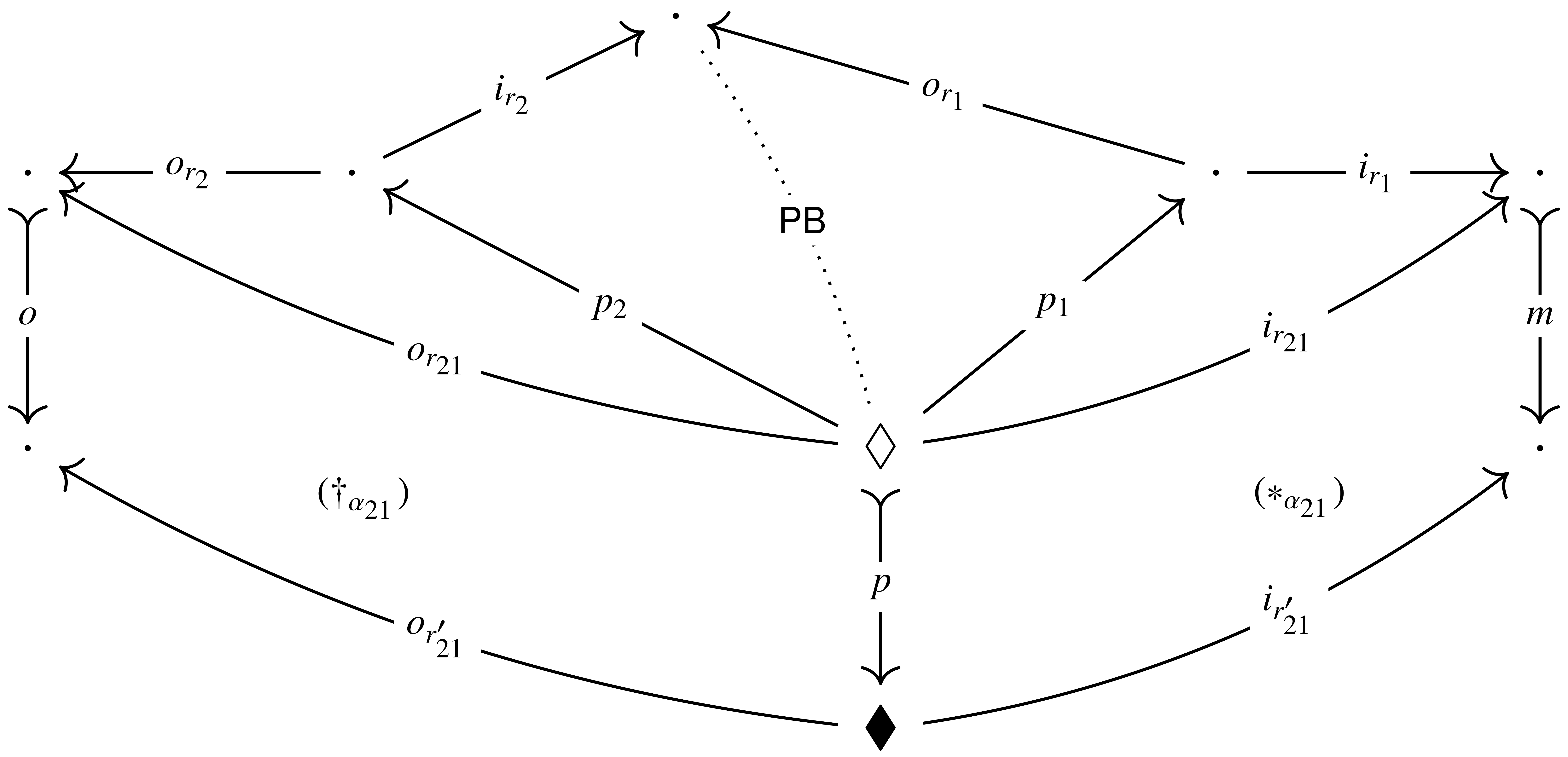
Horizontal composition



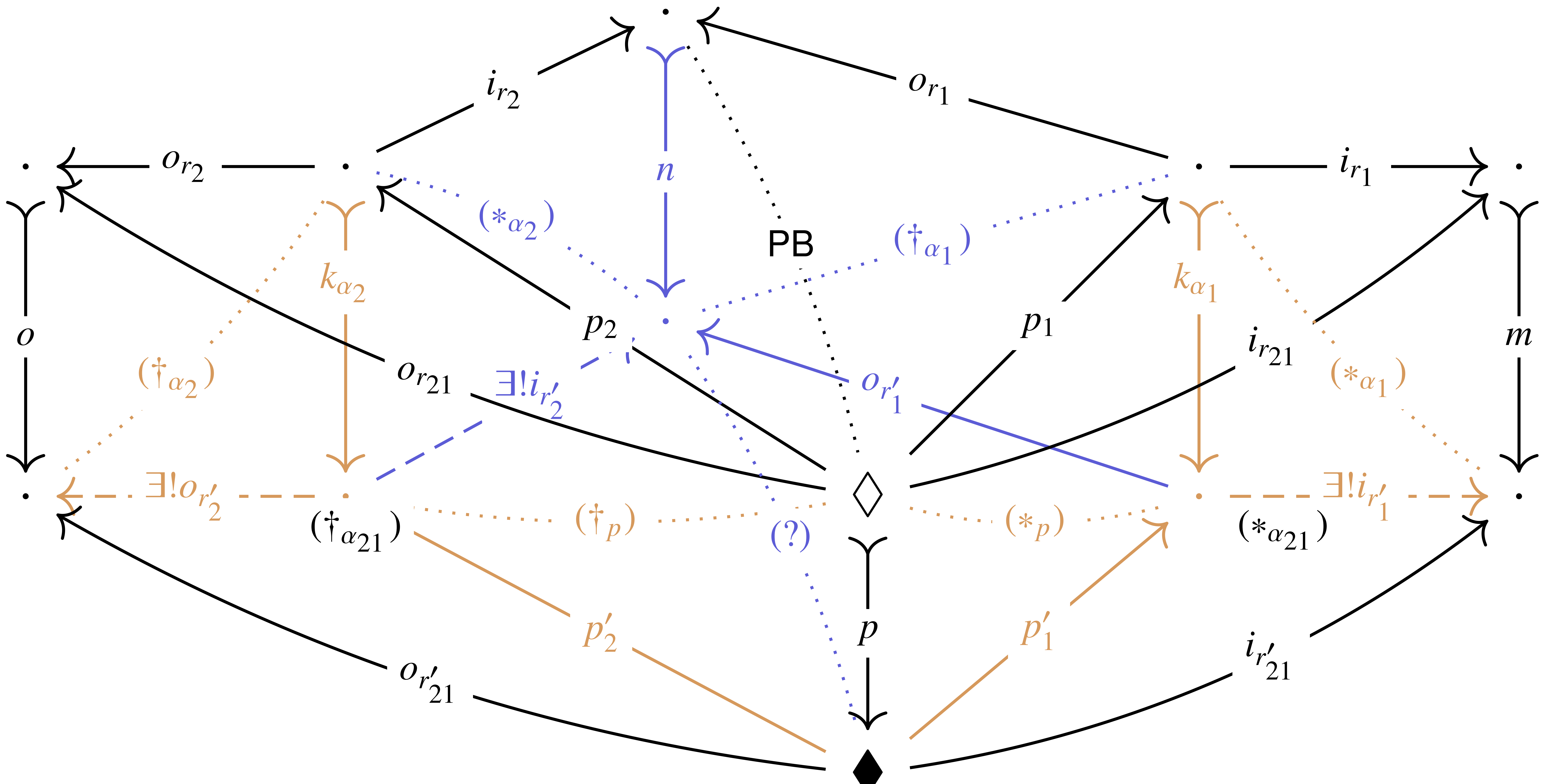


Proof relies upon **stability under pullbacks** of **POs/FPCs !**

Horizontal decomposition

