Homotopic and Compositional Aspects of (Hyper)graph Rewriting and Fundamental Physics

Mathematically Structured Programming (MSP) Seminar, University of Strathclyde

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November 24, 2021

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Background of this Talk

Much of the work presented here was performed in close collaboration with Xerxes Arsiwalla, Manojna Namuduri and Hatem Elshatlawy:

- J. Gorard, M. Namuduri, X. D. Arsiwalla (2021), https://arxiv.org/abs/2105.04057
- J. Gorard, M. Namuduri, X. D. Arsiwalla (2021), https://arxiv.org/abs/2103.15820
- J. Gorard, M. Namuduri, X. D. Arsiwalla (2020), https://arxiv.org/abs/2010.02752
- X. D. Arsiwalla, J. Gorard (2021), https://arxiv.org/abs/2111.03460
- X. D. Arsiwalla, J. Gorard, H. Elshatlawy (2021), https://arxiv.org/abs/2105.10822
- J. Gorard (2021), https://arxiv.org/abs/2102.09363
- etc.

Definition

A hypergraph, denoted H = (V, E), is a finite collection of (potentially ordered) hyperedges:

$$\mathsf{E}\subset\mathcal{P}\left(\mathsf{V}
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ight\},$$

where $\mathcal{P}(V)$ denotes the power set of V.

Definition

An *update rule*, denoted *R*, for a hypergraph H = (V, E) is an abstract rewriting rule of the form $H_1 = (V_1, E_1) \rightarrow H_2 = (V_2, E_2)$, where H_1 and H_2 are subhypergraphs of *H* (i.e. $V_1, V_2 \subseteq V$, $E_1, E_2 \subseteq E$).

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Hypergraph Rewriting Systems II



Figure: Hypergraphs corresponding to finite collections of ordered relations between elements, namely $\{\{1,2\},\{1,3\},\{2,3\},\{4,1\}\}$ and $\{\{1,2,3\},\{3,4,5\}\}$, respectively.



Figure: A hypergraph transformation rule corresponding to the set substitution system $\{\{x, y\}, \{y, z\}\} \rightarrow \{\{w, y\}, \{y, z\}, \{z, w\}, \{x, w\}\}$.

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Hypergraph Rewriting Systems III



Figure: The results of the first 10 steps in the evolution history of the set substitution system $\{\{x, y\}, \{y, z\}\} \rightarrow \{\{w, y\}, \{y, z\}, \{z, w\}, \{x, w\}\}.$



Figure: The result after 14 steps of evolution.

Compositional Structure of Hypergraph Rewriting I

Start from the definition of Kissinger and Fong:

Definition

A hypergraph category is a symmetric monoidal category (\mathbf{C}, \otimes, I) in which every object A in $ob(\mathbf{C})$ is equipped with a special commutative Frobenius algebra structure $(A, \mu, \eta, \delta, \epsilon)$, such that the Frobenius algebra structure of the monoidal product $A \otimes B$ (for A and B in $ob(\mathbf{C})$) is canonically induced from the Frobenius algebra structures of A and B.

Definition

A typed hypergraph production is a span of monomorphisms p:

$$p = \left(L \xleftarrow[l]{r} K \xrightarrow{r} R \right), \tag{2}$$

with L, K and R being typed hypergraphs, and I and r being injective typed hypergraph morphisms.

Definition

A direct typed hypergraph transformation $G \Rightarrow^{p,m} H$ is given by the following pair of pushout squares:

assuming production p and match $m: L \rightarrow G$.

Definition

A typed hypergraph transformation $G_0 \Rightarrow^* G_n$ is any sequence $G \Rightarrow G_1 \Rightarrow \cdots \Rightarrow G_n$ of direct typed hypergraph transformations.

Double-pushout (DPO) rewriting systems are conventionally defined over *adhesive categories*.

Definition

An *adhesive category* is a category that has *pushouts along monomorphisms*, that has pullbacks, and in which every pushout along a monomorphism satisfies the *van-Kampen square* condition.

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Definition

A pushout along a monomorphism is a pushout square:



of a span of the form:

$$B \xleftarrow[g]{g} A \xrightarrow{f} C$$
, (5)

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in which either f or g is a monomorphism.

Compositional Structure of Hypergraph Rewriting V

Definition

A pushout square satisfies the *van-Kampen square* condition if and only if, for every commutative diagram of the form:



for which certain subdiagrams are pullbacks, the pushouts and pullbacks are compatible.

