

Operadic Modeling of Dynamical Systems : Mathematics and Computation

Sophie Libkind, Andrew Baas,
Evan Patterson, and James Fairbanks

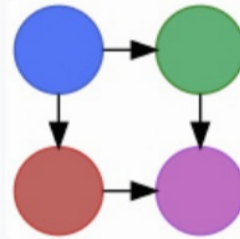
Applied Category Theory Conference, 2021

Introduction

FINDING
the right abstractions

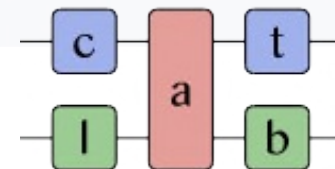


IMPLEMENTING
the right abstractions



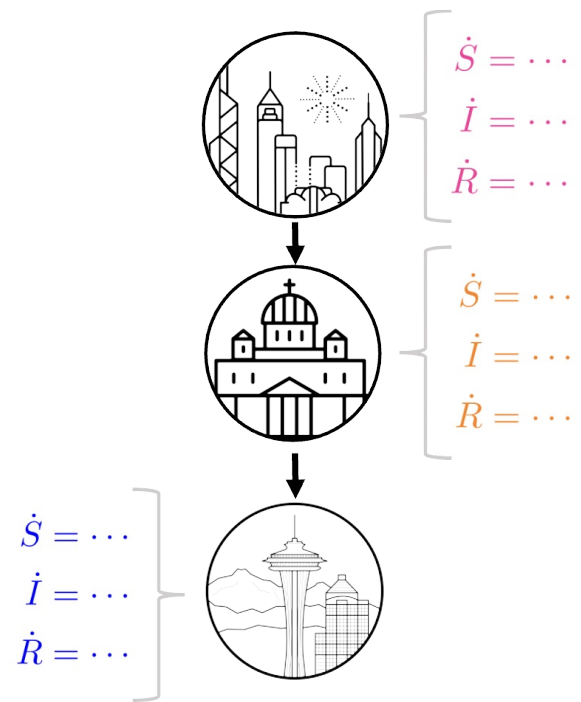
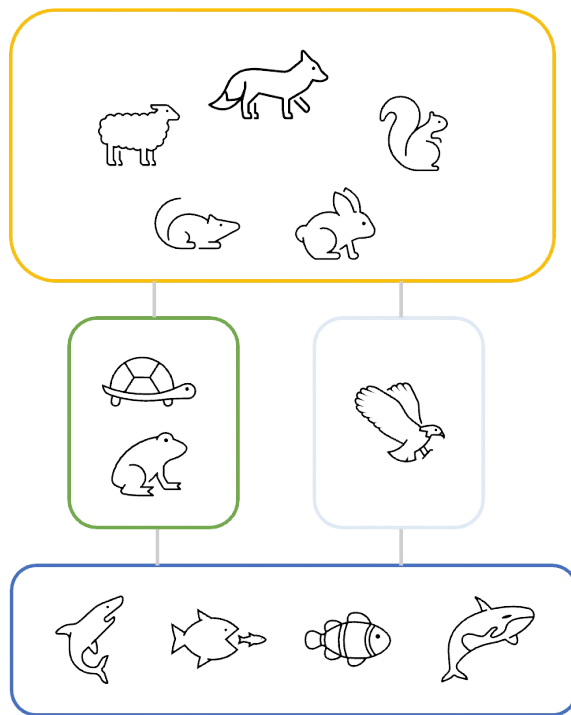
AlgebraicJulia

<https://www.algebraicjulia.org>




Introduction

systems have modular structure



Main idea


<p>Modeling terminology</p>	<p>mathematical abstractions</p> $F : \mathcal{O} \rightarrow \text{Set}$	<p>Julia implementation</p>  AlgebraicDynamics.jl
<p>system interface</p>	$t \in \text{ob } \mathcal{O}$	
<p>diagram of systems</p>	$\phi \in \mathcal{O}(s_1, \dots, s_n; t)$ $\phi_{\text{inner}} \in \mathcal{O}(r_1, \dots, r_m; s_i)$	<pre>diagram::ACSet{Theory0} inner_diagram::ACSet{Theory0}</pre>
<p>hierarchical diagram</p>	$\phi \circ_i \phi_{\text{inner}}$	<pre>ocompose(diagram, i, inner_diagram)</pre>
<p>elementary models</p>	$(m_1, \dots, m_n) \in F s_1 \times \dots \times F s_n$	<pre>models::Vector{T}</pre>
<p>composite model</p>	$F(\phi)(m_1, \dots, m_n) \in Ft$	<pre>oapply(diagram, models)</pre>