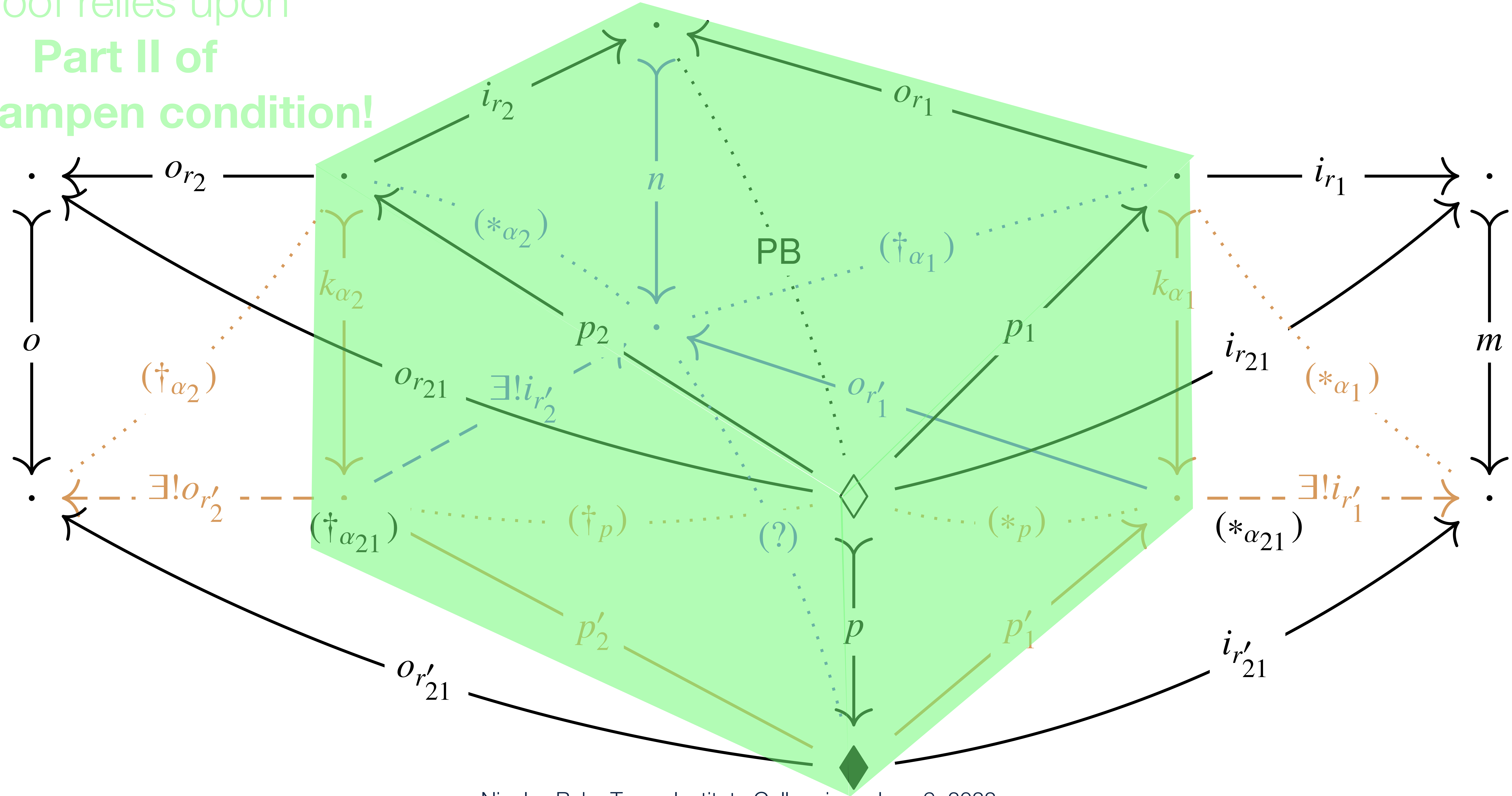


Horizontal decomposition — double-pushout semantics

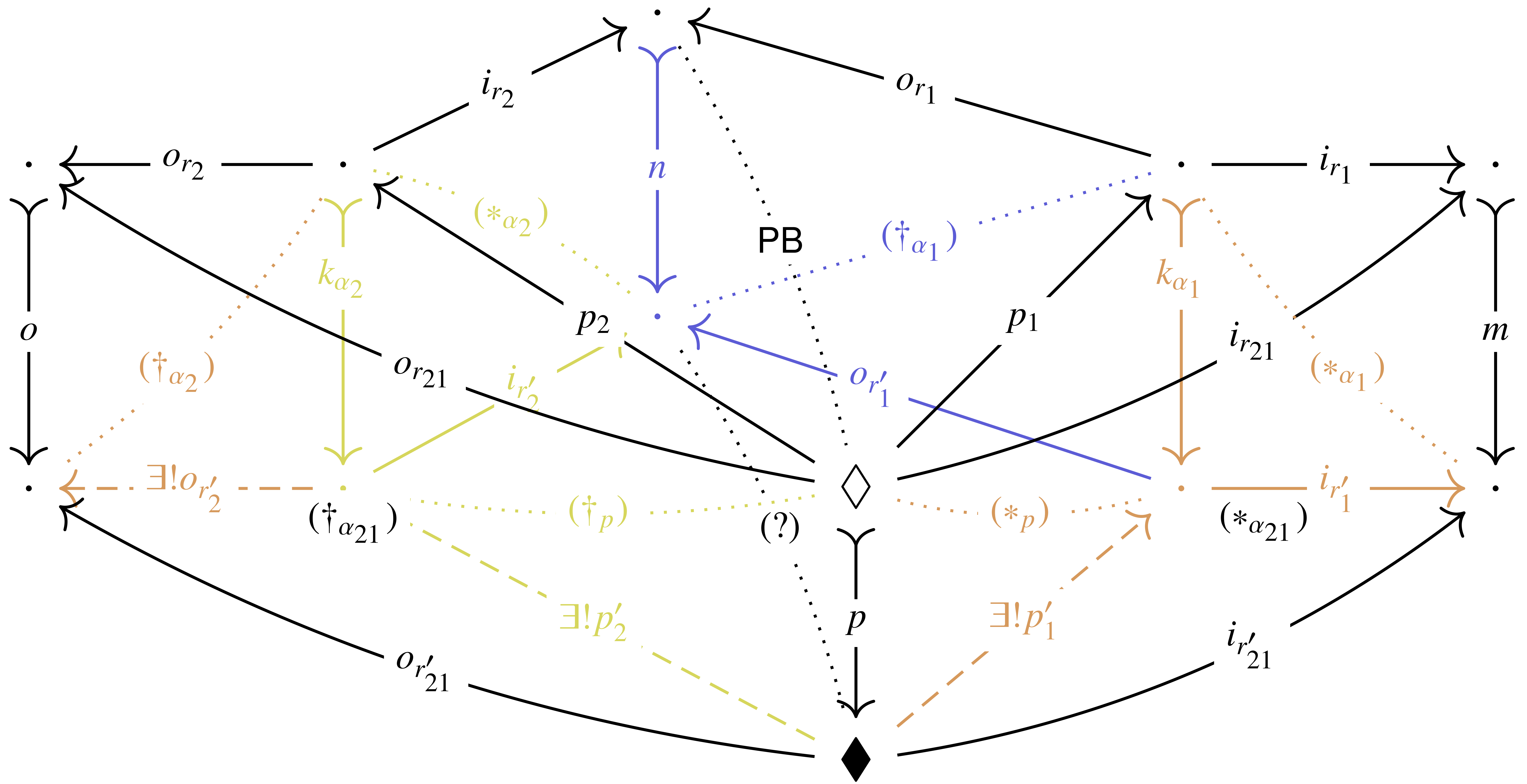


Horizontal decomposition — double-pushout semantics

Proof relies upon
Part II of
van Kampen condition!

