

AlgebraicABMs: An Emerging Next-Generation Categorical ABM Platform

Most diagrams from John Baez, Evan Patterson, Kris Brown,
Xiaoyan Li, Nathaniel Osgood

Separation of Concerns

Ontology (in physics, “kinematics”): Specifies what is changing over time (e.g., via a schema): The state

Governing processes (in physics, “dynamics”): Specifies the rules by which the situation changes

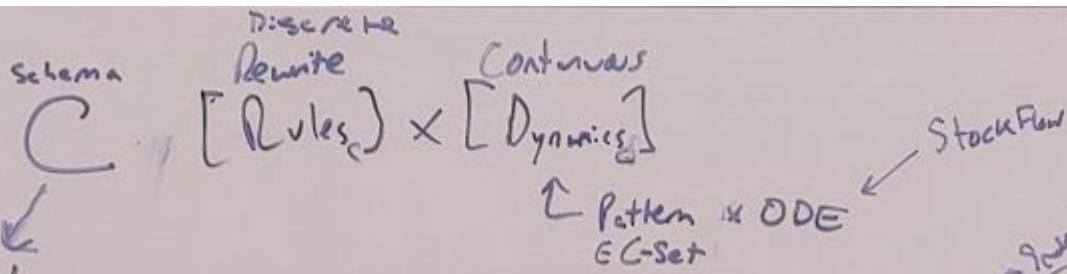
Runtime trajectory (in physics, “trajectory”): Evolution of the system for a single realization

Runtime trajectory distribution (in physics, “trajectory”): Evolution of the system; will be different for different purposes (e.g., single realization run, ensemble, sensitivity analysis, Particle Filtering/Particle MCMC, calibration)

Notable Characteristics of Technical Approach

- Continuous time setting; discrete time updates can occur at equidistant time points
- Intermixing of Discrete Events (CSet rewriting) with continuous (ODE) semantics
 - Talk to each other via attributes
- Metalinguistic abstraction: Each of discrete updates and continuous updates can be specified with multiple types of formalisms
- Declarative characterization of both continuous and discrete governing rules
- Minimize need to declare explicit rewrite rules via widespread use of higher level components
- Eliminating messages as ways of enabling actions based on context
- Weaving of relevant governing rules (continuous & discrete) into areas of the state schema via patterns, with dynamics updating attributes at those areas
- Data migration to translate rules between levels of context & with model evolution
- Planned: Piecing together continuous dynamics with OpenDynam, with dynamical systems coming from stock & flow, petri nets with mass-action semantics, AlgebraicDynamics (?)
- Statecharts.jl to encode statecharts
 - Statecharts as initially compiling to rewrite rules, but more restricted in semantics; potential for supporting explicitly via other high-efficiency mechanism
- Relational/contextual situations recognized as first-class entities for updating

Model Characterization



Current Code (in ABMs.jl in AlgebraicABMs.jl)

```
An agent-based model.  
"""  
@struct_hash_equal struct ABM  
    rules::Vector{ABMRule}  
    dyn::Vector{ABMFlow}  
    ABM(rules, dyn=[]) = new(rules, dyn)  
end
```

Statechart → Rules

How to specify ABM

Step 1: Pick Schema + Datatypes

Step 2: Pick discrete stochastic rules

Step 2a: Some are generated by Statecharts etc.

2b: Some are given as $L \rightarrow R$ in C-set

Step 3: Pick Continuous dynamics

For each: 3a: Pick a pattern C-set

3b: Pick an ODE

3c: ODE can be presented by StockFlow etc.

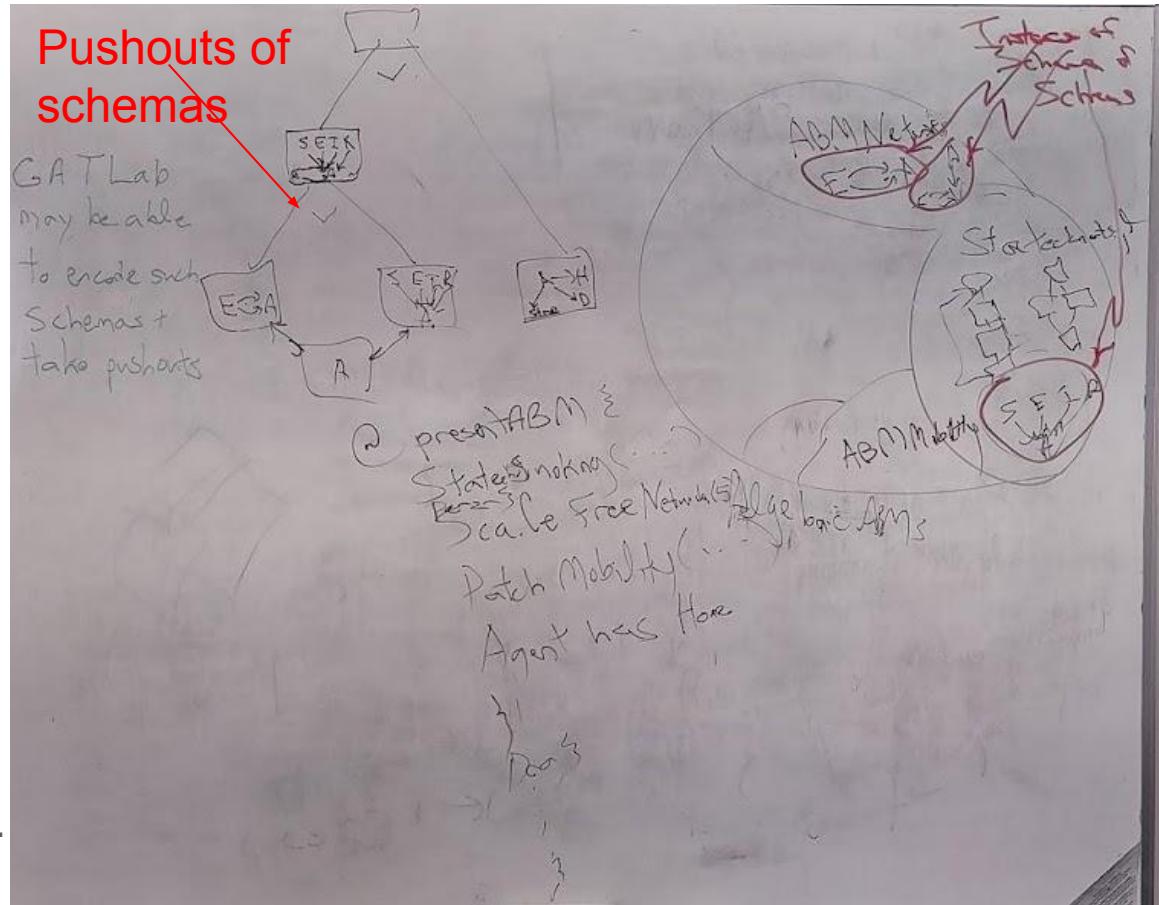
3d: Specify ODE variables correspond to variables in pattern

Layering in Context Via Schema Pushouts

-- Migrating Logic as Schema Grows

While GATLab can take pushouts of different theories, for legacy reasons, it cannot yet take pushouts of schemas for the same theory.

For now, Xiaoyan has implemented a schema of schemas. This will be replaced when GATLab's mechanisms are available.

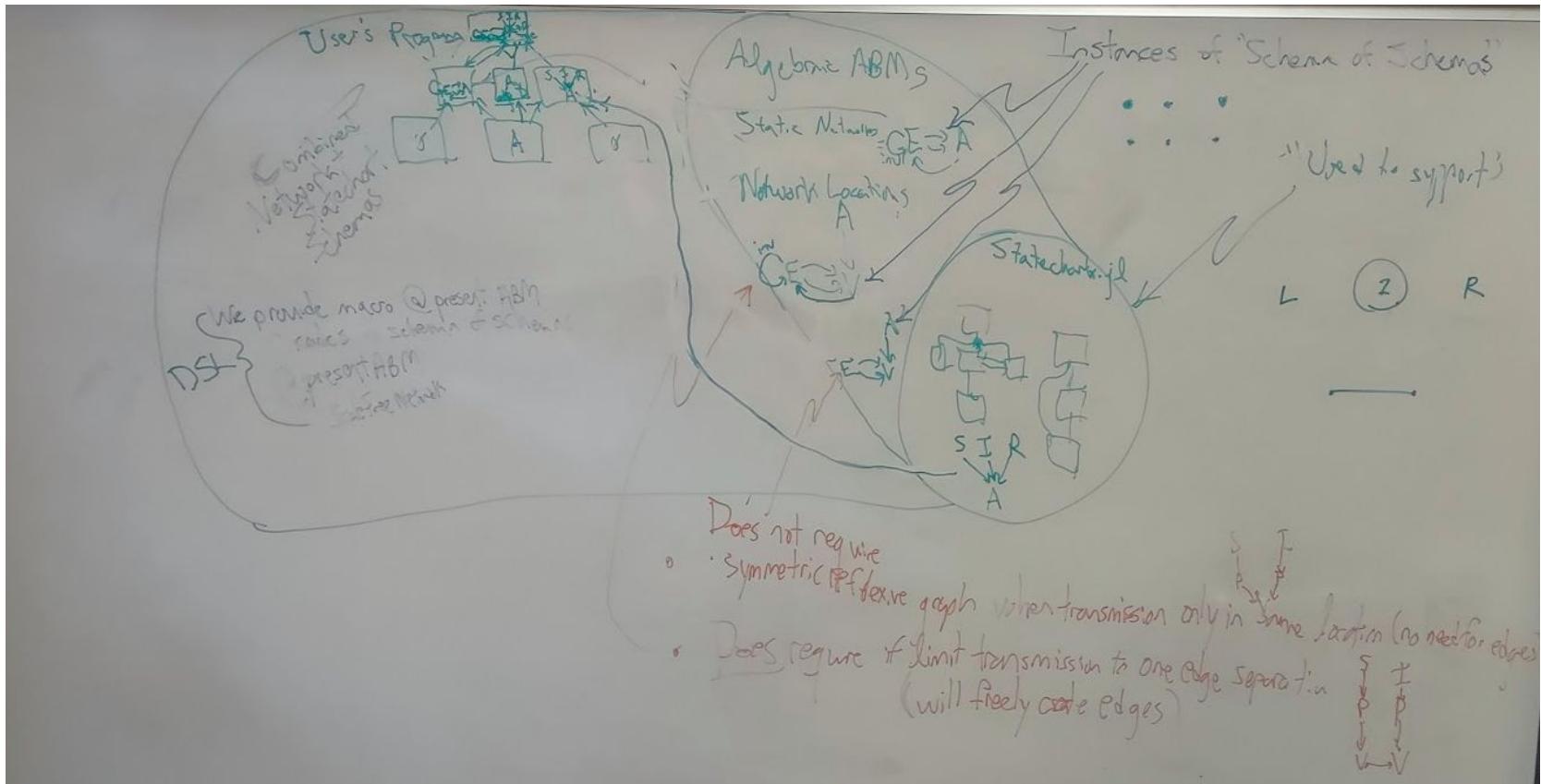


Use of C-Sets Supports Representing Higher Simplices

Assembly of Models out of Pre-Built Parts + Custom Pieces

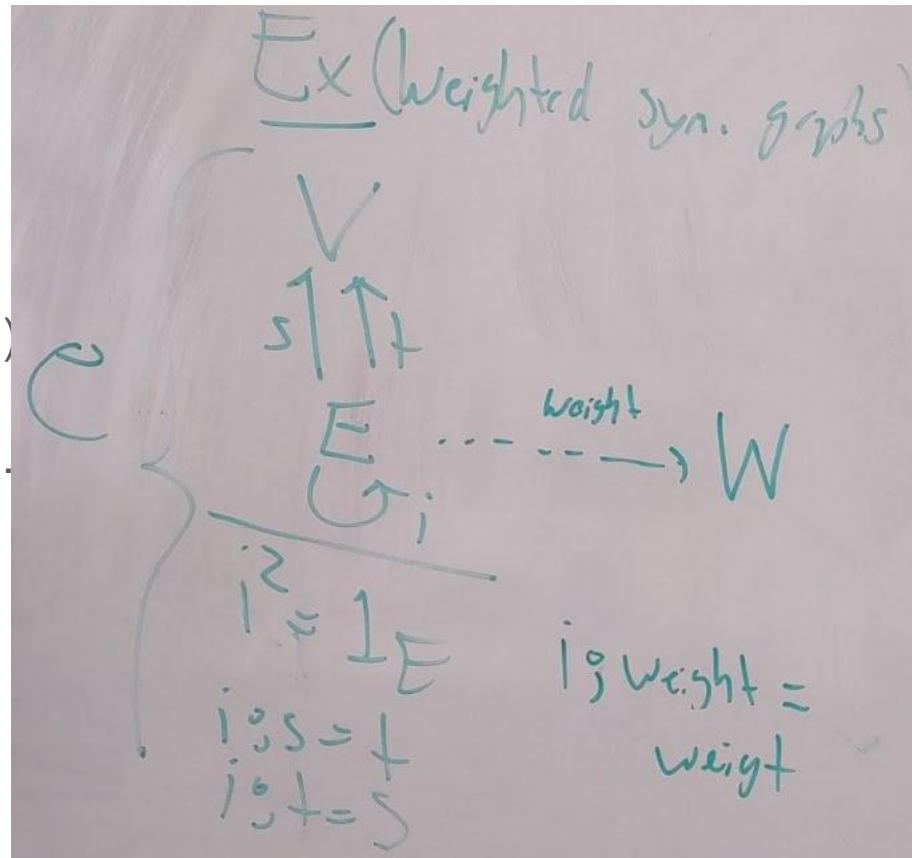
```
@abmAssembly {  
    elementalPerson(...)  
    home::Ob,  
    personHome::Hom(person,home),  
    NicotineUse(...),  
    HeartDisease(...),  
    Diabetes(...),  
    GeographicSpace(...),  
    DistanceBasedNetwork(...))  
}
```

Affordances in Some Relevant Areas of AlgebraicJulia



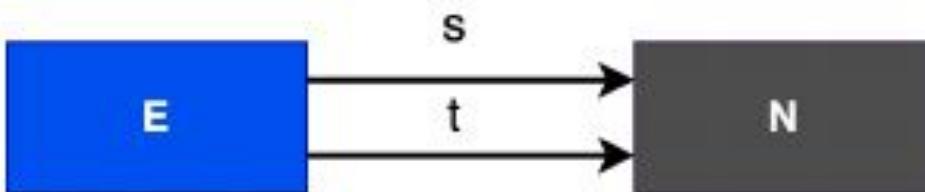
Issue -- Handling Equations

Our current workaround strategy of implementing our own schema-of-schemas (pending GATLab support for pushouts of presentations) does not support equations within schemas. For now, we need to put in place manually “fixups” that enforce such equations.

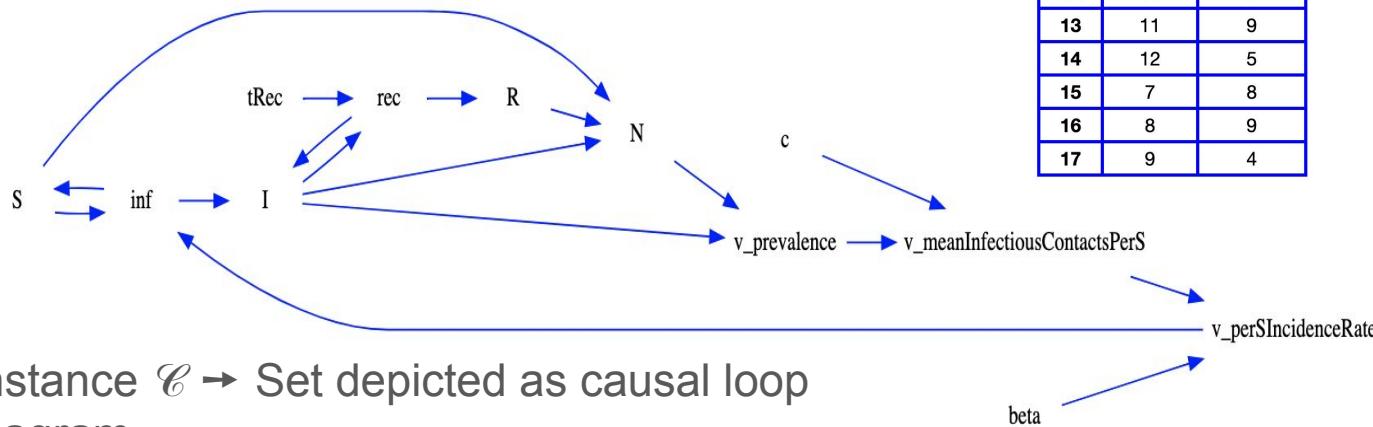


Fundamental Building Block: C-Sets

Schemas & their Instances 1



Schema category \mathcal{C}



Instance $\mathcal{C} \rightarrow$ Set depicted as causal loop diagram

E	s	t
1	1	6
2	2	6
3	3	6
4	6	7
5	2	7
6	1	4
7	2	5
8	4	2
9	5	3
10	4	1
11	5	2
12	10	8
13	11	9
14	12	5
15	7	8
16	8	9
17	9	4

Instance $\mathcal{C} \rightarrow$ Set depicted as database

N	nname
1	S
2	I
3	R
4	inf
5	rec
6	N
7	v_prevalence
8	v_meanInfectiousContactsPerS
9	v_perIncidenceRate
10	c
11	beta
12	tRec

Primitive Causal Loop Diagram Schema in AlgebraicJulia

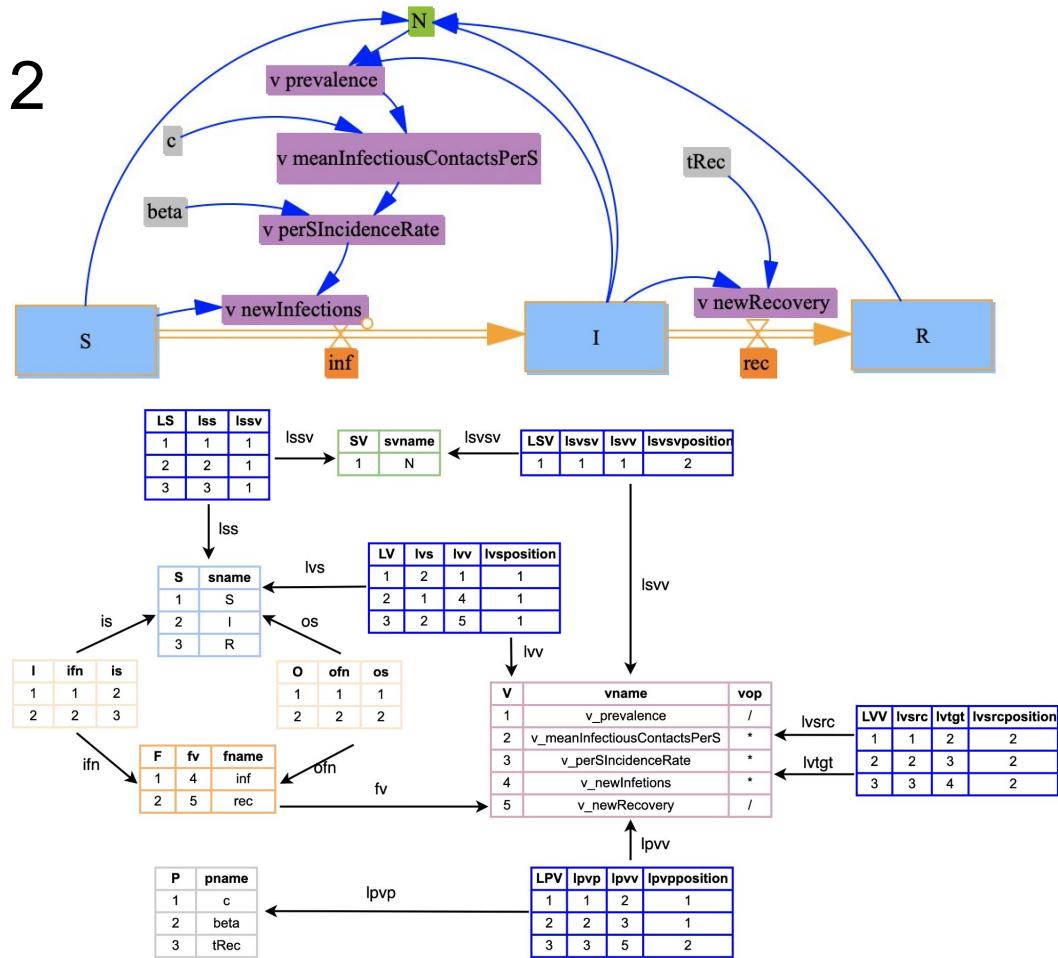
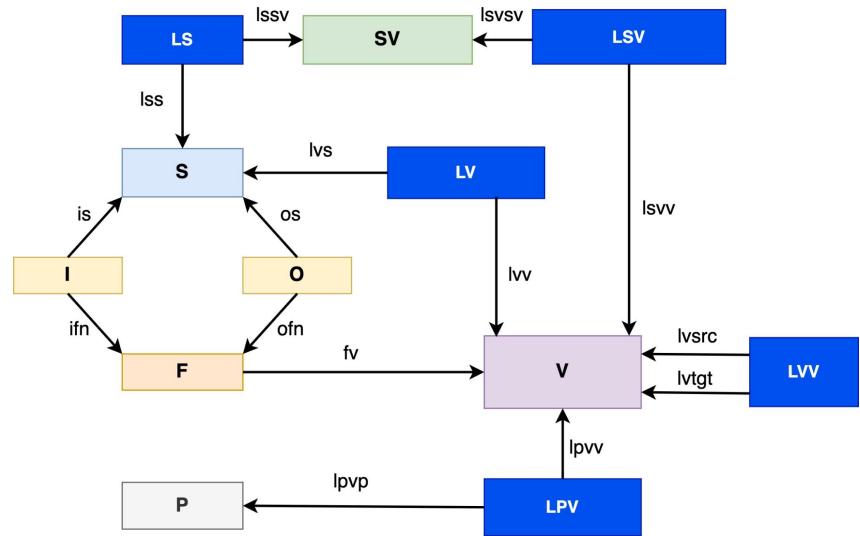
```
@present TheoryCausalLoop(FreeSchema) begin
    E::Ob
    N::Ob

    s::Hom(E, N)
    t::Hom(E, N)

    # Attributes:
    Name::AttrType

    nname::Attr(N, Name)
end
```

Schemas & their Instances 2



Representing Stock-Flow Schema in AlgebraicJulia

```
@present TheoryStockAndFlow(FreeSchema) begin
    S::Ob
    SV::Ob
    I::Ob
    O::Ob
    F::Ob
    V::Ob
    P::Ob
    LS::Ob
    LSV::Ob
    LV::Ob
    LVV::Ob
    LPV::Ob

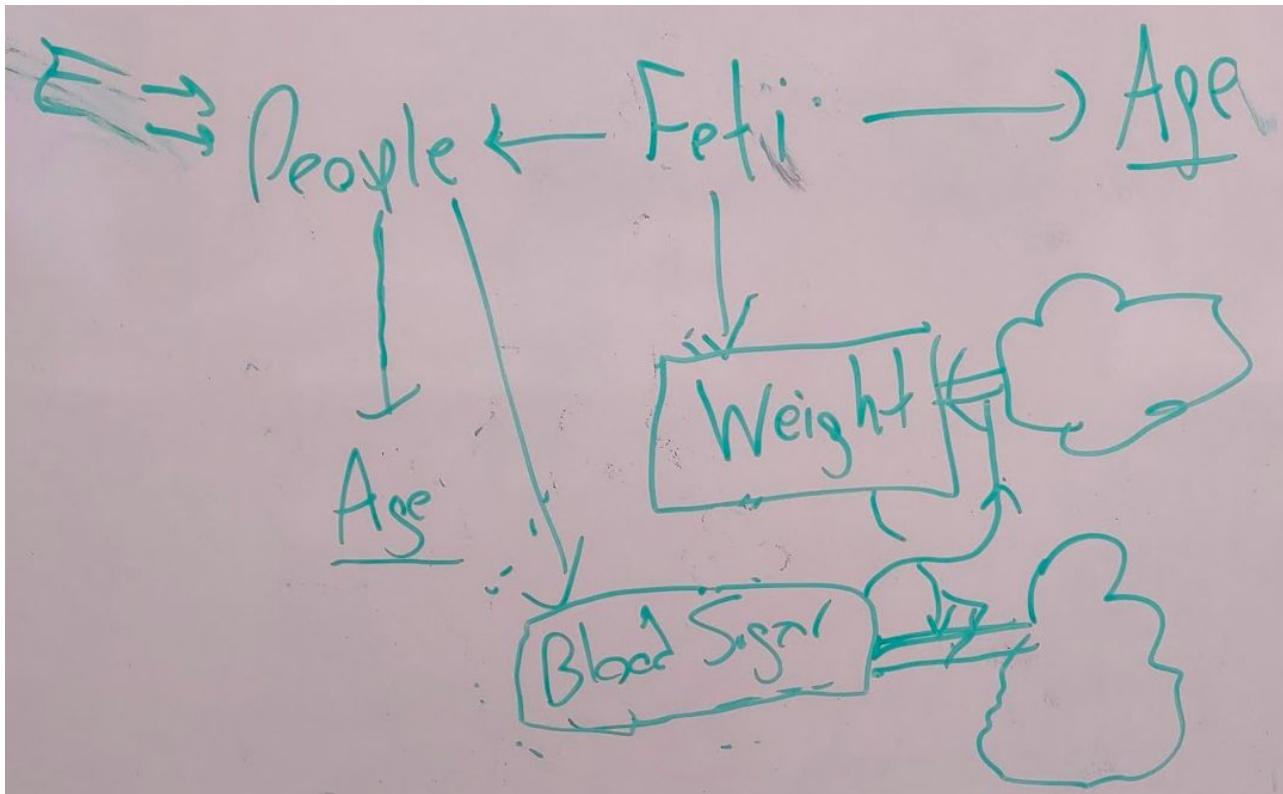
    lss::Hom(LS,S)
    lssv::Hom(LS,SV)
    ifn::Hom(I,F)
    is::Hom(I,S)
    ofn::Hom(O,F)
    os::Hom(O,S)
    fv::Hom(F,V)
    lvs::Hom(LV,S)
    lvv::Hom(LV,V)
    lsvsv::Hom(LSV,SV)
    lsvv::Hom(LSV,V)
    lsrc::Hom(LVV,V)
    lvtgt::Hom(LVV,V)
    lpvp::Hom(LPV,P)
    lpvv::Hom(LPV,V)
```

```
# Attributes:
    Name::AttrType
    Op::AttrType
    Position::AttrType

    sname::Attr(S, Name)
    svname::Attr(SV, Name)
    fname::Attr(F, Name)
    vname::Attr(V, Name)
    pname::Attr(P, Name)
    vop::Attr(V, Op)
    lvsposition::Attr(LV, Position)
    lsvsvposition::Attr(LSV, Position)
    lsrcposition::Attr(LVV, Position)
    lpvpposition::Attr(LPV, Position)
end
```

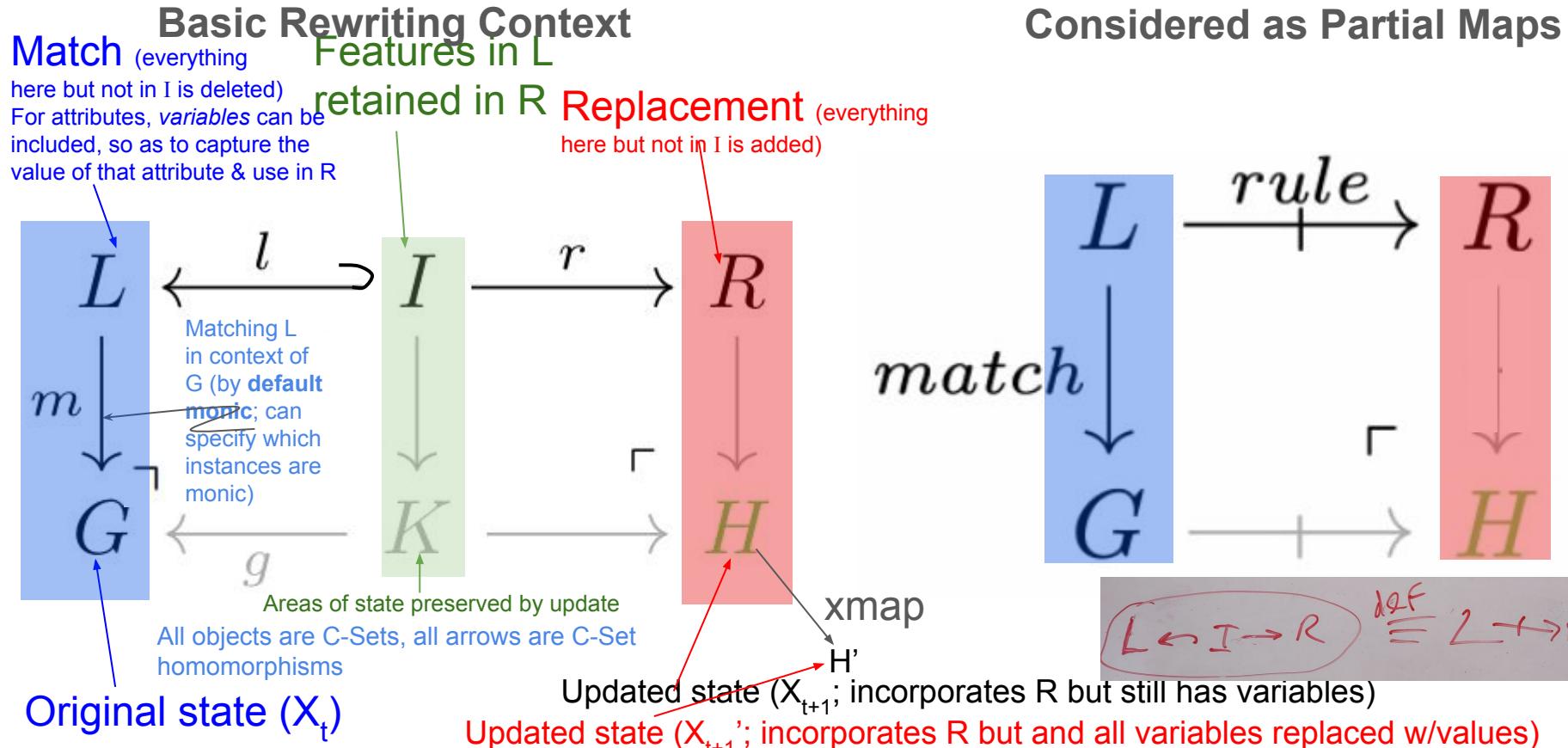
Associated attributes are as above.

C-Sets can encode Continuous & Discrete Attributes, Relational, Networks



Rewriting Essentials

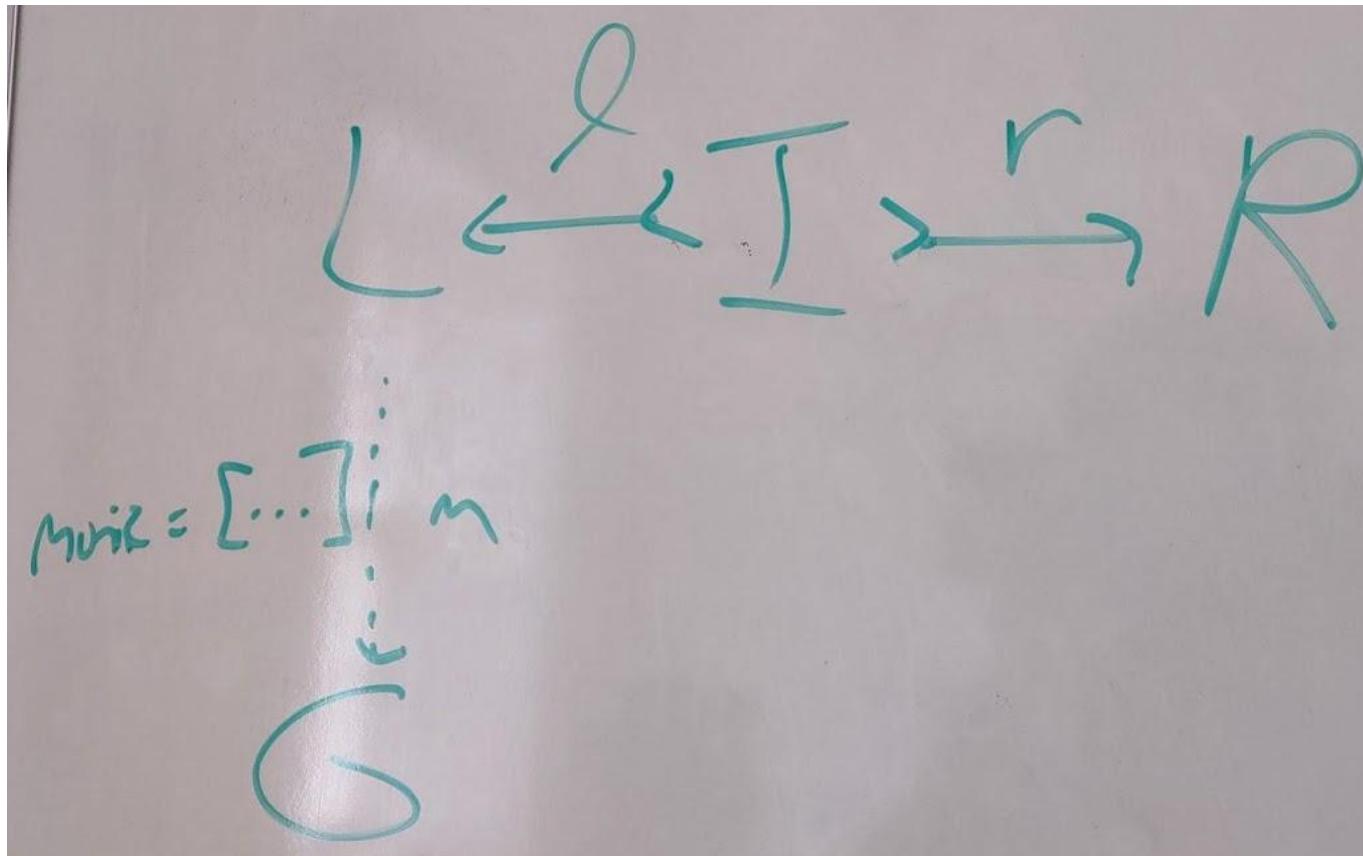
Basics of Rewriting: Double Pushout



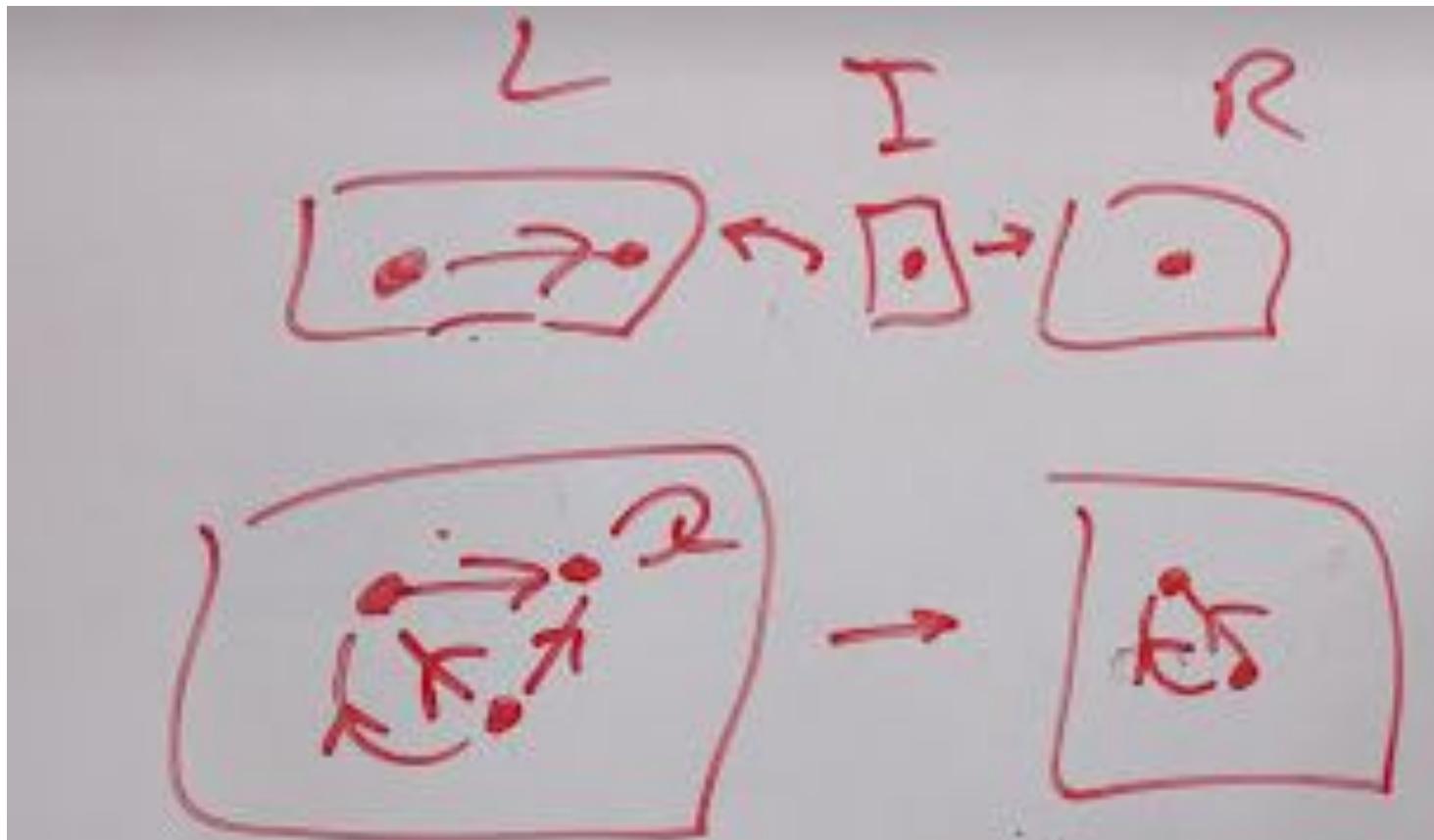
$$L \hookrightarrow I \rightarrow R \stackrel{\text{def}}{=} L \rightarrow R$$

Images adapted from Brown, K., Patterson, E., Hanks, T. and Fairbanks, J., 2022. Computational Category-Theoretic Rewriting. In International Conference on Graph Transformation (pp. 155-172). Springer, Cham. <https://arxiv.org/pdf/2111.03784.pdf>