Outline

I. undirected composition

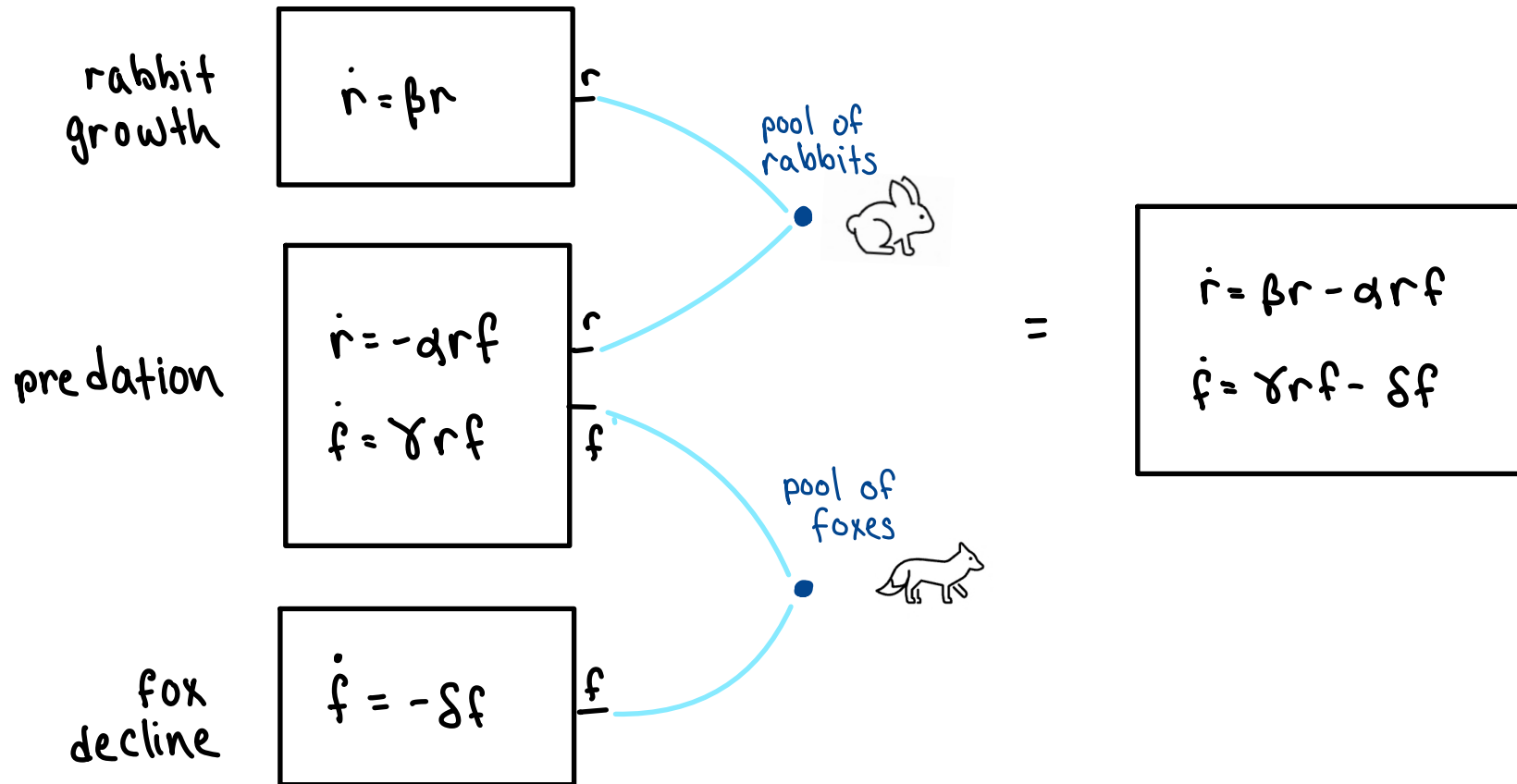
II. directed composition

III. conclusion

Modeling terminology	mathematical abstractions $F : \mathcal{O} \rightarrow \text{Set}$	Julia implementation  AlgebraicDynamics.jl
system interface	$t \in \text{ob } \mathcal{O}$	
diagram of systems	$\phi \in \mathcal{O}(s_1, \dots, s_n; t)$ $\phi_{\text{inner}} \in \mathcal{O}(r_1, \dots, r_m; s_i)$	<pre>diagram::ACSet{Theory0} inner_diagram::ACSet{Theory0}</pre>
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composite model	$F(\phi)(m_1, \dots, m_n) \in F t$	<pre>oapply(diagram, models)</pre>

I. Undirected composition - Motivation

Baez and Pollard (2017)



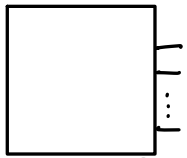
I. Undirected composition - abstractions for syntax

composition syntax (oper ad)
 $UWD := \mathcal{O}(\text{Cospan}_{\text{Finset}})$

composition semantics

system interface (types)

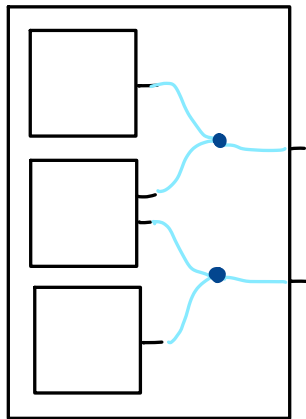
elementary models



$M \in \text{ob}(UWD)$

diagram of systems (terms)

composite model



$1+2+1 \rightarrow 2 \leftarrow 2 \in UWD(1, 2, 1; 2)$

I. Undirected composition - abstractions for syntax

composition syntax (operad)
 $UWD := \mathcal{O}(\text{Cospan}_{\text{Finset}})$

system interface (types)

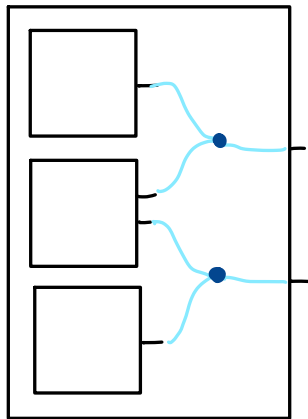


composition semantics (operad algebra)
 $\text{Dynam}_c^{\circ} : UWD \rightarrow \text{Set}$

elementary models

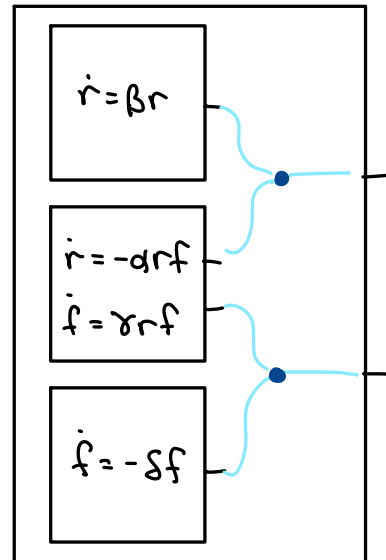
$$\text{Dynam}_c^{\circ}(M) = \left\{ \begin{array}{l} S \in \text{Finset} \\ v: \mathbb{R}^S \rightarrow T\mathbb{R}^S \\ p: M \rightarrow S \end{array} \right\}$$

diagram of systems (terms)



$$1+2+1 \rightarrow 2 \leftarrow 2 \in UWD(1, 2, 1; 2)$$

composite model



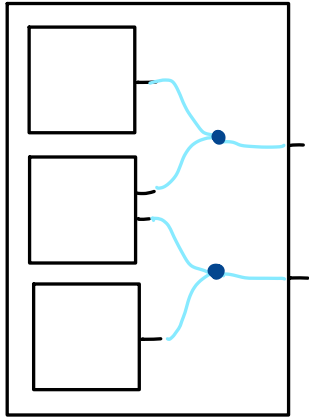
"add along shared coordinates"

$$= \begin{array}{l} \dot{r} = \beta r - \alpha r f \\ \dot{f} = \gamma r f - \delta f \end{array}$$

I. Undirected composition - implementation of syntax

def A \mathcal{C} -Set is a copresheaf $X: \mathcal{C} \rightarrow \text{Set}$

mathematical abstraction



data structure

def define a schema for undirected wiring diagrams by

$$\text{Th}(\text{UWD}) := \begin{array}{c} \\ \\ B \leftarrow P \rightarrow J \leftarrow Q \end{array}$$

prop undirected wiring diagrams

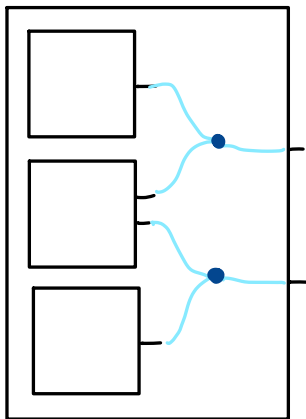
ie. terms of
 $\text{UWD} := \mathcal{O}(\text{Cospan}_{\text{Finset}})$



finite instances
of $\text{Th}(\text{UWD})$

I. Undirected composition - implementation of syntax

Mathematical Abstraction



$$1 + 2 + 1 \rightarrow 2 \leftarrow 2$$

$$\in \text{UWD}(1, 2, 1; 2)$$

Julia Code

```
rabbitfox_diagram = @relation (rabbits, foxes) begin
    growth(rabbits)
    predation(rabbits, foxes)
    decline(foxes)
end
```