These subdiagrams are of the form:

$$B' \xleftarrow{g_h} A' \qquad A \xleftarrow{h_A} A' \qquad \qquad A \xleftarrow{h_A} A' \qquad \qquad \\ \downarrow_{h_B} \qquad \downarrow_{h_A}, \qquad \text{and} \qquad \downarrow_f \qquad \downarrow_{f_h}. \qquad (7) \\ B \xleftarrow{g} A \qquad \qquad C \xleftarrow{h_C} C'$$

Note that the category of typed hypergraphs is not fully adhesive (due to arbitrary connectivity of hypergraph vertices, so pushouts along monomorphisms are not always guaranteed to exist). However, it is nevertheless *partial adhesive*, i.e. it forms a full subcategory \mathbf{C}' of an adhesive category \mathbf{C} for which the embedding functor $S : \mathbf{C}' \to \mathbf{C}$ preserves monomorphisms, which is sufficient to define a DPO system.

Multiway Hypergraph Rewriting I

Definition

A multiway evolution graph, denoted $G_{multiway}$, is a directed, acyclic graph corresponding to the evolution of a (generically non-confluct) abstract rewriting system (A, \rightarrow) , in which the set of vertices $V(G_{multiway})$ corresponds to the set of objects A, and the directed edge $a \rightarrow b$ exists in $E(G_{multway})$ if and only if there exists an application of the rewrite relation \rightarrow that transforms object a to object b.

Hence, a directed edge will connect vertices a and b in $G_{multiway}$ if and only if $a \rightarrow b$, and a directed path will connect vertices a and b if and only if $a \rightarrow^* b$, where \rightarrow^* denotes the reflexive transitive closure of \rightarrow , i.e. if and only if there exists a finite rewriting sequence of the form:

$$a \to a' \to a'' \to \dots \to b' \to b.$$
 (8)

Multiway Hypergraph Rewriting II



Figure: The multiway evolution graph corresponding to the first three steps in the non-deterministic evolution history of the hypergraph substitution system $\{\{x, y\}, \{y, z\}\} \rightarrow \{\{w, y\}, \{y, z\}, \{z, w\}, \{x, w\}\}$.

Multiway Hypergraph Rewriting III



Figure: The first three steps in the canonical evolution history (i.e. the evolution history with canonical updating order) for the hypergraph substitution system $\{\{x, y\}, \{y, z\}\} \rightarrow \{\{w, y\}, \{y, z\}, \{z, w\}, \{x, w\}\}$, as represented by a single path in the multiway evolution graph.

If the rewrite relation \rightarrow is an indexed union of subrelations $\rightarrow = \rightarrow_1 \cup \rightarrow_2 \cup \ldots$, with label set Λ , then the system $(A, \Lambda, \rightarrow)$ is simply a bijective function from A to a subset of the power set of A indexed by Λ , i.e. $\mathcal{P}(\Lambda \times A)$:

$$p \mapsto \{(\alpha, q) \in \Lambda \times A : p \to^{\alpha} q\}.$$
(9)

Recall that an *F*-coalgebra for an endofunctor $F : \mathbf{C} \to \mathbf{C}$ consists of an object *A* in ob(**C**), equipped with a morphism $\alpha : A \to FA$ in hom(**C**), hence denoted (A, α) .

The power set construction on **Set** is a covariant endofunctor $\mathcal{P} : \mathbf{Set} \to \mathbf{Set}$, such that the ARS (A, \to) consists of an object A equipped with an additional morphism of \to of **Set**:

$$\rightarrow: A \rightarrow \mathcal{P}A.$$
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The category **MuGraph** is symmetric monoidal.

The ordinary composition of morphisms in **MuGraph** arises from the fact that productions p_1 and p_2 , yielding an *E*-related transformation sequence $G \Rightarrow H \Rightarrow G'$, can be composed by means of the *concurrency theorem* in algebraic graph transformation theory to obtain an *E*-concurrent production $p_1 *_E p_2$, yielding the direct transformation $G \Rightarrow G'$:



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Likewise, the monoidal composition of morphisms in **MuGraph** arises from the fact that productions p_1 and p_2 , yielding sequentially-independent transformation sequences $G \Rightarrow H_1 \Rightarrow G'$ and $G \Rightarrow H_2 \Rightarrow G'$, can be composed by means of the *parallelism theorem* to obtain the parallel production $p_1 + p_2$, yielding the direct transformation $G \Rightarrow G'$:



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Definition

A causal network, denoted G_{causal} , is a directed, acyclic graph in which every vertex in $V(G_{causal})$ corresponds to an application of an update rule (i.e. an update 'event'), and in which the directed edge $a \rightarrow b$ exists in $E(G_{causal})$ if and only if:

$$\ln(b) \cap \operatorname{Out}(a) \neq \emptyset, \tag{13}$$

i.e. the input for event b makes use of hyperedges that were produced by the output of event a.