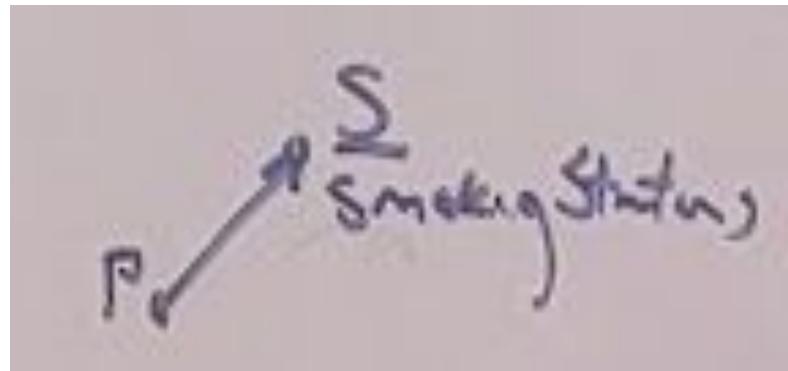
Selectively Monic Morphisms $L \rightarrow G$



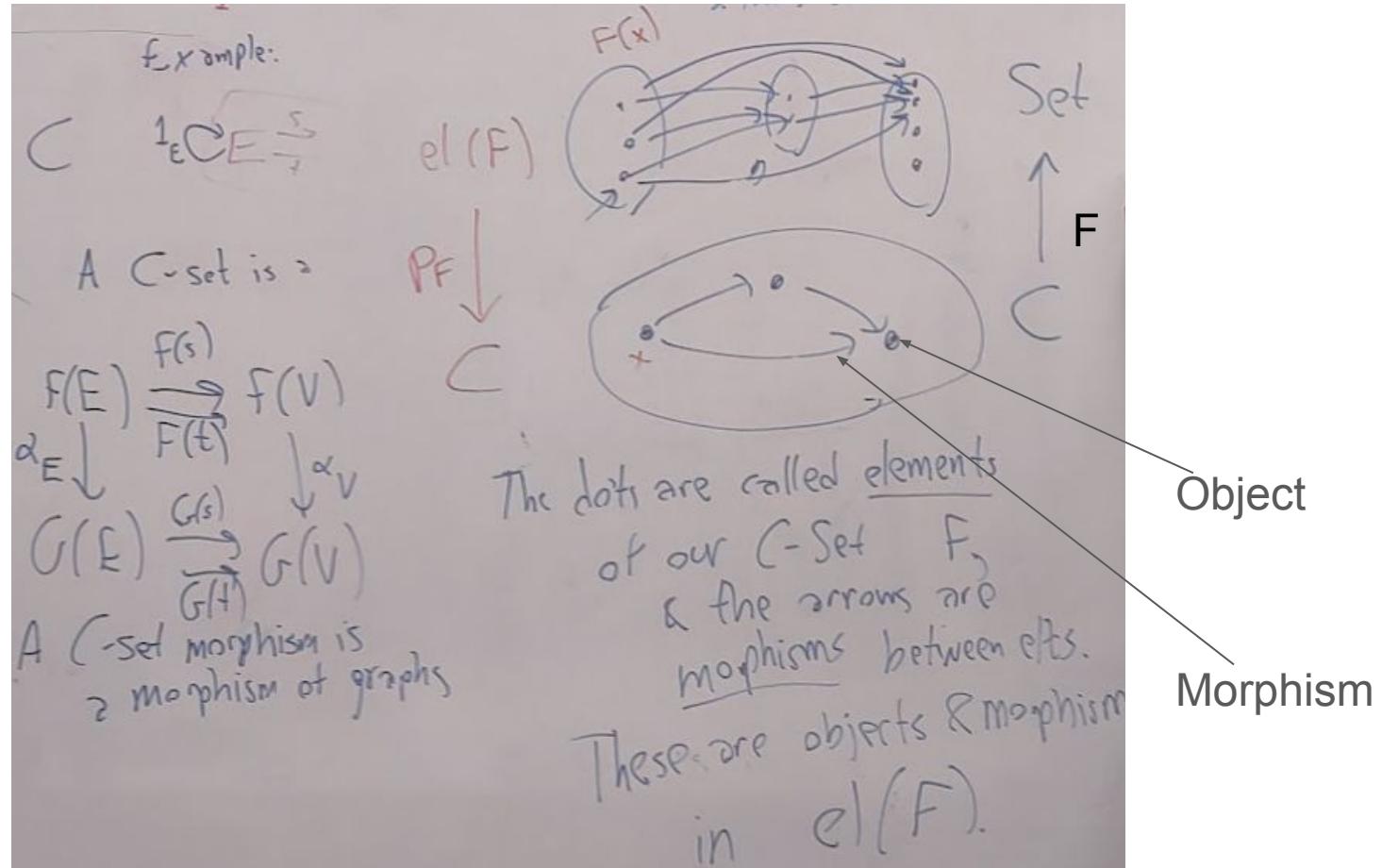
Commonly Rule Application Yields Multiple Matches



Simple Interpretation of Diagrams

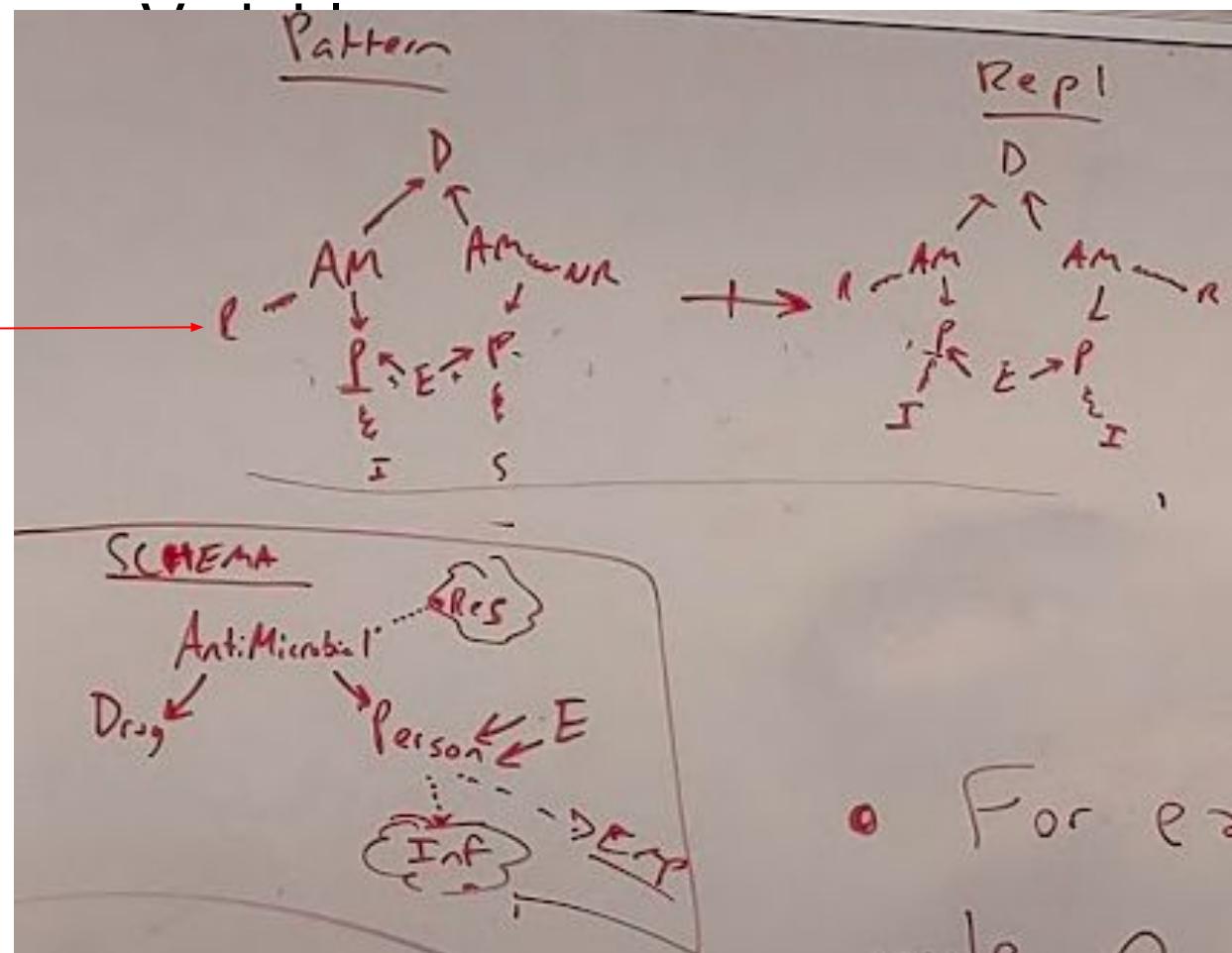


The Category of Elements $\text{el}(F)$ for a C-Set $F: \mathcal{C} \rightarrow \text{Set}$

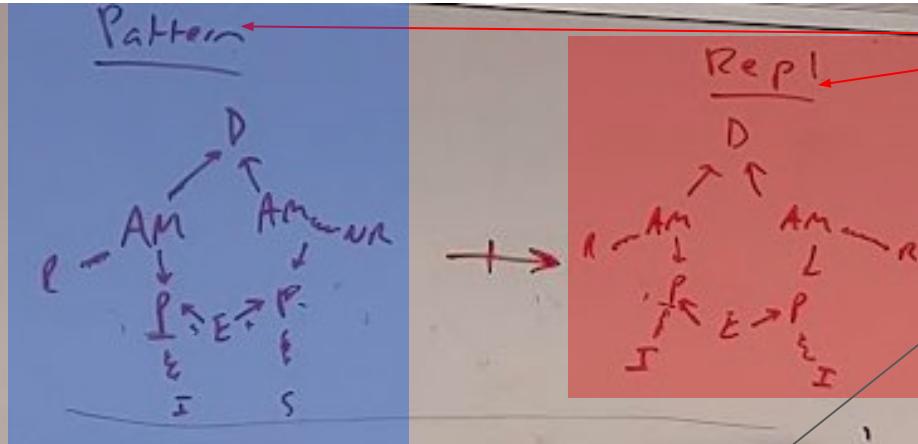


Patterns for Matching As Drawn from Category of Elements &

Note because these are C-Sets, the minimum that we can represent in this pattern is a representable.
In general, this is a colimit of representables.

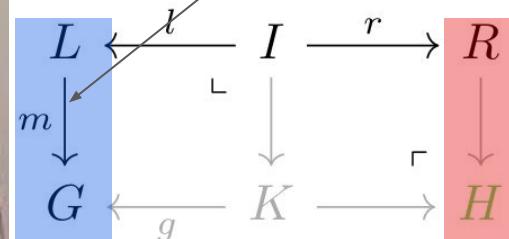
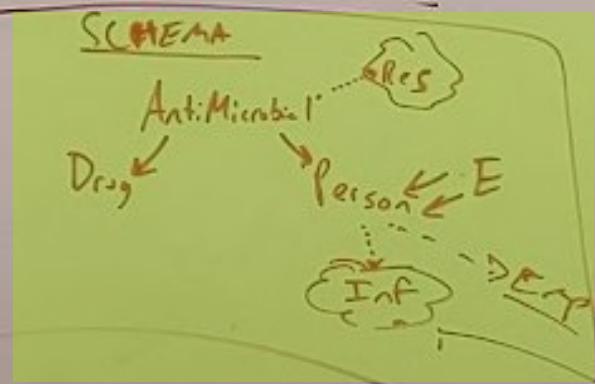


We Draw our **Pattern** & **Replacement** in the Category of Elements for C-Sets in the **Schema Category**

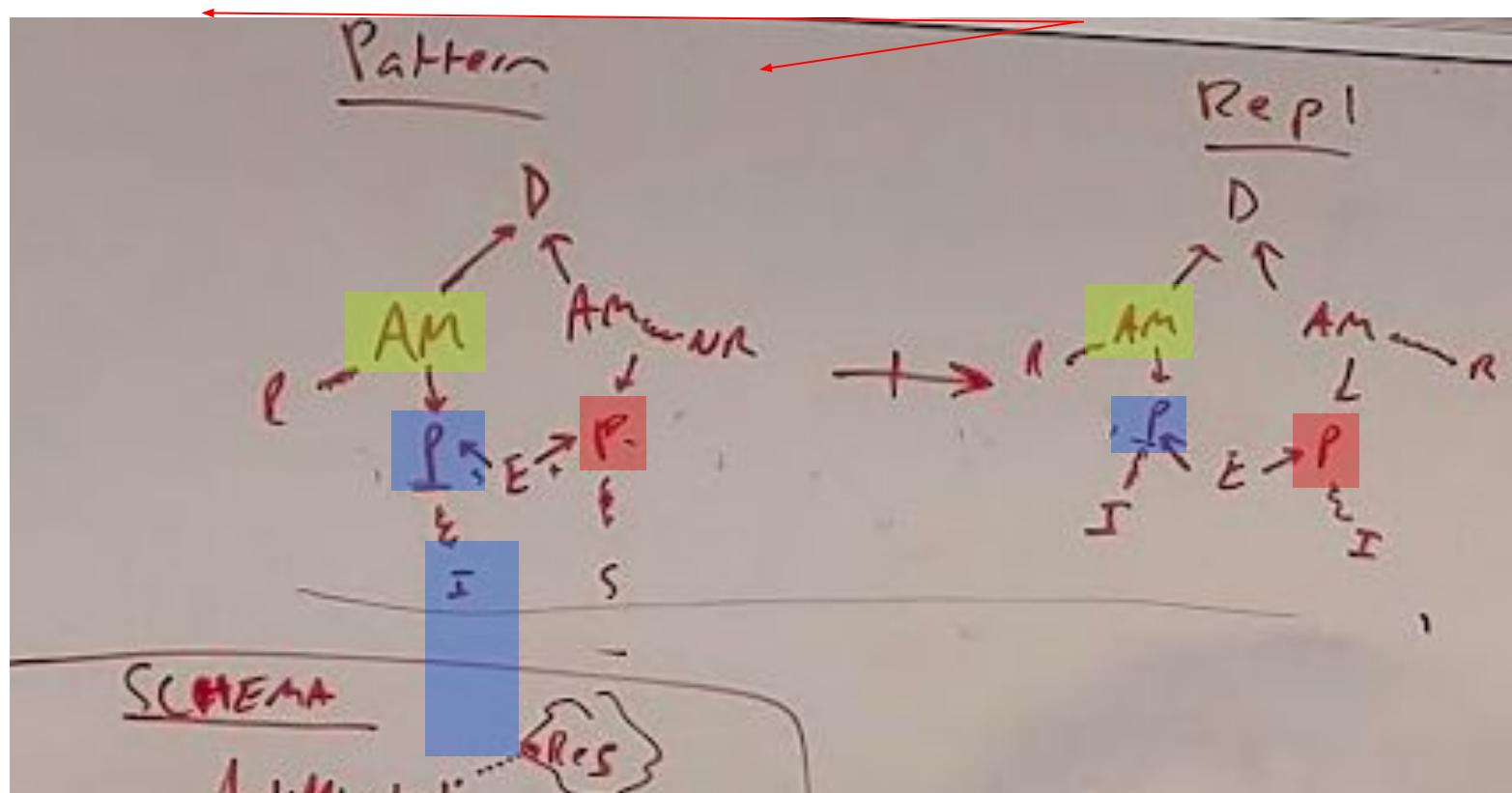


These are drawn in the category of elements for the schema; matching rewriting rules then searches for **homomorphisms** (structure preserving mappings) from such a C-Set into the state of the model (also encoded as a C-Set).

In practice, we can also use variables to capture the value of attributes in the **match** pattern, and use such values in formulating the **replacement**.



We Draw our **Pattern** & **Replacement** in the Category of Elements for C-Sets in the **Schema Category**



Interpretation?

Schema category \mathcal{C}

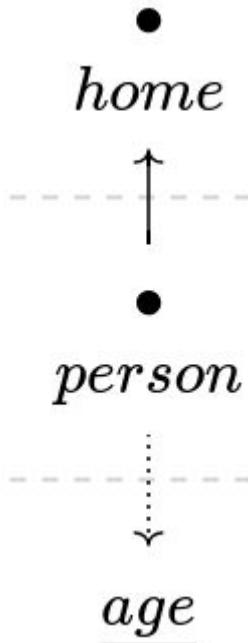
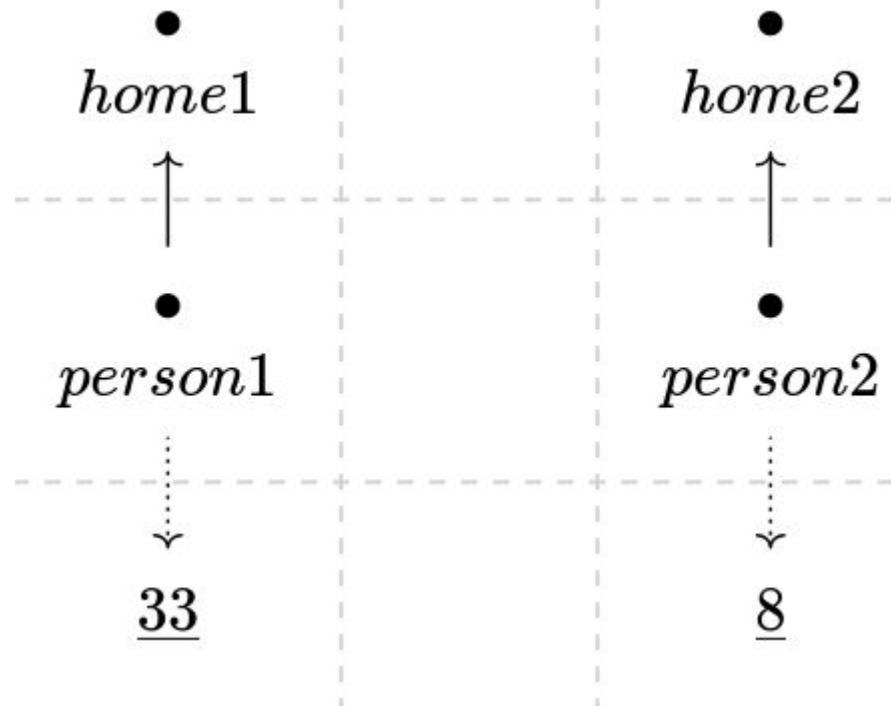


Diagram in category of elements



Interpretation?

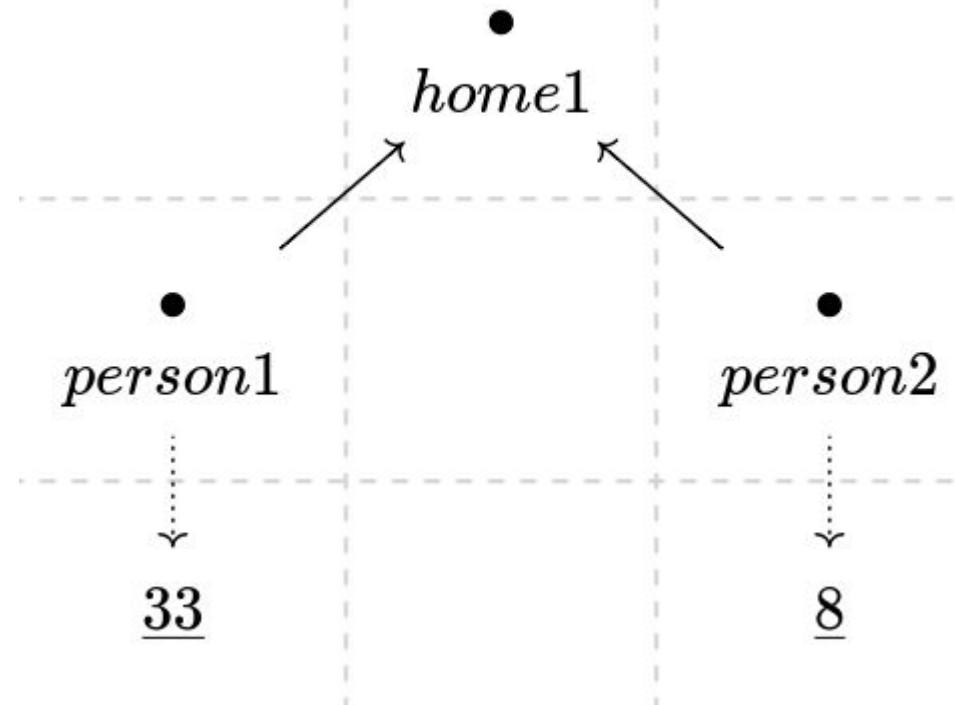
Schema
category \mathcal{C}

•
home

↑
•
person

age

Diagram in category of elements



Interpretation?

Schema
category \mathcal{C}

•
home



•
person



age

Diagram in category of elements

•
home1



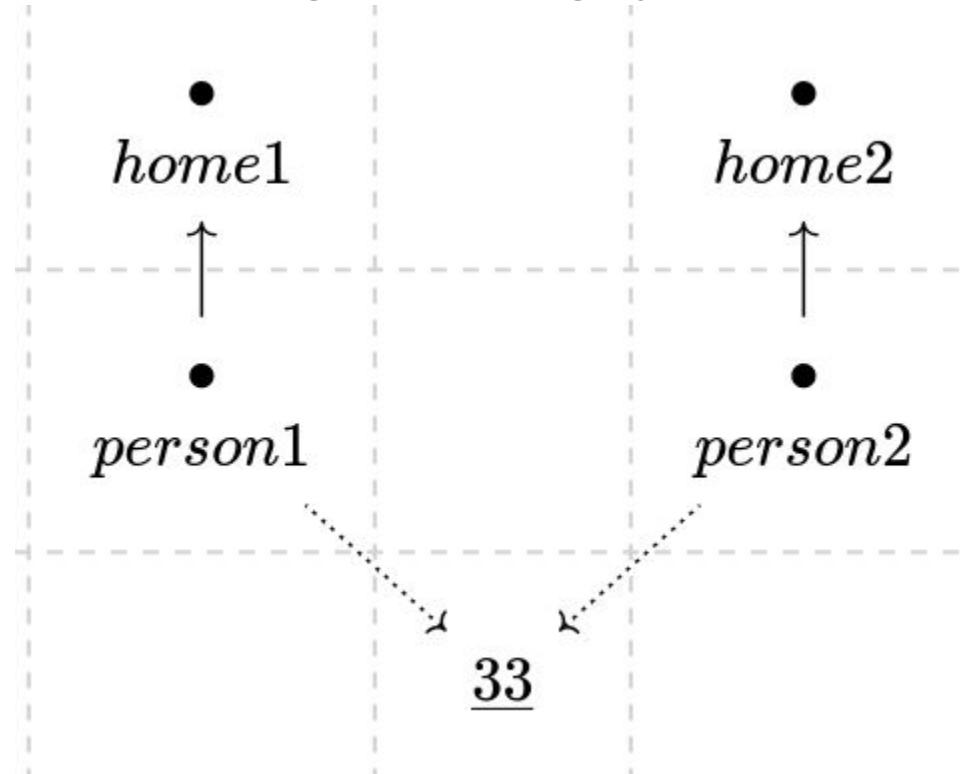
•
person1

•
home2



•
person2

33



Interpretation?

Schema
category \mathcal{C}

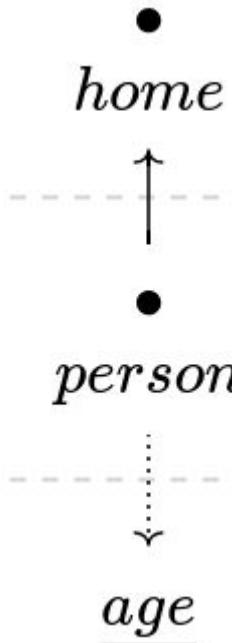
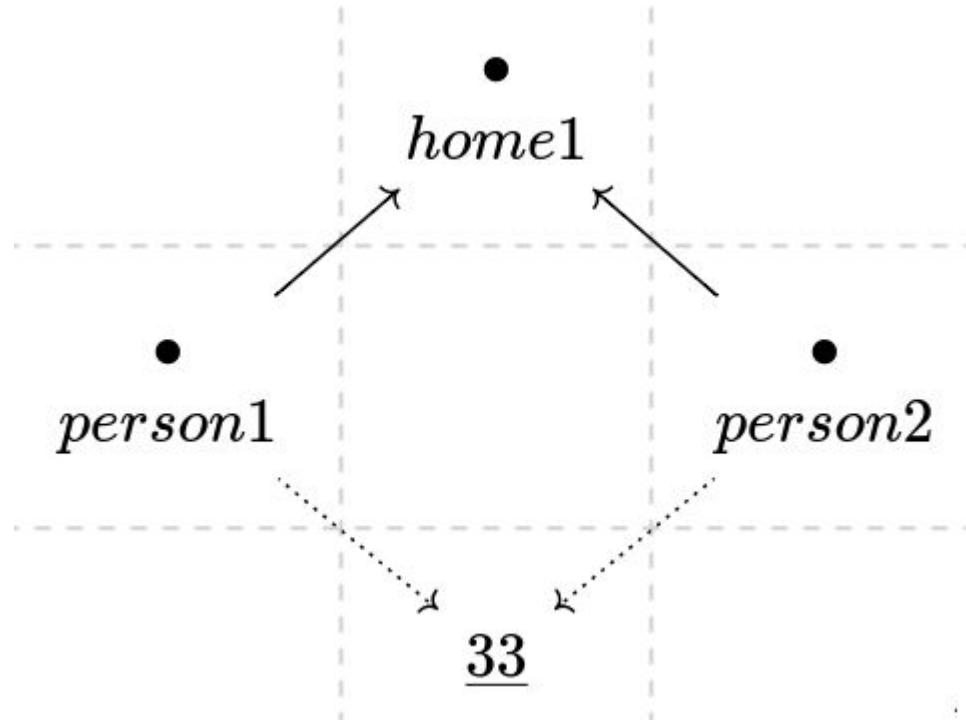
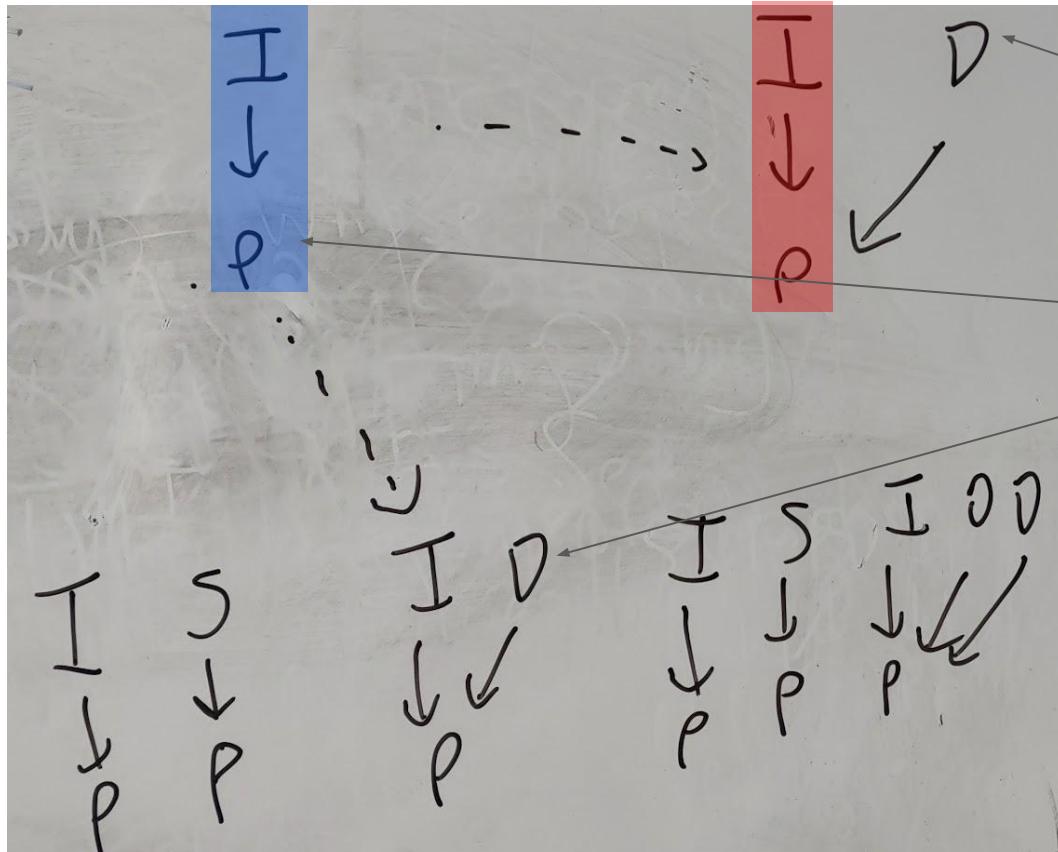


Diagram in category of elements



Understanding Pushouts of Patterns -- Take Pushout of the Image of the Match and State X_t Fibered by the Match



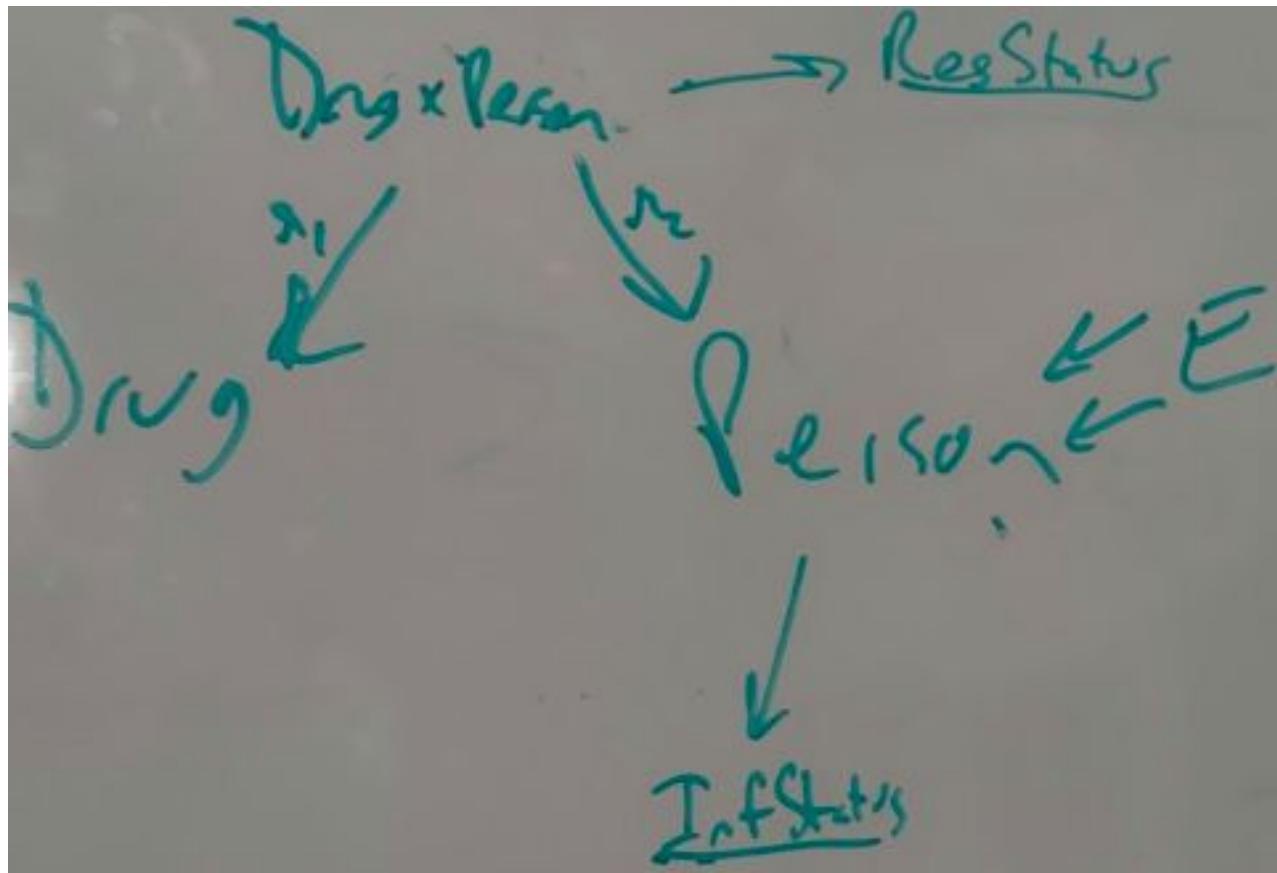
Even though have D in pattern B, and in X_t ,
because these are not in the homomorphism
match $I \rightarrow P$, get an addition of two dogs

Patterns Can Use *Attribute Variables*
to Bind & Propagate Values

Categorical Alternatives Offered

Traditional Construct	Our Construct
Messages	Context specific pattern matching
Agent as updated entity	Situations as matched
Nesting of agents	Relations between agents in patterns

Schema Capturing Drug-Specific Resistance for Person



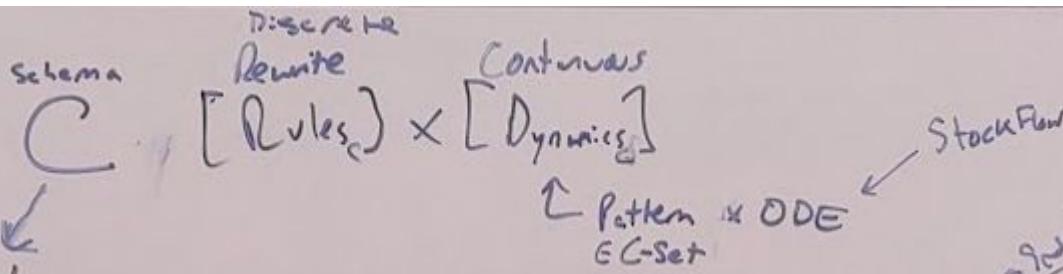
Recall: Use of ACSet_colim Eases Declarative Specification of Patterns

```
s_eat_pac = @acset_colim yLV begin s::Sheep; countdown(sheep_loc(s)) == 0 end;
```

```
w_eat_l = @acset_colim yLV begin  
    s::Sheep; w::Wolf  
    sheep_loc(s) == wolf_loc(w)  
end;
```

Recall: Model Constituents

Model Characterization



Current Code (in ABMs.jl in AlgebraicABMs.jl)

```
An agent-based model.  
"""  
@struct_hash_equal struct ABM  
    rules::Vector{ABMRule}  
    dyn::Vector{ABMFlow}  
    ABM(rules, dyn=[]) = new(rules, dyn)  
end
```

Statechart → Rules

How to specify ABM

Step 1: Pick Schema + Datatypes

Step 2: Pick discrete stochastic rules

Step 2a: Some are generated by Statecharts etc.
2b: Some are given as $L \rightarrow R$ in C-set

Step 3: Pick Continuous dynamics
For each: S1: Pick dynamics

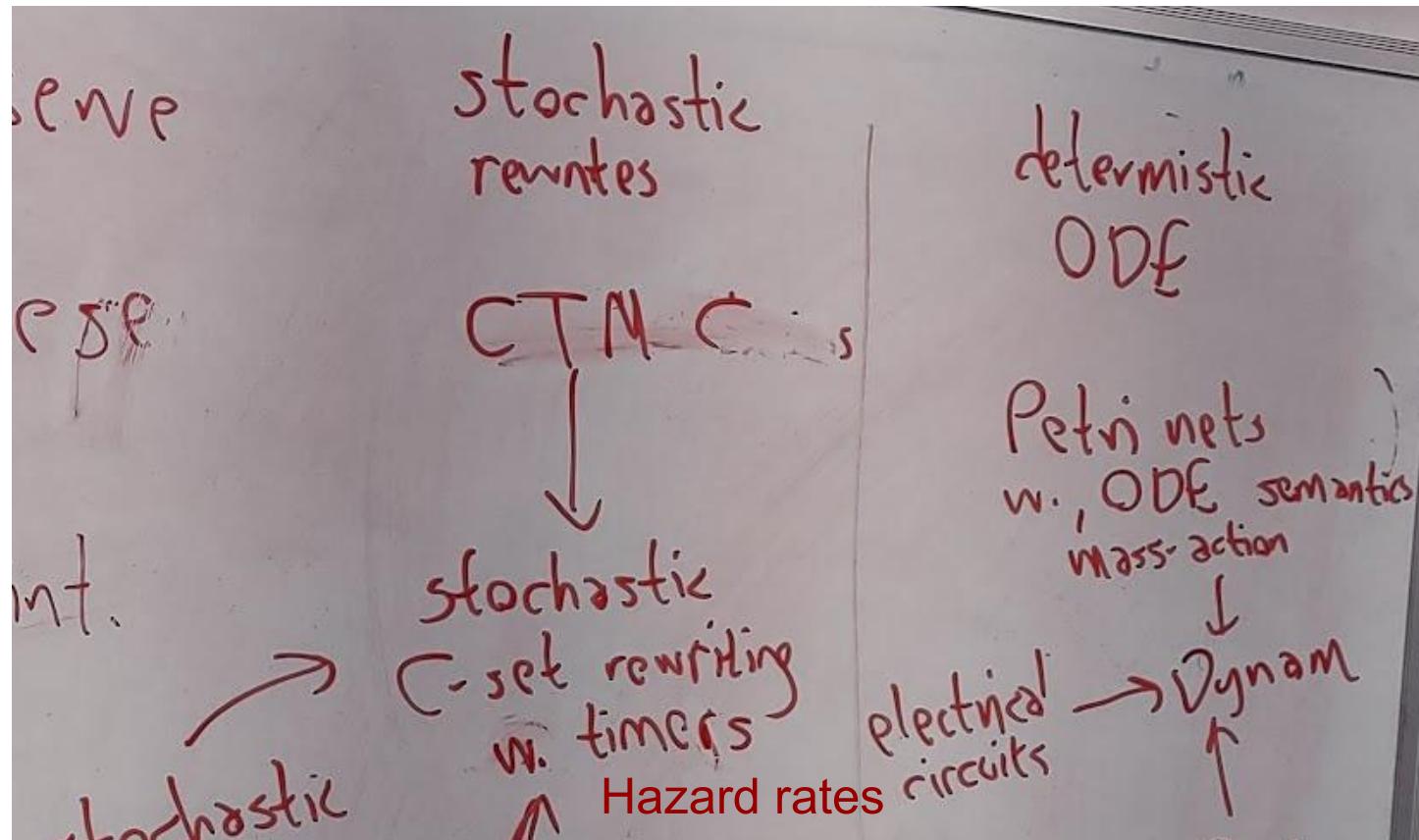
3a: Pick a pattern C-set
3b: Pick an ODE

3c: ODE can be presented by StockFlow etc.