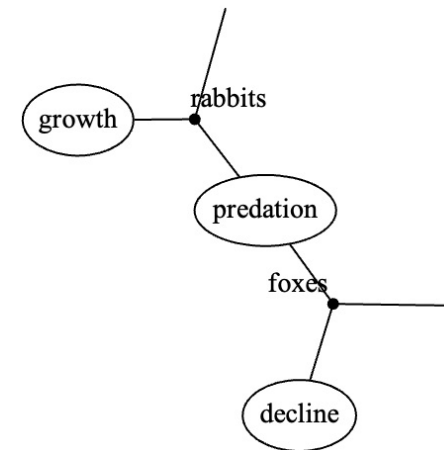
Julia Output

ACSet with elements Box = 1:3, Port = 1:4, OuterPort = 1:2, Junction = 1:2

Box	name	OuterPort	outer_junction
1	growth	1	1
2	predation	2	2
3	decline		

Junction	variable
1	rabbits
2	foxes

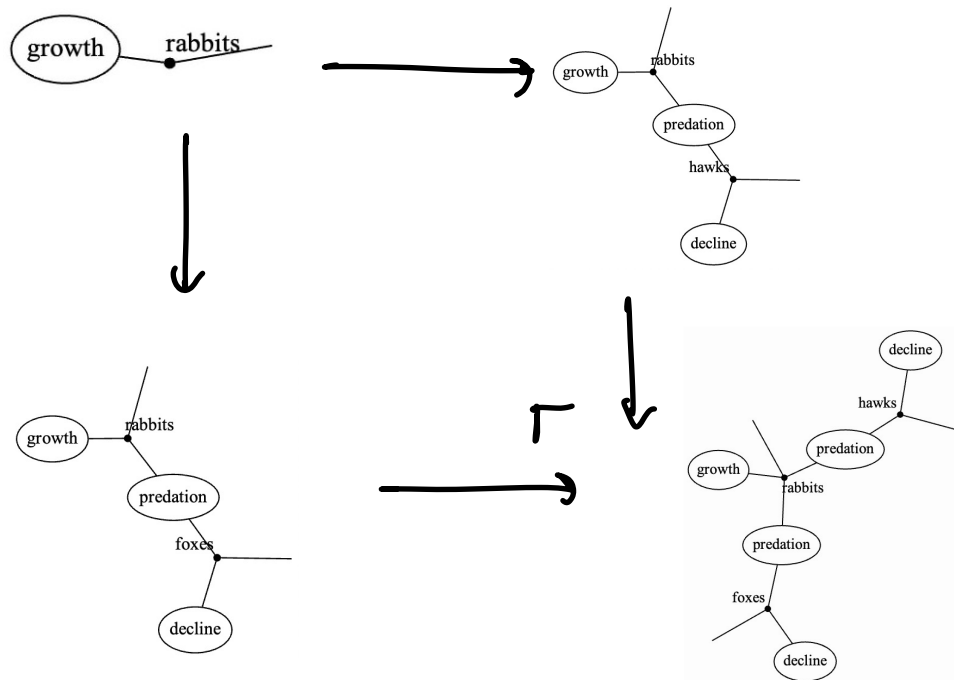
Port	box	junction
1	1	1
2	2	1
3	2	2
4	3	2



I. Undirected composition - Implementation of syntax

Advantages of \mathcal{C} -Set implementation:

1. Domain specific data structure
2. Apply features of $[\mathcal{C}, \text{Set}]$
 - limits / colimits
 - functorial data migration



```
# Define elementary diagrams of systems
rabbitfox_diagram = @relation (rabbits, foxes) begin
  growth(rabbits)
  predation(rabbits, foxes)
  decline(foxes)
end

rabbithawk_diagram = @relation (rabbits, hawks) begin
  growth(rabbits)
  predation(rabbits, hawks)
  decline(hawks)
end

rabbit_diagram = @relation (rabbits,) -> growth(rabbits)

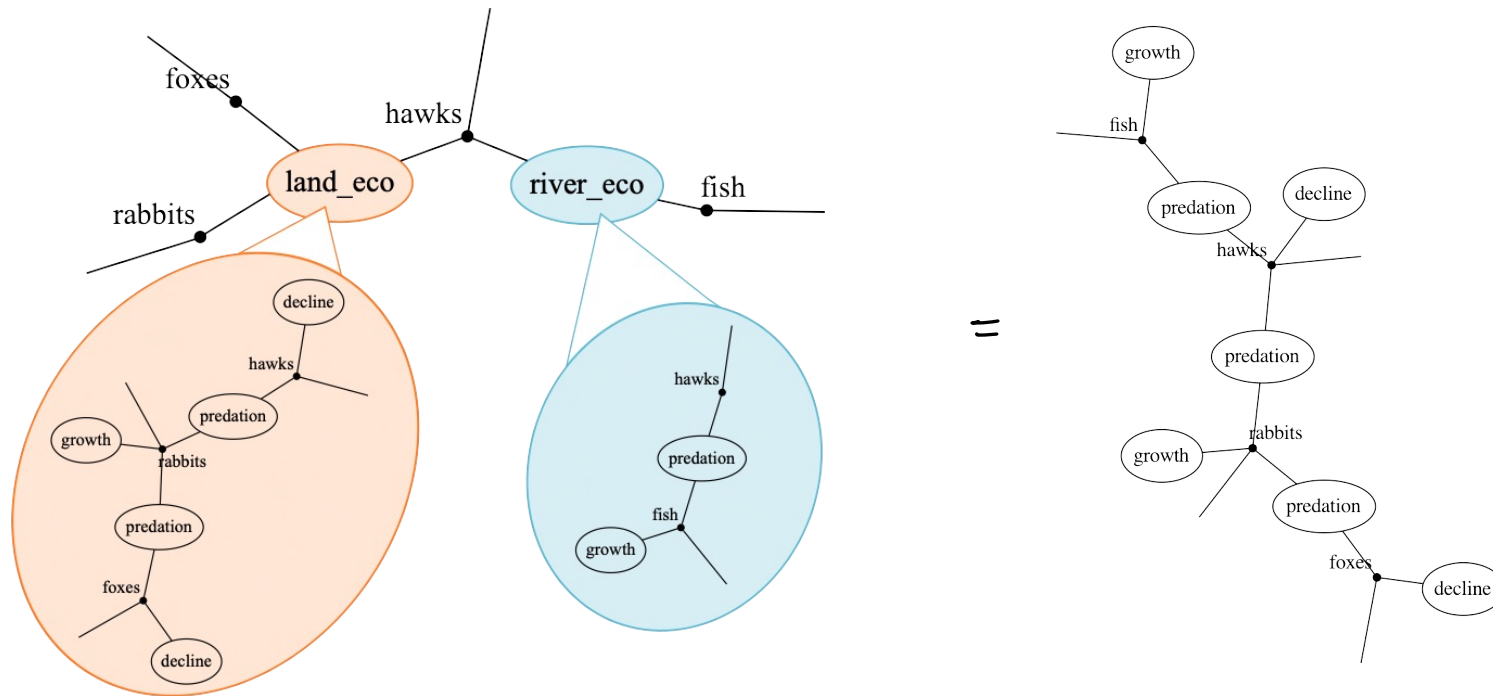
# Define transformations between the diagrams
rabbitfox_transform = ACSetTransformation(
  (Box=[1], Junction=[1], Port=[1], OuterPort=[1]),
  rabbit_diagram, rabbitfox_diagram
)

rabbithawk_transform = ACSetTransformation(
  (Box=[1], Junction=[1], Port=[1], OuterPort=[1]),
  rabbit_diagram, rabbithawk_diagram
)

# Take the pushout
land_diagram = ob(pushout(rabbitfox_transform, rabbithawk_transform))
```