The transitive reduction of the causal network corresponds to the Hasse diagram of a causal partial order relation, c.f. the conformal structure of spacetime.

Causal Structure II



Figure: The causal graphs corresponding to the first three and five steps in the deterministic evolution history for the set substitution rule $\{\{x, y\}, \{x, z\}\} \rightarrow \{\{x, y\}, \{x, w\}, \{y, w\}, \{z, w\}\}$, respectively.

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Causal Structure III



Figure: The multiway evolution causal graph (with evolution edges shown in gray, and causal edges shown in orange) for the set substitution system $\{\{x, y\}, \{z, y\}\} \rightarrow \{\{x, w\}, \{y, w\}, \{z, w\}\}.$

If we have productions p_1 and p_2 :

$$p_{1} = \left(\begin{array}{cc} L_{1} & \xleftarrow{r_{1}} & K_{1} & \xrightarrow{r_{1}} & R_{1} \end{array} \right), \quad (14)$$

$$p_{2} = \left(\begin{array}{cc} L_{2} & \xleftarrow{r_{2}} & K_{2} & \xrightarrow{r_{2}} & R_{2} \end{array} \right), \quad (15)$$

then they may be said to be *causally related* if $L_2 \setminus K_2$ (i.e. the "input" of production p_2) makes use of (hyper)edges that appear in $R_1 \setminus K_1$ (i.e. the "output" of production p_1):

$$(L_2 \setminus K_2) \cap (R_1 \setminus K_1) \neq \emptyset.$$
 (16)

The category **MuCauGraph** is now a weak 2-category (causal relationships between productions form 2-cells within **MuGraph**).

The category **MuCauGraph** is equipped with two distinct monoidal structures: \otimes_M , arising from parallel composition of productions (1-cells), and \otimes_C , arising from parallel composition of causal relationship between productions (2-cells). Strictly speaking, \otimes_C forms a *partial* monoidal structure in the sense of Coecke and Lal, i.e:

 $\otimes_{\mathcal{C}}$: CauGraph × CauGraph → CauGraph, (17)

is a *partial bifunctor*, namely a bifunctor:

$$\overline{\otimes_{\mathcal{C}}}$$
 : $\overline{\text{CauGraph}} \times \overline{\text{CauGraph}} \to \text{CauGraph},$ (18)

where **CauGraph** × **CauGraph** denotes a subcategory of **CauGraph** × **CauGraph** (known as the *domain of definition* of \otimes_C , denoted dd (\otimes_C)).

Evolution Causal Graphs as 2-Categories III

(**CauGraph**, \otimes_C , *I*) is a symmetric strict partial monoidal category, since every object *A* in ob (**CauGraph**) contains at least one element:

$$CauGraph(I, A) \neq \emptyset, \tag{19}$$

the unit object *I* in ob (**CauGraph**) is terminal, with unique morphism \top_A for each object *A* in ob (**CauGraph**):

$$\top_A : A \to I, \tag{20}$$

and the monoidal product $A \otimes_C B$ exists (for objects A and B in ob (**CauGraph**) if and only if:

$$CauGraph(A, B) = [CauGraph(I, B)] \circ \top_A, \quad (21)$$

 $\mathbf{CauGraph}(B,A) = [\mathbf{CauGraph}(I,A)] \circ \top_B. \tag{22}$

Homotopies in Abstract Rewriting Systems I



Figure: Multiway evolution graphs produced by the string substitution rule $A \rightarrow AB$ with red and yellow paths highlighted, illustrating the existence of multiple proofs of the proposition $AA \rightarrow ABBBABBB$.

Homotopies in Abstract Rewriting Systems II



Figure: A multiway evolution graph produced by the string substitution rule $A \rightarrow AB$, with purple edges corresponding to homotopy maps between two proofs of the proposition $AA \rightarrow ABBBABBB$.

Homotopies in Abstract Rewriting Systems III



Figure: Multiway evolution graphs produced by the string substitution rule $A \rightarrow AB$, with homotopy maps introduced in an ad hoc fashion (left) vs. homotopy maps introduced via explicit inclusion of additional/higher-order rewriting rules (right).

Homotopies in Abstract Rewriting Systems IV



Figure: A multiway evolution graph produced by the string substitution rule $A \rightarrow AB$, with four highlighted paths corresponding to two proofs of the proposition $AA \rightarrow ABBBABBBB$ and two further proofs of the proposition $ABAB \rightarrow ABBBABBBB$.