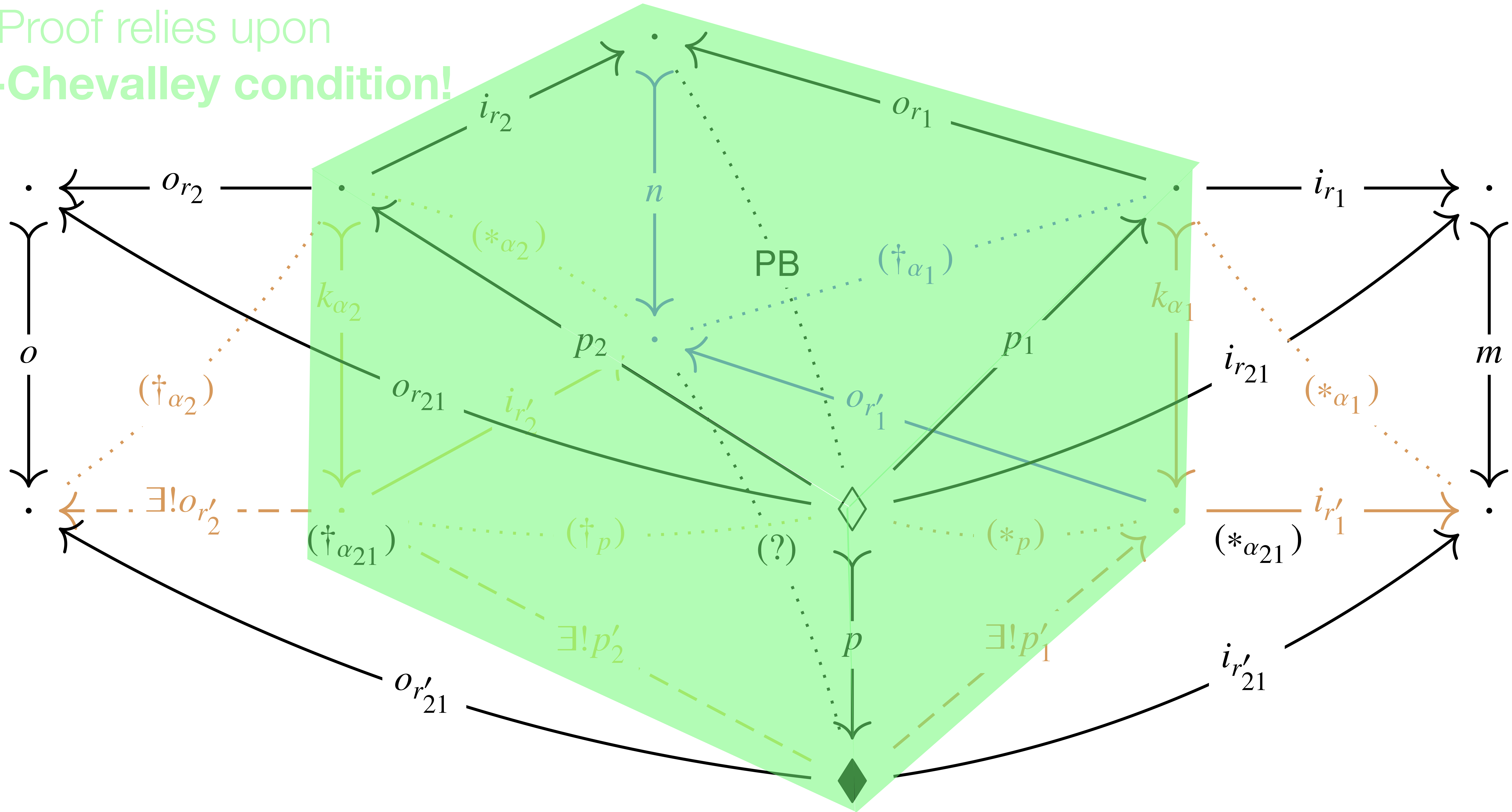


Horizontal decomposition — sesqui-pushout semantics

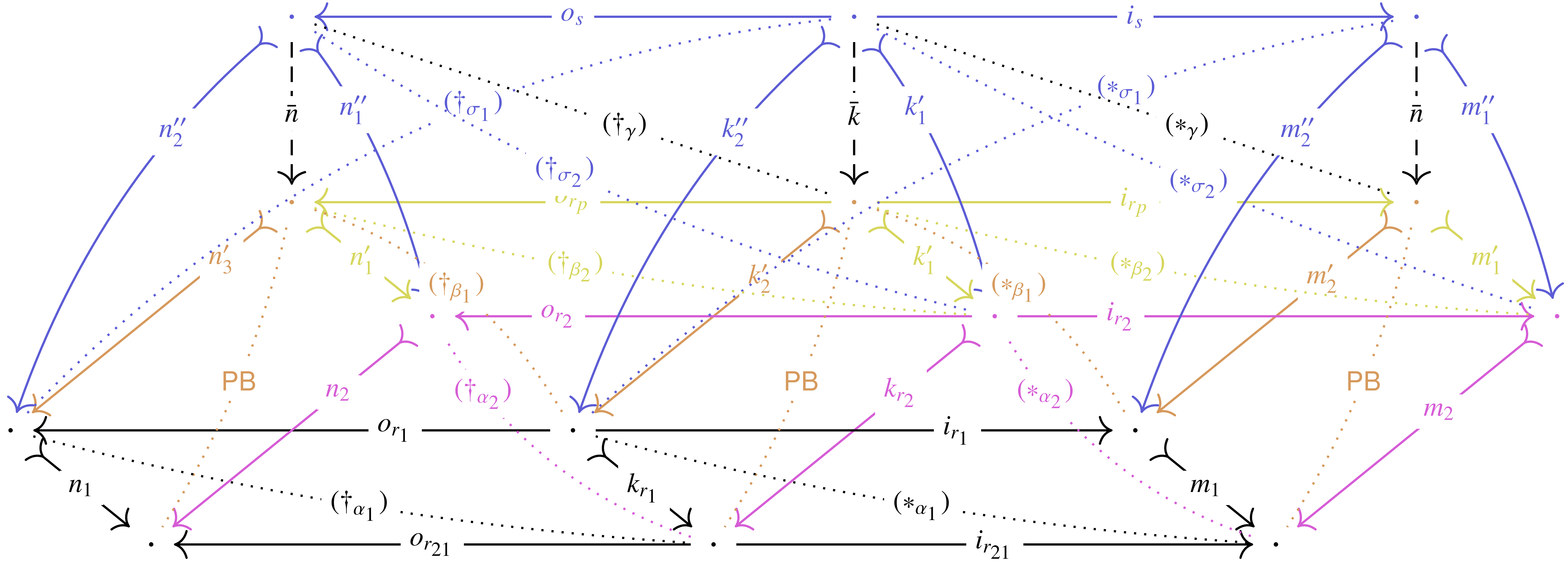


Horizontal decomposition — sesqui-pushout semantics

Proof relies upon
Beck-Chevalley condition!



$\mathbb{D}_1$ has pullbacks



(85)

Final result: table of **sufficient conditions** for **crDCs!**

<table>
<tr><th rowspan="2">Property</th><th colspan="3">Double-Pushout semantics</th><th colspan="4">Sesqui-Pushout semantics</th></tr>
<tr><th>linear</th><th>semi-linear</th><th>generic</th><th>linear</th><th>output-linear</th><th>input-linear</th><th>generic</th></tr>
<tr><td>$\mathbb{D}_0$ has multi-sums</td><td colspan="7">✓ (Lemma 8)</td></tr>
<tr><td>$\exists$ horizontal/vertical units</td><td colspan="7">✓ (Corollary 7)</td></tr>
<tr><td>vertical composition</td><td colspan="3">✓ (by pushout-pushout composition)</td><td colspan="4">✓ (by PO-PO- and vertical FPC composition)</td></tr>
<tr><td rowspan="2">horizontal composition (Proposition 8)</td><td colspan="2">**C** has pullbacks along $\mathcal{M}$-morphisms</td><td rowspan="2">**C** has pullbacks $\wedge$ (L-iii-a)</td><td colspan="4">**C** has pullbacks</td></tr>
<tr><td>$\wedge$ (V-iii-a)</td><td>$\wedge$ (W-iii-a)</td><td>$\wedge$ (V-iii-a)</td><td>$\wedge$ (H-iii-a)</td><td>$\wedge$ (V-iii-a)</td><td>$\wedge$ (L-iii-a)</td></tr>
<tr><td rowspan="3">horizontal decomposition (Proposition 9)</td><td colspan="3">**C** has pushouts along $\mathcal{M}$-morphisms</td><td colspan="4">**C** has pullbacks $\wedge$ has pushouts and FPCs along $\mathcal{M}$-morphisms</td></tr>
<tr><td colspan="2">$\wedge$ has pullbacks along $\mathcal{M}$-morphisms $\wedge$ (V-iii-b)</td><td>$\wedge$ has pullbacks $\wedge$ (L-iii-b)</td><td>$\wedge$ (V-iii-a) $\vee$ (H-iii-a)</td><td>$\wedge$ (H-iii-a)</td><td>$\wedge$ (V-iii-a)</td><td>$\wedge$ (L-iii-a)</td></tr>
<tr><td>$\mathbb{D}_1$ has pullbacks (Proposition 10)</td><td colspan="7">(V-iii-a)</td></tr>
<tr><td>S is a multi-opfibration (Theorem 15)</td><td colspan="3">**C** is a vertical weak adhesive HLR category</td><td colspan="4">**C** is vertical weak adhesive HLR and has FPCs along $\mathcal{M}$-morphisms</td></tr>
<tr><td>T is a residual multi-opfibration (Theorem 15)</td><td colspan="3">**C** is a vertical weak adhesive HLR category</td><td colspan="4">**C** is vertical weak adhesive HLR and has FPCs along $\mathcal{M}$-morphisms</td></tr>
</table>

Table 3: Requirements on the underlying category for giving rise to compositional rewriting semantics of the various kinds. For all cases, we minimally assume that **C** has a stable system of monics, with respect to which **C** is finitary, with respect to which the variants of adhesivity properties are required to hold, and such that $\mathbb{D}_0 := \mathbf{C}|_{\mathcal{M}}$ has pullbacks. The latter is equivalent to requiring that **C** has pullbacks of spans of $\mathcal{M}$-morphisms, which is true for all of the listed adhesivity properties. We moreover use the abbreviation *(W-iii)* to denote (V-iii) $\wedge$ (H-iii).