3d: Specify ODE variables correspond to variables in pattern

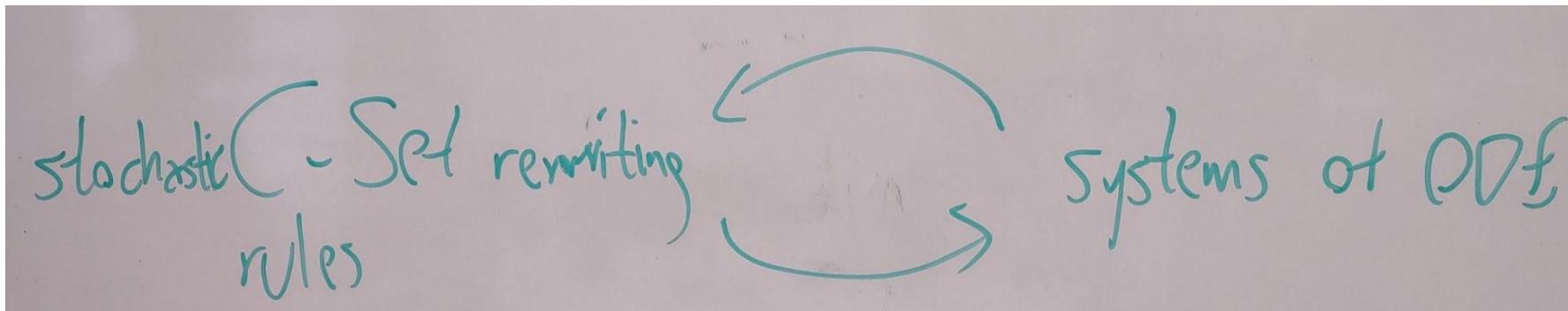
Basic Types of Dynamics

A Pluralistic Framework

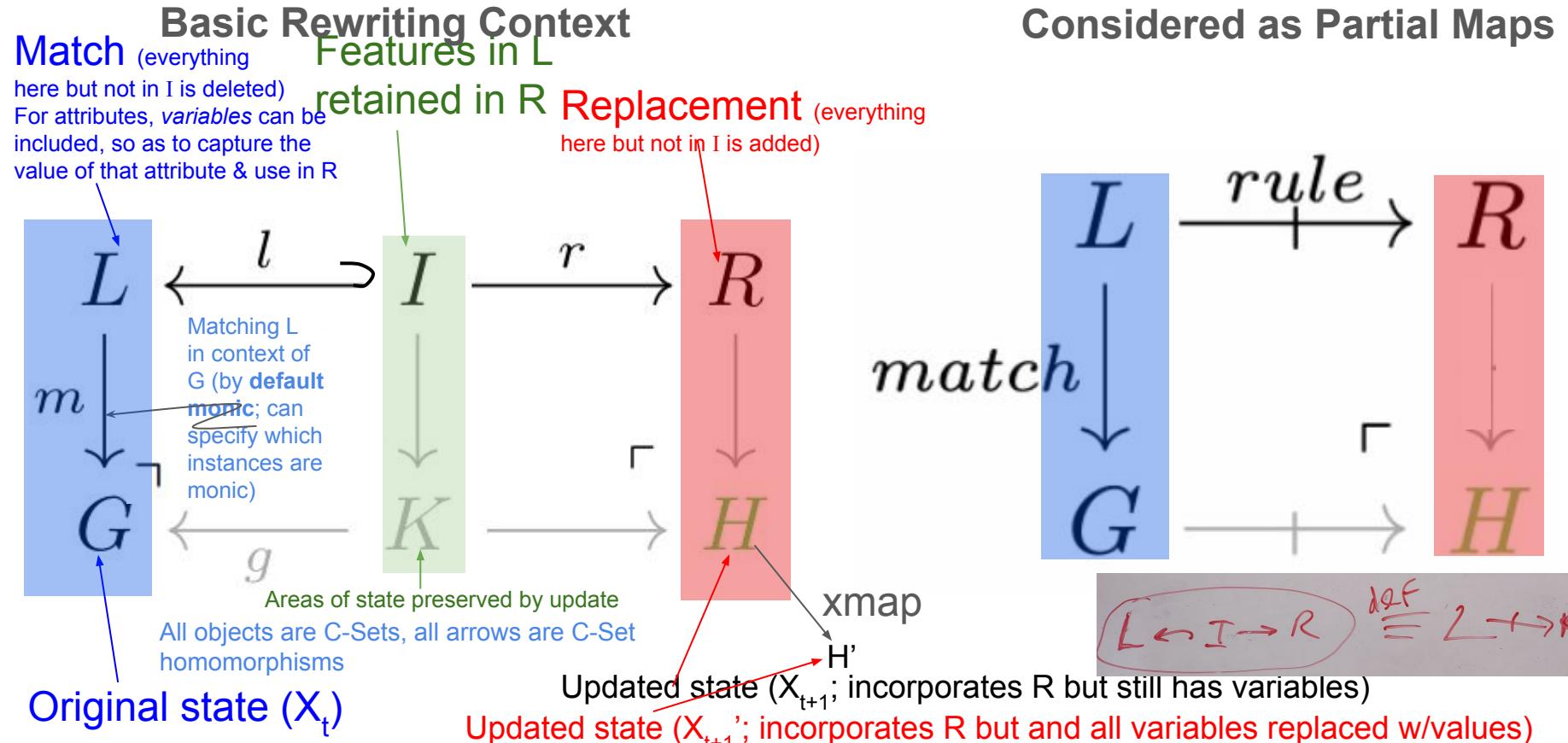


Two Types of Dynamics

- **Continuous over time:** Ongoing updates; Underlying framework: ODEs, e.g., through direct ODE specification, stock & flow, or Petri Net mass-action semantics
- **Discrete events:** Events occur at an instant, undertake atomic update to new state.



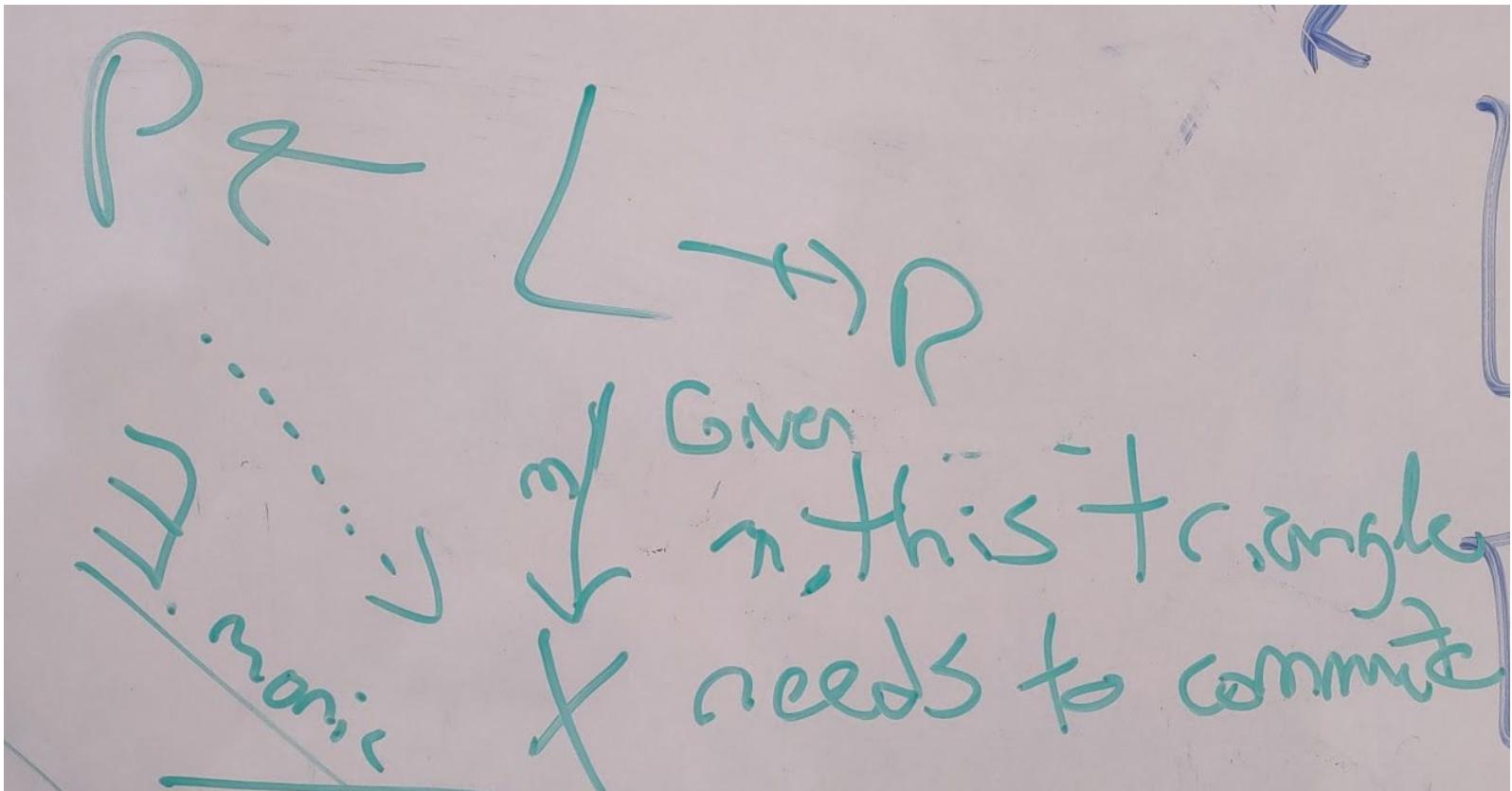
Rewriting Rules Triggered via Hazard Rates



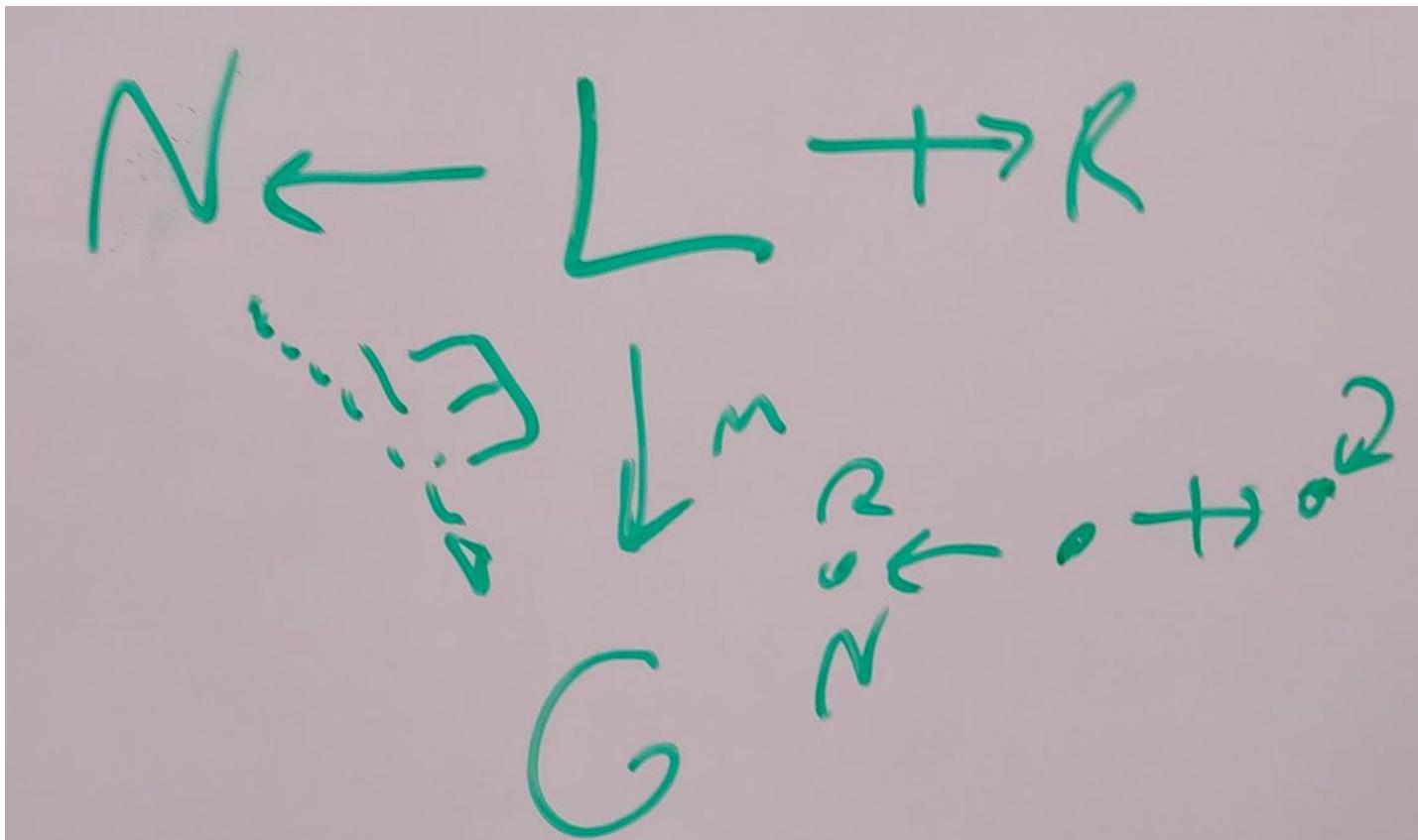
Images adapted from Brown, K., Patterson, E., Hanks, T. and Fairbanks, J., 2022. Computational Category-Theoretic Rewriting. In International Conference on Graph Transformation (pp. 155-172). Springer, Cham. <https://arxiv.org/pdf/2111.03784.pdf>

Application Conditions

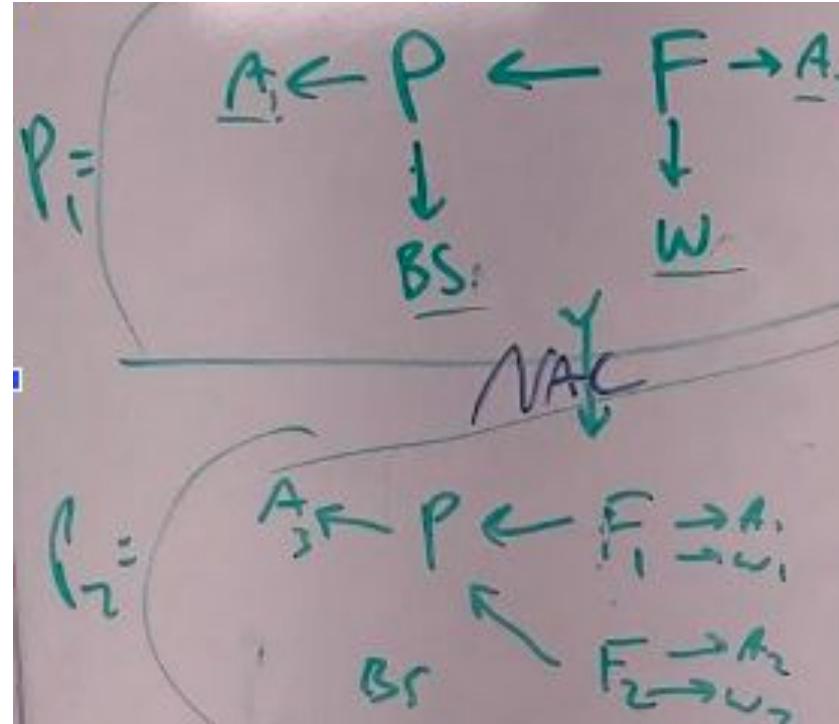
Positive Application Conditions



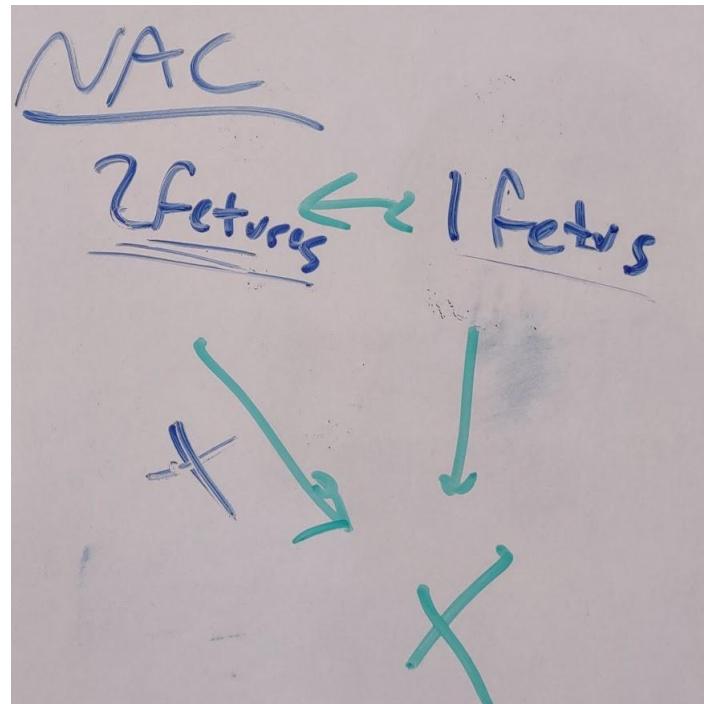
Negative Application Conditions



Example Need for Negative Application Condition -- P1 would normally apply if P2 matches, but NAC prevents this



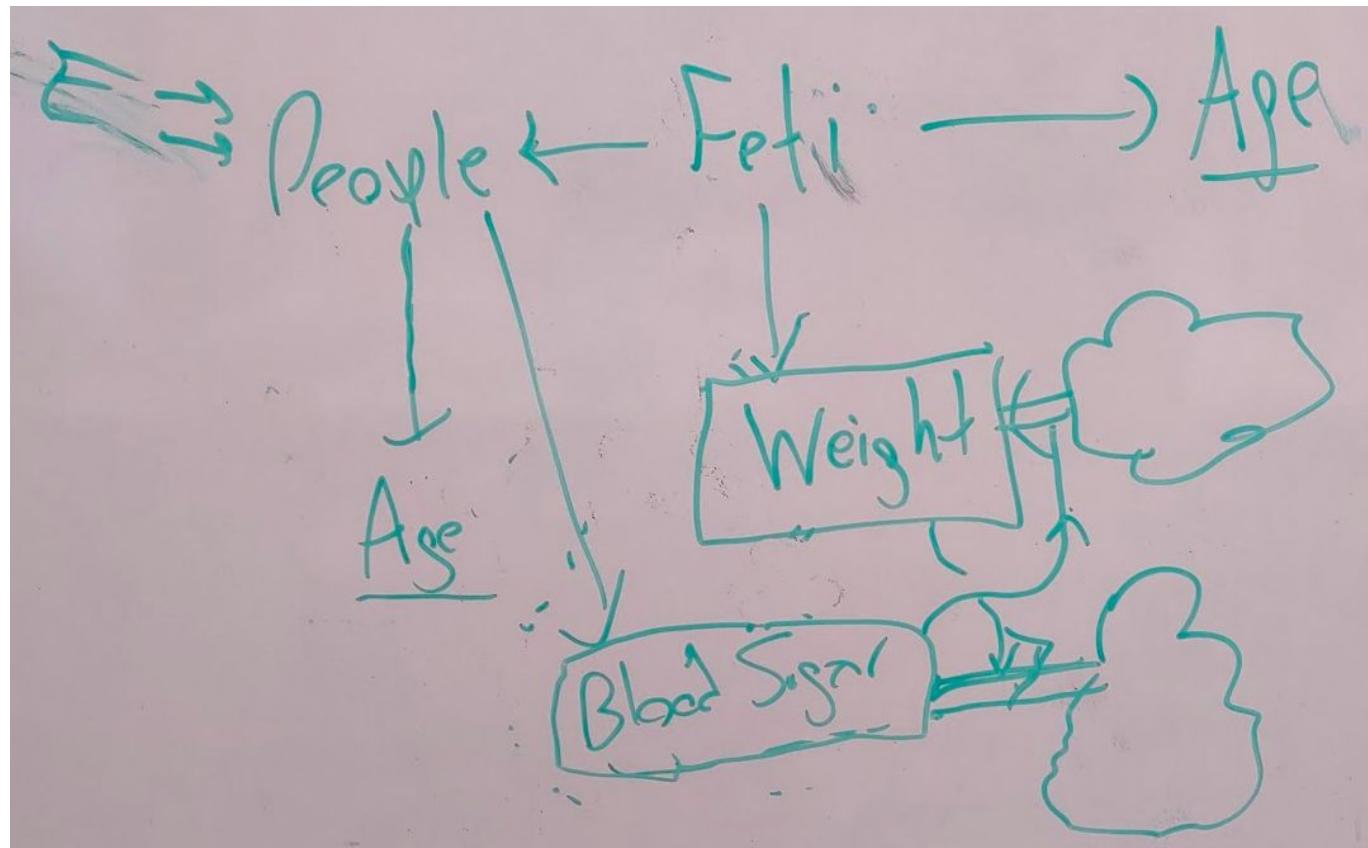
Example of Negative Application Condition



Underlying Rewriting Mechanisms -- Match & Schedule

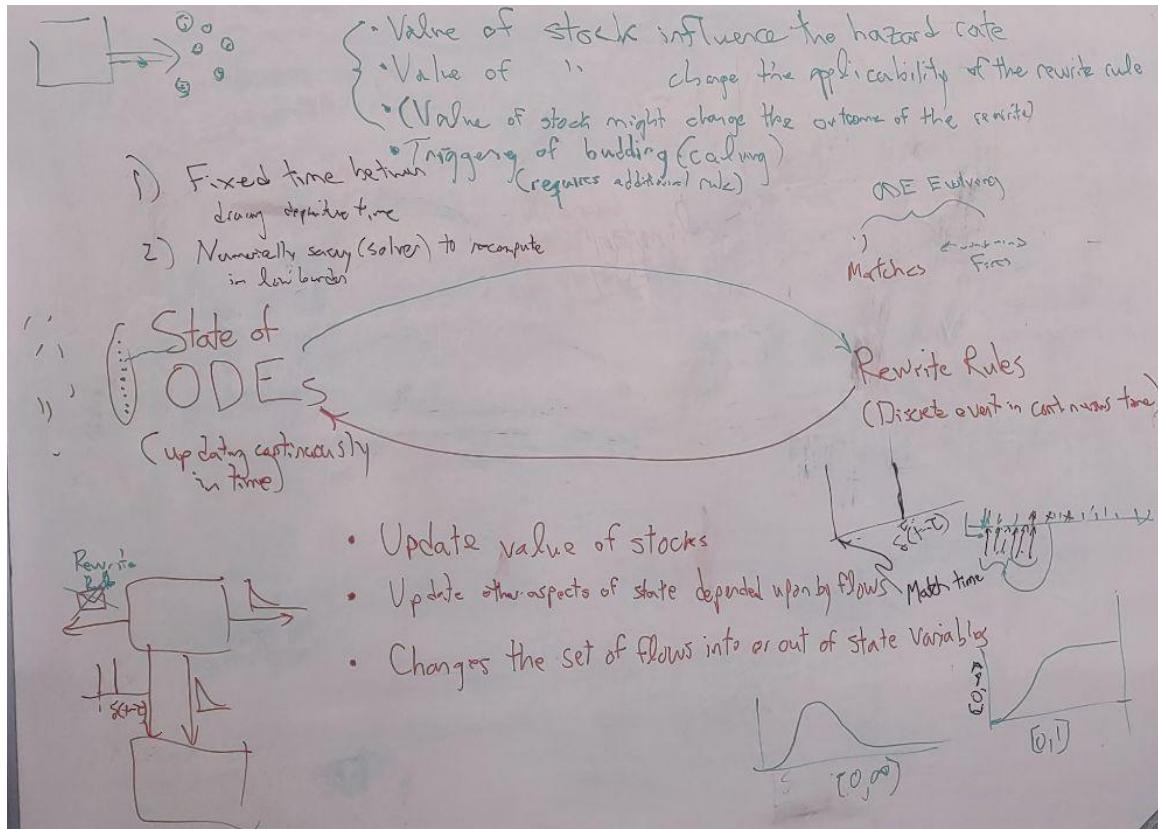
- Especially because there is no notion of “each agent” needing updates, we need to **match** pattern to find situations that can trigger dynamics via matching (e.g., that an agent is in a given state)
- These situations do not generally need to fire **immediately** -- for example, if an agent has entered a state; it could exhibits a hazard rate or timeout transition for leaving
- Using hazard rates (not PDF) lets us adjust firing rate as state evolves

Stock & Flow: Logic for Mother & Fetus



Interactions Between Types of Dynamics

Types of Interactions Between Rewriting & ODE Dynamics



C-Set rewrite impacts on evolution of ODE state variable X

- Directly updating the value of X
- Changing the value of attributes representing quantities depended upon by such flow functions (differentials) associated with X, so as to alter the value one or more flows compared to the value that it otherwise would have had; this could include e.g., other people who are neighbours of
- Changing (indirectly or directly) the value of other state variables depended upon by the flow functions (differentials) associated with X, so as to alter the value of one or more of the flows of compared to the value that they otherwise would have had
- Updating the collection of flows into or out of X

Pathways of ODEs Impact on C-Set Rewriting

- Affecting whether the pattern matches
- Affecting hazard rate
- Budding agents

Handling Contemporaneous Events

Different Notions of “Clashing” Rules for Discrete-Time ABMs

- Update order invariance for events that occur at the same time
 - Our framework achieves this because the homsets are updated after the time, allowing the updates to occur in lockstep
 - Note that the Game of Life is not itself naturally order invariant
- Clashing updates -- the rules issue clashing update requests for the same state (e.g., the same cell)
 - This is a more problematic issue, than can be **detected** by this framework with an error message given to the user, but ultimately needs to be handled by the user

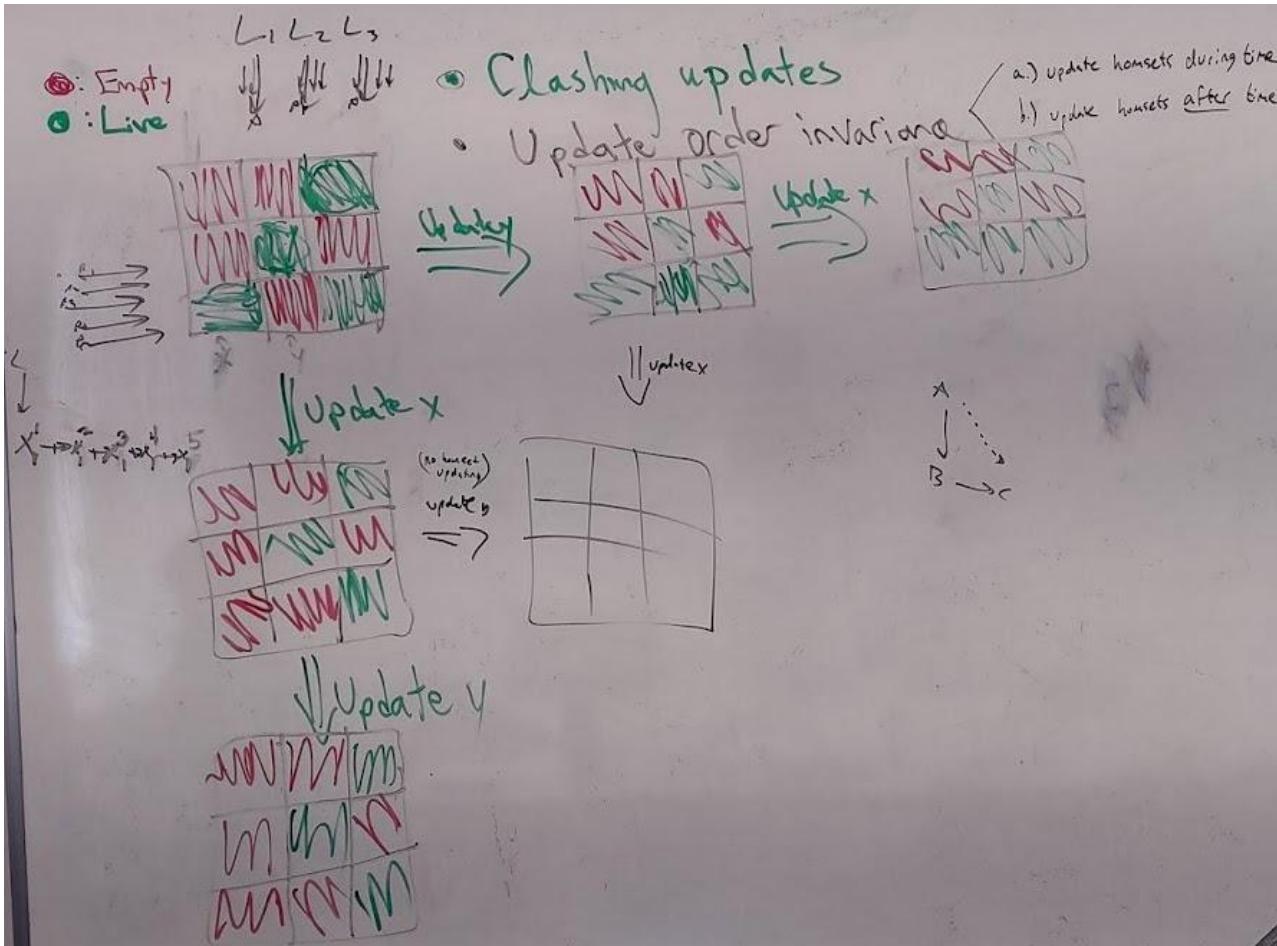
Contemporaneous Events Adhere to Lockstep Dynamics

- The formulated dynamics achieve capturing lockstep discrete time updates occurring at same time (e.g., for Game of Life), contingent on no clashes occurring

Handwritten mathematical equations in green ink on a whiteboard:

$$L_1 \rightarrow R_1$$
$$L_2 \rightarrow R_2$$
$$L_1 + l_2 \rightarrow R_1 + r_2$$

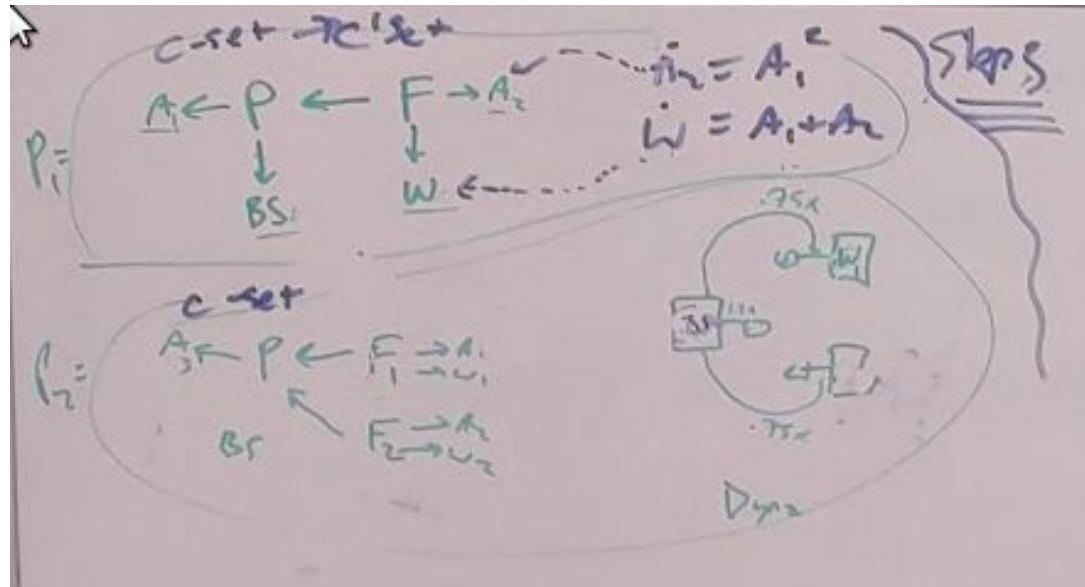
Invariance of Simultaneously Updating Rules



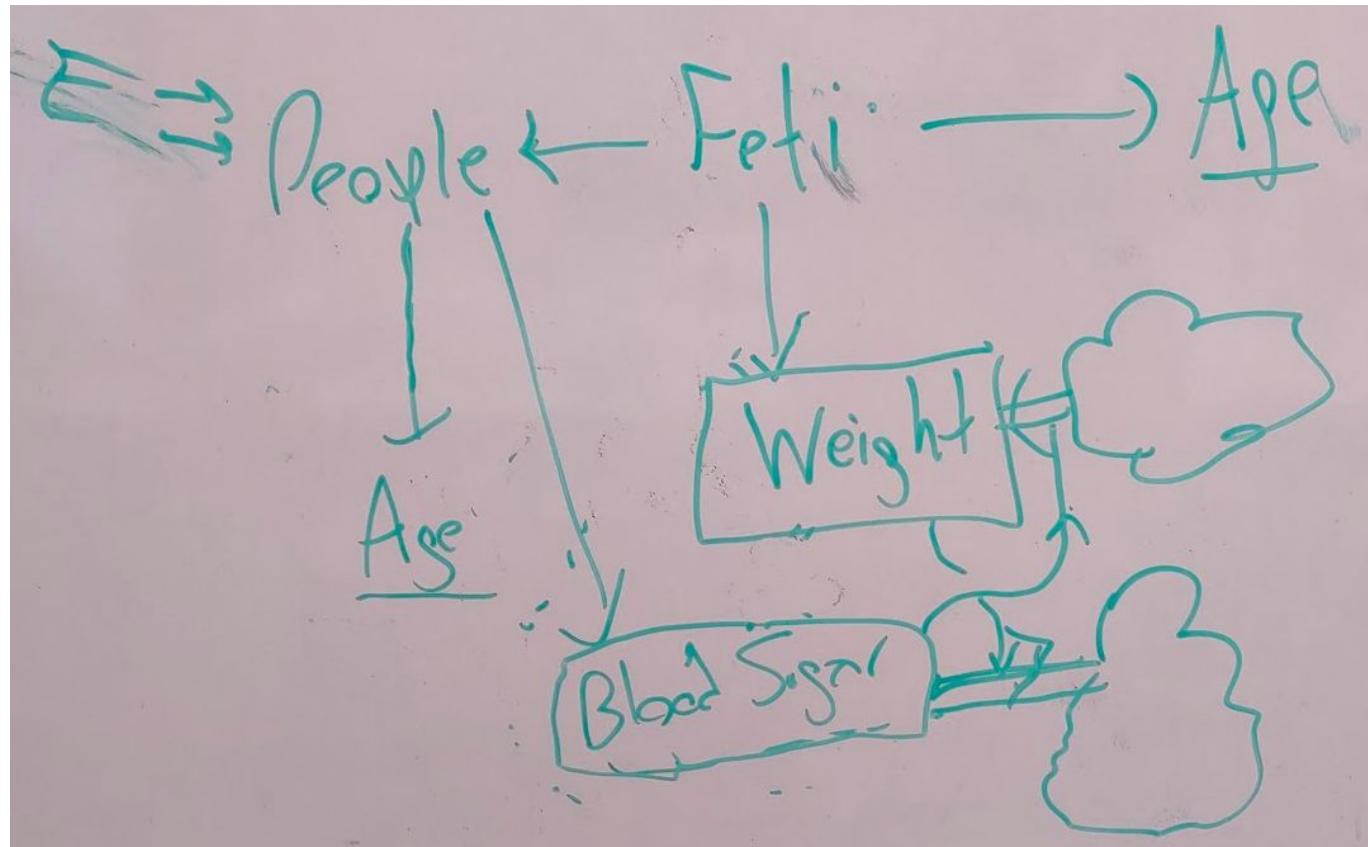
Pattern Matches Govern When & Where Continuous Dynamics is Placed within Running ABM

Matches Weave Governing Process Into Chosen Contexts

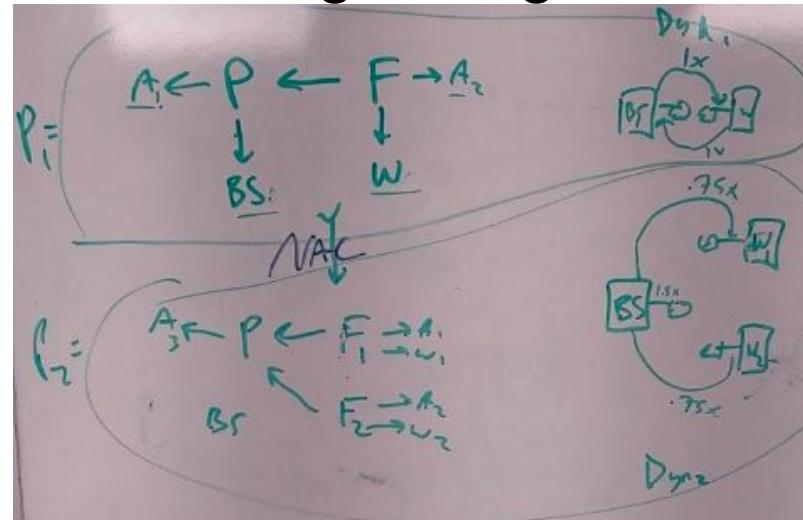
- We weave in dynamics at certain points based on where matches occur
- This can be done for either continuous or discrete event dynamics
- The mechanisms that govern this dynamics
- This allows for changing the governing dynamics as state evolves.