Homotopies in Abstract Rewriting Systems V



Figure: A multiway evolution graph produced by the string substitution rule $A \rightarrow AB$, with purple edges corresponding to homotopy 2-cells between red paths, and orange paths corresponding to homotopy 2-cells between yellow paths, such that the lighter arrows correspond to homotopy 3-cells between 2-cells.

Homotopies in Abstract Rewriting Systems VI



Figure: A multiway evolution graph produced by the string substitution rule $A \rightarrow AB$, with purple arrows corresponding to homotopy 3-cells between the 2-cells indicated by the red and yellow paths.

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Homotopies in Abstract Rewriting Systems VII



Figure: Multiway evolution graphs produced by the string substitution rule $A \rightarrow AB$, with higher homotopy maps introduced in an ad hoc fashion (left) vs. higher homotopy maps introduced via explicit inclusion of additional/higher-order rewriting rules (right).

Upon inclusion of 2-cells between paths, the resulting multiway system becomes a *double category*:



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2-cells in the double category **D** can be represented by the following commutative square (with ϕ being the 2-cell):



Upon inclusion of appropriate inversion rules, one obtains a *double* groupoid.

A Higher Categorical Approach III

Likewise, upon inclusion of 3-cells between paths, the resulting multiway system becomes a *3-fold category*:

Definition

- A 3-fold category, denoted $\mathbf{D}_2 \longrightarrow \mathbf{D}_1 \longrightarrow \mathbf{D}_0$, is any category in which:
 - The objects are the objects of D₀;
 - **②** The vertical arrows (1-morphisms) are the morphisms of D_0 ;
 - The horizontal arrows (1-morphisms)) are the objects of D₁;
 - The vertical squares (2-morphisms) are the morphisms of D_1 ;
 - The horizontal squares (2-morphisms) are the objects of D_2 ;
 - The cubes bounded by vertical and horizontal squares (3-morphisms) are the morphisms of D₂.

3-cells in a 3-fold category can be represented by the following commutative cube (with ϕ being the 3-cell):



(24)

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Continuation of this procedure (assuming admissibility of higher rewriting rules up to order n - 1) yields an *n*-fold category:



The $n \to \infty$ limit (assuming invertible rewriting rules, and assuming that all such rules are admissible) yields an ∞ -groupoid. The classifying space of these ∞ -groupoids is then an $(\infty, 1)$ -topos, as seen in classical homotopy theory. This has some potentially interesting implications regarding the emergence of spatial structure in fundamental physics(?)

Multiway systems inherit the compositional structure of a Hartle-Hawking wave function from the category **FdHilb**.



Figure: The default foliation of the multiway evolution graph for the set substitution system $\{\{x, y\}, \{y, z\}\} \rightarrow \{\{w, y\}, \{y, w\}, \{x, w\}\}$.

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Implications for General Relativity I

Hypergraphs inherit the compositional structure of Riemannian manifolds (and causal graphs inherit the structure of Lorentzian manifolds) from the category whose objects are Riemannian manifolds $(\mathcal{M}, g_{\mathcal{M}})$ and whose morphisms $f : (\mathcal{M}, g_{\mathcal{M}}) \to (\mathcal{N}, g_{\mathcal{N}})$ are smooth maps $\mathcal{M} \to \mathcal{N}$ (such that, for each $m \in \mathcal{M}$, the symmetric bilinear form $g_{\mathcal{M}} - f^*g_{\mathcal{N}}$ on the tangent fibre at m is positive-semidefinite).



Figure: Spatial hypergraphs corresponding to the initial hypersurface configuration of the head-on collision of two Schwarzschild black holes at time t = 0M, with resolutions of 200, 400 and 800 vertices, respectively, colored using the local curvature in the Schwarzschild conformal factor ψ .

Implications for General Relativity II



Figure: Spatial hypergraphs corresponding to the intermediate hypersurface configuration of the head-on collision of two Schwarzschild black holes at time t = 6M, with resolutions of 200, 400 and 800 vertices, respectively, colored using the local curvature in the Schwarzschild conformal factor ψ .

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Implications for General Relativity III



Figure: Spatial hypergraphs corresponding to the final hypersurface configuration of the head-on collision of Schwarzschild black holes at time t = 12M, with resolutions of 200, 400 and 800 vertices, respectively, colored using the local curvature in the Schwarzschild conformal factor ψ .

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Implications for General Relativity IV



Figure: Spatial hypergraphs corresponding to the post-ringdown hypersurface configuration of the head-on collision of Schwarzschild black holes at time t = 24M, with resolutions of 200, 400 and 800 vertices, respectively, colored using the local curvature in the Schwarzschild conformal factor ψ .