$\longleftarrow$ cf. **p. 60**

Final result: table of **sufficient conditions** for **crDCs!**

Property	Double-Pushout semantics: linear	Double-Pushout semantics: semi-linear	Double-Pushout semantics: generic	Sesqui-Pushout semantics: linear	Sesqui-Pushout semantics: output-linear	Sesqui-Pushout semantics: input-linear	Sesqui-Pushout semantics: generic
$\mathbb{D}_0$ has multi-sums	✓ (Lemma 8)						
∃ horizontal/vertical units	✓ (Corollary 7)						
vertical composition	✓ (by pushout-pushout composition)			✓ (by PO-PO- and vertical FPC composition)			

Final result: table of **sufficient conditions** for **crDCs!**

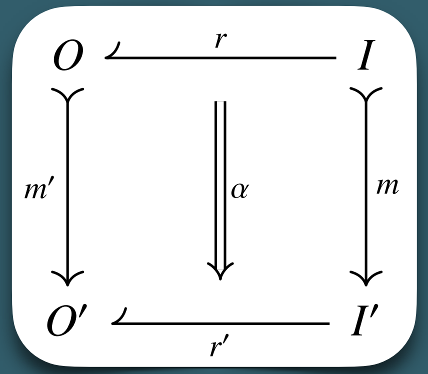
<table>
<tr><th rowspan="2">Property</th><th colspan="3">Double-Pushout semantics</th><th colspan="4">Sesqui-Pushout semantics</th></tr>
<tr><th>linear</th><th>semi-linear</th><th>generic</th><th>linear</th><th>output-linear</th><th>input-linear</th><th>generic</th></tr>
<tr><td rowspan="2">horizontal composition
(Proposition 8)</td><td colspan="2">C has pullbacks along $\mathcal{M}$-morphisms</td><td rowspan="2">C has pullbacks
$\land$ (L-iii-a)</td><td colspan="4">C has pullbacks</td></tr>
<tr><td>$\land$ (V-iii-a)</td><td>$\land$ (W-iii-a)</td><td>$\land$ (V-iii-a)</td><td>$\land$ (H-iii-a)</td><td>$\land$ (V-iii-a)</td><td>$\land$ (L-iii-a)</td></tr>
<tr><td rowspan="2">horizontal decomposition
(Proposition 9)</td><td colspan="3">C has pushouts along $\mathcal{M}$-morphisms</td><td colspan="4">C has pullbacks $\land$ has pushouts and FPCs along $\mathcal{M}$-morphisms</td></tr>
<tr><td colspan="2">$\land$ has pullbacks along $\mathcal{M}$-morphisms $\land$ (V-iii-b)</td><td>$\land$ has pullbacks $\land$ (L-iii-b)</td><td>$\land$ (V-iii-a) $\lor$ (H-iii-a)</td><td>$\land$ (H-iii-a)</td><td>$\land$ (V-iii-a)</td><td>$\land$ (L-iii-a)</td></tr>
</table>

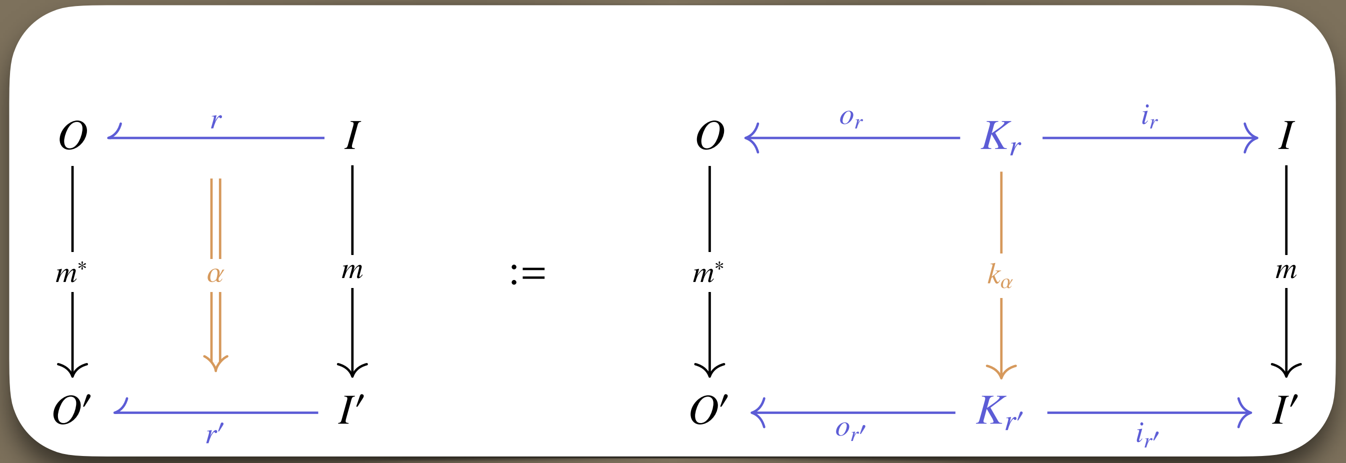
Final result: table of **sufficient conditions** for **crDCs!**

Property	Double-Pushout semantics: linear	Double-Pushout semantics: semi-linear	Double-Pushout semantics: generic	Sesqui-Pushout semantics: linear	Sesqui-Pushout semantics: output-linear	Sesqui-Pushout semantics: input-linear	Sesqui-Pushout semantics: generic
$\mathbb{D}_1$ has pullbacks (Proposition 10)	(V-iii-a)						
S is a multi-opfibration (Theorem 15)	**C** is a vertical weak adhesive HLR category			**C** is vertical weak adhesive HLR and has FPCs along $\mathcal{M}$-morphisms			
T is a residual multi-opfibration (Theorem 15)	**C** is a vertical weak adhesive HLR category			**C** is vertical weak adhesive HLR and has FPCs along $\mathcal{M}$-morphisms			

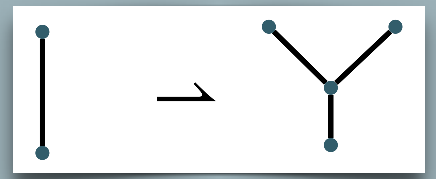
Table 3: Requirements on the underlying category for giving rise to compositional rewriting semantics of the various kinds. For all cases, we minimally assume that **C** has a stable system of monics, with respect to which **C** is finitary, with respect to which the variants of adhesivity properties are required to hold, and such that $\mathbb{D}_0 := \mathbf{C}|_{\mathcal{M}}$ has pullbacks. The latter is equivalent to requiring that **C** has pullbacks of spans of $\mathcal{M}$-morphisms, which is true for all of the listed adhesivity properties. We moreover use the abbreviation *(W-iii)* to denote (V-iii) $\wedge$ (H-iii).

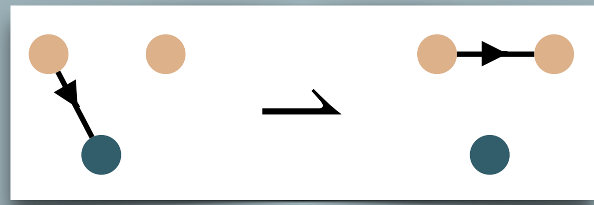
compositional rewriting double categories (crDCs)



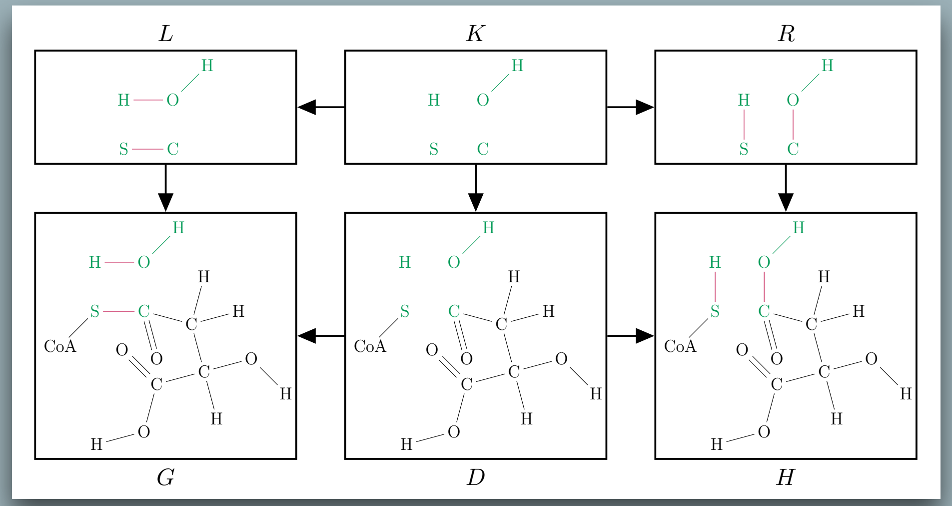


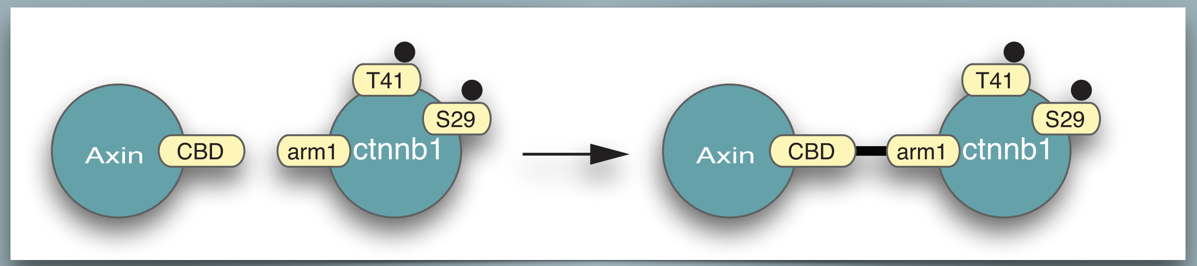
Explicit **rewriting semantics** (DPO, SqPO, …)