I. Undirected composition - implementation of syntax

Hierarchical Diagrams (substitution in UWD)



Julia
Code

```
ocompose(total_diagram, [land_diagram, river_diagram])
```

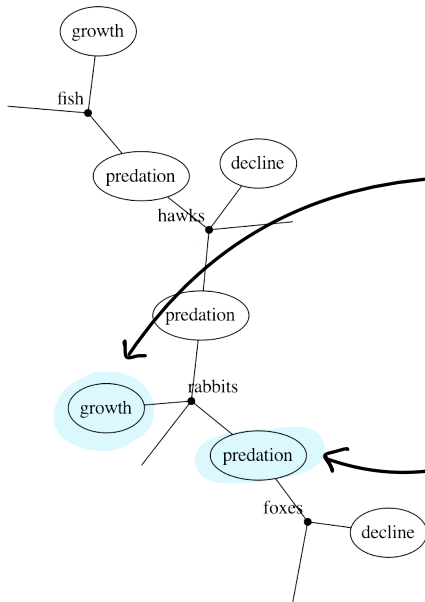
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I. Undirected composition - Implementation of semantics

Recall,

mathematical abstraction

Julia code



$$\dot{r} = \beta r$$

$$\begin{aligned} \dot{r} &= -\alpha r f \\ \dot{f} &= \gamma r f \end{aligned}$$

```
rabbit_growth = ContinuousResourceSharer{Float64}(  
    1, # exposed ports  
    1, # states  
    (u,p,t) -> p.β * u, # dynamics  
    [1] # port map  
)
```

```
rabbit_fox_predation = ContinuousResourceSharer{Float64}(  
    2, # exposed ports  
    2, # states  
    (u,p,t) -> [p.α*u[1]*u[2], p.γ*u[1]*u[2]], # dynamics  
    [1,2] # port map  
)
```