Another Example: Weaving Together Logic for Mother & Fetus



Application Conditions Support Added Refinement When Weaving in Logic



NAC

$(P_2) \text{ 2 futures} \leftarrow 1 \text{ future } (P_1)$

$\frac{dX_i}{dt} = \dots$

$33 \leftarrow \text{Mass} \xrightarrow{6\text{m}} \text{Entry} \xrightarrow{2\text{kg}} \dots \xrightarrow{1.5\text{kg}}$

$A \leftarrow P \leftarrow F_1$

F_2

As long as \exists ≥ 1 such commutative triangle $w(F) = 2.5$ $w(P) = 1.5$

do not apply P_1 (i.e., NAC applies)

Pre-scheduled and Dynamically Scheduled Events

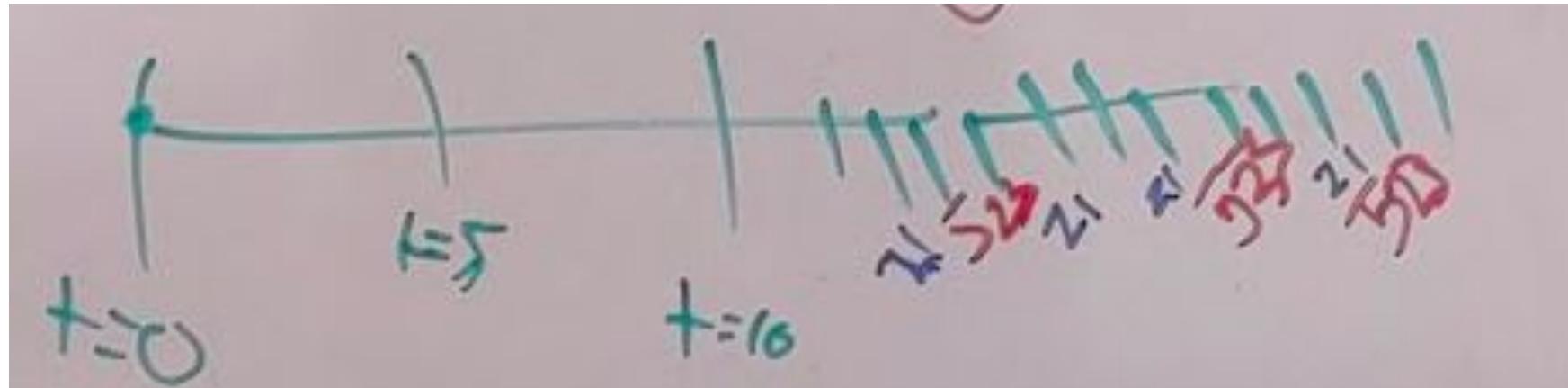
Underlying Rewriting Mechanisms -- Match & Schedule

- Especially because there is no notion of “each agent” needing updates, we need to **match** pattern to find situations that can trigger dynamics via matching (e.g., that an agent is in a given state)
- These situations do not generally need to fire immediately -- for example, if an agent has entered a state; it could exhibits a hazard rate or timeout transition for leaving
- Using hazard rates (not PDF) lets us adjust firing rate as state evolves
- [General case] For *state-dependent* events (hazard rates), we avoid **ongoing** need to reschedule by incrementally computing Bernoulli draws for the probability of firing, for a certain timestep
- For *state-independent* hazard, we **schedule** trigger, Check if match still applies when fires
- By default, if match still remains after rewriting, create new event in the schedule
 - A key exception -- when leaving state in a statechart (know that won’t match again)

Hybrid (Static-Dynamic) Scheduling

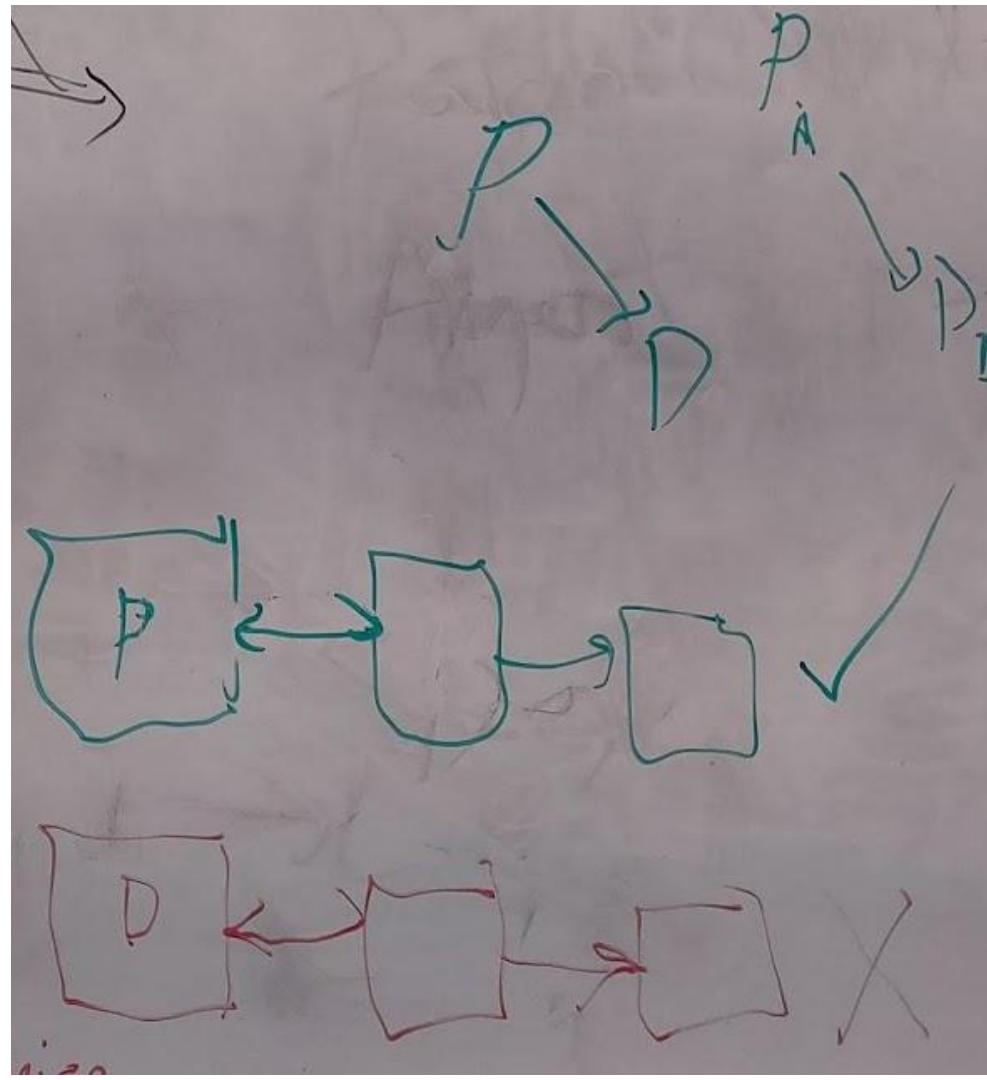
The Supporting Role of an Event Schedule (Queue)

- **Model state independent timing:** Pre-scheduled (both memoryless & memoryful)
- **Timing dependent on Model state:** Events whose scheduling is state dependent, dynamically schedule (Bernoulli draws as to firing)
- Regardless of type, scheduled events can be descheduled if they are preempted eg
 - Agent dies
 - Agent leaves because of matching a different pattern



Problem: Naive Rewrite Rule Apices
Could Violate CSet Rules

Consider:
Referential
integrity
constraints on
rewrites



Currently Planned Solution: Tweak Schema to Include Relation, rather than Direct Dependence so I can have no Link

$$\mathcal{C} = \{ E \Rightarrow V \leftarrow P \}$$

Like C-Par for

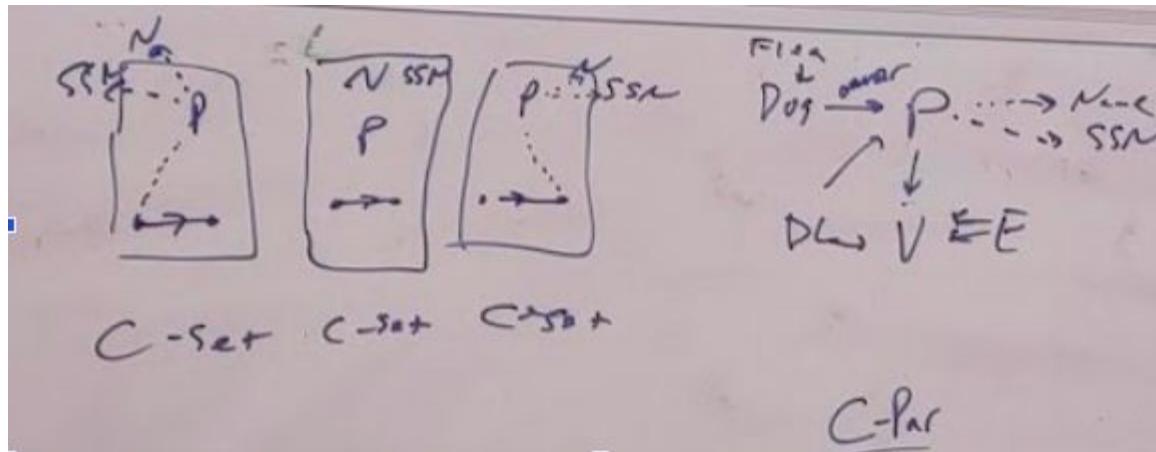
$$\mathcal{C}' = \{ E \Rightarrow V \leftarrow \cdot \leftarrow P \}$$

Possible Eventual Desire for Moving Rewriting to C-Par

We currently have a problem with rewriting needing to violate rules of valid CSet within conserved area I

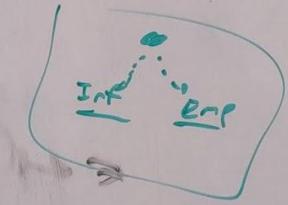
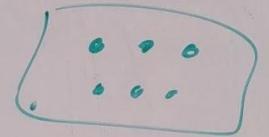
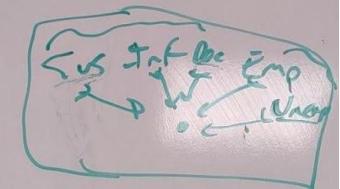
This problem crops up in each type of rewriting

Operating in C-Par allows for eliminating this problem



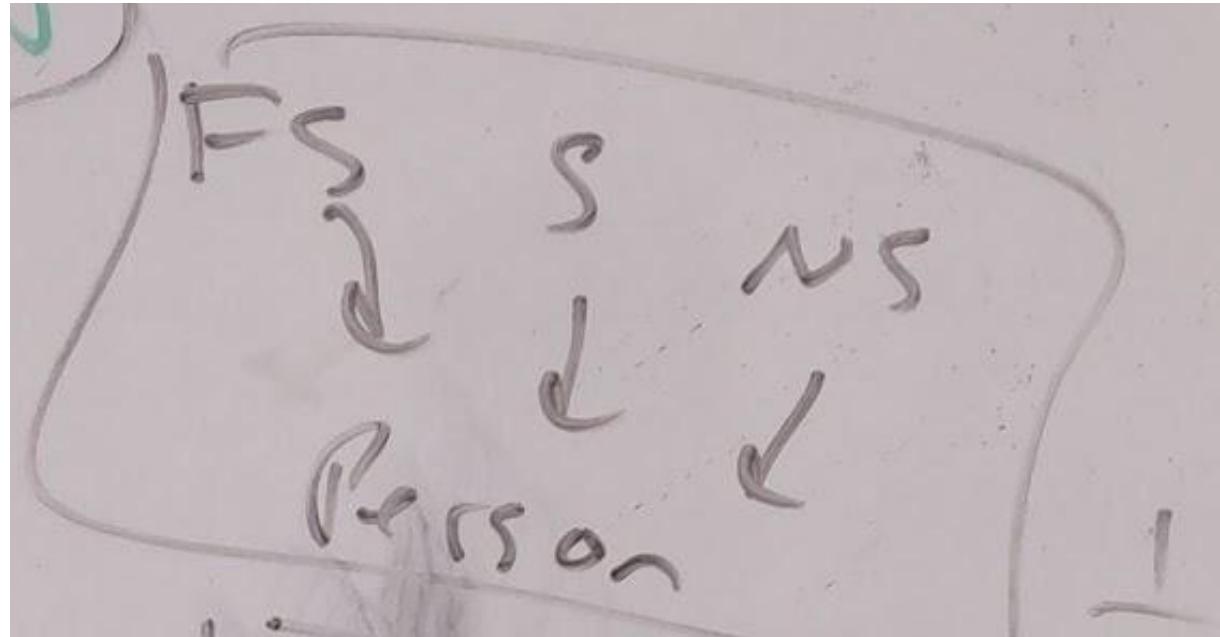
Dealing with Heterogeneity in Characteristics & State

4 Ways of Capturing Heterogeneity



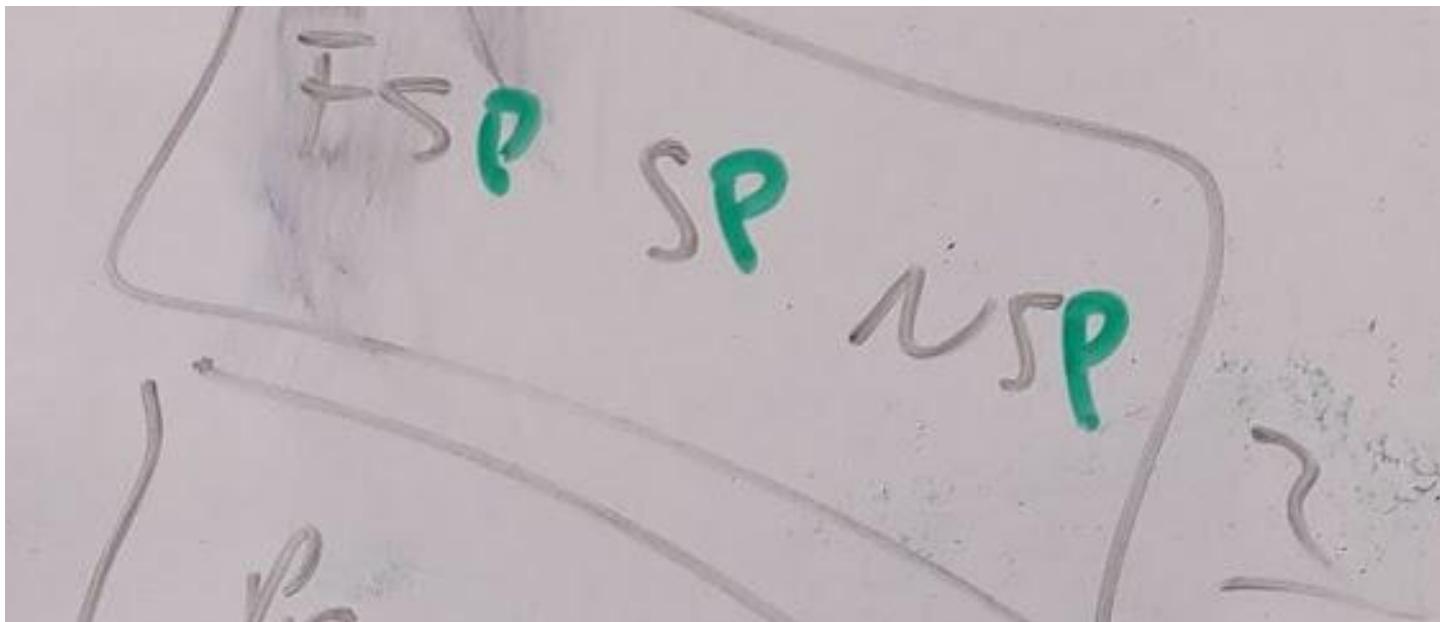
3 different ways of capturing nominal state information: 1

- Separate objects mapping into complete set
 - **Advantages:** Scales well with multiple dimensions of heterogeneity
 - **Disadvantages:** does not make clear the mutually exclusive and collectively exhaustive nature of the update



3 different ways of capturing nominal state information: 2

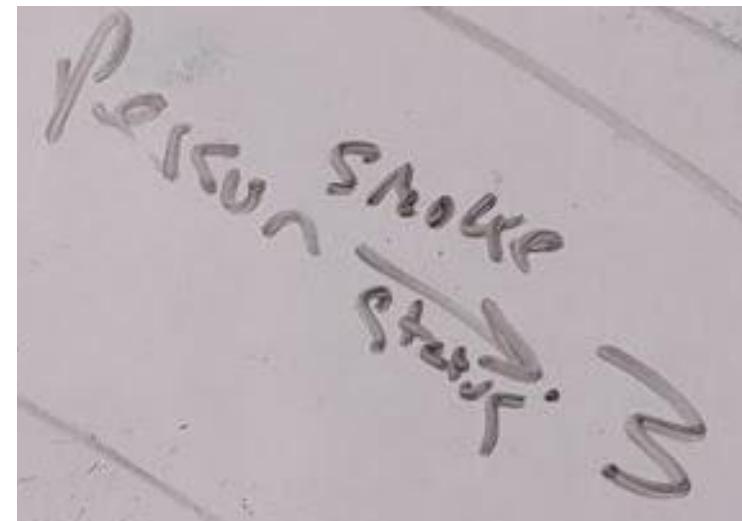
- Separate objects for each division of person
 - **Advantages:** Does make clear that covers all persons
 - **Disdvantages:** Suffers from Curse of Dimensionality with other heterogeneity dimensions



3 different ways of capturing nominal state information: 3

- Attributes

- **Advantages:** Handles both
 - curse of dimensionality
 - collectively exhaustive & mutually exclusive nature of the data
- **Disadvantages:**
 - Not as declarative in matching (but could be with enums?)
 - I believe that may not currently be as efficient for certain matching?? Ask Kris, but he seemed to think that it could be brought to a level that was as efficient.



Performance Investments

Performance Investments

- Incremental matching (“incremental hom search”) -- Alert rules when changes can trigger a pattern
 - Discrete event actions
 - More complicated with continuous dynamics
 - Descheduling events that no longer apply
- Staged computation: Build-time computation of constraints to optimize hom search
- Special match handling for
 - **Coproduct of Representables:** Due to Yoneda Lemma, know the number of matches (perhaps similar handling of each?); to match colimit, presumably need some match for each, so by Yoneda Lemma, rule out match if set mapped to by any of the representables whose colimit is taken are 0; detect change if count of any of “parts” has changed
 - Discrete category: This is a coproduct
- In-place rewriting
- Separation of positive application condition from patterns (reduces size of rewrite)
- Planned: Exploiting characteristics of statecharts
- Memoryless processes: Rather than scheduling n with rate λ , draw one with rate $n\lambda$
- Descheduling all events for a match when match fails

Successively Richer Opportunities for Optimization

- All transitions
- State independent transitions
- Memoryless state state independent transitions
- “Inevitable” memoryless state state independent transitions

Layering of Optimizations

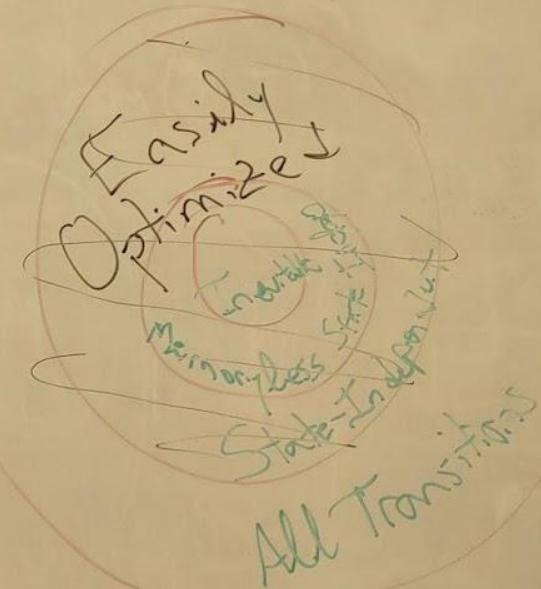
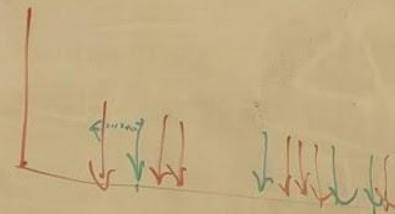
Initial 208-402

Λ

Preschedule state-independent transitions

Fixed Memoryless Transitions

Dirac Delta



Performance Investments

- Incremental matching (“incremental hom search”) -- Alert rules when changes can trigger a pattern
 - Discrete event actions
 - More complicated with continuous dynamics
 - Descheduling events that no longer apply
- Special match handling for
 - **Coproduct of Representables:** Due to Yoneda Lemma, know the number of matches (perhaps similar handling of each?); to match colimit, presumably need some match for each, so by Yoneda Lemma, rule out match if set mapped to by any of the representables whose colimit is taken are 0; detect change if count of any of “parts” has changed
 - **Discrete category:** This is a coproduct
- In-place rewriting
- Planned: Exploiting characteristics of statecharts
- Separation of positive application condition from patterns (reduces size of rewrite)
- Memoryless processes: Rather than scheduling n with rate λ , draw one with rate $n\lambda$
- Descheduling all events for a match when match fails
- HomSet type?

Flagging Coproducts of Representables for Optimization

A pattern match from a coproduct of representables is just a choice of parts in the codomain. E.g. matching $L = \bullet \rightarrow \bullet \cdot \bullet$ is just a random choice of edge and two random vertices.

The vector of ints refers to parts of L which are the counits of the left kan extensions that define the representables (usually this is just wherever the colimit leg sends 1, as there is often just one X part in the representable X).

WARNING: this is only viable if the timer associated with the rewrite rule is symmetric with respect to the disjoint representables and has a simple exponential timer.

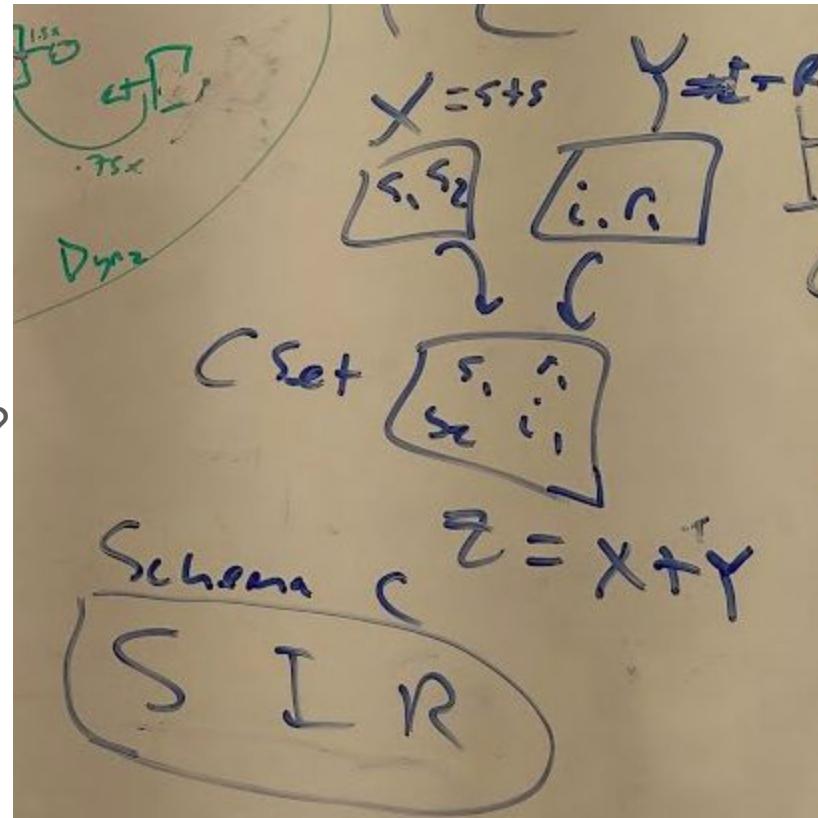
"""

```
@struct_hash_equal struct RepresentableP <: PatternType
| parts::Dict{Symbol, Vector{Int}}
end
```

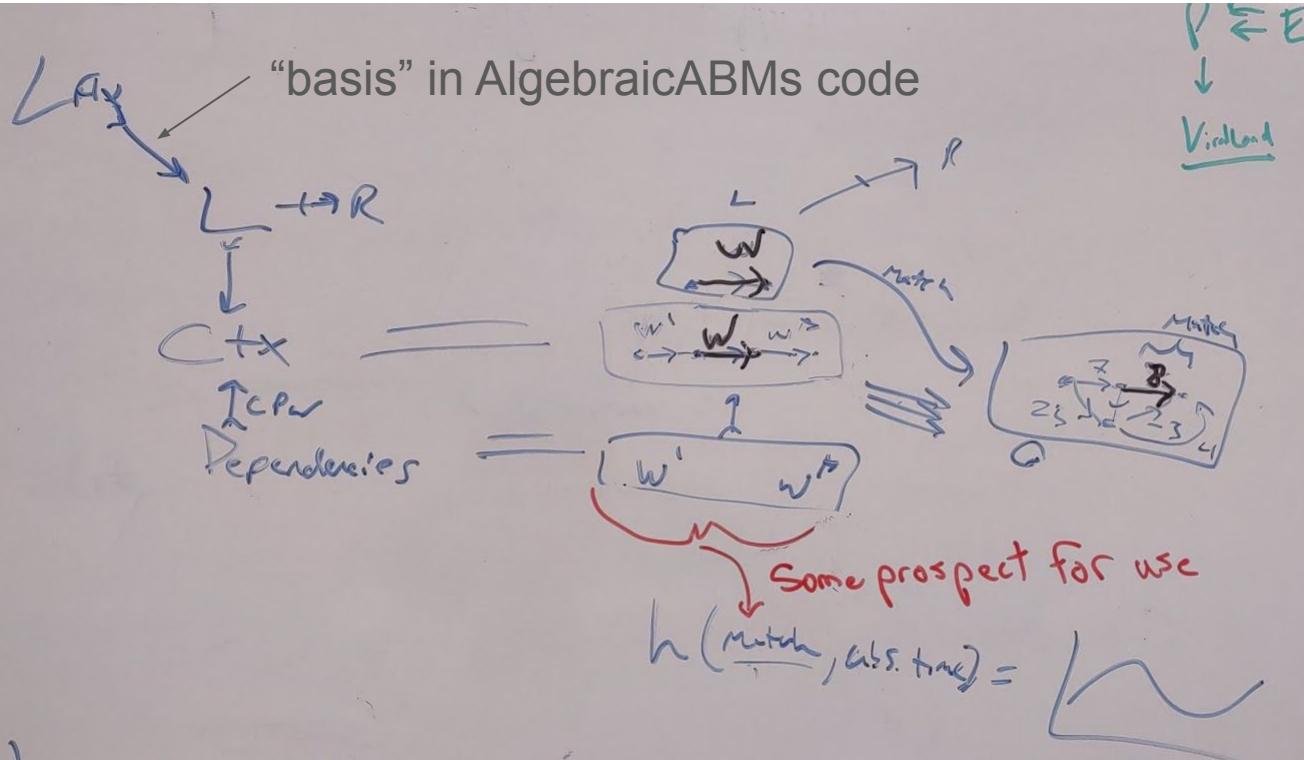
```
Base.keys(p::RepresentableP) = keys(p.parts)
```

Discrete Case

I believe the idea is perhaps that the coproduct of discrete cases is itself discrete?

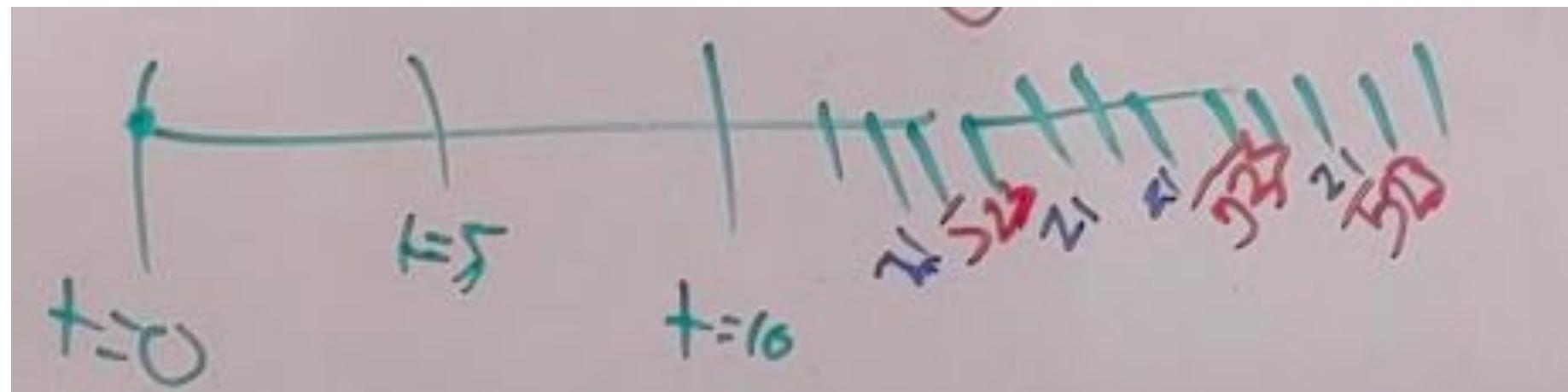


L_{fix} limits what Changes Are of Concern in Pattern Matching

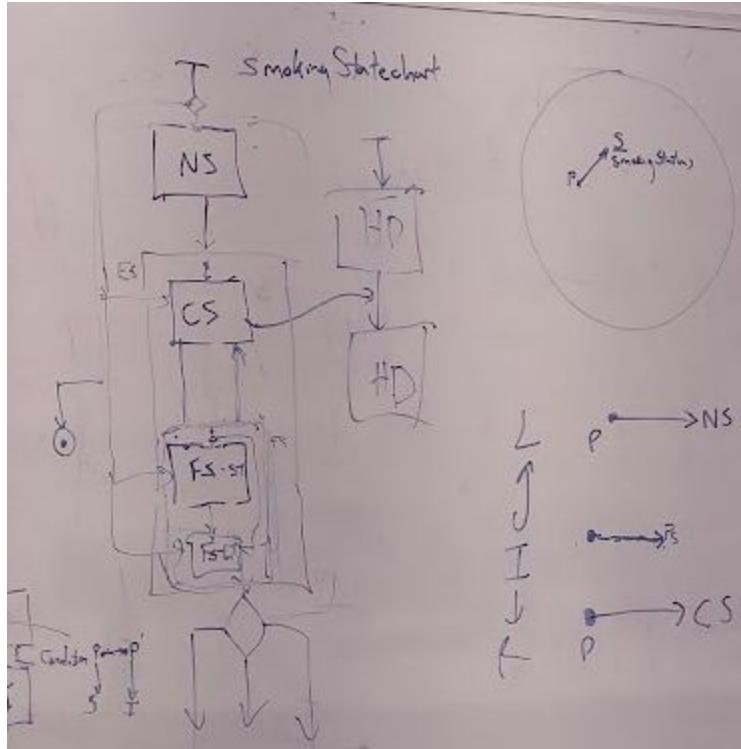


$$\text{List}(R \times R) \rightarrow [0, \infty]^{R^2}$$

Recall: Role of an Event Schedule (Queue)



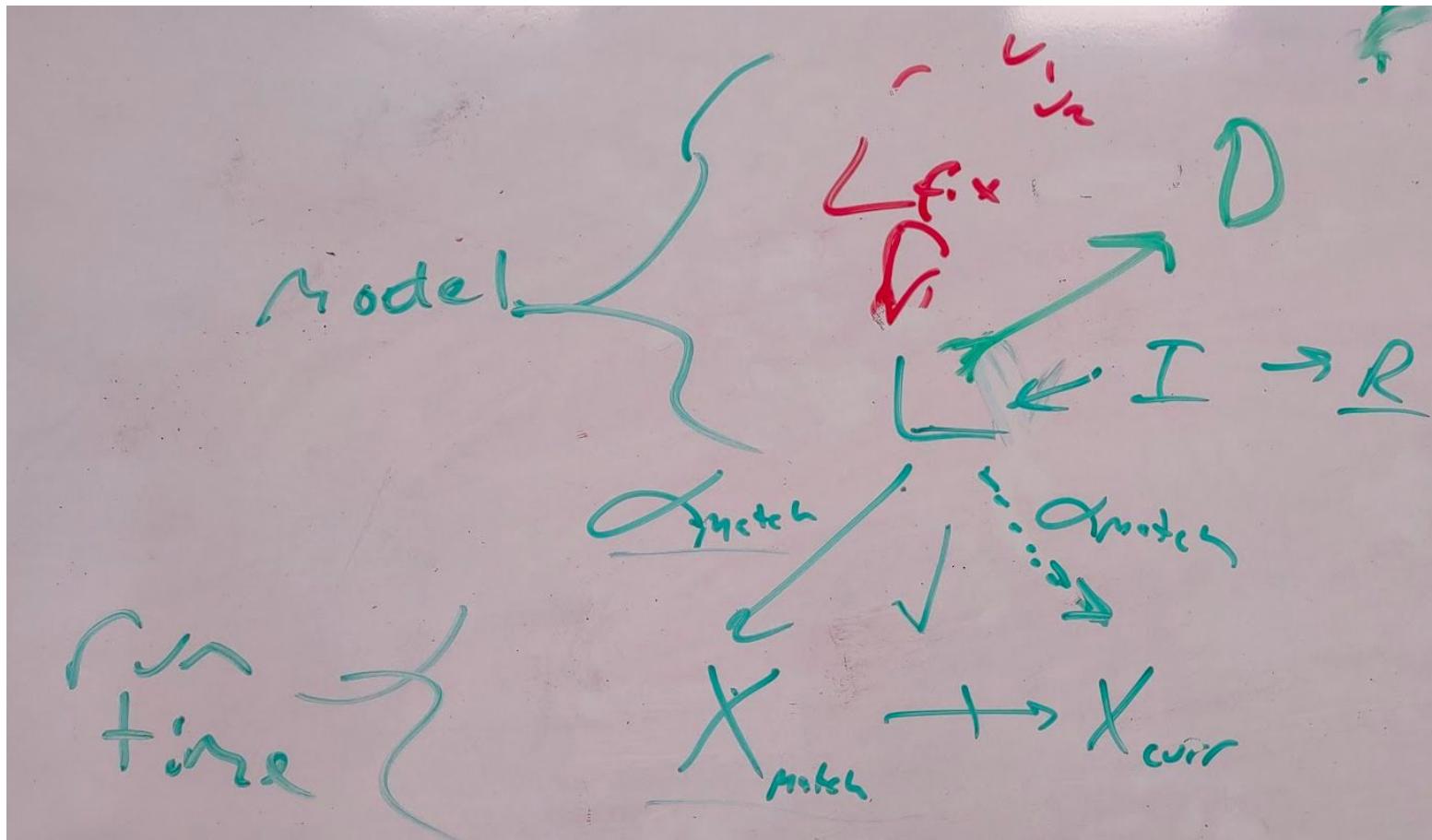
Statecharts Can Compile to Rewrite Rules



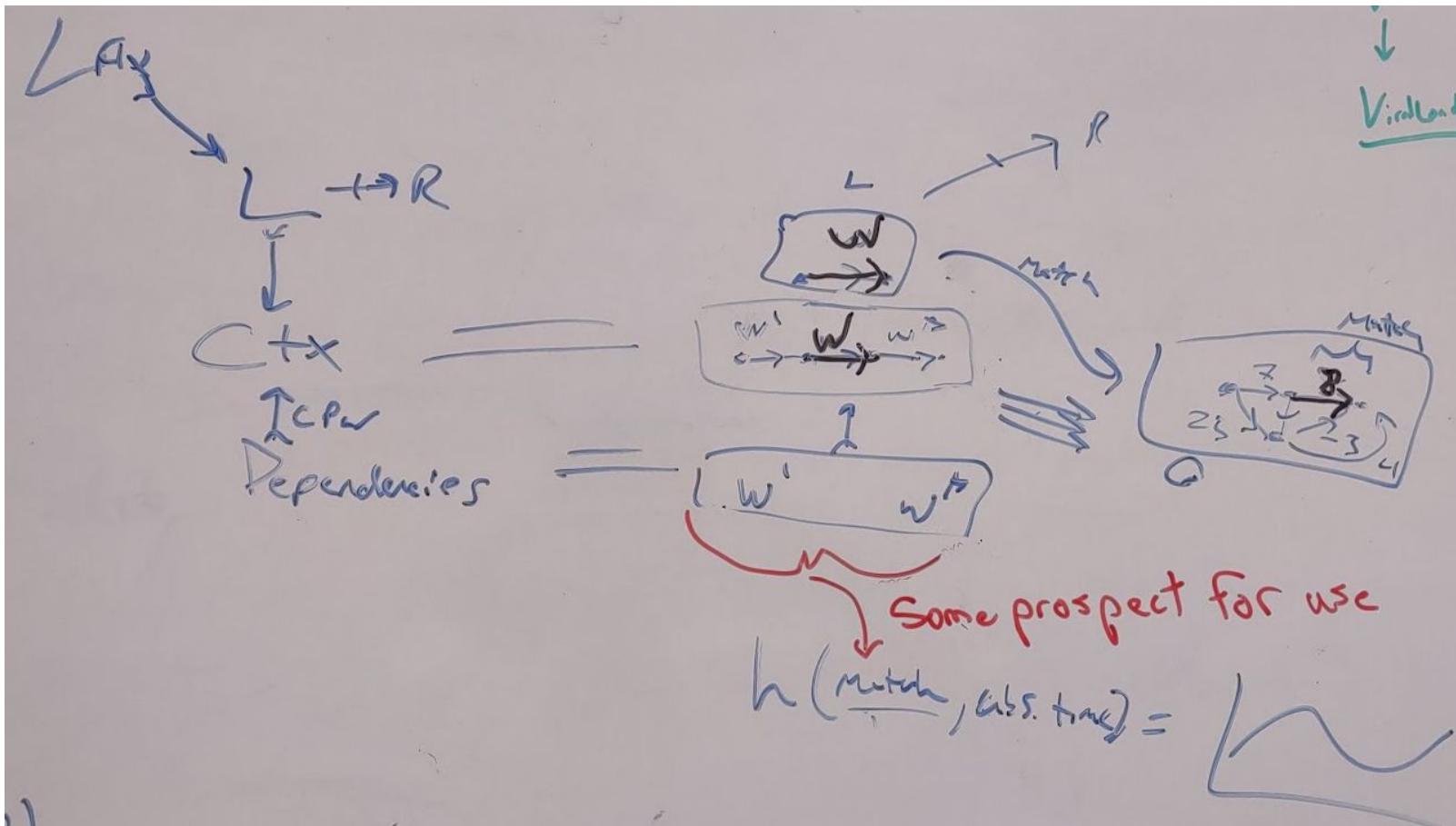
Anticipated Optimizations

- Moving to observation processes rather than all changes in state

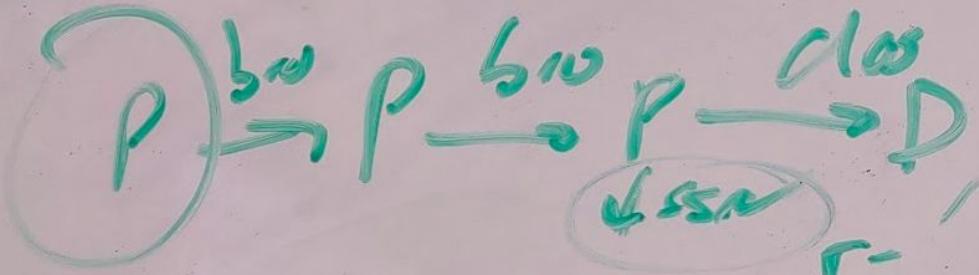
Separating out Context that Need not be Matched or Rewritten



Extracting Further Information on Selected Dependencies



D_{Sub}



D

Statecharts

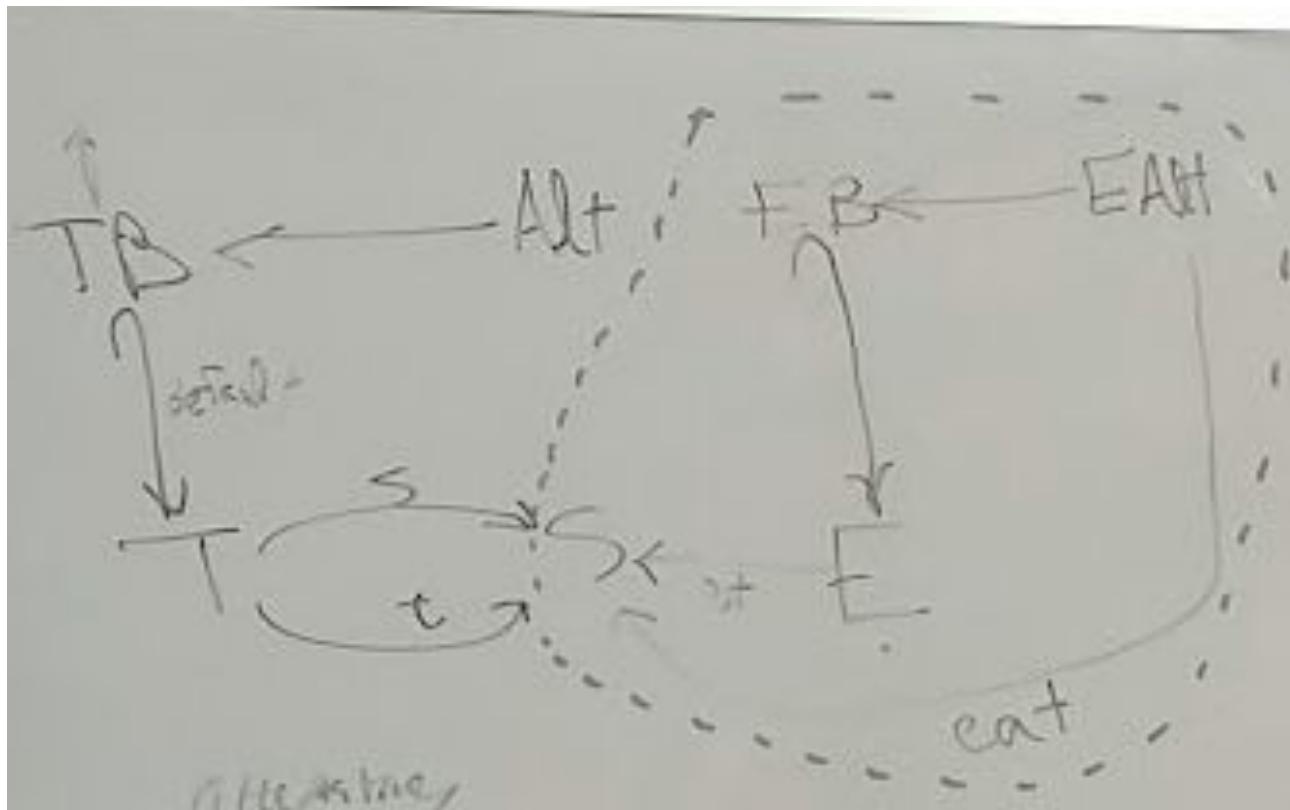
Currently Planned Statechart Transition Types