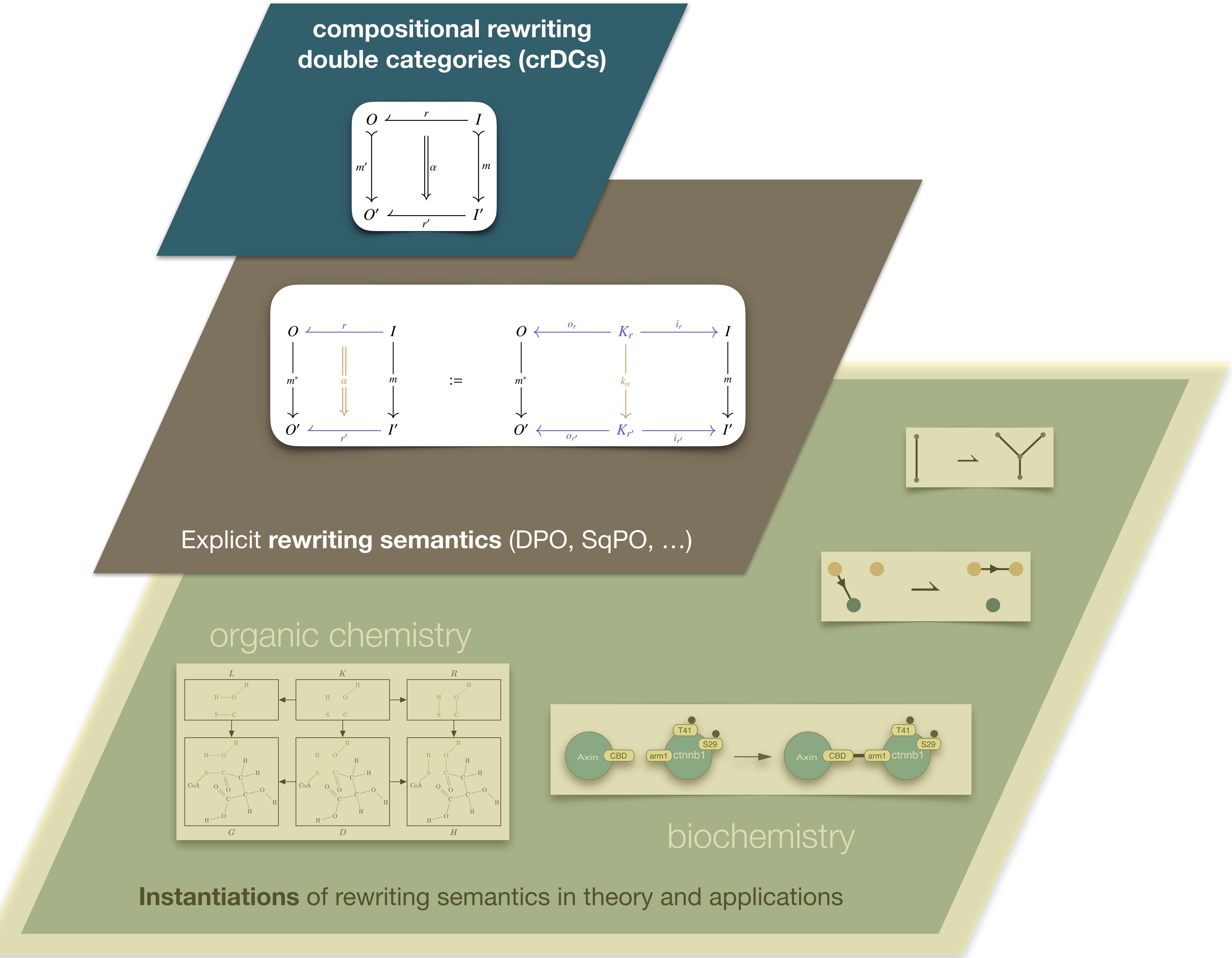
organic chemistry





biochemistry

Instantiations of rewriting semantics in theory and applications


compositional rewriting
double categories (crDCs)
O
r
I
m′
α
m
O′
r′
I′
O
r
I
m*
α
m
O′
r′
I′
:=
O
o_r
K_r
i_r
I
m*
k_α
m
O′
o_r′
K_r′
i_r′
I′
Explicit rewriting semantics (DPO, SqPO, …)
organic chemistry
L
K
R
G
D
H
CoA
Axin
CBD
arm1
ctnnb1
T41
S29
biochemistry
Instantiations of rewriting semantics in theory and applications

≈ "DPO → adhesivity properties", "SqPO → quasi-topoi"

Category (underlying data type)	quasi-topos	adhesive	quasi-adhesive	adhesive HLR	hor. weak adh. HLR	vert. weak adh. HLR	references
Set (sets)	✓	✓	✓	✓	✓	✓	[5]
Graph (directed multigraphs)	✓	✓	✓	✓	✓	✓	[5]
HyperGraph (directed ordered hypergraphs)	✓	✓	✓	✓	✓	✓	[7, Ex. 7]
Sig (algebraic signatures)	✓	✓	✓	✓	✓	✓	[7, Ex. 6]
$\hat{\mathbf{S}}$ (presheaves on category **S**)	✓	✓	✓	✓	✓	✓	[58, 54]
$\hat{\mathbf{T}}_\Sigma$ (term graphs over a signature Σ)	?		✓	✓	✓	✓	[41]
TripleGraph (functor category $[\mathbf{S}_3, \mathbf{Graph}]$)	?			✓	✓	✓	[3, Fact 4.18]
$\mathbf{AGraph}_\Sigma$ (attributed graphs over signature Σ)	?			✓	✓	✓	[3, Thm. 11.11], [8, 54]
$\mathbf{SymbGraph}_D$ (symbolic graphs over Σ-algebra D)	?			✓	✓	✓	[59, Thm. 2], [54]
uGraph (undirected multigraphs)	?				✓	✓	[29]
ElemNets (elementary Petri nets)	?			(!)	✓	✓	[8]
PTnets (place/transition nets)	?				✓	✓	[3, Fact 4.21], [8]
Spec (algebraic specifications)	✓				✓	✓	[7, Ex. 6], [3, Fact 4.24]
SGraph (directed simple graphs)	✓				✓	✓	[7, Prop. 17], Corollary 5(q-v)
$\mathbf{Set}_F$ (coalgebras for $F : \mathbf{Set} \to \mathbf{Set}$)	(∗)					(†)	[7], [57, Thm. 1]
lSets (list sets)	?					✓	[39]

Table 2: Examples of categories exhibiting various forms of adhesivity properties. The symbol ? indicates when a certain property is (to the best of our knowledge) not known to hold. Note that for the HLR variants of adhesivity properties, the information not contained in the table is the precise nature (cf. references provided) of the stable system of monics $\mathcal{M}$ for which the adhesivity properties hold. Moreover, the precise conditions (∗) and (†) under which the category $\mathbf{Set}_F$ of F-coalgebras has quasi-topos or adhesivity properties are provided in [7] and [57, Thm. 1], respectively.