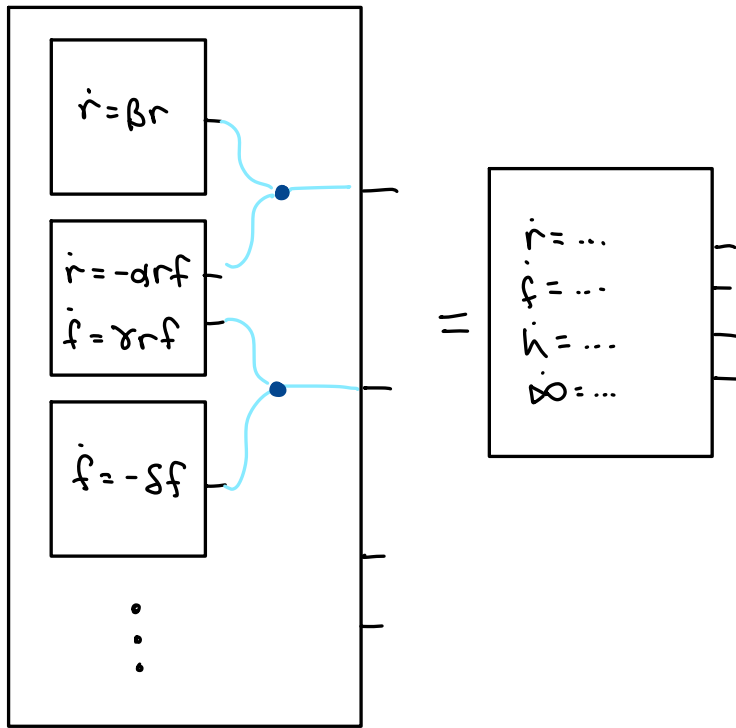
diagram of systems

elementary models

I. Undirected composition - Implementation of semantics

mathematical abstraction

Julia code + output

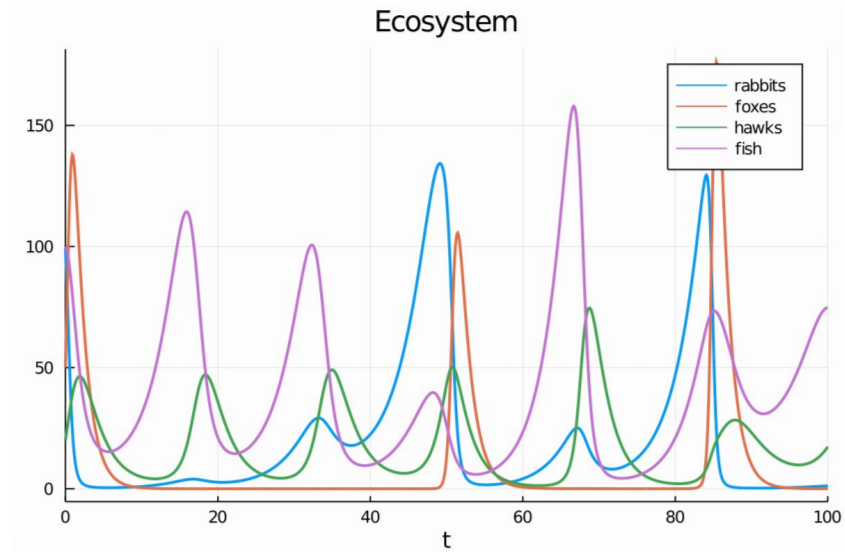


composite model

```
# compose models
eco_sys = oapply(eco_diagram, vcat(land_models, river_models))

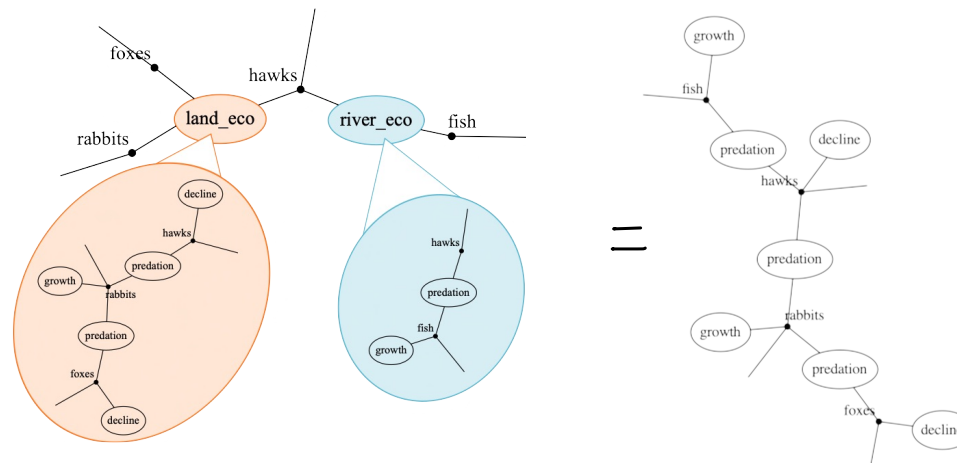
# solve and plot
tspan = (0.0, 100.0)
u0 = [100.0, 50.0, 20.0, 100.0]

prob = ODEProblem(eco_sys, u0, tspan, params)
sol = solve(prob, Tsit5())
```



I. Undirected Composition - Highlights of Algebraic Dynamics

#1: Compositional and Hierarchical Model Specification and Analysis



```
# flattened model specification
```

```
eco_diagram = ocompose(total_diagram, [land_diagram, river_diagram])
```

```
eco_sys     = oapply(eco_diagram, vcat(land_models, river_models))
```


```
# hierarchical model specification
```

```
land_sys   = oapply(land_diagram, land_models)
```

```
river_sys  = oapply(river_diagram, river_models)
```

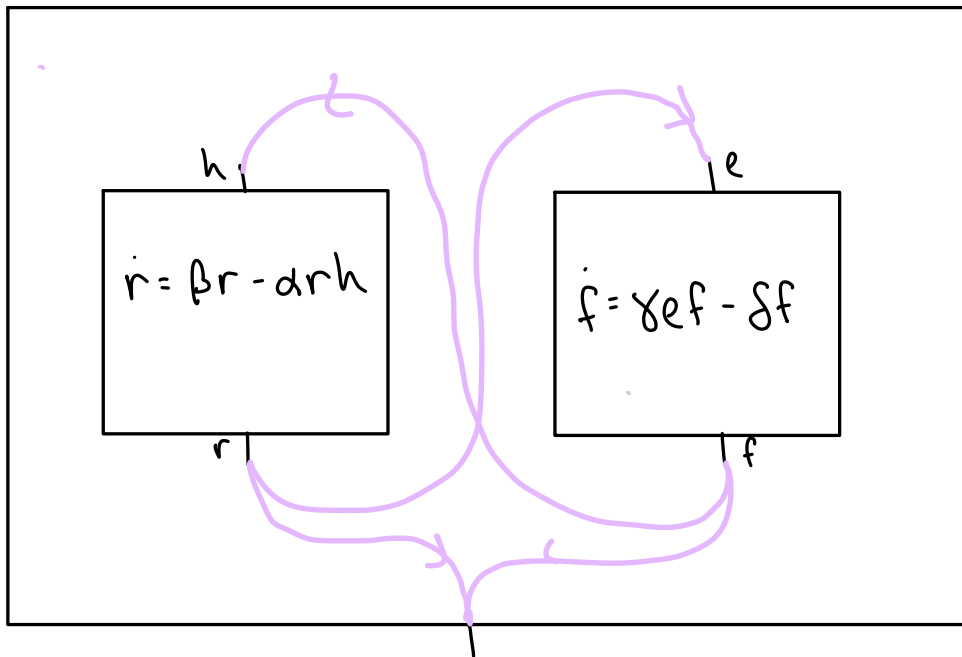
```
eco_sys    = oapply(total_diagram, [land_sys, river_sys])
```

Main idea

<p>Modeling terminology</p>	<p>mathematical abstractions</p> $F : \mathcal{O} \rightarrow \text{Set}$	<p>Julia implementation</p>  AlgebraicDynamics.jl
<p>system interface</p>	$t \in \text{ob } \mathcal{O}$	
<p>diagram of systems</p>	$\phi \in \mathcal{O}(s_1, \dots, s_n; t)$ $\phi_{\text{inner}} \in \mathcal{O}(r_1, \dots, r_m; s_i)$	<pre>diagram::ACSet{Theory0} inner_diagram::ACSet{Theory0}</pre>
<p>hierarchical diagram</p>	$\phi \circ_i \phi_{\text{inner}}$	<pre>ocompose(diagram, i, inner_diagram)</pre>
<p>elementary models</p>	$(m_1, \dots, m_n) \in F s_1 \times \dots \times F s_n$	<pre>models::Vector{T}</pre>
<p>composite model</p>	$F(\phi)(m_1, \dots, m_n) \in Ft$	<pre>oapply(diagram, models)</pre>

II. Directed composition - Motivation

vagner, spivak, lerman (2015)



=

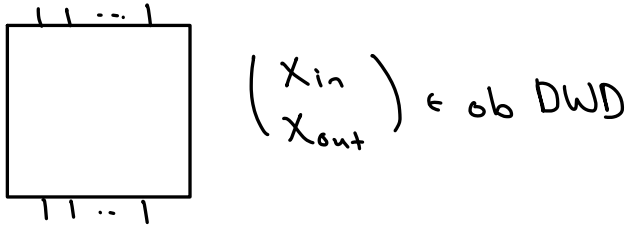
$$\begin{array}{l} \dot{r} = \beta r - \alpha r f \\ \dot{f} = \gamma r f - \delta f \\ \hline | r + f \end{array}$$

II. Directed composition - abstractions for syntax and semantics

composition syntax (operad) $DWD := \mathcal{O}(\text{Lens}_{\text{cospan}(\text{Finset}^{\text{op}})})$

composition semantics (operad algebra) $\text{Dynam}_c^{\rightarrow} : DWD \rightarrow \text{Set}$

system interface (types)