- Condition (fires immediately upon pattern match)
- Arrival (fires immediately upon arrival)
- For each of {Hazard rate, Timeout [Dirac delta]}, variants that have the following; guards here can make use of both positive & negative application conditions
 - Plain
 - Eligibility Guard
 - Triggering Guard
 - Both Eligibility & Triggering Guard

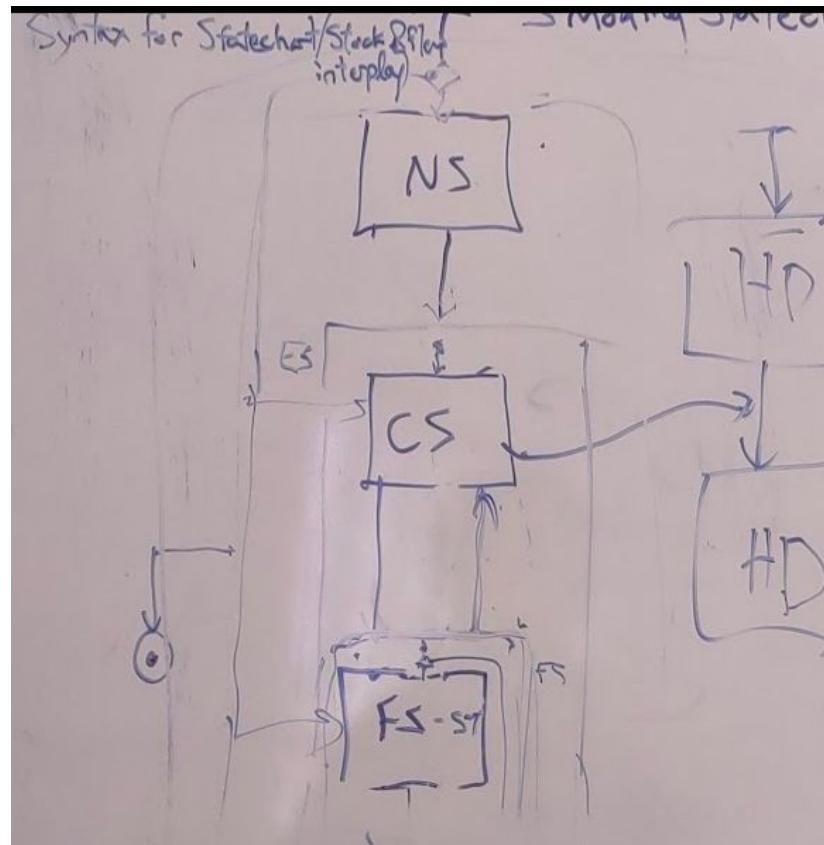
Statechart Affordances for Optimization

- All transitions emerging from state S are conditional on remaining in state S
- Can readily dequeue events departing a state if leave via other mechanisms
- For events without conditions other than presence in the originating state
 - Can determine events candidate timing for all departure transitions, and pre-schedule only earliest of them -- not all
 - Need not check any conditions at start than presence on state, and nothing when leave since would be dequeued if left state
- When have only eligibility-guarded transition, by definition need only check that condition when first matching; would be removed if left before firing, and fires unconditionally if remain
- When have only triggered-guarded transition, need only check presence in state as match, and then check condition when would fire; would be removed if left before firing
- When have both eligibility-guarded and triggered-guarded transition, we have the usual case: Need to check full match initially (including that in state), and then check match when would fire
- Don't have to reschedule a new firing time when departing state -- know won't match

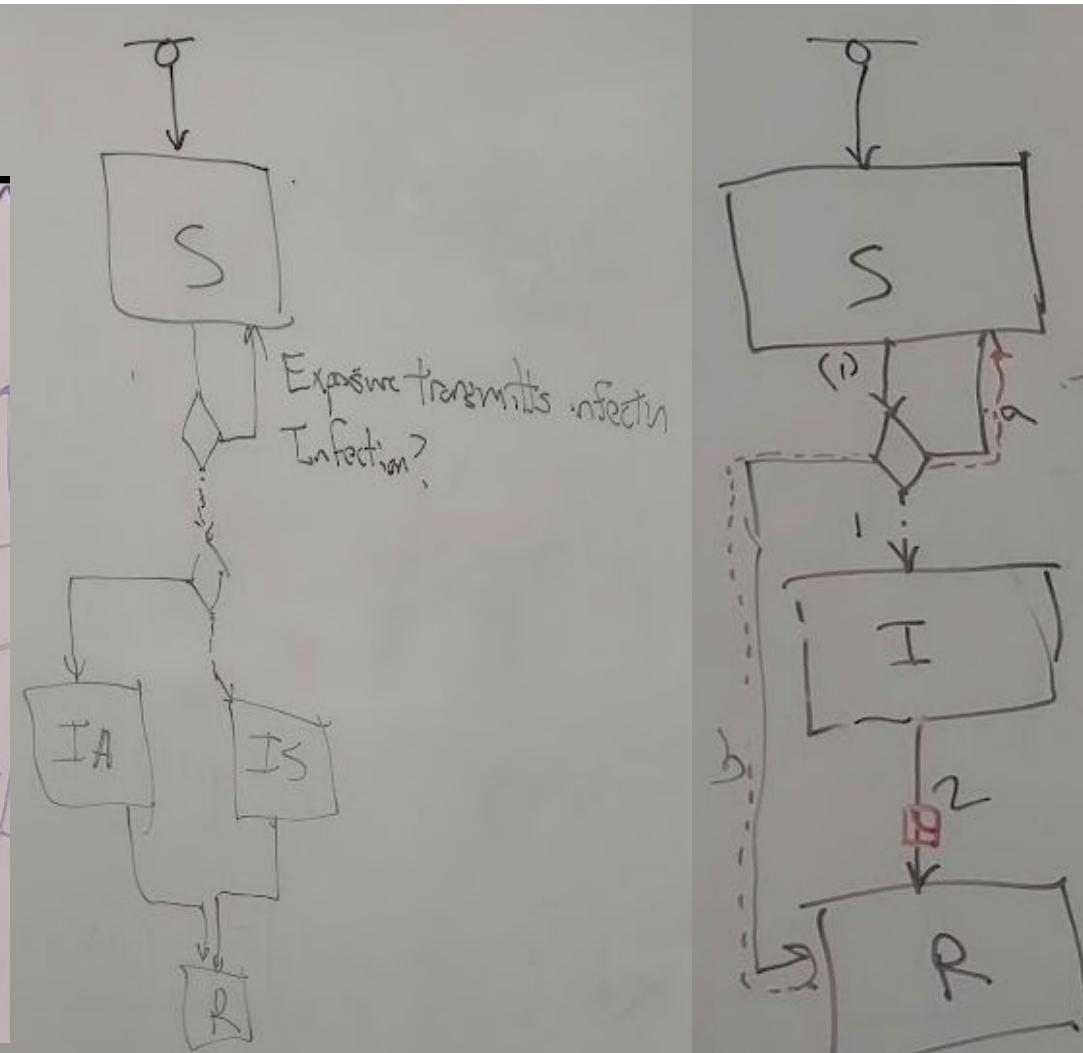
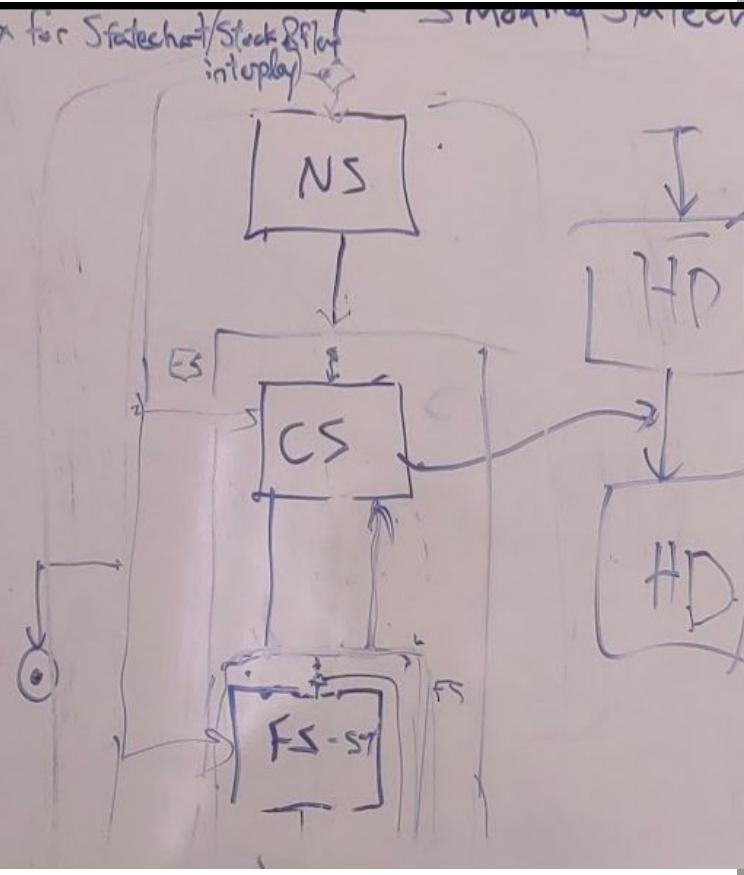
Early Idea for Statechart Schema



Forgoing Hierarchical Statecharts for Now



Example Statecharts



Statecharts and Dependencies

- Pattern matching rules for contextual dependencies not CONSUMING
 - Will seek negative or positive application condition alongside a rule that would otherwise fire
- application conditions can be nicely combined with statecharts when don't require resource to be consumed -- can't just take the boolean negation of boolean for application
- for contextual dependencies dependent on an agent's state that are required for a transition which require CONSUMING or CHANGING other aspects of state, we can often either a
 - petri net
 - arbitrary rewrite conditoons

Statechart Hazard Rate Expressions via GATLab

- We will represent the hazard rate rules for statecharts via GATLab
- A GATExpr (and subtypes) can be represented as an attribute in schemas
- Using GATLab in this way will let us track added semantic information -- e.g., dimensions/units, domains of values
- GATLab is already planned for explicit use in taking pushouts of schemas

Example Starting Theory for Statechart Schemas

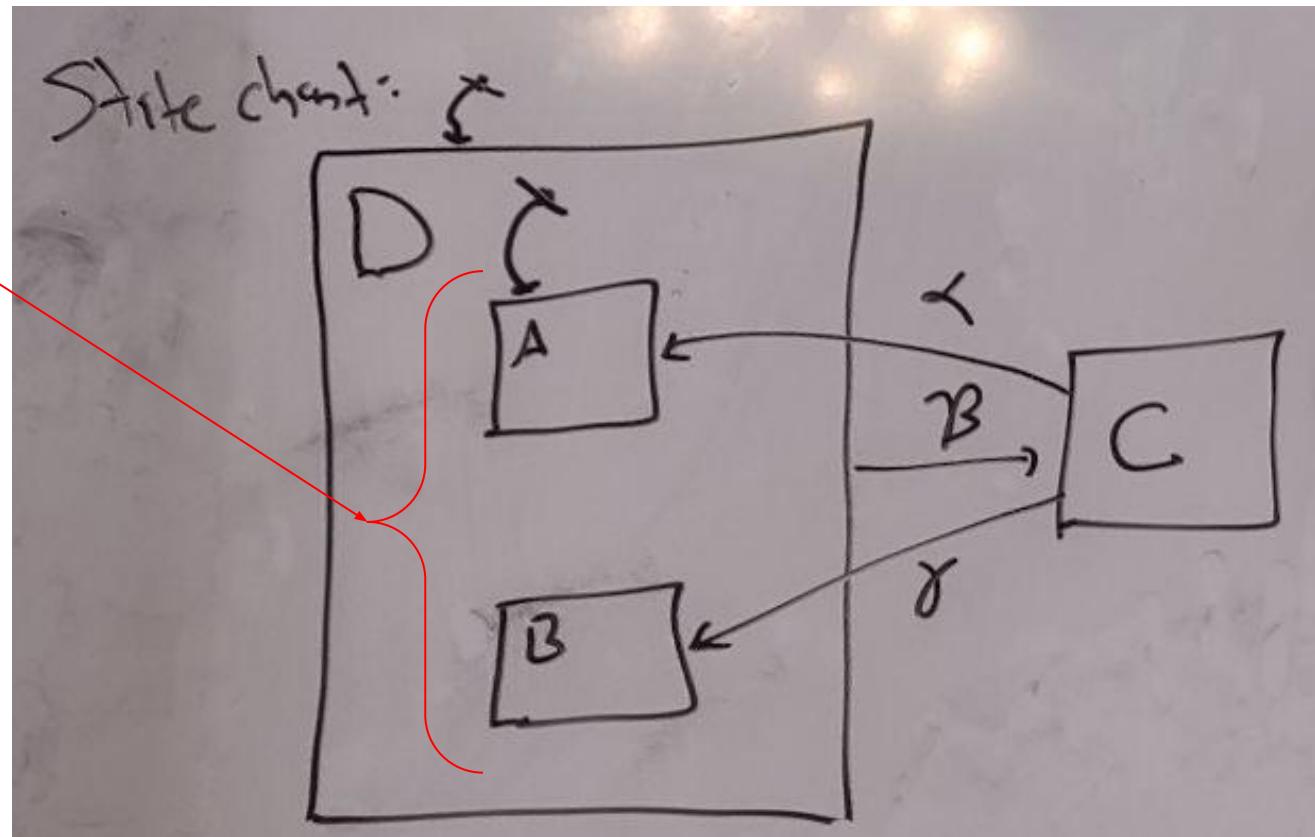
```

1 import Base.::
2 import Catlab.::
3
4 @theory ThStatechartAlgebra begin
5   State::TYPE
6   Quantity::TYPE
7
8   # Multiplicative commutative monoid.
9   @op (.) := times
10  times(x::Quantity, y::Quantity)::Quantity
11  unit()::Quantity
12
13  x . (y . z) == (x . y) . z -> [(x,y,z)::Quantity]
14  x . unit() == x -> [x::Quantity]
15  unit() . x == x -> [x::Quantity]
16  x . y == y . x -> [(x,y)::Quantity]
17
18   # Additive abelian group.
19   @op (+) := plus
20   plus(x::Quantity, y::Quantity)::Quantity
21   zero()::Quantity
22
23   @op (~) := neg
24   neg(x::Quantity)::Quantity
25   # TODO: Axioms of abelian group.
26
27   # Convenience term for subtraction.
28   @op (-) := minus
29   minus(x::Quantity, y::Quantity)::Quantity
30   x - y == x + (~y) -> [(x,y)::Quantity]
31 end
32
33 @symbolic_model FreeStatechartAlgebra{GATExpr, GATExpr} ThStatechartAlgebra {
34   times(x::Quantity, y::Quantity) = associate_unit(new(x,y), unit)
35   minus(x::Quantity, y::Quantity) = plus(x, neg(y))
36 }
37
38 a, b, c = [Quantity(FreeStatechartAlgebra.Quantity, name) for name in [:a,
39
40 #=
41 @present ExStatechartAlgebra(FreeStatechartAlgebra) begin
42   (a, b, c)::Quantity

```

Theory for Hierarchical Statecharts (Evan Patterson)

$D := A + B$



Distributive Categories -- Category \mathcal{C} with

- Finite coproducts
- Finite products
- Products distribute over coproducts: For all $A, B, C \in \text{Ob}(\mathcal{C})$ have isomorphism
 $(C \times A) + (C \times B) \xrightarrow{\sim} C \times (A + B)$
 - A canonical forward map is present for any category
 - For a distributive category, the reverse map must be the inverse of the forward map

Guaranteed, Canonical Map $(C \times A) + (C \times B) \rightarrow C \times (A + B)$

- As a map out of a coproduct, $(C \times A) + (C \times B) \rightarrow C \times (A + B)$ is equivalent to the pair of maps
 - $(C \times A) \rightarrow C \times (A + B)$
 - $(C \times B) \rightarrow C \times (A + B)$
- $(C \times A) \rightarrow C \times (A + B)$ is given by
 - $\pi_C: (C \times A) \rightarrow C$
 - $\pi_A; \iota_A: (C \times A) \rightarrow A + B$
- $(C \times B) \rightarrow C \times (A + B)$
 - $\pi_C: (C \times B) \rightarrow C$
 - $\pi_B; \iota_B: (C \times B) \rightarrow A + B$

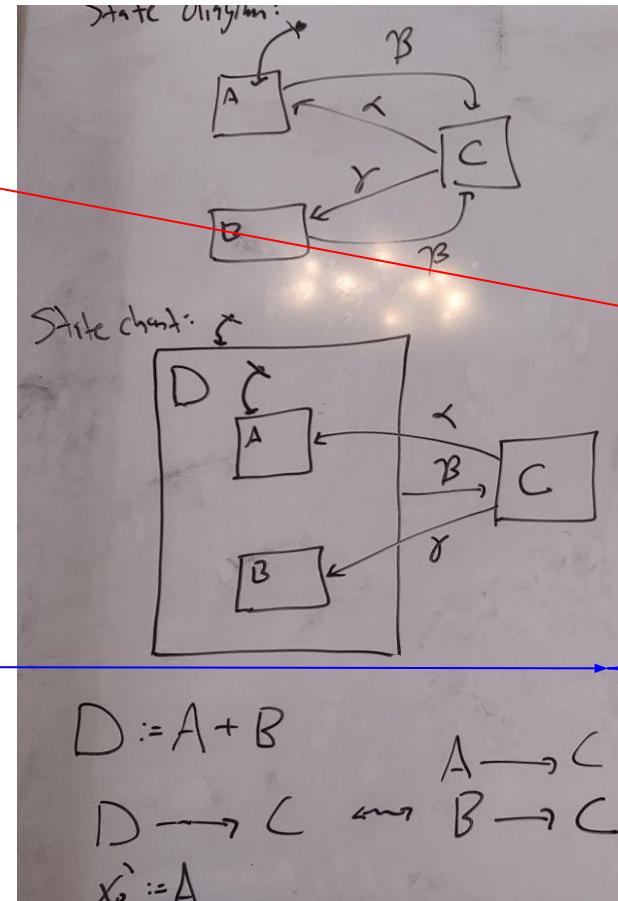
Statecharts as Distributive Categories: “Top-down” Expansion

- Multiple (mutually exclusive and collectively exhaustive) substates within a state (or overall statechart) as combined via **coproduct**
- Parallel statecharts combined via **product**
- **Morphisms:** Coproduct-preserving “refinement functor” maps coarser statechart to more detailed statechart (expanding hierarchically to do so)
- Additional features
 - Shared transitions (inputs) between statecharts
 - Initial states

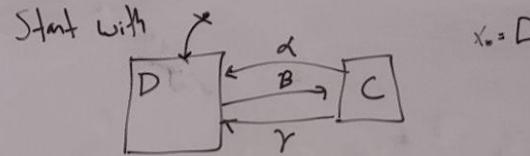
Co-Product Components: “Refinement” Relation

Coproduct preserving “refinement functor” maps coarser diagram into finer-grained (“refined”) diagram

Mapping of objects & morphisms



Refinement: top-down approach to hierarchical specifications



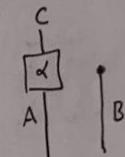
Refine via a Morphism between cocartesian categories
(coproduct-preserving functor)

$$\begin{cases} D \mapsto A + B \\ C \mapsto C \end{cases}$$

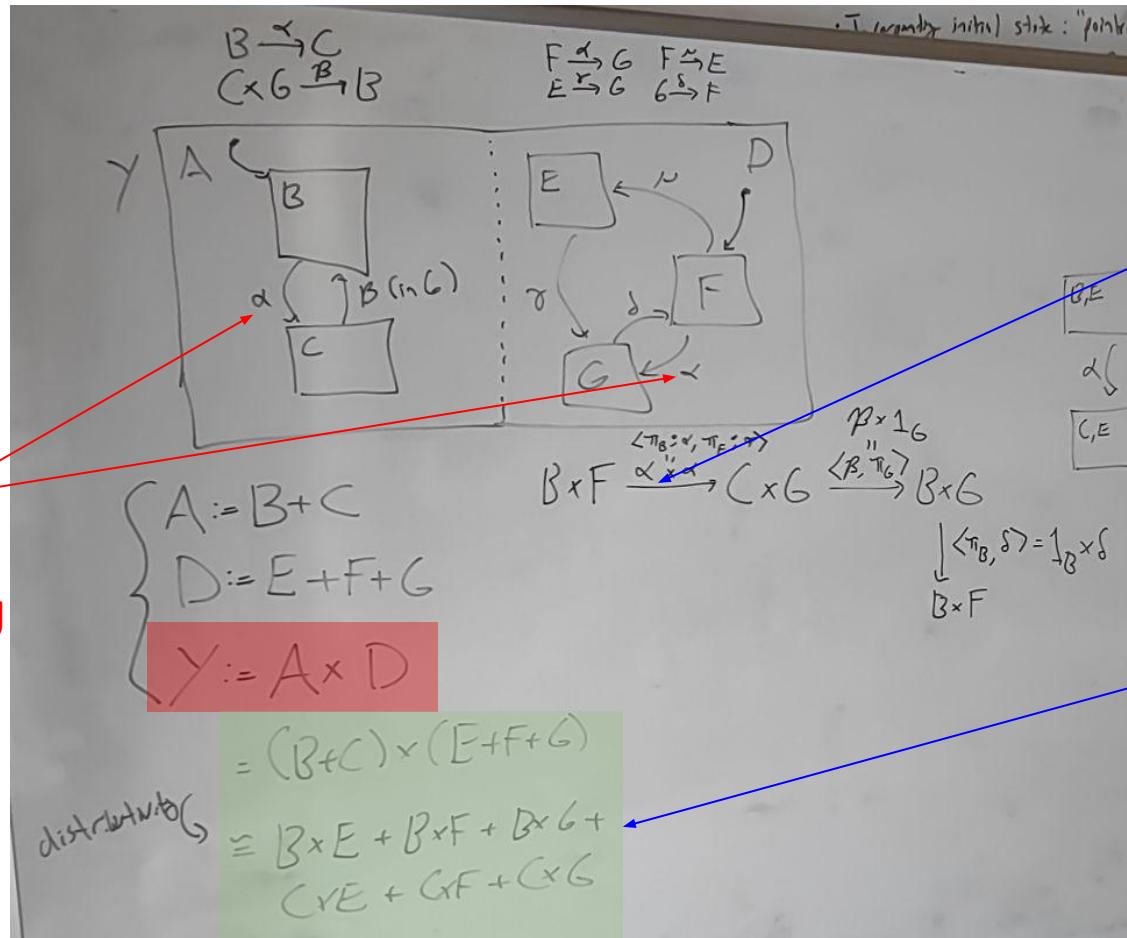
$$\begin{cases} (\alpha: C \rightarrow D) \mapsto (C \xrightarrow{\alpha} A \xrightarrow{c_A} A + B = D) \end{cases}$$

$$\begin{cases} \gamma \mapsto \gamma \circ c_B \\ \beta \mapsto \beta \end{cases}$$

$$A = x_0 \xrightarrow{c_A} x_0 = D$$



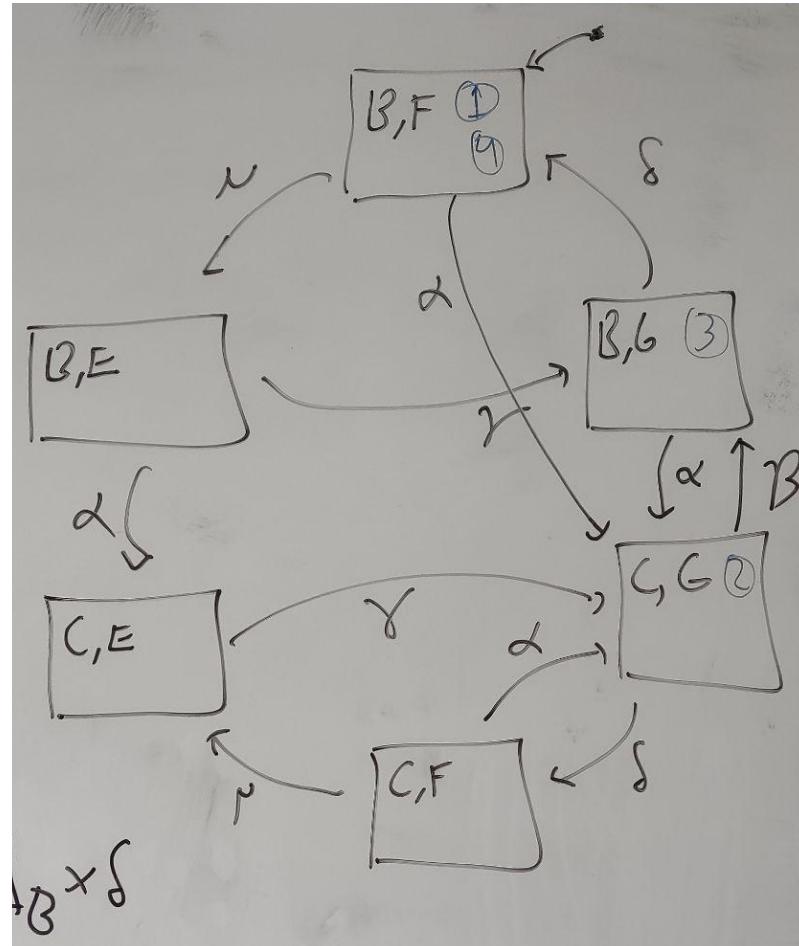
Product Components: Parallel Statecharts



Transitions from one state to another

Application of distributive law

Equivalent Fully Expanded (Non-Hierarchical) Statechart



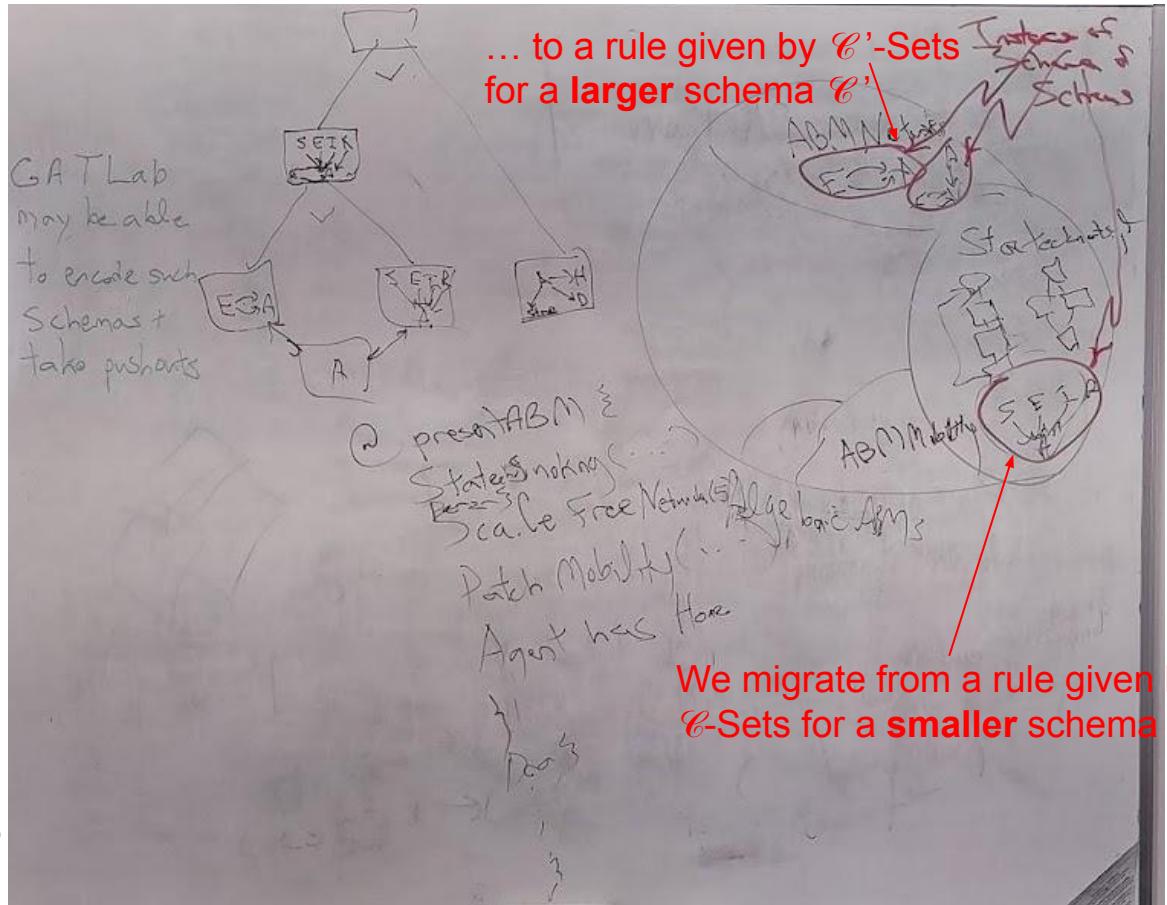
Lifting of Rewrite Rules & Patterns to Successively Larger Schemas

Layering in Context Via Schema Pushouts

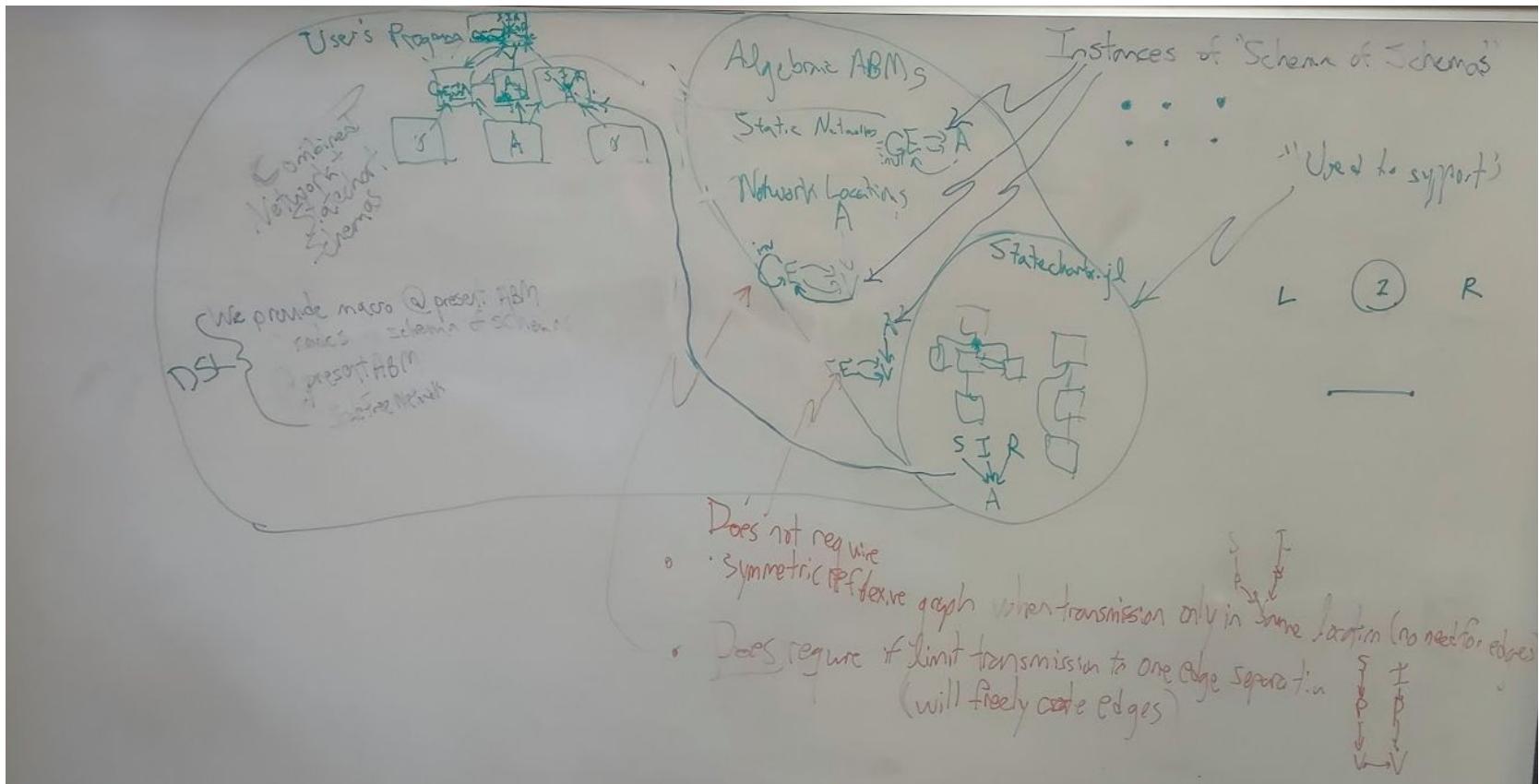
-- Migrating Logic as Schema Grows

While GATLab can take pushouts of different theories, for legacy reasons, it cannot yet take pushouts of schemas for the same theory.

For now, Xiaoyan has implemented a schema of schemas. This will be replaced when GATLab's mechanisms are available.