⟵ cf. **p. 45**

Some constructions for categories with **adhesivity properties**

$$\begin{array}{ccccccc} E & \xrightarrow{\iota} & F(V)\times F(V) & \xleftarrow{\Delta} & F(V) & \xleftarrow{F} & V \\ \downarrow{\scriptstyle \varphi_E} & & \downarrow{\scriptstyle \Delta\circ F(\varphi_V)} & & \downarrow{\scriptstyle F(\varphi_V)} & & \downarrow{\scriptstyle \varphi_V} \\ E' & \xrightarrow{\iota'} & F(V')\times F(V') & \xleftarrow{\Delta} & F(V') & \xleftarrow{F} & V' \end{array}$$

F	Description
$Id_{\mathbf{Set}}$	directed multigraphs
$\square^*$	directed “ordered” hypergraphs with multiple incidences (**HyperGraph** [3, Fact 4.17] aka **PNet** [7, Ex. 7])
$\mathcal{M}$	directed “unordered” hypergraphs with multiple incidences (= **PTNets** of [3, Fact 4.21])
$\mathcal{P}$	directed “unordered” hypergraphs with simple incidences (= **ElemNets** of [3, Fact 4.20])

$$\begin{array}{ccccc} E & \xrightarrow{\iota} & F(V) & \xleftarrow{F} & V \\ \downarrow{\scriptstyle \varphi_E} & & \downarrow{\scriptstyle F(\varphi_V)} & & \downarrow{\scriptstyle \varphi_V} \\ E' & \xrightarrow{\iota'} & F(V') & \xleftarrow{F} & V' \end{array}$$

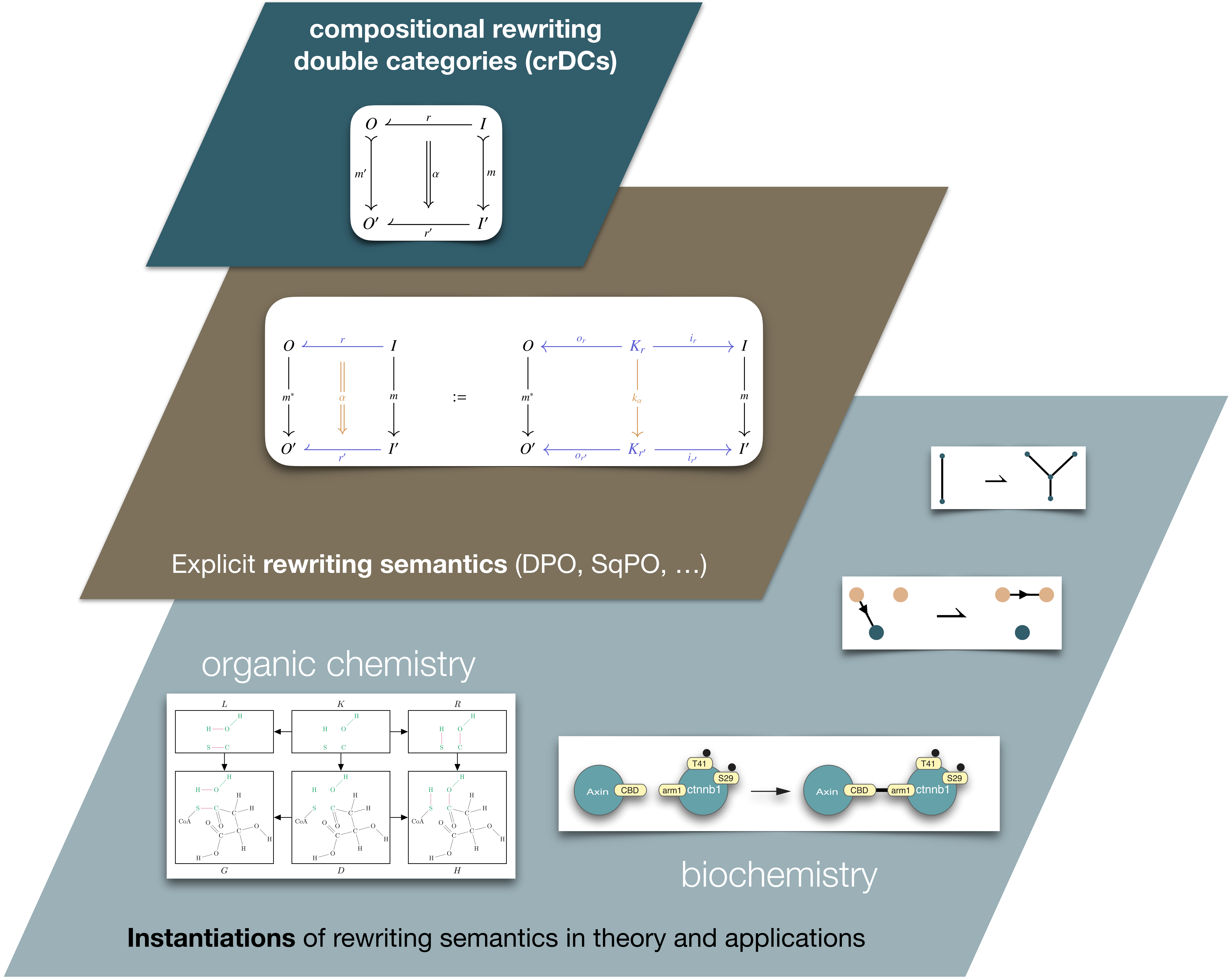
F	Description
$\mathcal{P}^{(1,2)}$	*undirected multigraphs* [29]
$\square^*$	undirected “ordered” hypergraphs with multiple incidences (i.e. lists)
$\mathcal{M}$	undirected “unordered” hypergraphs with multiple incidences
$\mathcal{P}$	undirected “unordered” hypergraphs with simple incidences

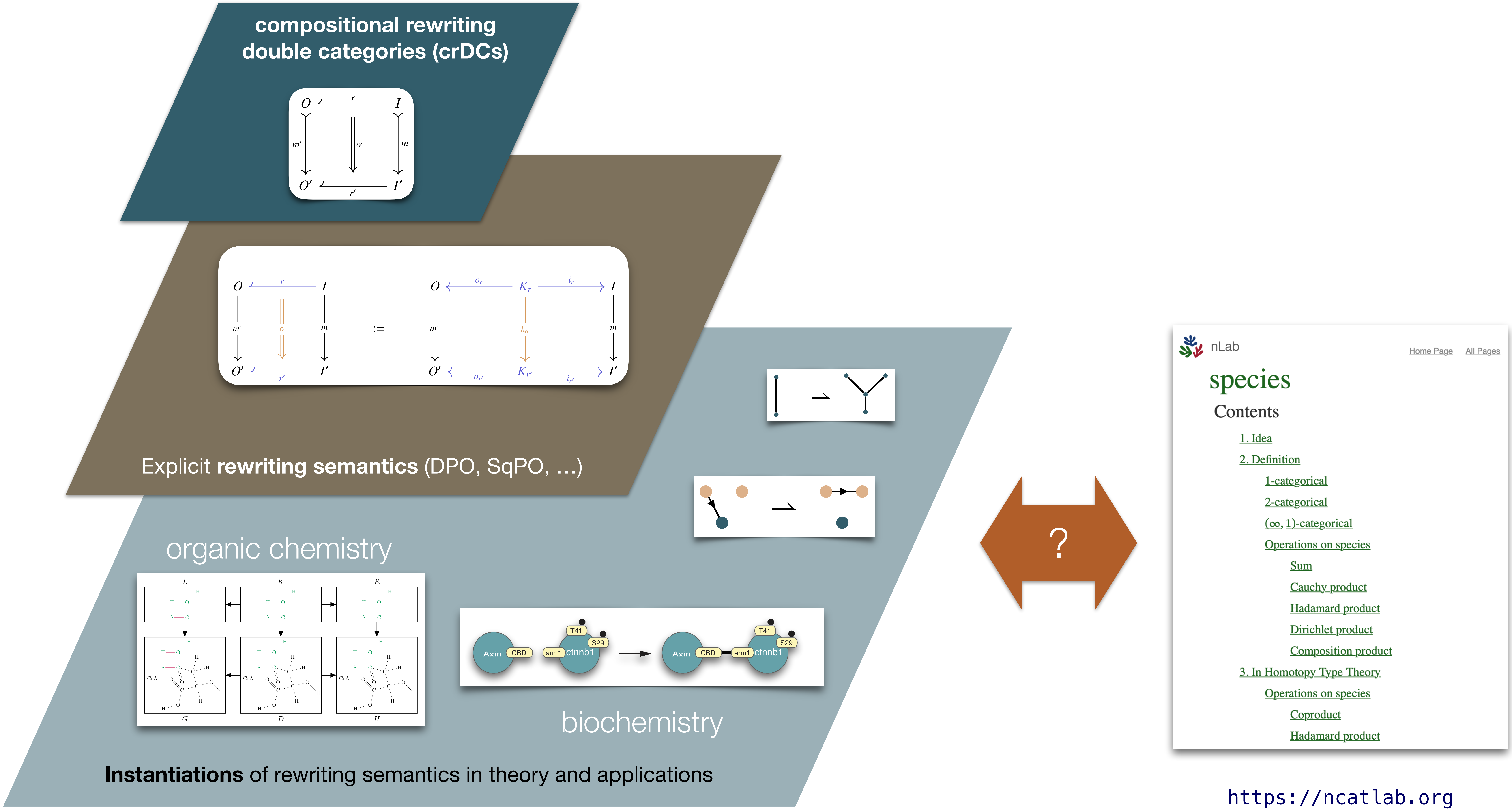
Table 1: Collection of examples for categories with adhesivity properties based upon two “schemas” of comma category constructions. Here, we employ the notations $\square^*$ for the free monoid functor, $\mathcal{M}$ (also denoted $\oplus^*$ in [3]) for the free commutative monoid functor, $\mathcal{P}$ for the covariant powerset functor, and $\mathcal{P}^{(1,2)}$ for the restricted version thereof (cf. e.g. [57]).