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Applications to Diagrammatic Theorem-Proving I



Figure: Multiway evolution causal graphs corresponding to the first five steps in the non-deterministic evolution history for the hypergraph substitution rule $\{\{x, y\}, \{x, z\}\} \rightarrow \{\{x, z\}, \{x, w\}, \{w, y\}\}$, with a highlighted path (right) between vertices $\{\{0, 0\}, \{0, 0\}\}$ and $\{\{0, 1\}, \{1, 2\}, \{2, 0\}, \{0, 3\}, \{3, 4\}, \{4, 5\}, \{5, 0\}\}$.

Applications to Diagrammatic Theorem-Proving II

Here, we exploit the causal structure \otimes_C of **MuCauGraph** to construct a refutation-complete proof calculus (based on the construction of Bachmair and Ganzinger) for diagrammatic logic, with inference rules of *selective resolution*:

$$\frac{\Lambda \cup \{u \approx v\} \implies \Pi}{\Lambda \sigma \implies \Pi \sigma},$$
(26)

selective superposition:

$$\frac{\Gamma \implies \Delta \cup \{s \approx t\}}{\{u[t] \sigma \approx v\sigma\} \cup \Gamma\sigma \cup \Lambda\sigma \implies \Delta\sigma \cup \Pi\sigma},$$
(27)

and ordered resolution:

$$\frac{\Gamma \implies \Delta \cup \{P(s_1, \dots, s_n) \approx tt\}}{\Gamma \sigma \cup \Lambda \sigma \implies \Delta \sigma \cup \Pi \sigma} \xrightarrow{\{P(t_1, \dots, t_n) \approx tt\} \cup \Lambda \implies \Pi} (28)$$

Applications to Diagrammatic Theorem-Proving III

Here, $u \approx v$ is any occurrence of an equation within the clause:

$$\{u\approx v\}\cup\Lambda\implies\Pi,\tag{29}$$

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that is maximal with respect to the (causal) selection function S.

Applications to Diagrammatic Theorem-Proving IV



Figure: The proof graph corresponding to the proof of the proposition $\{\{0,0\},\{0,0\}\} \rightarrow \{\{0,1\},\{1,2\},\{2,0\},\{0,3\},\{3,4\},\{4,5\},\{5,0\}\},$ subject to the hypergraph substitution rule $\{\{x,y\},\{x,z\}\} \rightarrow \{\{x,z\},\{x,w\},\{w,y\}\}.$

Applications to Quantum Circuit Simplification I

Both open and closed hypergraphs are special cases of full typed hypergraphs.

For every hypergraph G, there exists a distinct hypergraph TG (the *type hypergraph*), with a total hypergraph morphism $type_G$ (the *typing morphism*):

$$type_G: G \to TG.$$
 (30)

The following type graph, denoted $2_{\mathcal{G}}$, can be used to distinguish between "true" vertices and "dummy" vertices:

$$V \underbrace{\frown}_{\epsilon \not\supseteq} \epsilon \not\supseteq . \tag{31}$$

The category **OHGraph** of open hypergraph string diagrams is therefore given by a subcategory of the slice category (**HGraph** $\downarrow 2_G$), where **HGraph** designates the category of closed hypergraph string diagrams. A construction of Kerber allows us to extend this calculus to higher-order diagrammatic logics by defining a morphism Θ from the *n*th-order diagrammatic logic \mathcal{L}^n to the first-order multisorted logic (with equality) \mathcal{L}^1_{sort} :

$$\Theta: \mathcal{L}^{n}(S) \to \mathcal{L}^{1}_{sort}(\Theta(S)), \qquad (32)$$

with S and $\Theta(S)$ denoting the signatures of the logics \mathcal{L}^n and \mathcal{L}^1_{sort} , respectively, such that sets of formulas \mathcal{F} in the higher-order logic $\mathcal{L}^n(S)$ are always mapped to sets of formulas in the first-order multisorted logic $\mathcal{L}^1_{sort}(\Theta(S))$:

$$\Theta: \mathcal{F}\left(\mathcal{L}^{n}\left(S\right)\right) \to \mathcal{F}\left(\mathcal{L}^{1}_{sort}\left(\Theta\left(S\right)\right)\right).$$
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Applications to Quantum Circuit Simplification III



Figure: The statement of unitarity of the CNOT gate (left), represented as a diagrammatic equality theorem in the ZX-calculus, along with the corresponding proof graph for this theorem (right).

Applications to Quantum Circuit Simplification IV



Figure: Plots showing the time complexity (in seconds) of the automated theorem-proving algorithm when reducing randomly-generated Clifford circuits with sizes up to 3000 gates down to pseudo-normal form, both with (right) and without (left) causal optimization.

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