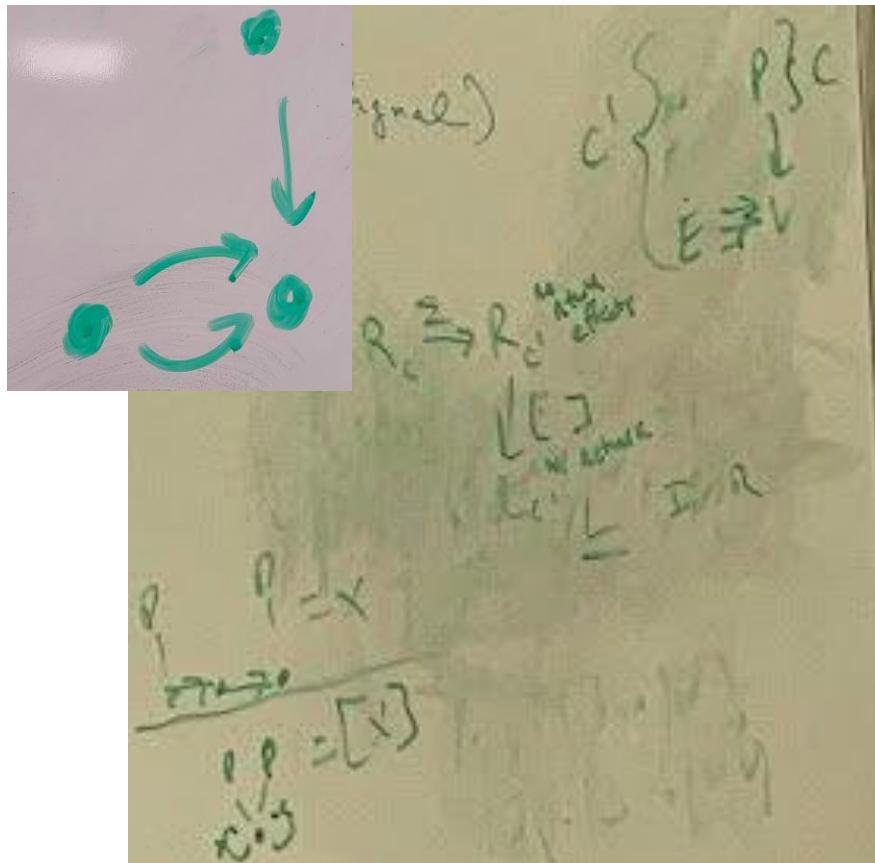
Successive Layering



Weaving in Common Location Logic into an Arbitrary Rule

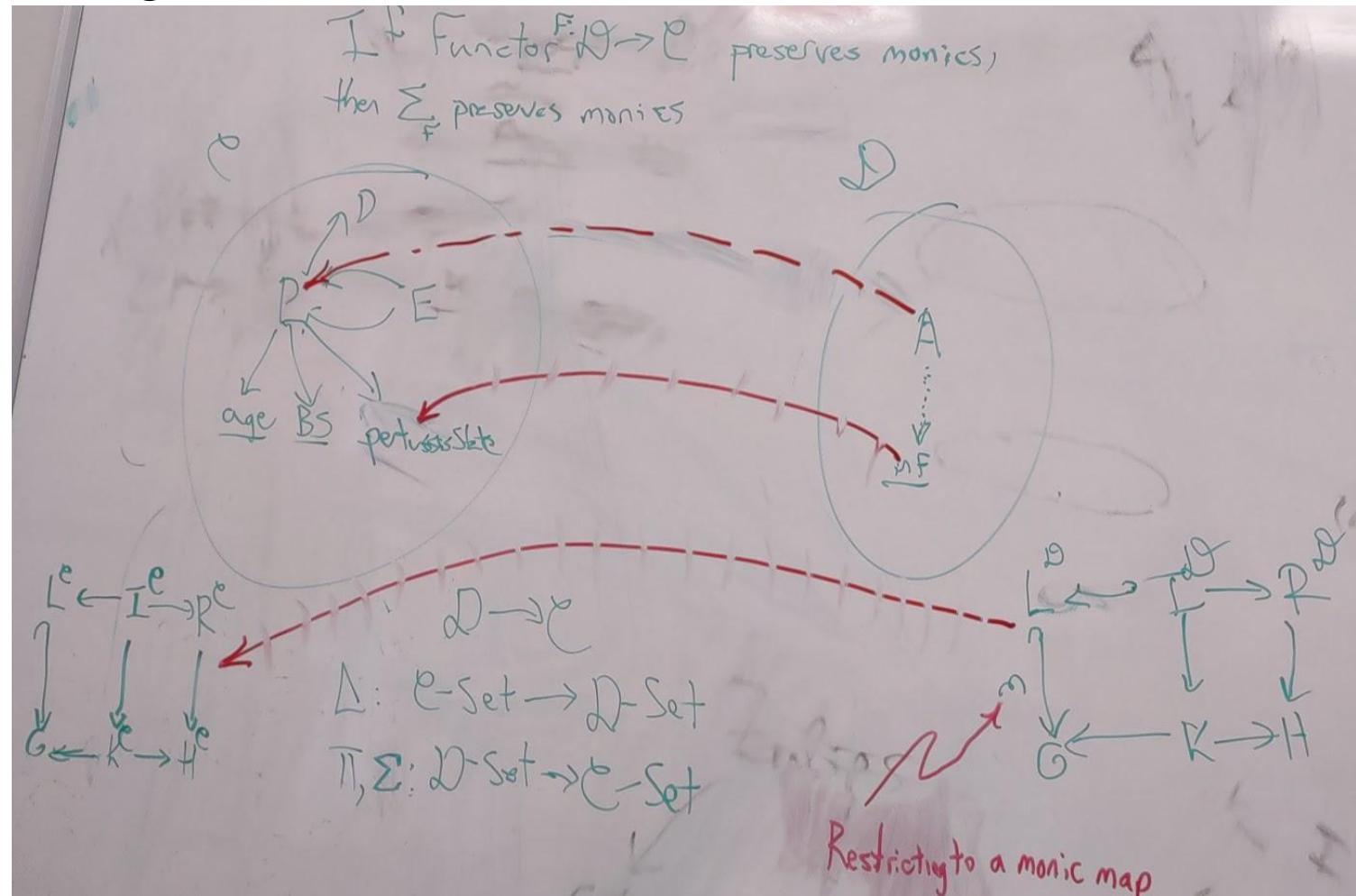
For example can readily weave rewrite rule logic for these cases:

- without regards to network
- at the same location
- for agents with n distance of each other



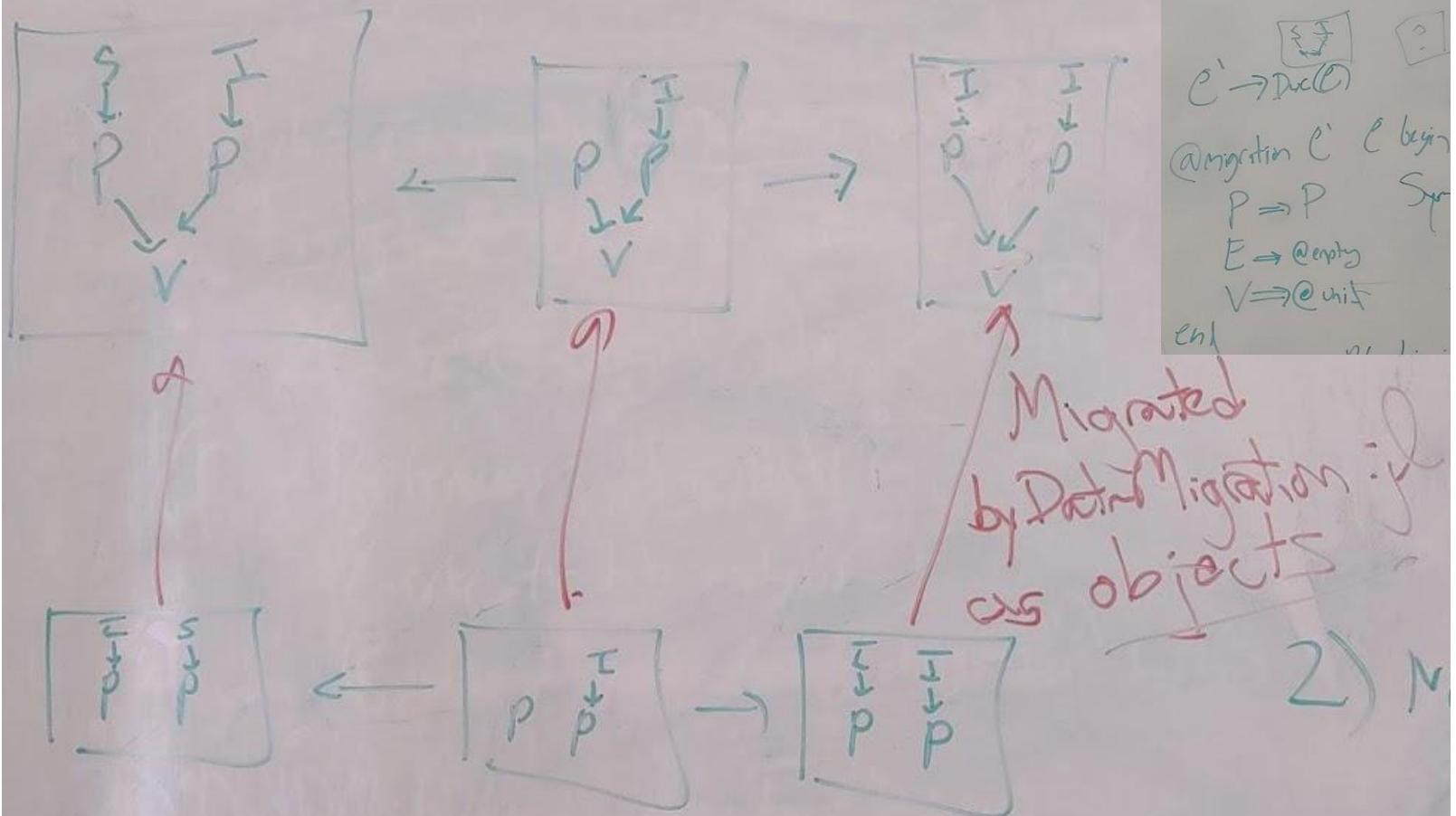
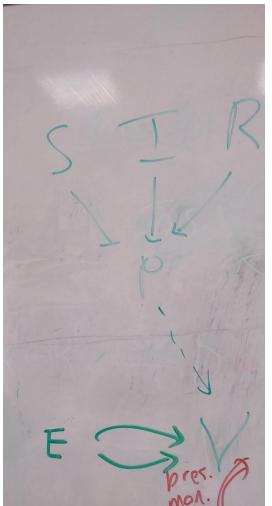
Data Migrations -- Canonical and Otherwise

Whilst such canonical data migrations are useful, there are many times we will seek other forms of data migrations that cannot be expressed in terms of simple maps between schemas. DataMigrations.jl gives us far greater flexibility.



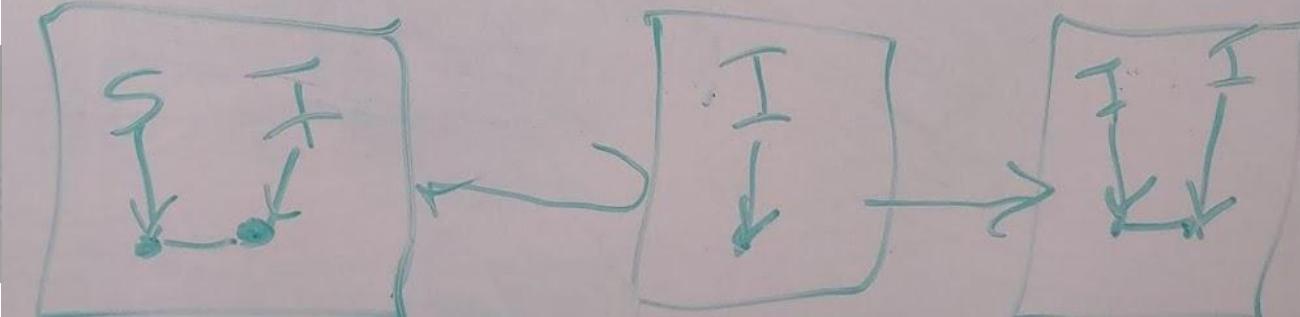
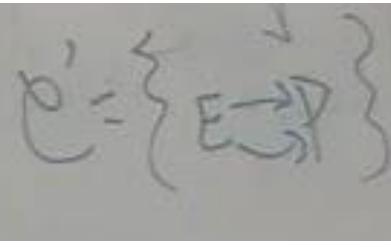
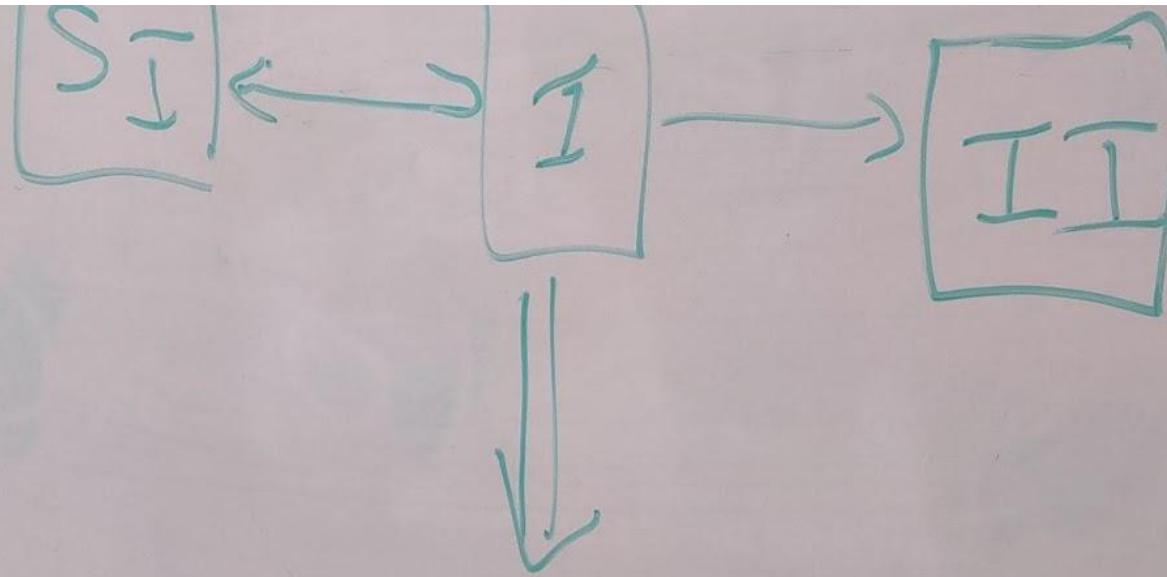
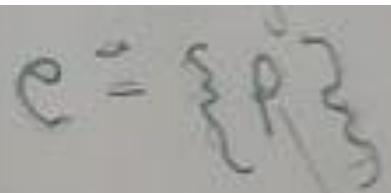
Migrating to Default Network Behaviour

Schema



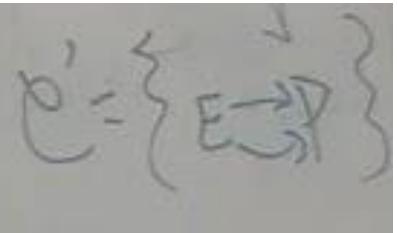
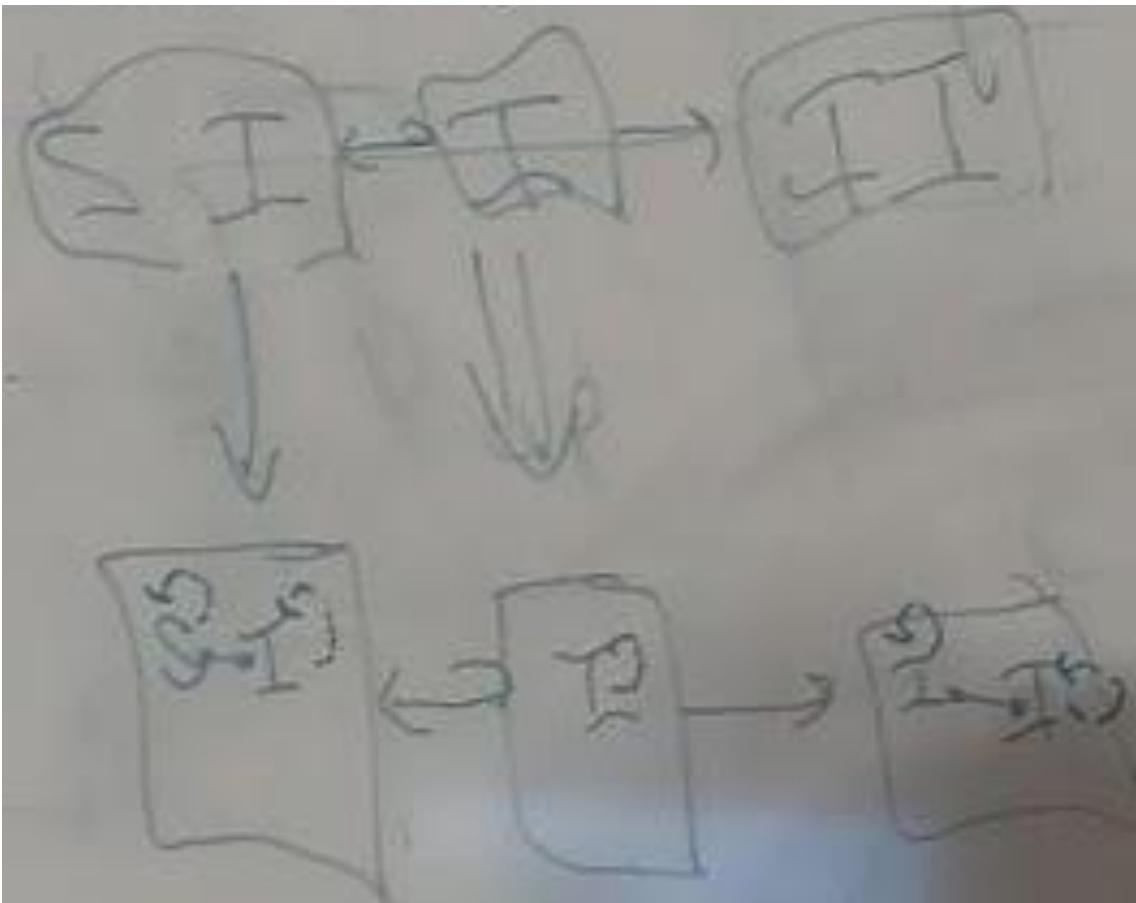
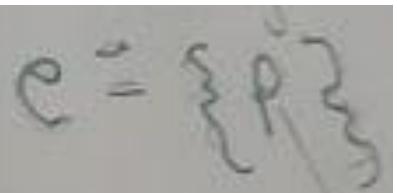
Schema

Logical Limits on Behaviour: Infeasible Migration

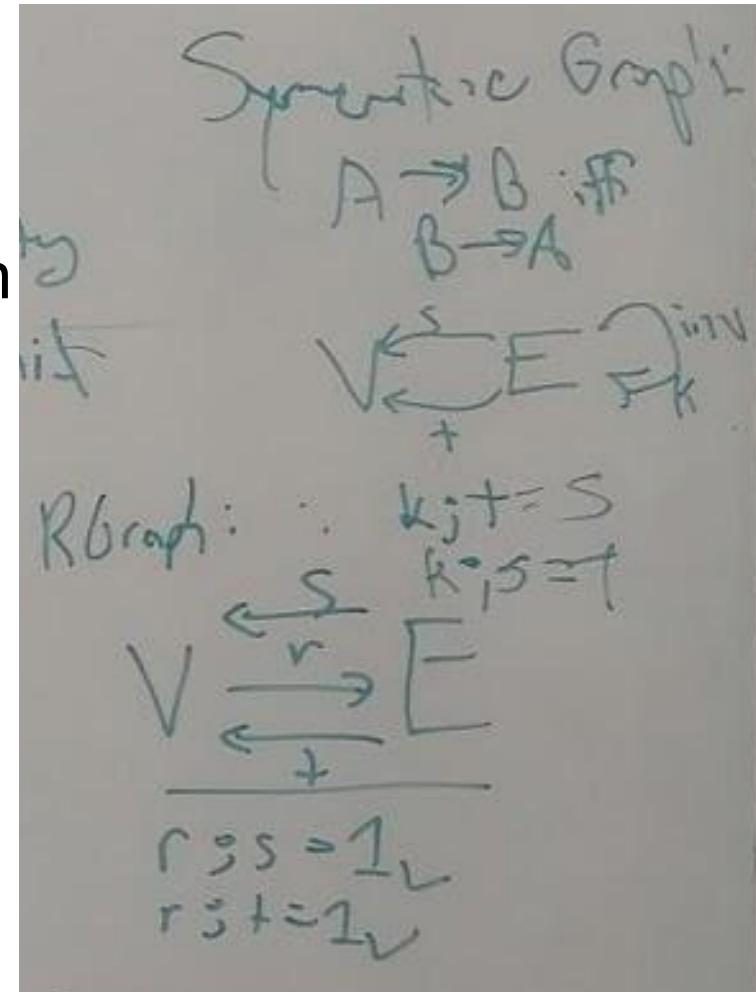


Schema

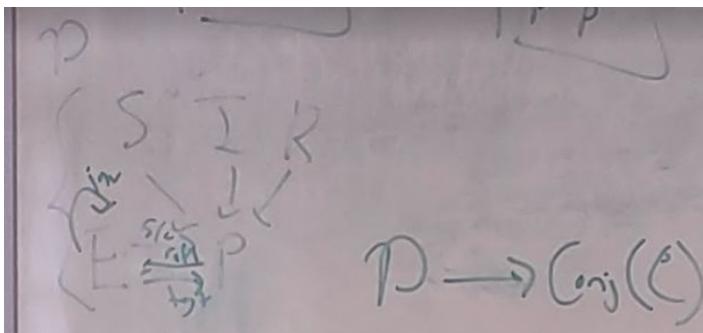
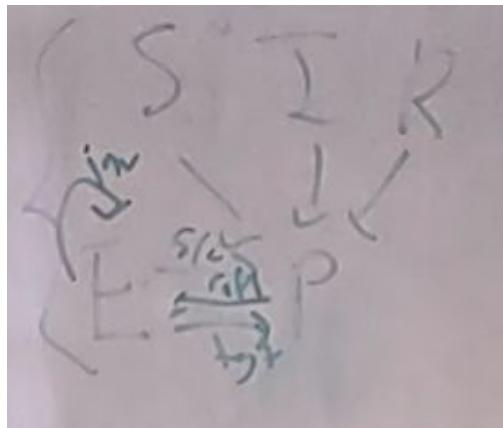
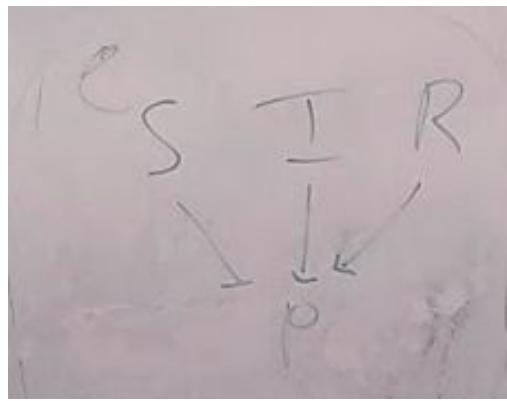
Logical Limits on Behaviour: Feasible Variant



Suggestion: Make what would otherwise be artefactual behaviour (and could be missed in rewriting patterns) standard, so that it is assured in all matches



Additional Detail



@partition DC begin

$P \Rightarrow P$

$E \rightarrow$ @product begin

$P_1 :: P$
 $P_2 :: P$

end

$Sr_C \Rightarrow P_1$

$Tg_C \Rightarrow P_2$

$inv \Rightarrow begin$

$I_1 \Rightarrow I_2$

$P_2 \Rightarrow P_1$

Sigma Migration Gives “Free” Migration

$\Sigma(\omega)$



$\Sigma(\omega) : \ell\text{-Set} \rightarrow \ell\text{-Set}$

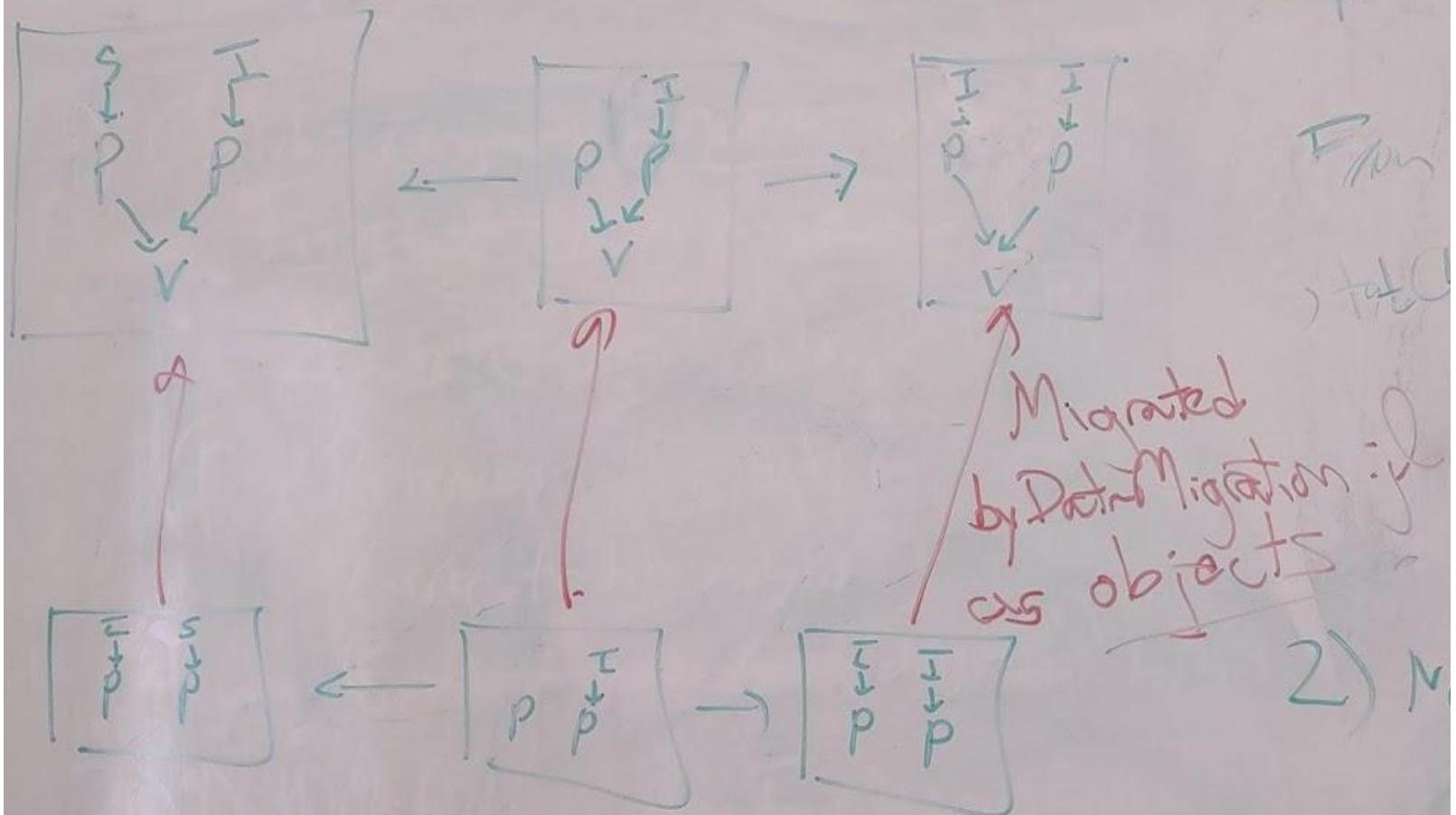
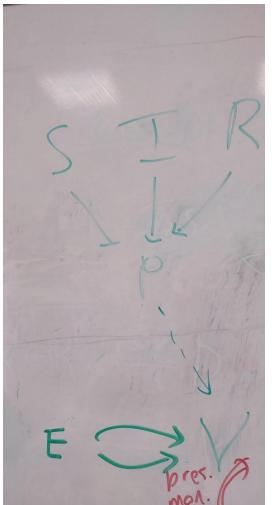
Gives n distinct copies of rep'table for P

Add what have to but no more

These are distinct unless fixed equal

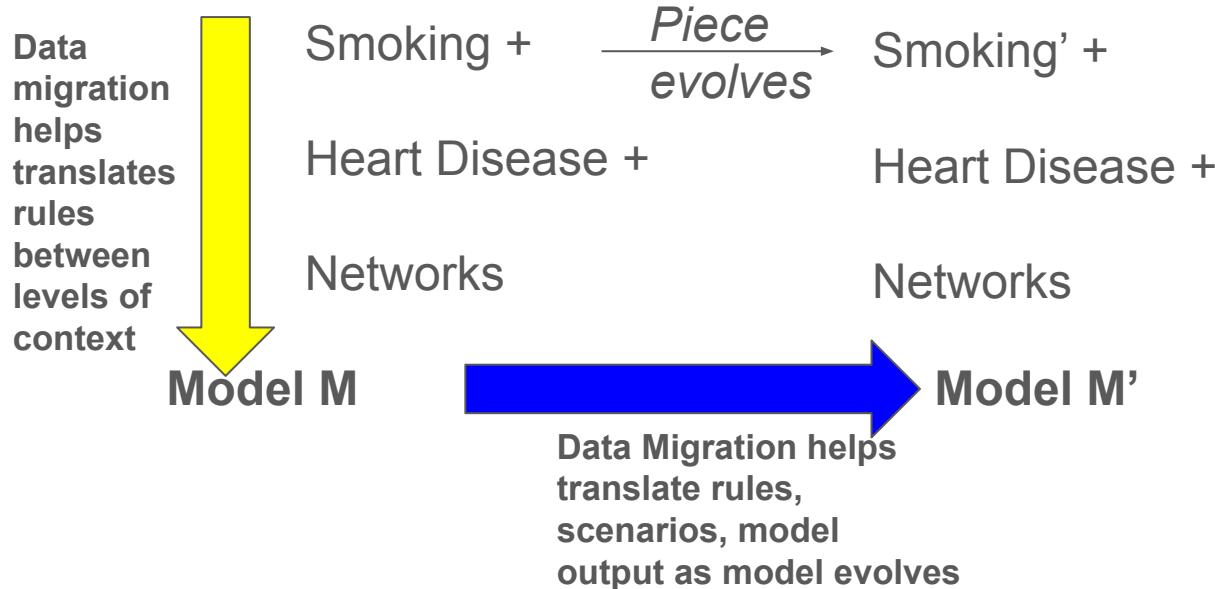
Migrating to Default Network Behaviour

Schema



Data Migration Supports Translation
Across Level of Model & Evolution of Model

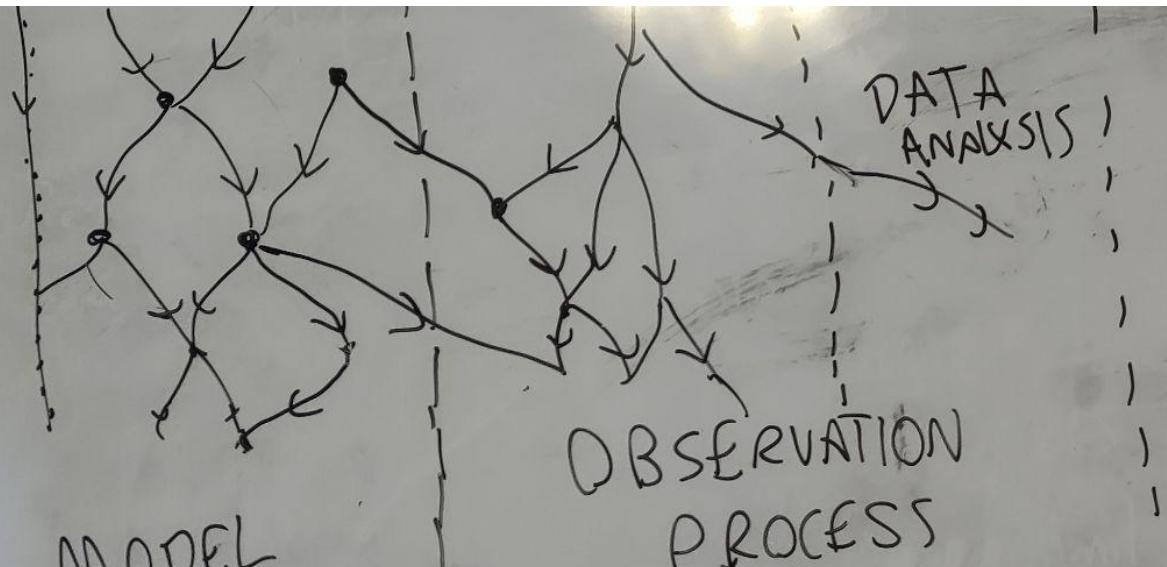
Data Migration Helps Translate with Model Context & Evolution



Observation Processes

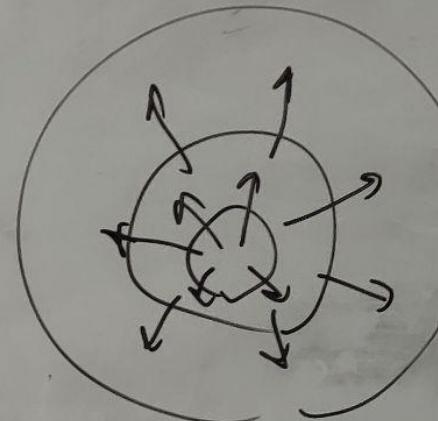
Observation Processes: Aggregation over the Population & Current State

Observation Processes Separated from Governing Processes



Characterization of
governing processes.

Characterized with a simpler
domain-specific language



Characterizing Observation Processes -- Desiderata

- Mathematically transparent
- Declarative
- Modular definition
- Modular use
- Per-run, user-specific enablement without model structure change
- Supports different levels of aggregation
- Supports summaries over time
- Evolves w/model structure (where possible, automatically)
- Affords staged computation
- Computationally efficient
- Accessible to non-modelers
- Exportable

Common Needs

- **Cross-sectional:** Summarizing model current state at varying levels of aggregation (including histogram by agent state in statechart)
- **Longitudinal:** Summarizing or more model events over time (potentially w/context), broken down by time interval

Common Structure to Capture

Both cross-sectional & longitudinal data

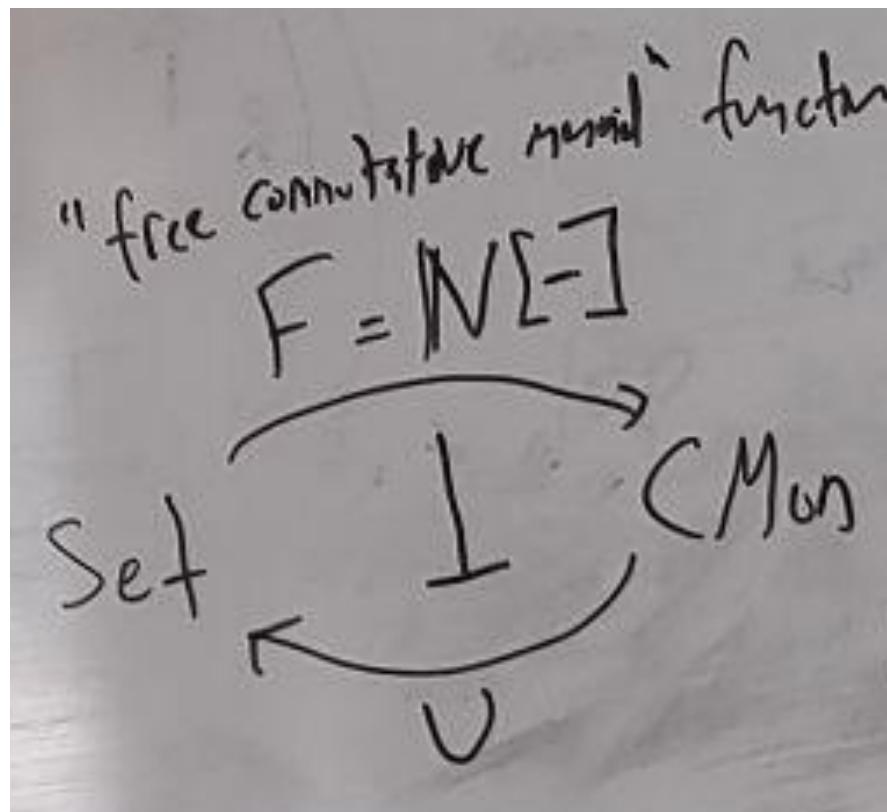
Longitudinal data

- Measurand
 - Operator
 - **Predicate measurand:** count, proportion
 - **Continuous measurand:** max/min, average, median, mode
 - Breakdown: support varying levels of aggregation
 - Subpopulation to consider
- Different time interval to consider

Optimizations

- Incremental computational of quantities
 - Incrementally counting number in state(s) by recording (discrete) in & out transitions (inflows and outflows) for such state(s)
- Hierarchical computation based on subpieces (exploiting topological structure)
 - subintervals of time (Computed per-day incidence contributes to computed per-week incidence)
 - subcategories of cross-tabulation breakdown

There is an adjunction between **Set** and Commutative Monoids



One example of the correspondence

$$\begin{array}{ccc} \mathbb{R} & \xrightarrow{\text{id}} & \mathcal{U}(\mathbb{R}, +) \quad \text{in Set} \\ \hline & \cong & \\ N[\mathbb{R}] & \xrightarrow{\text{id}^\#} & (\mathbb{R}, +) \quad \text{in } \text{CMon} \end{array}$$

Aggregation 1

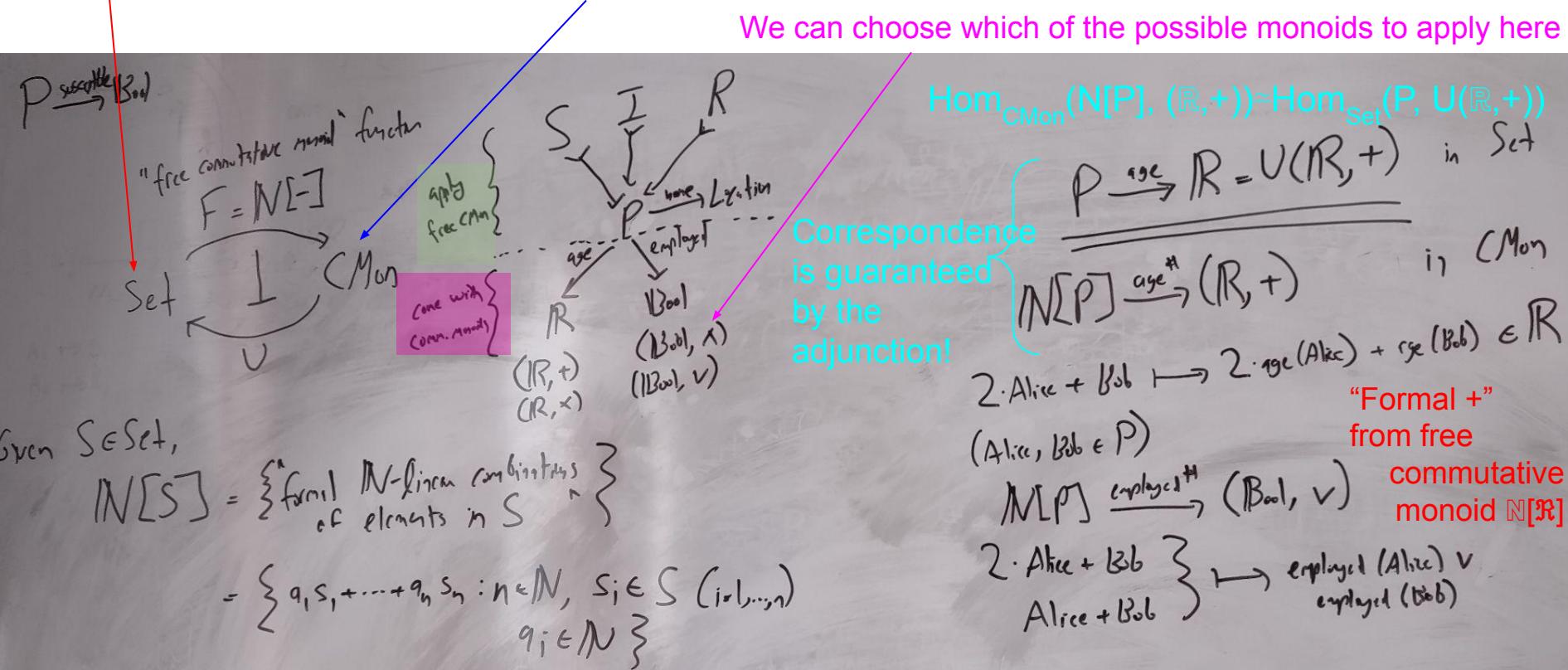
Objects are sets

Morphisms are functions

Objects are commutative monoids

Morphisms are monoid homomorphisms (preserving monoid structure)

We can choose which of the possible monoids to apply here



Adjunction Guarantees Natural Isomorphism

$N[City] \xrightarrow{\eta_{N[City]}} N[S] \xrightarrow{\epsilon_{N[S]}} N[Intervention]$ in \mathbf{CAlg}
is fully specified by $\{S\}$
 $City \rightarrow N[Intervention]$ in \mathbf{Set}

Because $\mathbb{N}[S]$ is a **Free** Monoidal Category, Maps out of it are Completely Determined by its Generators (Bases)

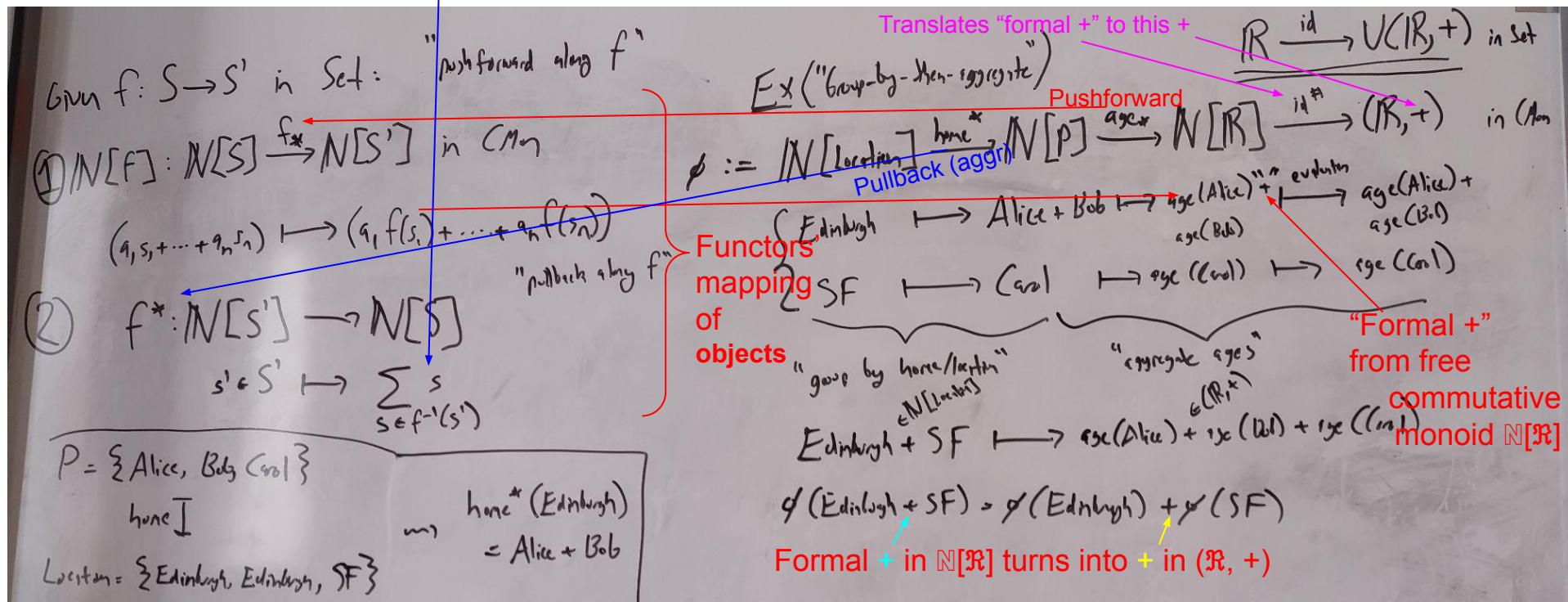
Determined by a map in \mathcal{M}

$$\mathbb{N}[C_i] \rightarrow \mathbb{N}[\text{Intents}] \quad \text{in } \mathcal{M}$$
$$Z_{NY} + S_{F} \quad \left\{ \begin{array}{l} \\ \\ \end{array} \right.$$
$$\text{City} \longrightarrow u(\mathbb{N}[\text{Intents}]) \quad \text{in } \text{Set}$$

SF

Aggregation 2: Functors from Morphisms

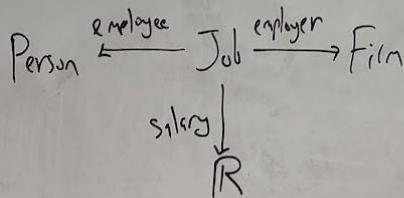
A key component of why this works is that, while in general, for element $s' \in S'$, $f^1(s')$ gives an **entire set**, the order in which these are inserted into is irrelevant, as $N[S]$ is a **commutative monoid**!