elementary models

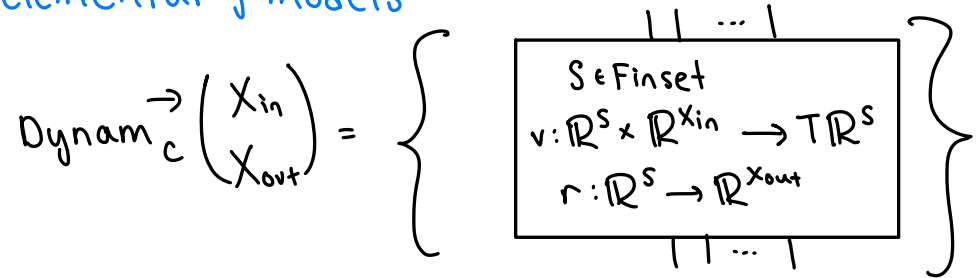
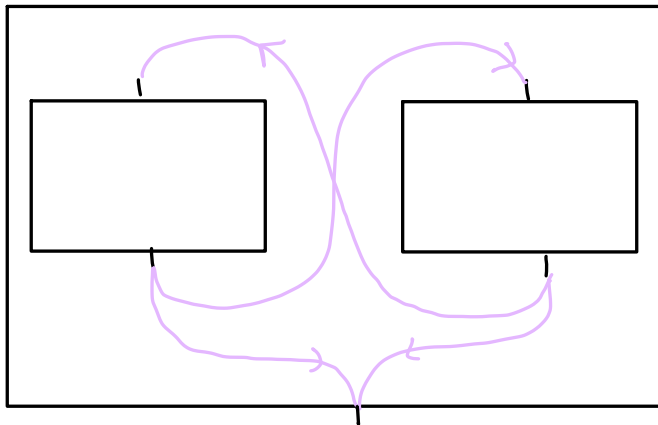
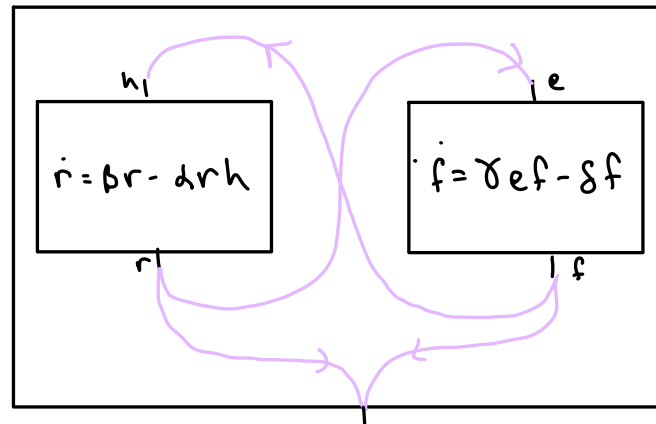


diagram of systems (terms)

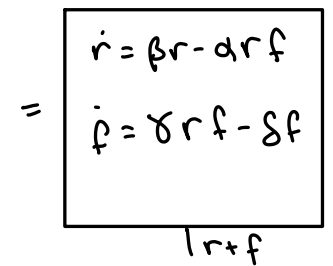


$\in DWD((!), (!); (!))$

composite model

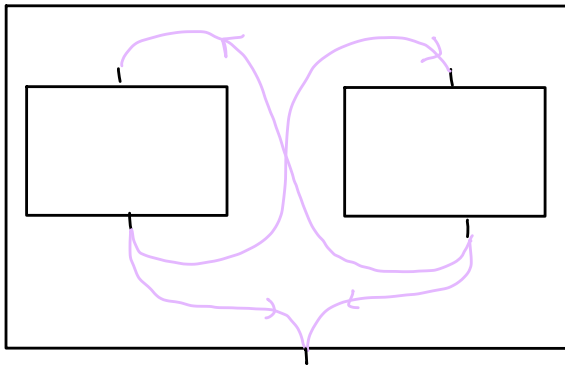


"send information along wires"



II. Directed composition - Implementation of syntax

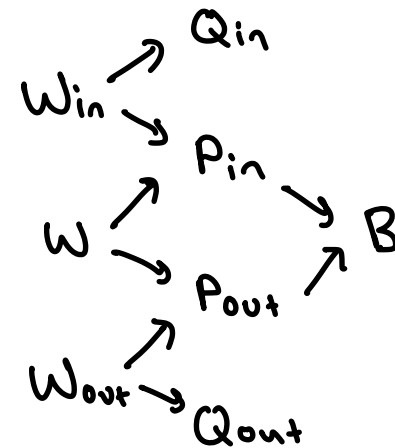
mathematical abstraction



data structure

def define a schema for directed wiring diagrams by

$\text{Th}(\text{DWD}) :=$



PROP directed wiring diagrams

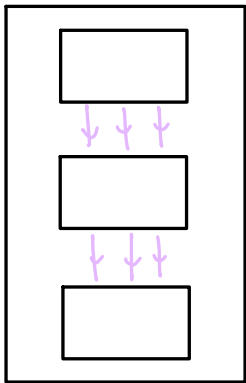
ie. terms of
 $\text{DWD} := \text{Lens}(\text{Cospan}_{\text{FinSet}^{\text{op}}})$



finite instances
of $\text{Th}(\text{DWD})$

II. Directed composition - Implementation of syntax

Mathematical Abstraction



$\in \text{DWD} \left(\begin{pmatrix} 3 \\ 0 \end{pmatrix}, \begin{pmatrix} 3 \\ 3 \end{pmatrix}, \begin{pmatrix} 0 \\ 3 \end{pmatrix}; \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right)$

Julia Code

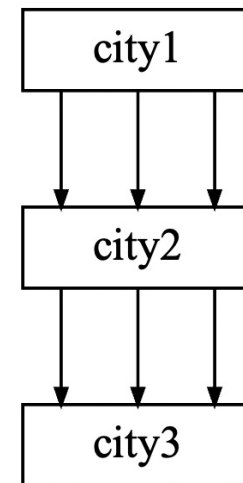
```
function get_city_diagram(ncities, roads)
    nout_roads = map(i -> count(r -> r.first == i, roads), 1:ncities)

    city_diagram = WiringDiagram([], [])
    cities = map(1:ncities) do i
        add_box!(city_diagram,
            Box(Symbol("city", i), [:S, :I, :R], [:S, :I, :R]))
    end

    wires = map(Base.Iterators.product(roads, 1:3)) do ((src, tgt), j)
        add_wire!(city_diagram, (cities[src], j) => (cities[tgt], j))
    end
    return city_diagram
end

ncities = 3
roads = [1 => 2, 2 => 3]
city_diagram = get_city_diagram(ncities, roads)
```