⟵ cf. **p. 44**

PART 3: OUTLOOK

The COREACT project


compositional rewriting
double categories (crDCs)
Explicit rewriting semantics (DPO, SqPO, …)
organic chemistry
biochemistry
Axin
CBD
arm1
ctnnb1
T41
S29
Instantiations of rewriting semantics in theory and applications


compositional rewriting
double categories (crDCs)
Explicit **rewriting semantics** (DPO, SqPO, …)
organic chemistry
biochemistry
Instantiations of rewriting semantics in theory and applications
?
nLab
Home Page
All Pages
species
Contents
1. Idea
2. Definition
1-categorical
2-categorical
(∞, 1)-categorical
Operations on species
Sum
Cauchy product
Hadamard product
Dirichlet product
Composition product
3. In Homotopy Type Theory
Operations on species
Coproduct
Hadamard product
https://ncatlab.org

CoREACT

Coq-based Rewriting: towards Executable Applied Category Theory

Consortium: IRIF (UP), LIP (ENS-Lyon), LIX (École Polytechnique), Sophia-Antipolis (Inria)

Partner	Last name	First name
Université Paris Cité	BEHR	Nicolas
	GALLEGO	Emilio
	GHEERBRANT	Amélie
	HERBELIN	Hugo
	MELLIÈS	Paul-André
	ROGOVA	Alexandra
	PhD student	(to recruit)
ENS-Lyon	HARMER	Russell
	HIRSCHOWITZ	Tom
	POUS	Damien
	PostDoc	(to recruit)
École Polytechnique	MIMRAM	Samuel
	WERNER	Benjamin
	ZEILBERGER	Noam
	PostDoc	(to recruit)
Inria Sophia-Antipolis	BERTOT	Yves
	COHEN	Cyril
	TASSI	Enrico
	PostDoc	(to recruit)
Cambridge University	LAFONT	Ambroise

coreact.wiki

Category theory

- **Special types of categories:**
  - adhesive/quasi-adhesive/adhesive HLR/weak adhesive HLR/…
  - quasi-topoi
- **Double categories**
- **Universal constructions:**
  - stable systems of monics, factorisation systems, multi-sums, …
  - pushouts, pullbacks, final pullback complements, multi-initial pushout complements, final pullback complement augmentations, …
  - Grothendieck fibrations/multi-opfibrations/residual multi-opfibrations …
- **Lemmata on special properties of universal constructions:**
  - (De-)composition properties
  - fibrational properties
  - Beck-Chevalley conditions

Diagrammatic reasoning

- **Commutative diagrams**
- **Reasoning moves**
  - from universal properties
  - from diagrammatic lemmata
- **Compositionality of reasoning moves**

Formalisations for `coreact.workbench`

- **Auxiliary tactics** to convert between **drawings** and **Coq expressions**
- From **drawing transformations** to **reasoning moves**
- From **drawing transformations** to **Cypher queries**

Foundations of compositional rewriting theory

- **Compositional rewriting double categories (crDCs)**
- **Concurrency Theorems**
- **Associativity Theorems**
- **Rule Algebra and Stochastic Mechanics**
- **Tracelet Hopf Algebras and Decomposition Spaces**

Collection of rewriting semantics

- **Double Pushout/Sesqui-Pushout/Single-Pushout/AGREE/PBPO+/…**
  - linear/input-linear/output-linear/non-linear/…
- **Theory of constraints and application conditions:**
  - nested application conditions
  - constraint-guaranteeing/-preserving semantics
- **Compositional rewriting for rules with conditions**
  - shift and transport constructions
  - Concurrency and associativity theorems
  - Rule algebras/stochastic mechanics/tracelets/…

Executable Applied Category theory (ExACT)

- **Constructive characterization of categories with adhesivity/quasi-topoi:**
  - Artin gluing/slice/coslice/product/sum/**functor and comma categories**/…
  - **collection** of practically relevant examples (**Graph** as **presheaf topos**, **SimpleGraph** via **Artin gluing**, **HyperGraph** as **comma category**, …)
- **Translation** from **rewriting semantics** to **SMT solvers/theorem provers**
- **Reference prototype algorithms for concrete rewriting semantics**

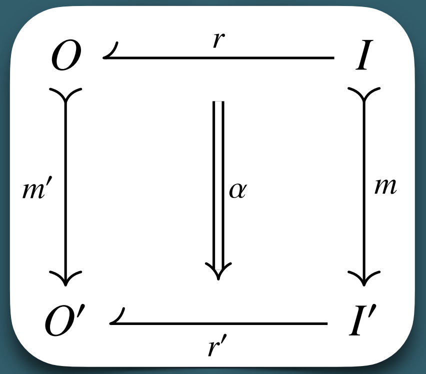
Category theory

- **Special types of categories:**
  - adhesive/quasi-adhesive/adhesive HLR/weak adhesive HLR/…
  - quasi-topoi
- **Double categories**
- **Universal constructions:**
  - stable systems of monics, factorisation systems, multi-sums, …
  - pushouts, pullbacks, final pullback complements, multi-initial pushout complements, final pullback complement augmentations, …
  - Grothendieck fibrations/multi-opfibrations/residual multi-opfibrations …
- **Lemmata on special properties of universal constructions:**
  - (De-)composition properties
  - fibrational properties
  - Beck-Chevalley conditions

Executable Applied Category theory (ExACT)

- **Constructive characterization of categories with adhesivity/quasi-topoi:**
  - Artin gluing/slice/coslice/product/sum/**functor and comma categories**/…
  - **collection** of practically relevant examples (**Graph** as **presheaf topos**, **SimpleGraph** via **Artin gluing**, **HyperGraph** as **comma category**, …)

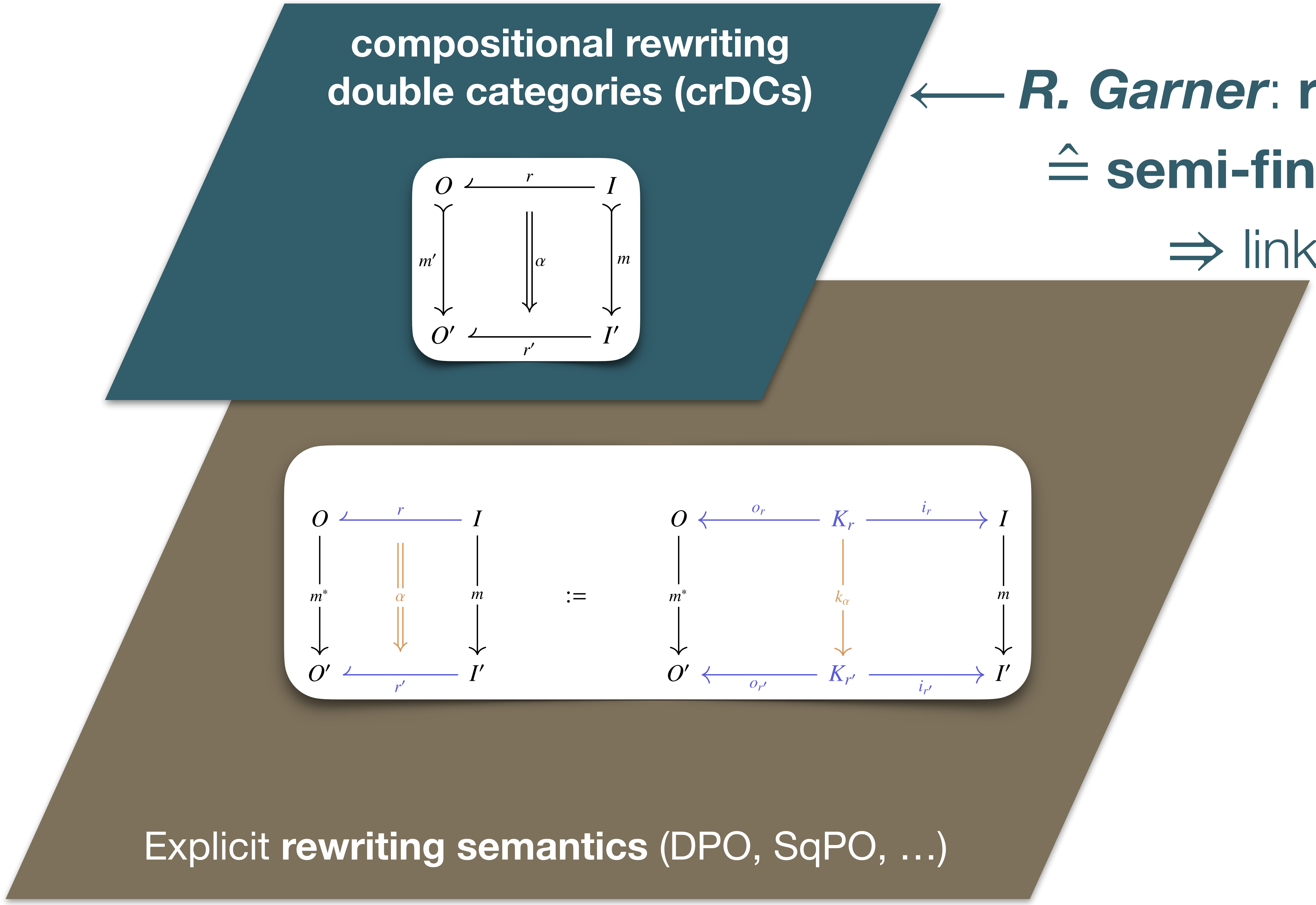
compositional rewriting double categories (crDCs)