Another example: Counting via the Terminal Object

$$\begin{array}{ccc} \mathcal{F} = \mathbb{N}[-] & & \\ \downarrow & \nearrow & \\ \text{Set} & \perp & \subset \text{Mon} \end{array}$$

Dat:



$$\text{Person} = \{\text{Alice}, \text{Bob}, (\text{C}_0)\}$$

$$Job > \begin{cases} Alice_{-it} \\ Alice_{-it} \end{cases}$$

at each film:

$$N[\text{Firm}] \xrightarrow{\text{employer}^*} N[\text{Job}] \xrightarrow{\text{employee}} N[\text{Person}] \quad \text{in } \text{Obj}$$

↓
 $\text{Firm} \longrightarrow \bigcup(N[\text{Person}]) \quad \text{in } \text{Set}$

Ex (Counting)

The number of jobs held by each person: using $\text{Job} \rightarrow 1 = \{*\}$

$$\mathbb{N}[\text{Person}] \xrightarrow{\text{employee}^*} \mathbb{N}[\text{Job}] \xrightarrow{!} \mathbb{N}[1] \cong (\mathbb{N}, +)$$

Alice → Alice+!-ACME → * + * = 2 *

$$\mathcal{T}_{\text{ob}} > \begin{cases} \text{Alice} \rightarrow \text{-ACME}, \quad \text{Bob} \rightarrow \text{-ACME}, \\ \text{Alice} \rightarrow \text{-Uni.Ed.}, \quad \text{Carol} \rightarrow \text{-Uni.Ed.} \end{cases}$$

$$\text{Person} = \{\text{Alice}, \text{Bob}, \text{Carlo}\}$$

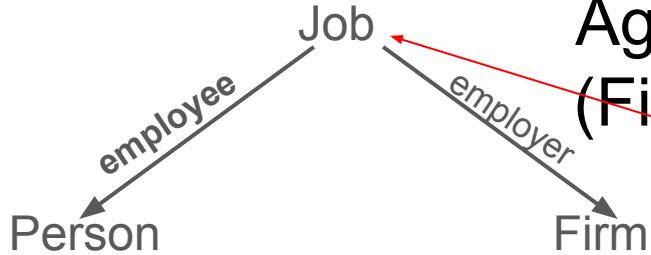
Firn = { ACME, Univ. Ed. }
, ICMS

Total number of firms: using $\text{Firm} \xrightarrow{!} 1$,

$$N[1] \xrightarrow{!^*} N[Film] \xrightarrow{!^*} N[1] \cong (N,+)$$

* \mapsto ACME + Univ. Edi \mapsto 3 *

Aggregation of Pairs of (Firm, Person) for Jobs



A span

Pushforward

$$f: \mathbb{J}_{\text{Job}} \rightarrow \mathbb{J}_{\text{Job}}^2$$

$$\mathbb{N}[\mathbb{J}_{\text{Job}}] \xrightarrow{f_*} \mathbb{N}[\mathbb{J}_{\text{Job}}^2]$$

$$j \mapsto f(j)$$

$$q_1 j_1 + \dots + q_n j_n \mapsto q_1 f(j_1) + \dots + q_n f(j_n)$$

Choose $f = \Delta_{\text{Job}}$
 $f(j) = (j, j)$

in CMon

Ex (Aggregation of pairs)

Find all employee-employer pairs (with multiplicity):

$$\mathbb{N}[1] \xrightarrow{!^*} \mathbb{N}[\mathbb{J}_{\text{Job}}] \xrightarrow{\Delta^*} \mathbb{N}[\mathbb{J}_{\text{Job}} \times \mathbb{J}_{\text{Job}}] \xrightarrow{(\text{employee} \times \text{employer})_*} \mathbb{N}[\text{Person} \times \text{Firm}]$$

(using $\text{Job} \xrightarrow{!} 1$)

(using diagonal map
 $\Delta: \mathbb{J}_{\text{Job}} \rightarrow \mathbb{J}_{\text{Job}} \times \mathbb{J}_{\text{Job}}$
 $j \mapsto (j, j)$)

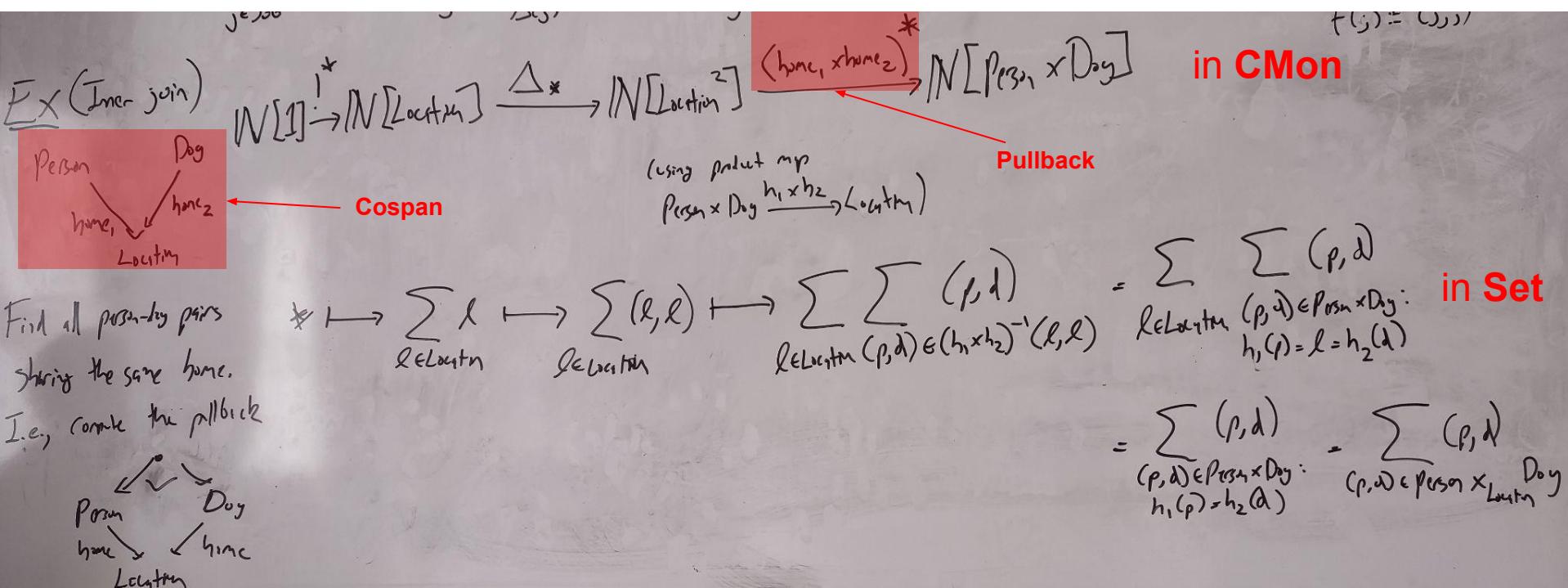
(using product
 $\text{employee} \times \text{employer}: \mathbb{J}_{\text{Job}}^2 \rightarrow \text{Person} \times \text{Firm}$)

$$* \mapsto \sum_{j \in \mathbb{J}_{\text{Job}}} j \mapsto \sum_{j \in \mathbb{J}_{\text{Job}}} (j, j) \mapsto \sum_{j \in \mathbb{J}_{\text{Job}}} (\text{employee}(j), \text{employer}(j))$$

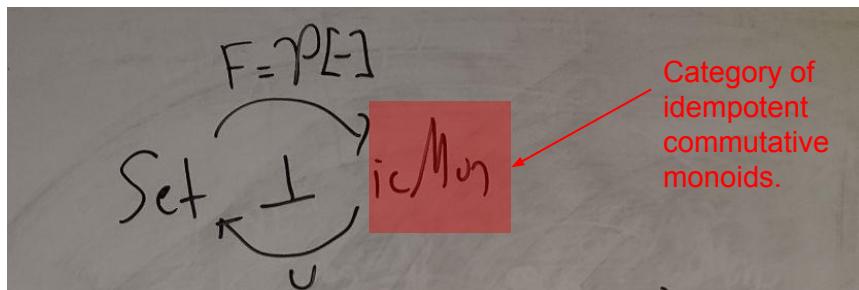
in Set

Inner Join Example: Persons & Dogs Sharing Same Home

Previous example featured a **span**; this features a **cspan** & is similar to a **conjunctive query**



Handling Commutative Idempotent Monoids: Case of (Set, \cup)



$\mathcal{P}[S] = (\text{powerset of } S, \cup_{\text{int}}, \emptyset)$

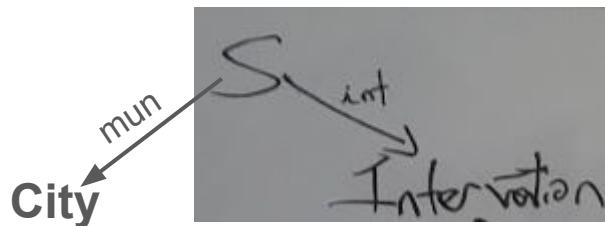
Given $f: S \rightarrow T$:

1) Pushforward:

$$f_*: \mathcal{P}[f]: \mathcal{P}[S] \rightarrow \mathcal{P}[T]
A \mapsto f(A) = \{f(s) : s \in A\}$$

2) Pullback:

$$f^*: f^{-1}: \mathcal{P}[T] \rightarrow \mathcal{P}[S]
B \subseteq T \mapsto f^{-1}(B) \subseteq S$$

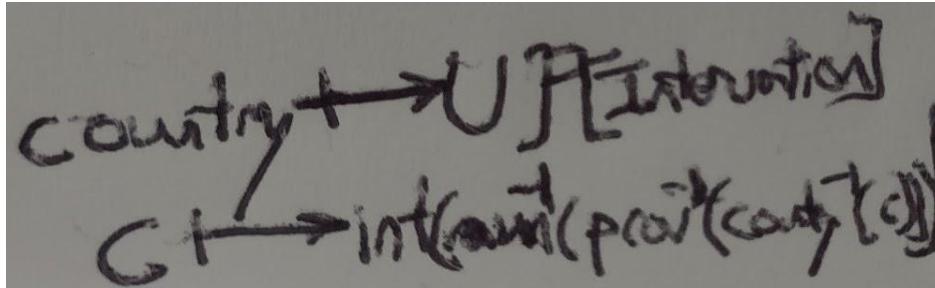
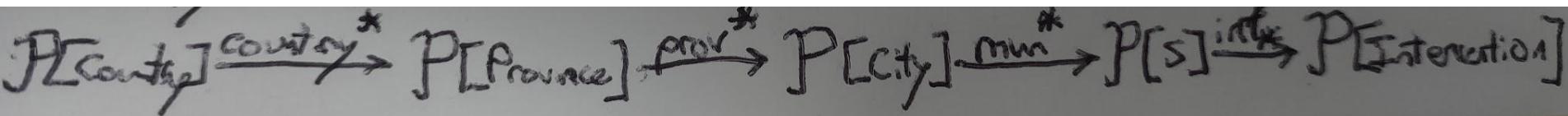
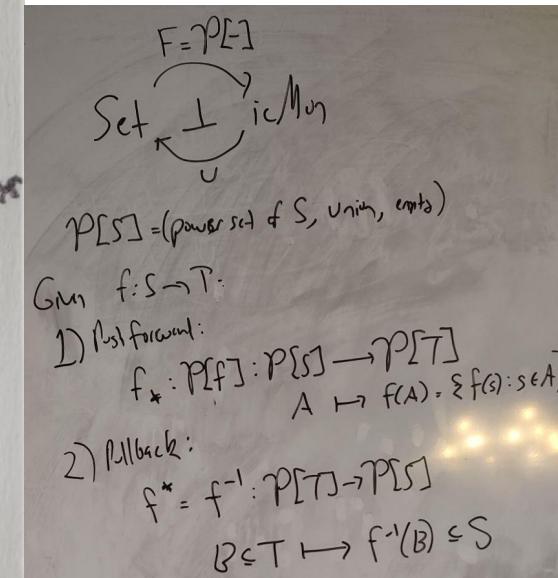
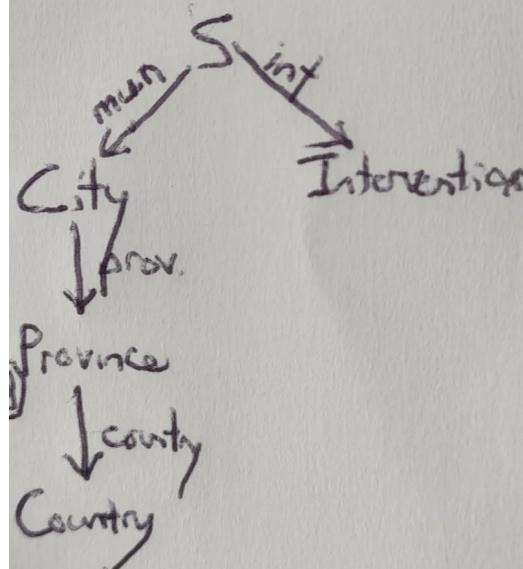


$$\mathcal{P}[\text{City}] \xrightarrow{\text{mun}^*} \mathcal{P}[S] \xrightarrow{\text{int}^*} \mathcal{P}[\text{Intervention}]$$

$$\text{City} \rightarrow \vee \mathcal{P}[\text{Intervention}]$$

$$c \mapsto \text{int}(\text{mun}^{-1}(c))$$

Multi-Level (Hierarchical) Aggregation



General Non-Commutative Monoids: \mathbf{Mon}

$$\begin{array}{ccc} \text{Set} & \xrightarrow{\quad F = \text{List}[-] \quad} & \text{Mon} \\ \downarrow \perp & \curvearrowright & \downarrow \perp \\ \text{List}(S) & \xrightarrow{\quad S \mapsto \underline{U(M, \cdot)} \quad} & \text{in } \text{Set} \\ & \Rightarrow & \\ & \text{String} & \xrightarrow{\quad \text{id} \quad} \underline{U(\text{String}, \cdot)} \quad \text{in } \text{Set} \\ & \text{List}(\text{String}) & \xrightarrow{\quad \text{id}^n = \text{concat} \quad} (\text{String}, \cdot) \quad \text{in } \text{Mon} \end{array}$$

A key problem is that, in general, for element $s' \in S'$, $f^{-1}(s')$ gives an **entire set**, and there is **no canonical ordering for those** -- and yet order matters for a **non-commutative monoid!**

$$s' \in S' \mapsto \sum_{s \in f^{-1}(s')} s$$

General Non-Commutative Monoids: \mathbf{Mon}

$$\text{Person} \xrightarrow{\text{name}} \text{String} \\ (\text{String}, \cdot)$$

$$\begin{array}{ccc} \text{Set} & \xrightarrow{\quad F = \text{List}[-] \quad} & \mathbf{Mon} \\ & \downarrow I & \leftarrow \text{in } \mathbf{Mon} \\ & & \end{array}$$

$$\begin{array}{ccc} S & \xrightarrow{\quad U(M, \cdot) \quad} & \text{in } \text{Set} \\ \underline{\text{List}(S)} & \longrightarrow & (M, \cdot) \quad \text{in } \mathbf{Mon} \end{array}$$

$$\Rightarrow \begin{array}{ccc} \text{String} & \xrightarrow{\quad id \quad} & U(\text{String}, \cdot) \\ \underline{\text{List}(\text{String})} & \xrightarrow{\quad id^n = \text{concat} \quad} & (\text{String}, \cdot) \quad \text{in } \mathbf{Mon} \end{array}$$

$(CMon \hookrightarrow M_{\text{Mon}})$ The category of commutative monoids is a subcategory of the category of monoids.

$$(N[R]) \xrightarrow{\text{Sort} \leq} \text{List}[R] \quad \underline{\text{not in } M_{\text{Mon}}}$$

$$\text{Sort}((1+c)+b) = [s, b, c]$$

$$\text{Sort}((1+c) \cdot \text{sort}(b)) = [1, c, b]$$

Handling of
Non-commutative monoids
requires more study

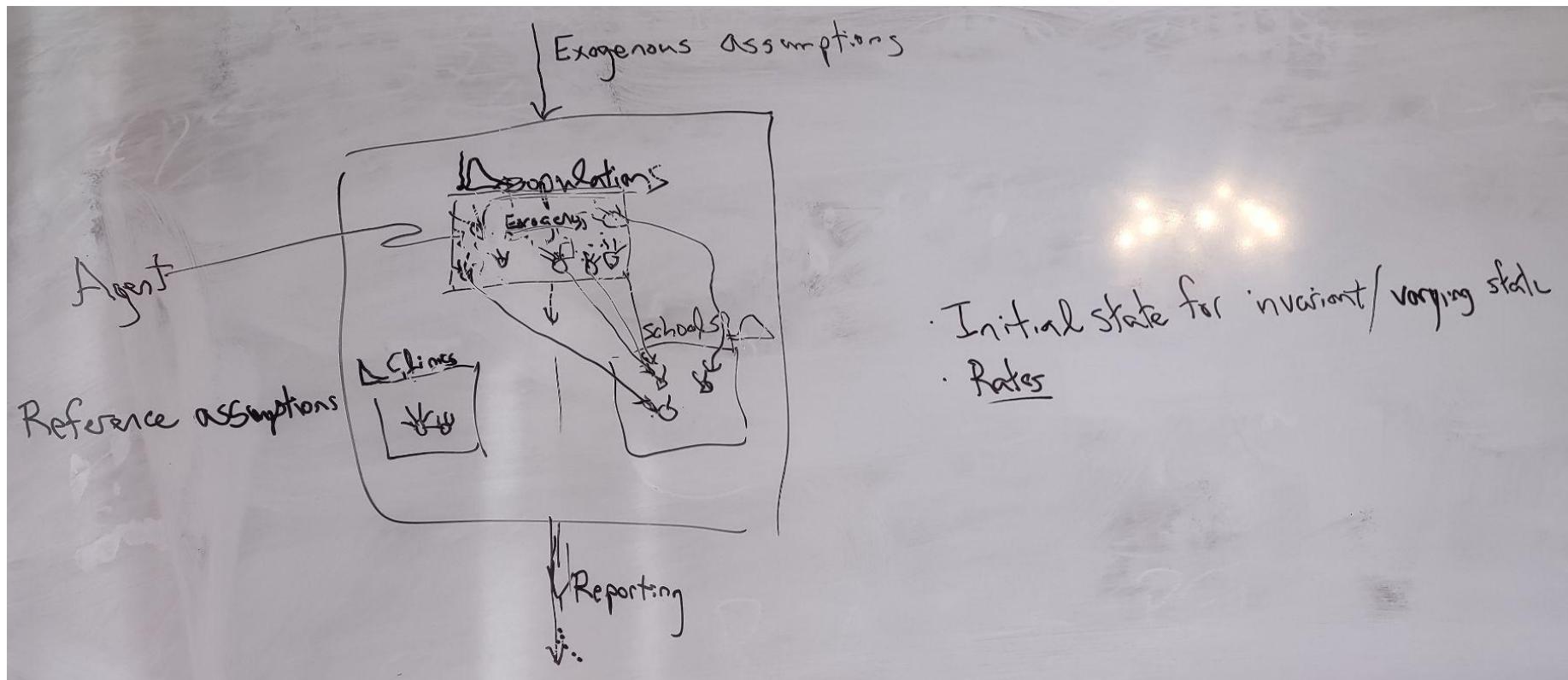
Observation & History Processes: Aggregation Over Time

Strategies for Time Aggregation

- Built-in knowledge of the nested nature of different timespans
- Instrumentation of rules via data migration functors to a schema augmented by
 - “counters” for the types of events
 - For non-counter events (e.g., log messages), attributes as needed to accrete the information
- Use of temporal sheaves to aggregate up such data over broader time periods
 - Ability to compute values for broader timespans from those for smaller, without being forced separately

Exogenous Assumptions

Capturing Exogenous Assumptions



- Initial state for invariant/varying scale
- Rates

Scenarios

Variety in Scenarios

Outputs considered: Model quantities vs. Scenario tradeoffs

- Simple scenario: Single set of exogenous assumptions
- Stochastic sensitivity ensemble: Many simulations of model with different stochastic realizations
- Scenario with randomly drawn initial state (network structure)
- Monte Carlo sensitivity: Draw designated parameters from specified distributions
- Optimization
 - "Parameter sweep": Systematic sensitivity analysis (deterministically vary parameter values)
 - N-way
 - Latin hypercube
 - Orthogonal array
 - Empirically informed scenarios
 - Calibrations
 - MCMC
 - ABC
 - Statistically filtering (PF, KF, PMCMC)
 - Structural sensitivity analysis

Distinguishing Two Distinct Notions of Hierarchy

- **In model specification:** Hierarchy use of exogenous assumptions: Scope & aggregation level at which model assumptions apply (across entire model, at level of population of agents, at level of a particular agent)
- **During model simulation:** Hierarchy in nesting of agents (e.g., family members are nested in a family context, nested in a neighbourhood, nested in a city, nested in a province, and in a country).
 - This may relate to run-time structures: There would seem to be a choice as to whether this is captured through nesting of structures at runtime vs. capturing inclusions via monomorphisms
 -

Duality Between (Model Assumptions & Behaviour) and (Model Behaviour & Model Observer Processes)

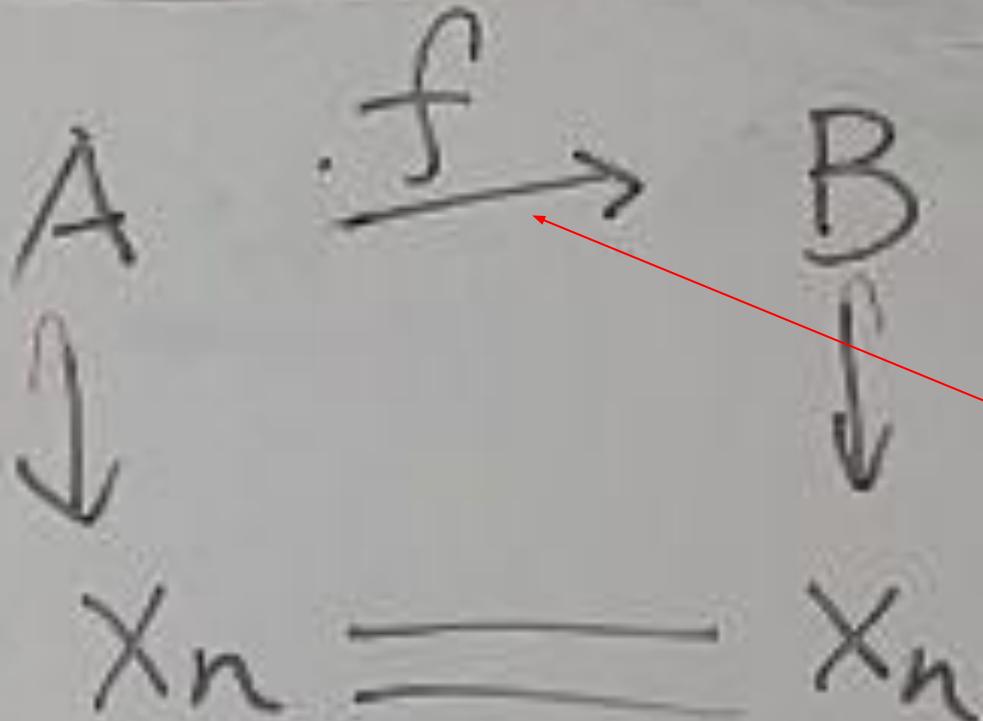
- Model exogenous assumptions affect but aren't shaped by governing behaviour of a model
- Epiphenomenal observation processes observe but don't modify governing behaviour of a model

Questions

- Could this be used for non-commutative (and, indeed, non-symmetric) monoids? (e.g., for string concatenation)?
- What is the mechanism to get back the pre-image (elements that map to each value via f)?

Wiring Diagrams & their Operators

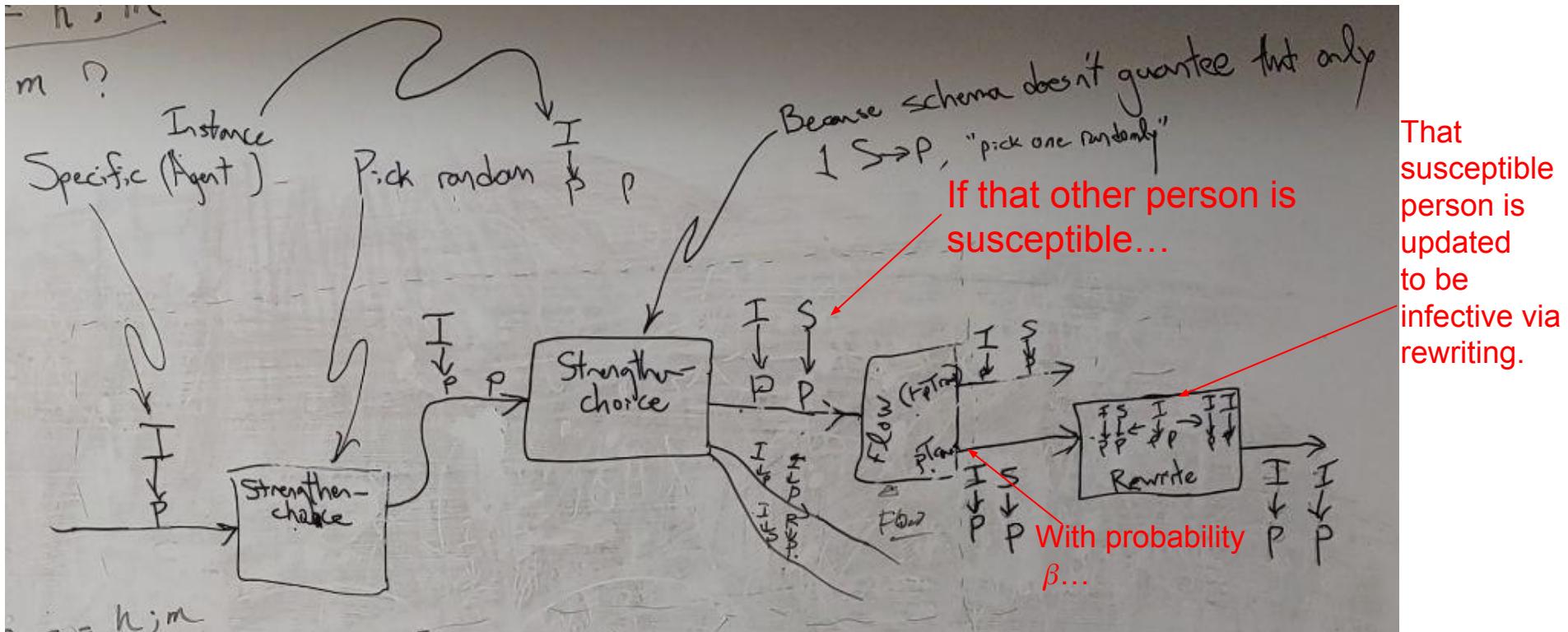
“Strengthen Choice” -- Get a (Randomly Chosen) Instance of this Pullback in X_n , Failing If Doesn’t Exist



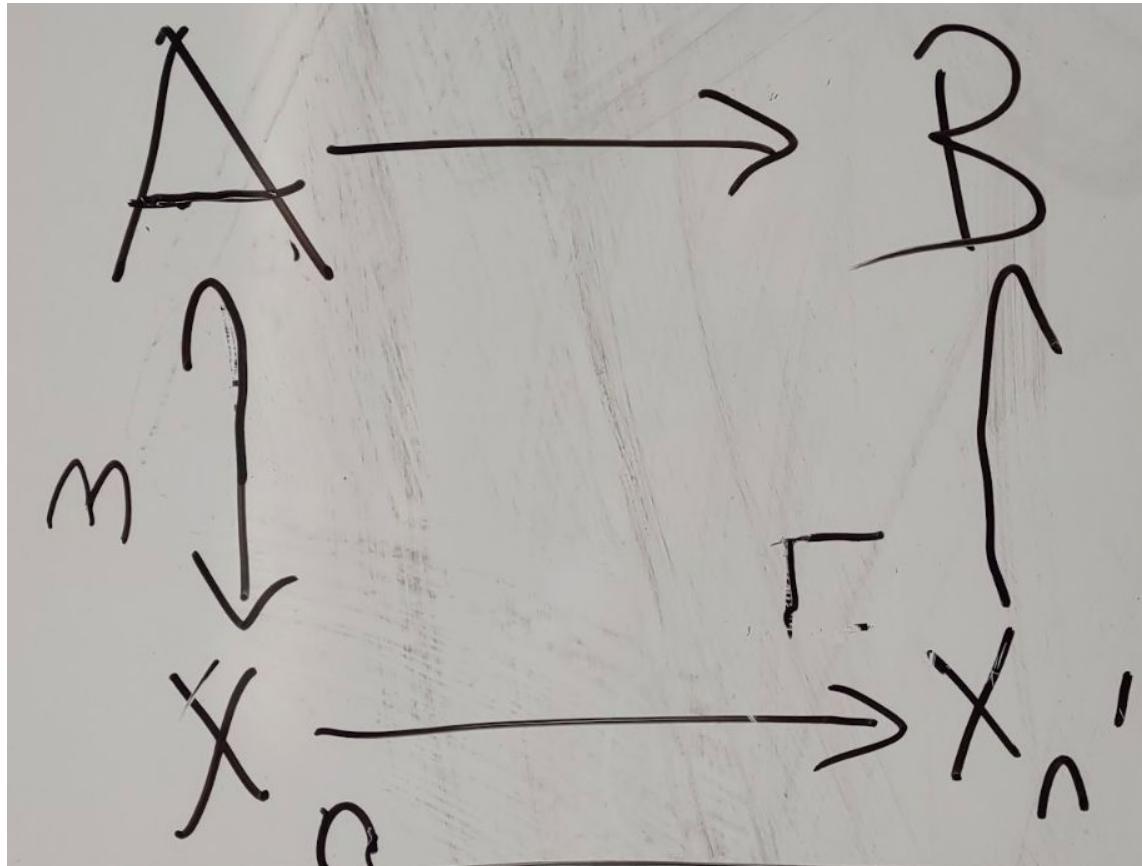
If $f: A \rightarrow B$.
If $\nexists B \hookrightarrow X_n$, “fail”, and we get A out
If $\exists! B \hookrightarrow X_n$, we have that
If \exists many $B \hookrightarrow X_n$, we choose one randomly

Remember that each morphism here is a C-Set homomorphism.

Capturing Random Mixing via Strengthen_Choice, Flow & Rewrite Blocks



“Strengthen Force” -- X_n , is the Result of the Pushout

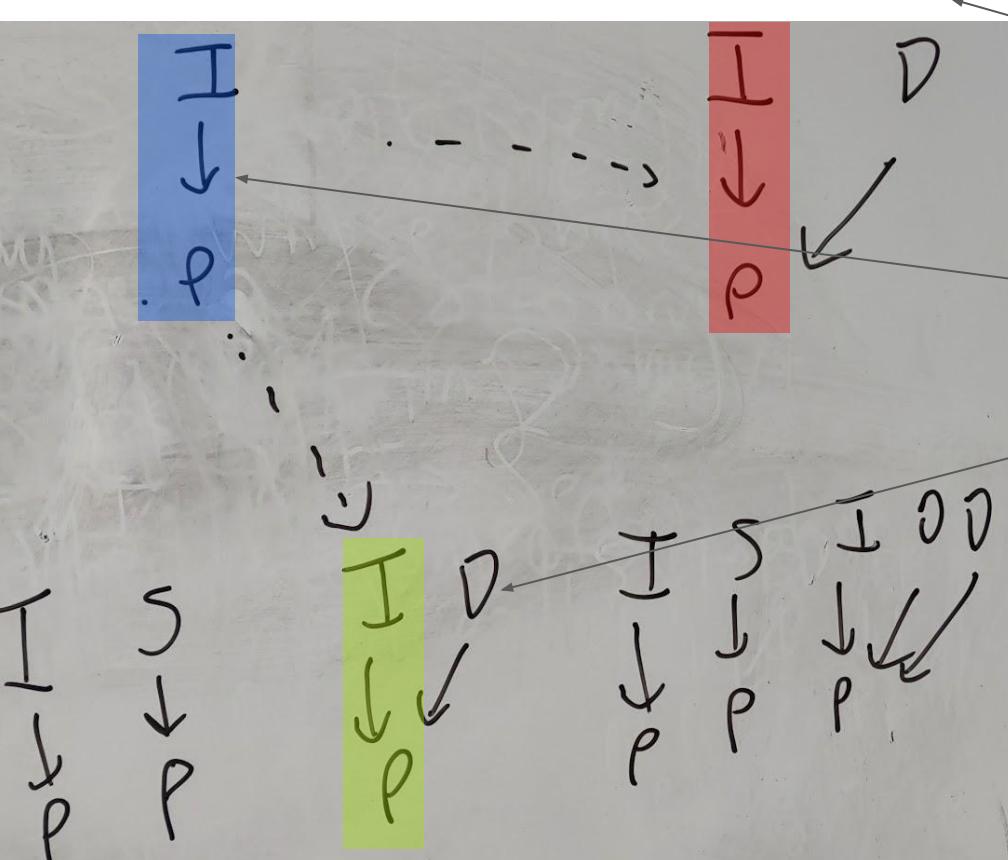


We glue X_n & B together at the image of A in each.

$X_n \rightarrow X_{n'}$ undergoes the same homomorphism seen in $A \rightarrow B$;

B in X_n is put in the same context as is A in X_n

Understanding Pushouts of CSets -- Take Pushout of the Image of the Match Hom and State X_t Fibered by the Match



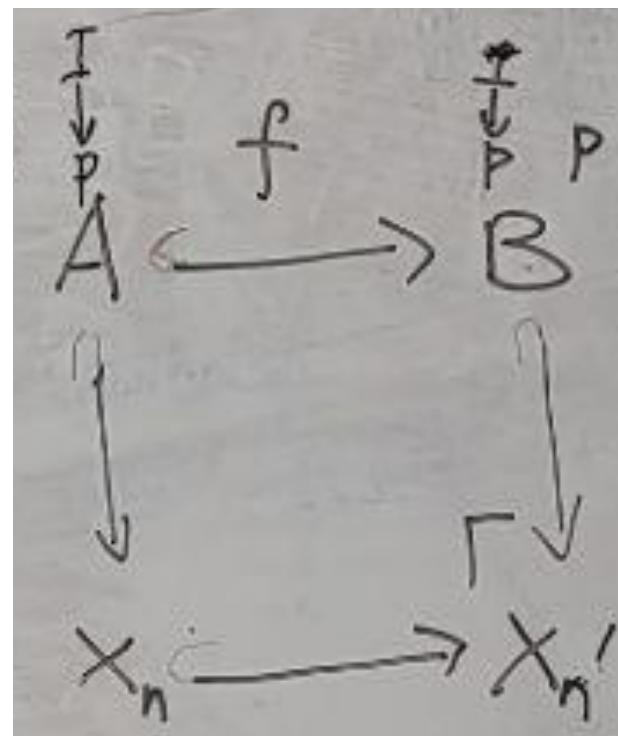
Even though have D in pattern B, and in X_n ,
because these are not in the homomorphism
~~match $I \rightarrow P$, get an addition of two dogs~~

We glue X_n & B together at the image of A in each.