Julia Output



II. Directed composition - Implementation of semantics

Recall,

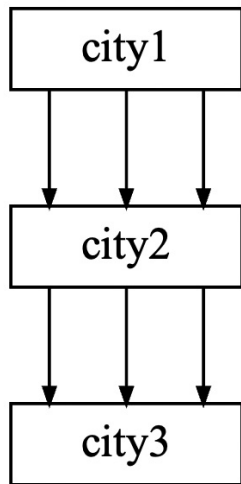
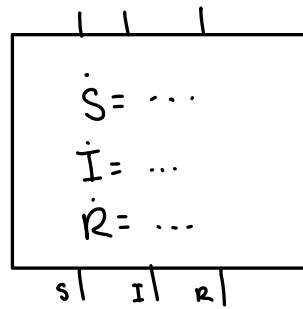


diagram of systems

mathematical abstraction



Julia code

```
city_models = map(1:ncities) do i

  ContinuousMachine{Float64}(
    3, # inputs
    3, # states
    3, # outputs
    (u,x,p,t) -> p.μ*(x - nout_roads[i]*u) + [
      -p[β(i)]*u[1]*u[2], # Ḡ
      p[β(i)]*u[1]*u[2] - p[γ(i)]*u[2], # İ
      p[γ(i)]*u[2]], # Ṛ
    u -> u)

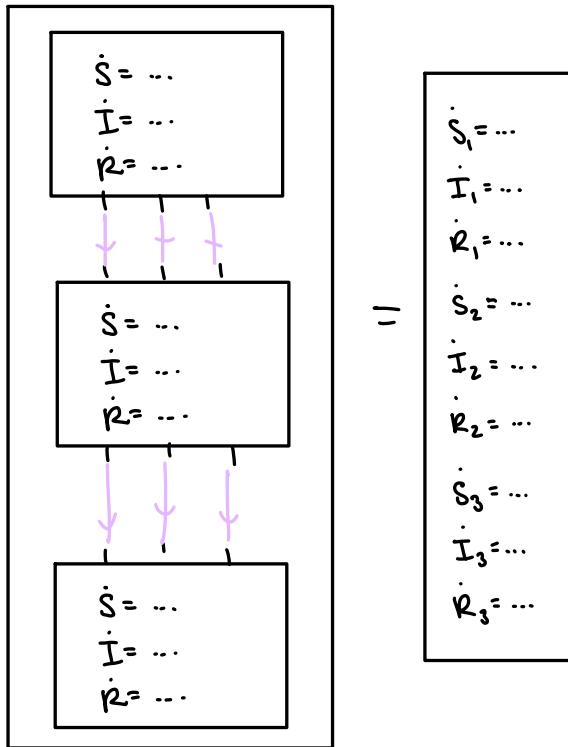
end
```

elementary models

II. Directed composition - Implementation of semantics

mathematical abstraction

Julia Code + Output



```
# compose models
sir_model = oapply(city_pattern, city_models)

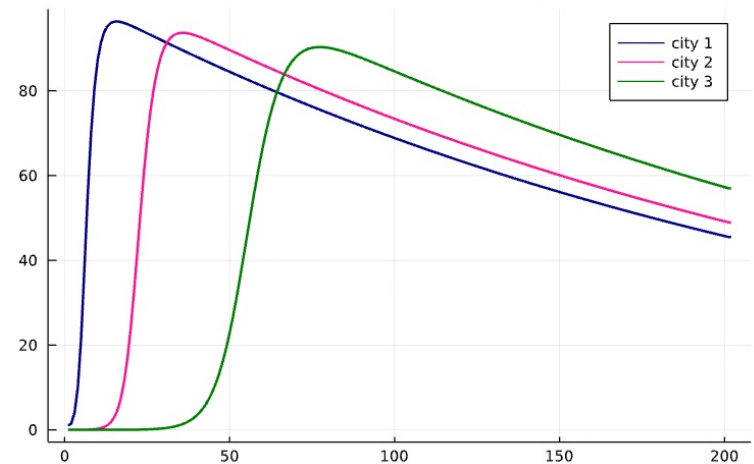
# solve and plot
params = LVector(μ = 0.01,
                β1 = 0.7, γ1 = 0.4,
                β2 = 0.4, γ2 = 0.4,
                β3 = 0.2, γ3 = 0.4
            )

u0 = [100.0, 1.0, 0.0, 0.0, 0.0,
      100.0, 0.0, 0.0, 0.0, 0.0,
      100.0, 0.0, 0.0, 0.0, 0.0] # initial populations

tspan = (0.0, 2.0)

prob = ODEProblem(sir_model, u0, tspan, params)
sol = solve(prob, Tsit5(); dtmax = 0.01)
```

Infected populations of multi-city SIR model

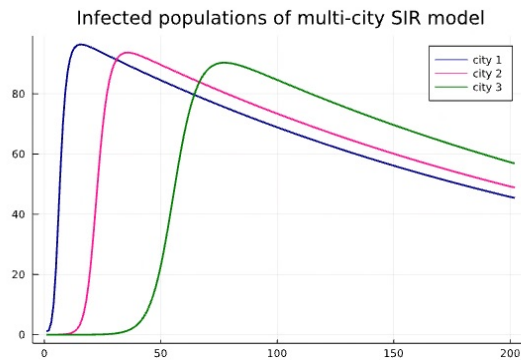
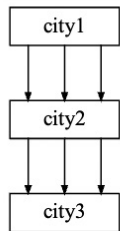


composite model

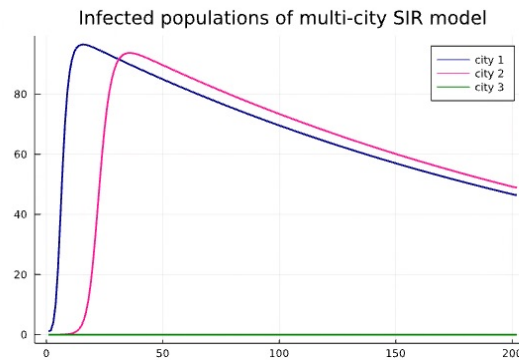
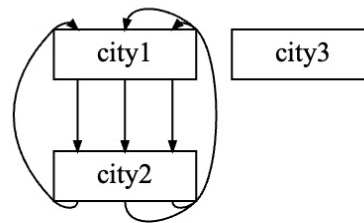
II. Directed composition - Highlights of Algebraic Dynamics

#2: independence of model syntax and model semantics

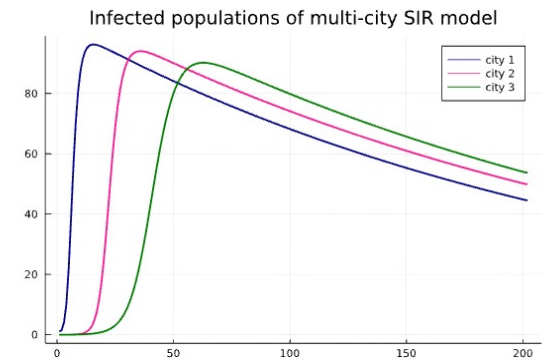
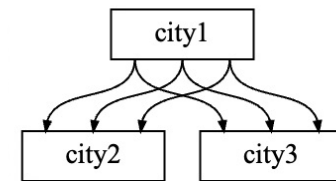
```
ncities = 3  
roads = [1 => 2, 2 => 3]  
city_pattern1 = get_city_pattern(ncities, roads)  
  
sir_model = oapply(city_pattern1, city_models)
```



```
ncities = 3  
roads = [1 => 2, 2 => 1]  
city_pattern2 = get_city_pattern(ncities, roads)  
  
sir_model = oapply(city_pattern2, city_models)
```