⟵ ***R. Garner*: residual multi-opfibrations**

≙ **semi-final liftings (Tholen, 1950s)**

⇒ link to **algebraic topology?**



⟵ ***R. Garner***: **residual multi-opfibrations**

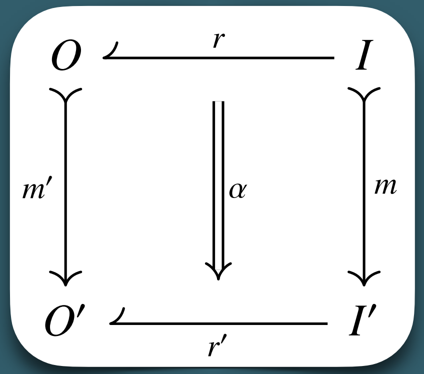
≙ **semi-final liftings (Tholen, 1950s)**

⇒ link to **algebraic topology?**

⟵ other ***semantics (PBPO+, AGREE, …)***,

*extension to **rewriting with constraints & conditions, …***

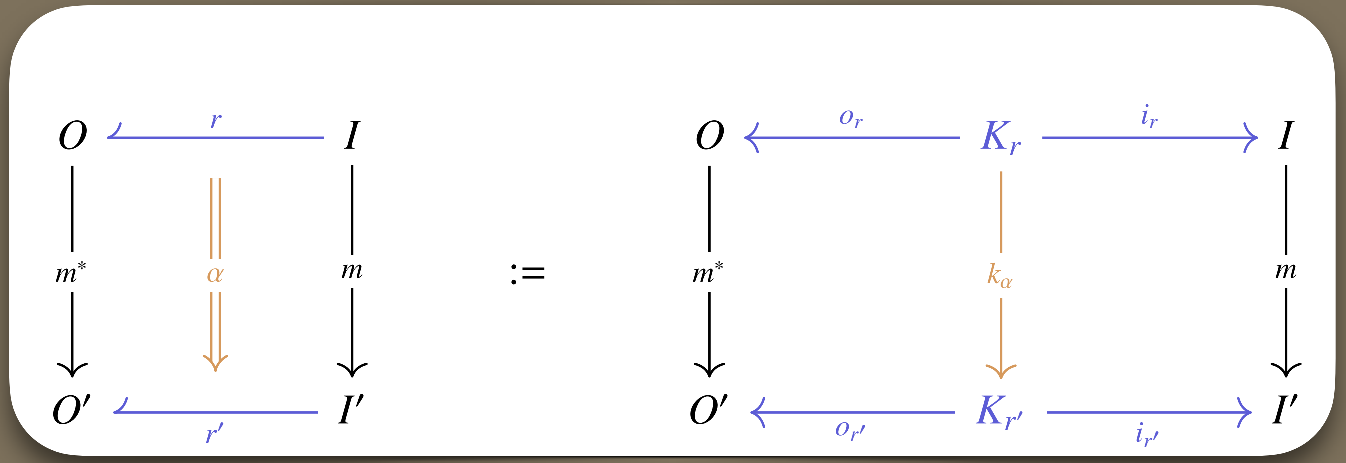
compositional rewriting double categories (crDCs)



⟵ ***R. Garner*: residual multi-opfibrations**

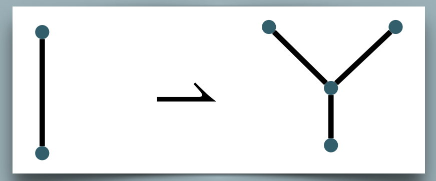
≙ **semi-final liftings (Tholen, 1950s)**

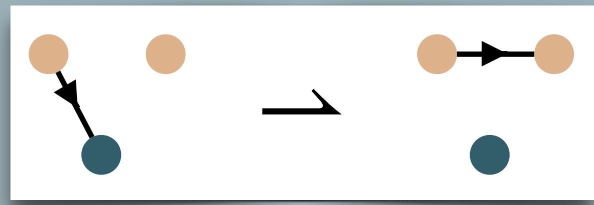
⇒ link to **algebraic topology?**



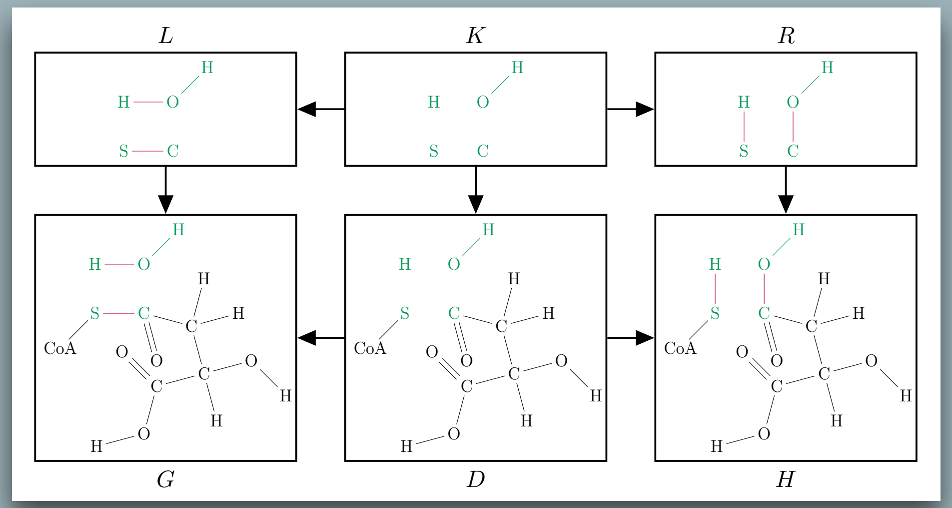
Explicit **rewriting semantics** (DPO, SqPO, …)

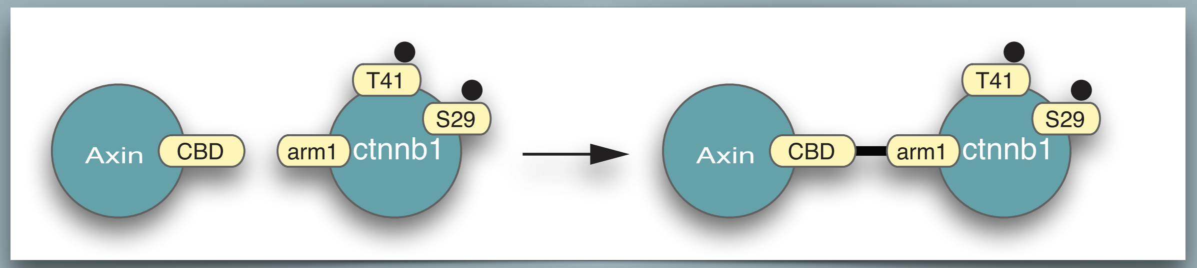
⟵ other ***semantics (PBPO+, AGREE, …)***, *extension to* ***rewriting with constraints & conditions, …***





organic chemistry





biochemistry

Instantiations of rewriting semantics in theory and applications

⟵ search for a better **classificaiton** of suitable categories (especially in terms of **existence guarantees** for factorization systems, FPCs, …), **constructions** for suitable categories (**comma categories, Artin gluing**, …)

References, additional slides and videos available at nicolasbehr.com

Merci beaucoup !

INSTITUT DE RECHERCHE EN INFORMATIQUE FONDAMENTALE

cnrs

Université Paris Cité

Fundamentals of Compositional Rewriting Theory

Topos Institute Colloquium, June 9, 2022

Nicolas Behr

CNRS, Université Paris Cité, IRIF (UMR 8243)