$X_n \rightarrow X_{n'}$ undergoes the same homomorphism seen
in $A \rightarrow B$;

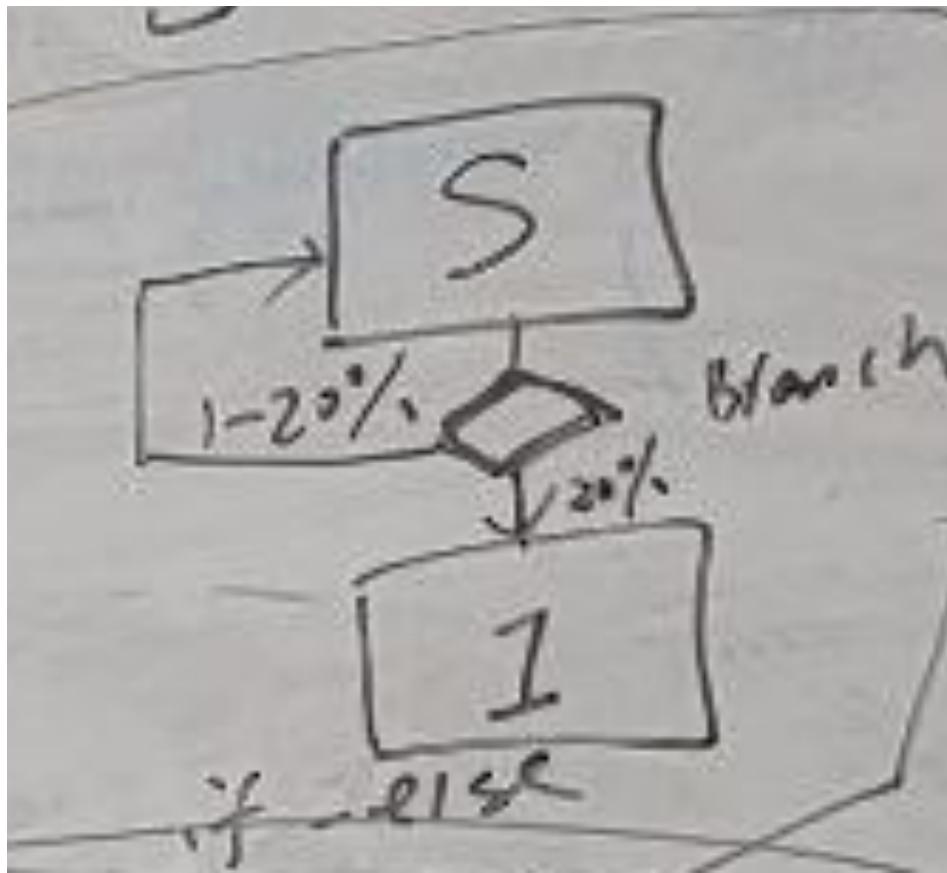
B in $X_{n'}$ is put in the same context as is A in X_n

“Strengthen Force”



If $f: A \rightarrow B$, then X_{n+1} contains $B + X_n$ glued around a common a ie.) with a as a common subspace

Capturing Branching Logic with a “Flow” Block



Forthcoming Theoretical Foci

Areas of Theory to be Further Elucidated

- Model composition
- Logically linked aspects of model inputs/outputs
 - Exogenous quantities/Parameters
 - Scenarios (single realizations, ensembles, sensitivity analyses, calibrations, optimizations, ABC, PF, PMCMC, etc.)
- Integration of numerical integration and occurrence of stochastic transitions
- Mapping to different semantics
- Handling stochastic differential equations (rather than strictly deterministic ODEs)
- Hierarchical models
- Clearer formulation of hybrid continuous/discrete interaction

Implementation: Key Mechanisms for Running

Central Implementation Abstractions

- ABM -- keeps rules (ABMRules), ABMFlows, index of names of ints
- ABMRule -- “A stochastic rewrite rule with a **dependent hazard rate**”
- AbsTimer & types thereof (including stateless, time-invariant AbsHazard, both continuous & discrete)
- AbsDynamics -- for ODEs
- ABMFlow
- Sampler
- PatternType (Regular, Empty, Representable)
- RuntimeABM -- the ABM runtime structures: current state & time, cum. events, sampler, rng, rule names=>int & ODE structures
- Traj

ABMRule -- Algebraic Rewriting Rule Plus Timer (Type)

```
"""
A stochastic rewrite rule with a dependent hazard rate

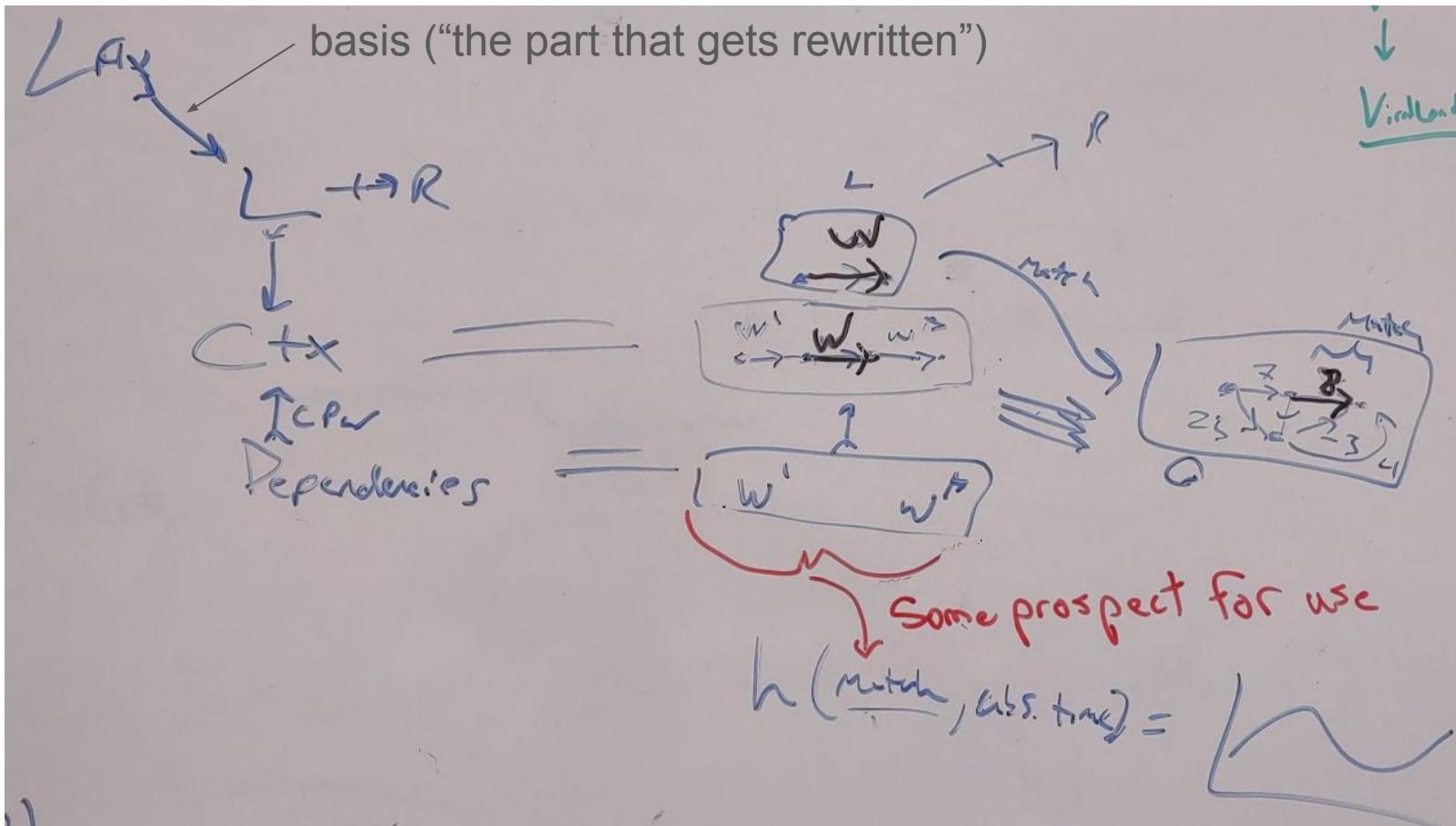
A basis is a subobject of the pattern of the rule for which we want a timer
per match. By default, the basis [] pattern map is just id(pattern).

NB: A "basis" corresponds to the map from "L_fix" in the Edinburgh discussions
(See "Lfix limits what Changes Are of Concern in Pattern Matching" in
AlgebraicABMs slides)

"""

@struct_hash_equal struct ABMRule
    rule::Rule
    timer::AbsTimer
    basis::Maybe{ACSetTransformation}
    name::Maybe{Symbol}
    pattern_type::PatternType
    ABMRule(r::Rule, t::AbsTimer; basis=nothing, name=nothing) =
        new(r, t, basis, name, pattern_type(r, is_exp(t)))
end
```

Extracting Further Information on Selected Dependencies



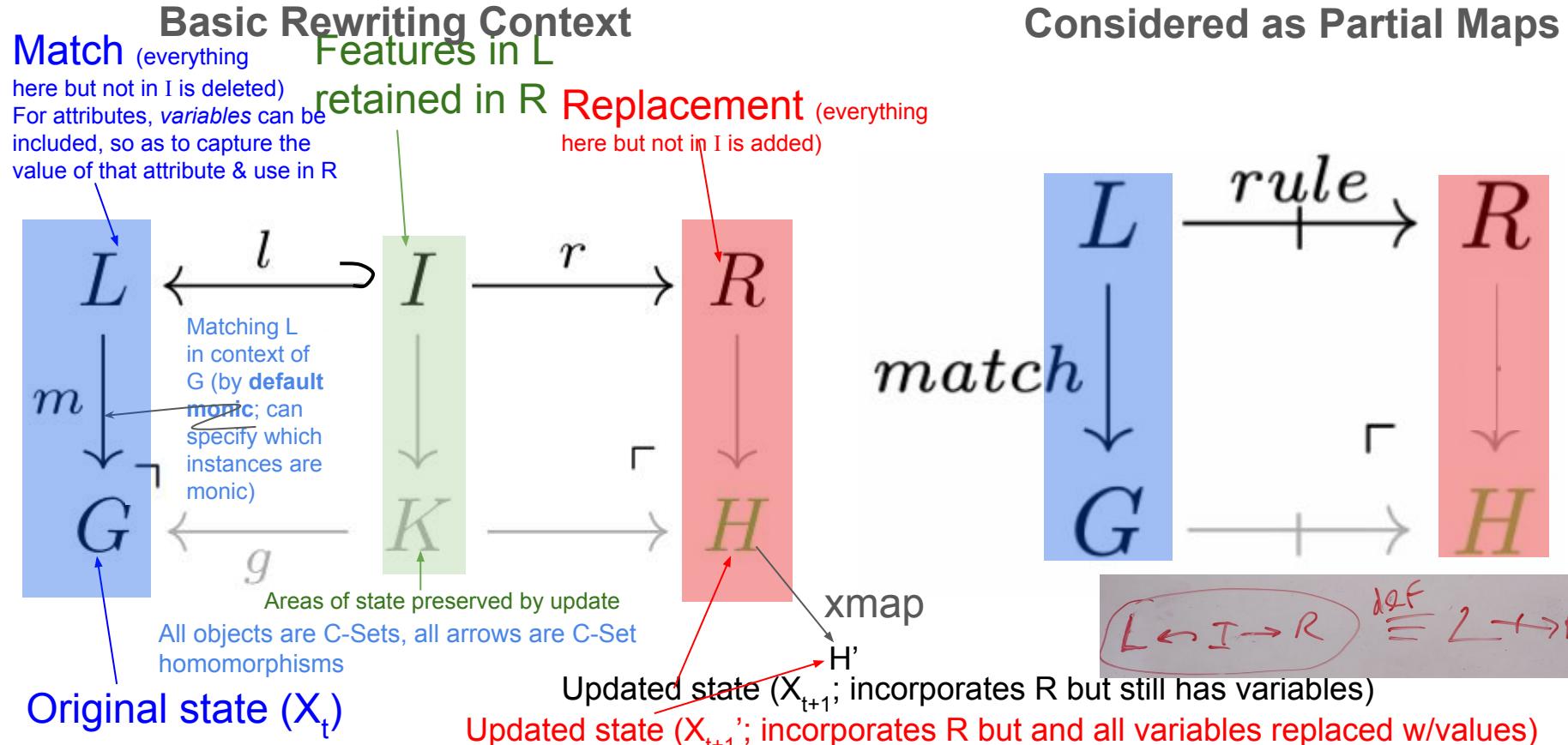
ABM -- Static Features of the Agent-Based Model

```
"""
An agent-based model.
"""
#*** Key structure for an ABM -- rules, continuous dynamics, names (what are these?)
#*** ASK: Are the names associated with the variables in the patterns in the rewrite rule?
@struct_hash_equal struct ABM
    rules::Vector{ABMRule}
    dyn::Vector{ABMFlow}
    #*** A map from the name of a rule to its index in "rules".
    names::Dict{Symbol, Int}
    function ABM(rules, dyn[])
        names = Dict(n=>i for (i,n) in enumerate(nameof.(rules)) if !isnothing(n))
        new(rules, dyn, names)
    end
end
end
```

Key Summary

- **ABM** keeps track of key static data structures (e.g., rules with timers [hazard rate generators])
- **RuntimeABM** keeps track of dynamic data structures (current state, time, scheduler) and initializes the state & event queue
- **Timers** provide ways of generating hazard rates&thus potentially draw an event time
- The `run!` function actually performs successive handling of events, and accumulating a trajectory (via the `Traj` structure) of output, calling `get_match` with the pattern type
- The **sampler** basically keeps track of events (each at a time drawn from a `hazardDistribution`, and identified merely by a key, which commonly relates them to a rule and then necessary information about them to process the event).
- **Coproducts of representables** provide key optimizations, because Yoneda Lemma lets us know how many we have at any one time, and instead of enqueueing a n corresponding rules for drawing a hazard & thus events, if we have a stateless, memoryless time invariant, rule `@rate λ`, we successively sample the first at rate $nλ$, and consider as coming from a random tuple of values from each representable.

Rewriting Rules Triggered via Hazard Rates



Images adapted from Brown, K., Patterson, E., Hanks, T. and Fairbanks, J., 2022. Computational Category-Theoretic Rewriting. In International Conference on Graph Transformation (pp. 155-172). Springer, Cham. <https://arxiv.org/pdf/2111.03784.pdf>

Underlying Rewriting Mechanisms -- Match & Schedule

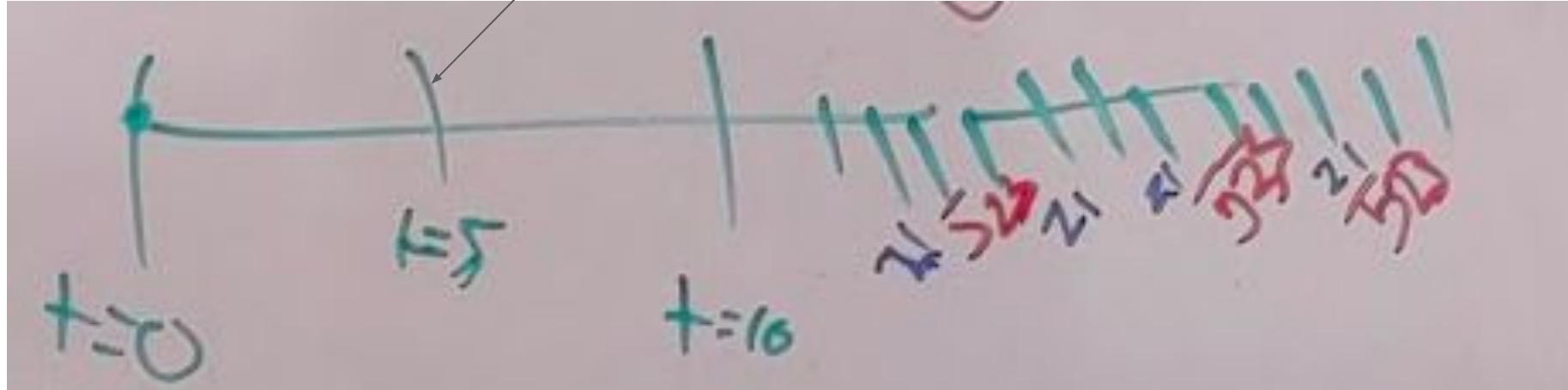
- Especially because there is no notion of “each agent” needing updates, we need to **match** pattern to find situations that can trigger dynamics via matching (e.g., that an agent is in a given state)
- These situations do not generally need to fire immediately -- for example, if an agent has entered a state; it could exhibits a hazard rate or timeout transition for leaving
- Using hazard rates (not PDF) lets us adjust firing rate as state evolves
- [General case] For *state-dependent* events (hazard rates), we avoid **ongoing** need to reschedule by incrementally computing Bernoulli draws for the probability of firing, for a certain timestep
- For *state-independent* hazard, we **schedule** trigger, Check if match still applies when fires
- By default, if match still remains after rewriting, create new event in the schedule
 - A key exception -- when leaving state in a statechart (know that won’t match again)

Hybrid (Static-Dynamic) Scheduling

The Supporting Role of an Event Schedule (Queue)

- **Model state independent timing:** Pre-scheduled (both memoryless & memoryful)
- **Timing dependent on Model state:** Events whose scheduling is state dependent
- Regardless of type, scheduled events can be descheduled if they are preempted eg
 - Agent dies
 - Agent leaves because of matching a different pattern

Event is associated with a “key” uniquely identifying it (e.g., rule id and any required information on the particular morphism m with which it is associated). The timing is determined by a draw from a function giving the hazard rate (?).



Functions

- **pattern_type** -- determine type of a pattern (currently, EmptyP, RegularP, RepresentableP)
- **get_hazard** -- gets the hazard for a pattern, returning a UnivariateDistribution. Note that this includes taking into account the faster sampling for state-independent, memoryless, time-invariant coproducts of representables
- **get_match** -- gets a match for the given pattern type and event information (schedule key). This handles any basis (L_{fix}), and can draw randomly from matches for representables
- **pops!(rt::RuntimeABM)** -- “Pop the next random event, advance the clock”
- **run!**

Key Competing Clocks Functions

- For a sampler, competing clocks maintains a set of events
- **enable!(sampler, key, hazardDistr, ?, ?, rng)**: Creates an event with a draw from that key
- **next(sampler, tnow, rng)**: Gets the next event (pure function -- no change to queue)
- **disable!(sampler, key, time)**: simply delete something from the queue
- **transition_entry** -- dictionary (maps from key to an Int used in a queue); useful for asking if this haskey of a key

Helper functions in [Upstream.jl](#)

- **pops!(sampler, rng, time)**: collates all events from the queue occurring at the next time, deletes such events (via pop!) and returns pair of next time & vector of the keys at that time
- **pop!(sampler, rng, time)**: gets & deletes first event from the queue via calling next & disable! in competing clocks, and returns pair of next time and that event's key (defined in [Upstream.jl](#))

Rewrites

- Multiple events (and thus rewrites) at specific points in time have to superimpose their effects, which they do so through pullback mechanisms together with composition
-

Major Concepts

```
"""
An agent-based model.
"""
#*** Key structure for an ABM -- rules, continuous dynamics, names (what are these?)
#*** ASK: Are the names associated with the variables in the patterns in the rewrite rule?
@struct_hash_equal struct ABM
    rules::Vector{ABMRule}
    dyn::Vector{ABMFlow}
    #*** A map from the name of a rule to its index in "rules".
    names::Dict{Symbol, Int}
    function ABM(rules, dyn[])
        names = Dict(n=>i for (i,n) in enumerate(nameof.(rules)) if !isnothing(n))
        new(rules, dyn, names)
    end
end
end
```

Representation of Current State of ABM

```
@struct_hash_equal struct ABM
    rules::Vector{ABMRule}
    dyn::Vector{ABMFlow}
    ABM(rules, dyn=[]) = new(rules, dyn)
end
```

NB: *clocks* is
always in 1-to-1
correspondence with
abm.rules.

```
"""
Data @struct_hash_equal structure for maintaining simulation information while running an ABM
"""

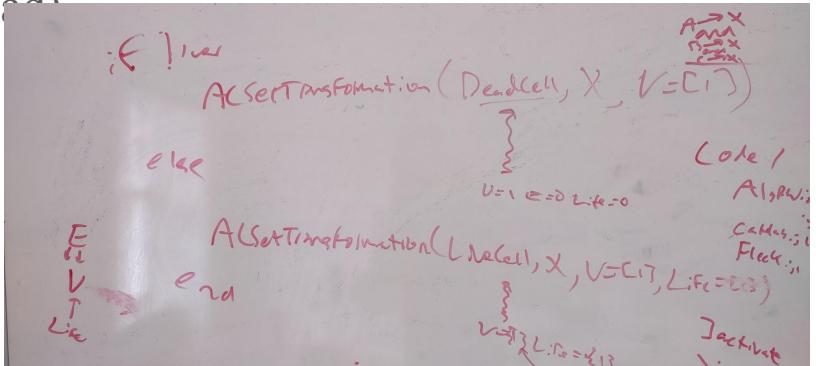
mutable struct RuntimeABM
    state::ACSet
    const clocks::Vector{AbsHomSet}
    tnow::Float64
    nevent::Int
    const sampler::SSA # stochastic simulation algorithm
    const rng::Distributions.AbstractRNG
    function RuntimeABM(abm::ABM, init::T; sampler=default_sampler) where T<:ACSet
        rt = new(init, init_homset.(abm.rules, Ref(init), Ref(additions(abm))),
                0., 0, sampler(), Random.RandomDevice())
        for (i, homset) in enumerate(rt.clocks)
            kv = homset isa ExplicitHomSet ? pairs(homset) : [nothing => create(init)]
            for (key, val) in kv
                haz = get_hazard(val, 0., abm.rules[i].timer)
                enable!(rt.sampler, i => key, haz, 0., 0., rt.rng)
            end
        end
        rt
    end
end
```

```

"""Create a context of n living neighbors for either a dead or alive cell"""
function living_neighbors(n::Int; alive=true)::ACSetTransformation
    X = LifeState(1)
    alive && add_part!(X, :Life, live=1)
    for v in 1:n
        v = add_part!(X, :V)
        add_part!(X, :Life, live=v)
        add_edge!(X, v, 1)
    end
    homomorphism(alive ? LiveCell : DeadCell, X; initial=(v=[1],))
end;

```

- we have a central cell (as created by `LifeState(1)`)
- We create n living neighbours of this central cell, each marked live and with an edge going to it from the central cell
- Because this is used in a morphism $L \leftarrow I$, we have to return an `ACSetTransformation` from I (given as `live` or `dead`)
- The last line is essentially equivalent to this:
`initial` basically constrains the map to ensure that we are making the morphism to the central cell



Trajectories of Event-Vectors and the $X_t + X_{t'}$ ACSets

The apex is the span the K in the match, but rather unimportant

```
A trajectory of an ABM: each event time and result of `save`.  
"""  
@struct _hash_equal struct Traj  
    init::ACSet  
    events::Vector{Tuple{Float64, Int, Any}}  
    hist::Vector{Span{<:ACSet}}  
end  
  
Traj(x::ACSet) = Traj(x, Pair{Float64, Any}[], Span{ACSet}[])  
  
function Base.push!(t::Traj, τ::Float64, rule::Int, v::Any, sp::Span{<:ACSet})  
    push!(t.events, (τ, rule, v))  
    isempty(t.hist) || codom(left(sp)) == codom(right(last(t.hist))) || error(  
        "Bad history\n$(codom(left(sp)))\n!=\n$(right(last(t.hist))))"  
    )  
    push!(t.hist, sp)  
end
```

Running the ABM

```
function run!(abm::ABM, rt::RuntimeABM, output::Traj;
    save=deepcopy, maxevent=MAXEVENT, maxtime=Inf)

    # Helper functions that automatically incorporate the runtime `rt`
    log!(rule::Int, sp::Span) = push!(output, rt.tnow, rule, save(rt.state), sp)
    disable = disable!(rt.sampler, key, rt.tnow)
    disable = disable
    function enable
        haz = get_hazard(m, rt.tnow, abm.rules[rule].timer)
        enable!(rt.sampler, rule => key, haz, rt.tnow, rt.tnow, rt.rng)
    end

    # Main loop
    while rt.nevent < maxevent && rt.tnow < maxtime
        # get next event + update clock time
        which = next(rt)

        if isnothing(which)
            @info "Stochastic scheduling algorithm ran out of events"
            return output
        end

        # Unpack data associated with the current event
        event::Int, key::Maybe{KeyType} = which
        rule::ABMRule, clocks::AbsHomSet = abm.rules[event], rt.clocks[event]
        rule_type::Symbol = ruletype(rule) # DPO, SPO, etc.
```

Updating after each update while handling simultaneous updates

NB: Despite superficial similarity,
this is not itself depicting a rewrite rule!

If nothing in Pat is deleted when transitioning $G_t \rightarrow G_{t+\frac{1}{2}}$ by **previous simultaneous rule**, then

have $m_{t+\frac{1}{2}} = \text{pull_back}(\ell, m_t) \circ r$

Otherwise, there is no hom of Pat into the apex

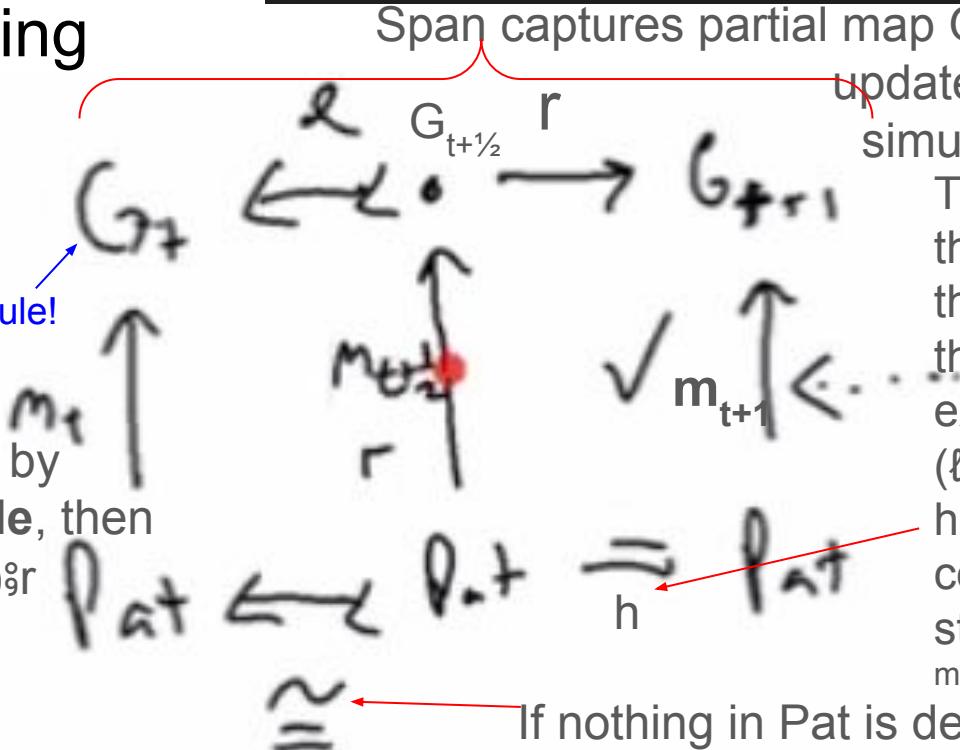
$$\text{pull_back}(\ell, m_t) = \text{not } m \text{ or } m_{t+\frac{1}{2}}$$

```
# bring the match 'up to speed' given the previous (simultaneous) updates
for (l, r) in first.(update_data)
    m = pull_back(l, m) □ r
end
```

Span captures partial map $G_t \rightsquigarrow G_{t+1}$ after updates by series of simultaneous rules

This is the match that we seek to the match AFTER this previous executed rule (ℓ, r) . B/c

h is id & square commutes, if Pat still \exists after (ℓ, r) , $m_{t+1} = \text{pull_back}(\ell, m_t) \circ r$



If nothing in Pat is deleted when transitioning $G_t \rightarrow G_{t+1}$, then this monic arrow will be an isomorphism, otherwise, it will not be

Recall: For Representables, we Count the “Parts”

What is the notion of the “parts” here is a general notion for CSets (not just representables); this is the same notion as add_part! for CSets; each element of the Set mapped to y an object in the schema is termed a “representable”. For representables, there is one main “Driver” for the representable; the others follow through from that -- for example, might have the representable for “ E ”, where object “ E ” maps to a set of size 1; others then follow of necessity from this (due to naturality). KB notes that for representables, often the Set for the “driver” of the representable only has a single element, but not always -- consider the case of reflexive graphs, where the “driver” has 3 elements.

```
"""
A pattern match from a coproduct of representables is just a choice of parts
in the codomain. E.g. matching L = •→• •• is just a random choice of edge and
two random vertices.

The vector of ints refers to parts of L which are the counits of the left kan
extensions that define the representables (usually this is just wherever the
colimit leg sends 1, as there is often just one X part in the representable X).

WARNING: this is only viable if the timer associated with the rewrite rule is
symmteric with respect to the disjoint representables and has a simple
exponential timer.
"""

@struct_hash_equal struct RepresentableP <: PatternType
| parts::Dict{Symbol, Vector{Int}}
end
```

```
m = get_match(pattern_type(rule), pattern(rule), rt.state, clocks, key;  
            basis=basis(rule))
```

Ideas for Future Work

Ideas for Dimensional Quantities

- Derive units when calculating aggregate totals
- Ensure dimensional consistency when calculating
 - Stock & flow models
 - Observables (when totalling up, has to be consistent)
 - Hazard rates (here, know needs to be dimension 1/Time)
 - Conditionals (e.g., for branches in statecharts)
- For Petri Nets, rates
- For observables: When know units, could ask for automatic conversion between units (e.g., report in per month values)
- When comparing output
- Dimensional consistency supported for parameters

Questions

Questions

- This doesn't have {SchLifeGraph} in part because in terms of syntax, it is a macro being applied, not a type being declared directly with this line `@acset_type`

```
LifeState(SchLifeGraph) <: AbstractSymmetricGraph;
```

Questions

E
L
T
Life

- The game of life has the following schema, specifying cell information
- This creates a dead cell: `const DeadCell = LifeState(1) # a single dead cell` because we just have a cell where we have only a vertex (as specified by the argument “1”, due to a constructor for graphs that uses the only integer argument for the size of V).
- We thus get $V=[1]$, $\text{Life}=\emptyset$, and $\text{Hom}(V, \text{Life}) = \emptyset$
- By contrast, we have

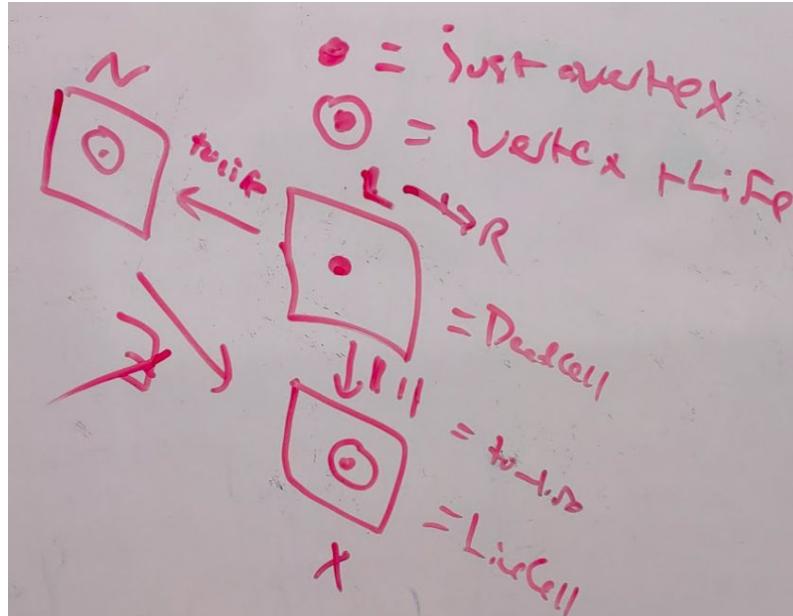
```
const LiveCell = @acset LifeState begin V=1; Life=1; live=1 end # a single living cell
```

and thus $V=[1]$, $\text{Life}=[1]$, and $\text{Hom}(V, \text{Life}) = 1 \mapsto 1$

A Required Application Condition

- This needs the last application condition:
- To ensure that “DeadCell” doesn’t simply match the “empty” part of a “LiveCell”, that is, we want to ensure that:

```
# A cell is born iff it has three living neighbors
birth = TickRule(id(DeadCell), to_life;
                  ac=[PAC(living_neighbors(3; alive=false)),
                      NAC(living_neighbors(4; alive=false)),
                      NAC(to_life)]);
```



Questions

- this creates a dead cell, because for graphs (from whose schema this schema is derived), we have a special constructor that can take just an integer, and create a graph with a single vertex. This creates a cell with just a vertex, and empty “Life”

```
const DeadCell = LifeState(1) # a single dead cell
```

- Meaning of “initial” here: homomorphism(alive ? LiveCell : DeadCell, x; initial=(v=[1],))
- Why does this have the last application condition:

```
129 |  
130 | # Create an initial state  
131 | G = make_grid([1 0 1 0 1;  
132 |           0 1 0 1 0;  
133 |           0 1 0 1 0;  
134 |           1 0 1 0 1;  
135 |           1 0 1 0 1])  
136 | view_life(G);  
137 | G = make_grid(ones(1,1))  
138 | # Run the model  
139 | res = run!(AddCoords(GoL), G; maxevent=2);  
140 |
```

```
# A cell is born iff it has three living neighbors  
birth = TickRule(id(DeadCell), to_life;  
                  ac=[PAC(living_neighbors(3; alive=false)),  
                        NAC(living_neighbors(4; alive=false)),  
                        NAC(to_life)]);
```

Questions

- this create a dead cell, because for graphs (from whose schema this schema is derived), we have a special constructor that can take just an integer, and create a graph with a single vertex. This creates a cell with just a vertex, and empty “Life”

```
const DeadCell = LifeState(1) # a single dead cell
```

- Meaning of “initial” here: homomorphism(alive ? LiveCell : DeadCell, X; initial=(v=[1],))
- Why does this have the last application condition:

```
129 |  
130 | # Create an initial state  
131 | G = make_grid([1 0 1 0 1;  
132 |           0 1 0 1 0;  
133 |           0 1 0 1 0;  
134 |           1 0 1 0 1;  
135 |           1 0 1 0 1])  
136 | view_life(G);  
137 | G = make_grid(ones(1,1))  
138 | # Run the model  
139 | res = run!(AddCoords(GoL), G; maxevent=2);  
140 |
```

```
# A cell is born iff it has three living neighbors  
birth = TickRule(id(DeadCell), to_life;  
                  ac=[PAC(living_neighbors(3; alive=false)),  
                        NAC(living_neighbors(4; alive=false)),  
                        NAC(to_life)]);
```

Questions

- this creates a dead cell, because for graphs (from whose schema this schema is derived), we have a special constructor that can take just an integer, and create a graph with a single vertex. This creates a cell with just a vertex, and empty “Life”

```
const DeadCell = LifeState(1) # a single dead cell
```

- Meaning of “initial” here: homomorphism(alive ? LiveCell : DeadCell, X; initial=(v=[1],))
- Why does this have the last application condition:

```
129
130 # Create an initial state
131 G = make_grid([1 0 1 0 1;
132 |           0 1 0 1 0;
133 |           0 1 0 1 0;
134 |           1 0 1 0 1;
135 |           1 0 1 0 1])
136 view_life(G);
137 G = make_grid(ones(1,1))
138 # Run the model
139 res = run!(AddCoords(GoL), G; maxevent=2);
```

```
# A cell is born iff it has three living neighbors
birth = TickRule(id(DeadCell), to_life;
                  ac=[PAC(living_neighbors(3; alive=false)),
                       NAC(living_neighbors(4; alive=false)),
                       NAC(to_life)]);
```

Recall: for each of the “parts”, we have a Symbol count associated with the RepresentableP.

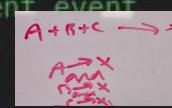
Don’t bother enabling if any are 0 -- for this case, there will be 0 pairs; see:

Question: Seeking Understanding on this Code

Here, we are checking if the size of the set mapped to by any of the objects have changed. (Here, we quantify over symbols ob, and compare the size of each; Ref(ob) just duplicates to be of equal size as the vector of parts.)

Question: Is it possible that the # remains invariant but identity changes?

```
# All other rules can potentially update in response to the current event
for (i, (rulei, clocks_i)) in enumerate(zip(abm.rules, rt.clocks))
    pt = pattern_type(rulei)
    if pt == RegularP() # update explicit nom-set w/r/t span X_n -> X_{n+1}
        for d in deletion!(clocks_i, lft)
            disable # disable clocks which are invalidated
        end
        for a in addition!(clocks_i, event, rmap, rght) # rght: R -> X_{n+1}
            enable
        end
    elseif pt isa RepresentableP
        relevant_obs = keys(pt)
        # we need to update current timer if # of parts has changed
        if !all(ob -> allequal(nparts.(codom.(pmap), Ref(ob)), relevant_obs)
            currently_enabled = haskey(rt, i)
            currently_enabled && disable # Disable if active
            # enable new timer if possible to apply rule
            if all(>(0), nparts.(Ref(rt.state), relevant_obs))
                enable, i)
            end
        end
    end
end
end
```



Question: Confirm Understanding for the Below

rmap_ is R->H, and rmap is R->H' (thus that rt.state is set to codom(rmap))

xmap is
a variable binding
morphism?

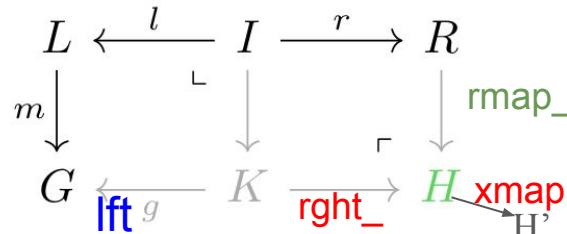
```

441 # If RegularPattern, we have an explicit match, otherwise randomly pick one
442 m = get_match(pattern_type(rule), pattern(rule), rt.state, clocks, key)
443
444 # Execute rewrite rule and unpack results
445 rw_result = (rule_type, rewrite_match_maps(getrule(rule), m))
446 rmap_ = get_rmap(rw_result...)
447 xmap_ = get_expr_binding_map(getrule(rule), m, rw_result[2])
448 (lft, rght_) = get_pmap(rw_result...)
449 rmap, rght = compose.([rmap_, rght_], Ref(xmap_))
450 pmap = Span(lft, rght)
451 rt.state = codom(rmap) # update runtime state
452 log!(event, pmap)     # record event result

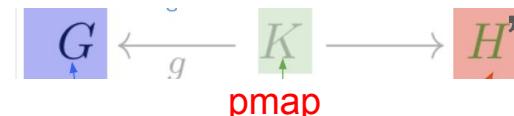
```

lft is and rght are as follows:

rght is rght_
with variables
substituted in



pMap is the span below



Questions 2

- For single pushout, is $R \rightarrow H$ a partial map? No
- What is the thinking on optimizing use of discrete cases?

Optimizing Memoryless Processes

Here, when scheduling
we don't need to
enumerate explicit
homs for
representables
when we have a
memoryless
transition -- we can
just use counts.

```
"""A collection of timers associated at runtime w/ an ABMRule"""
abstract type AbsHomSet end

@struct_hash_equal struct EmptyHomSet <: AbsHomSet end

@struct_hash_equal struct DiscreteHomSet <: AbsHomSet end

@struct_hash_equal struct ExplicitHomSet <: AbsHomSet val::IncHomSet end

Base.keys(h::ExplicitHomSet) = keys(h.val)

Base.pairs(h::ExplicitHomSet) = pairs(h.val)

Base.getindex(h::ExplicitHomSet, i) = h.val[i]

deletion!(h::ExplicitHomSet, m) = deletion!(h.val, m)

addition!(h::ExplicitHomSet, k, r, u) = addition!(h.val, k, r, u)

"""Initialize runtime hom-set given the rule and the initial state"""
function init_homset(rule::ABMRule, state::ACSet, additions::Vector{<:ACSetTransformation})
    p, sd = pattern_type(rule), state_dep(rule.timer)
    p == EmptyP() && return EmptyHomSet()
    (sd || p == RegularP()) && return ExplicitHomSet(IncHomSet(pattern(rule)), additions, state)
    @assert p isa RepresentableP  "$(typeof(p))"
    return DiscreteHomSet()
end
```

Pleasing Symmetry in Game of Life

```
# A previously empty cell is colonized iff it has three living neighbors
birth = TickRule(id(DeadCell), to_life;
                  ac=[PAC(living_neighbors(3; alive=false)),
                      NAC(living_neighbors(4; alive=false)),
                      NAC(to_life)]);
# A living cell remains alive iff it has ≥ 2 living neighbors but < 4 living neighbors
death = TickRule(to_life, id(DeadCell));
                  ac=[PAC(living_neighbors(2)),
                      NAC(living_neighbors(4))]);
```