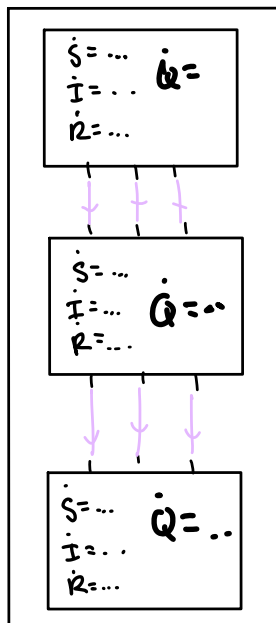


```
ncities = 3  
roads = [1 => 2, 1 => 3]  
city_pattern3 = get_city_pattern(ncities, roads)  
  
sir_model = oapply(city_pattern3, city_models)
```



II. Directed composition - Highlights of Algebraic Dynamics

#2: independence of model syntax and model semantics



```

sir_city_models = map(1:ncities) do i

  ContinuousMachine{Float64}(
    3, # inputs
    3, # states
    3, # outputs
    (u,x,p,t) -> p.u*(x - nout_roads[i]*u) + [
      -p[β(i)]*u[1]*u[2], # S
      p[β(i)]*u[1]*u[2] - p[γ(i)]*u[2], # I
      p[γ(i)]*u[2], # R
    ]
    u -> u
  )
end

sir_model = oapply(city_pattern, sir_city_models)

```

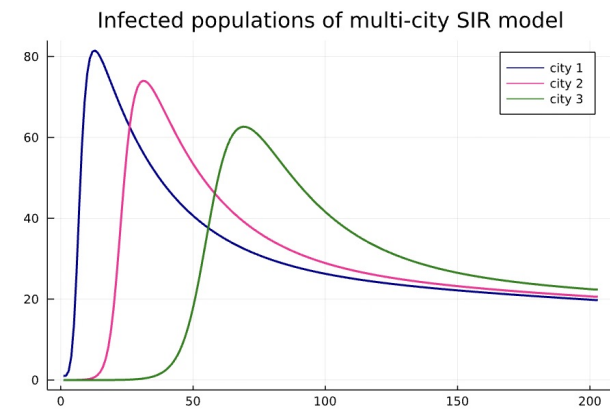
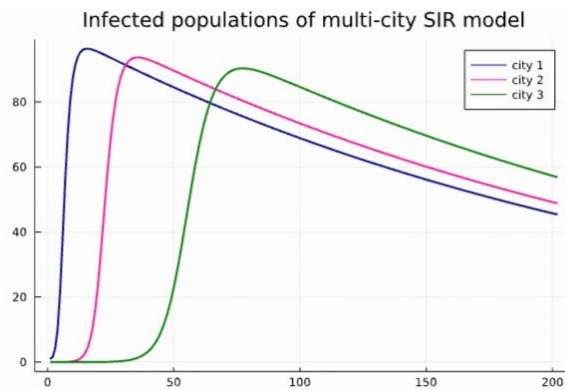
```

sirq_city_models = map(1:ncities) do i

  ContinuousMachine{Float64}(
    3, # inputs
    5, # states
    3, # outputs
    (u,x,p,t) -> begin
      q_rate = 0.025 * u[2]
      return p.u*([x..., 0,0] - nout_roads[i]*u) + [
        -p[β(i)]*u[1]*u[2] - q_rate*u[1] + (1 - q_rate)*u[4], # S
        p[β(i)]*u[1]*u[2] - p[γ(i)]*u[2] - q_rate*u[2] + (1 - q_rate)*u[5], # I
        p[γ(i)]*(u[2] + u[5]), # R
        q_rate * u[1] - (1 - q_rate) * u[4], # Qs
        q_rate * u[2] - (1 - q_rate) * u[5] - p[γ(i)]*u[5] # Qi
      ]
    end,
    u -> u[1:3]
  )
end

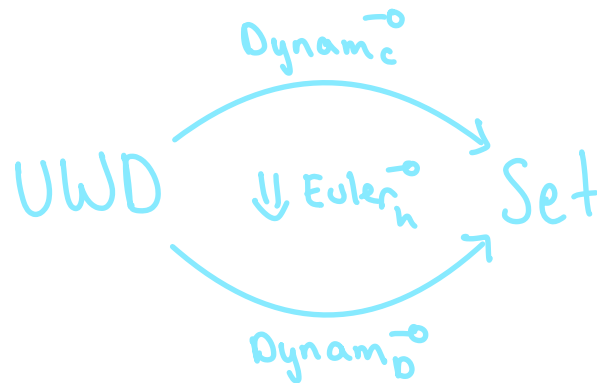
sirq_model = oapply(city_pattern, sirq_city_models)

```



III. Conclusion - contributions

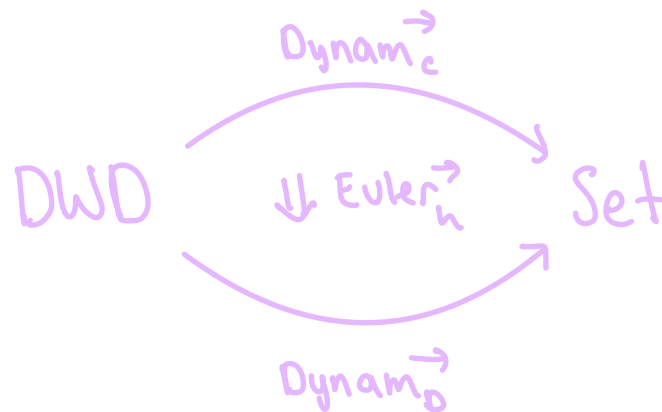
undirected
composition



- implementation of operads + operad algebras in Julia

- new algebras for composing dynamical systems

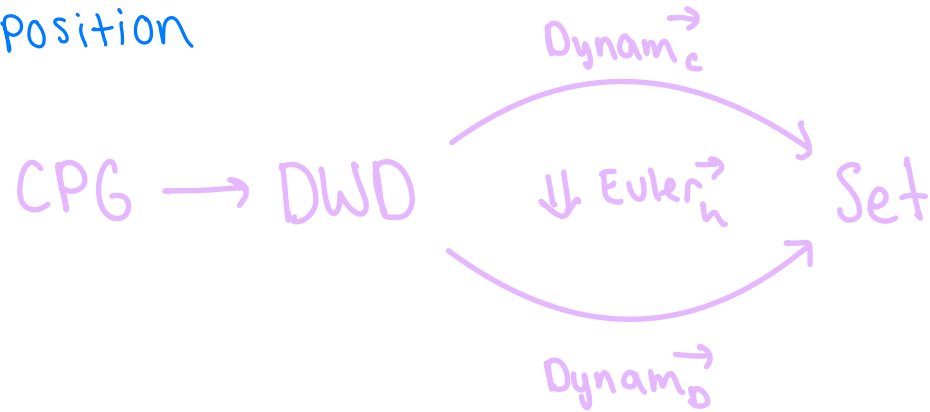
directed
composition



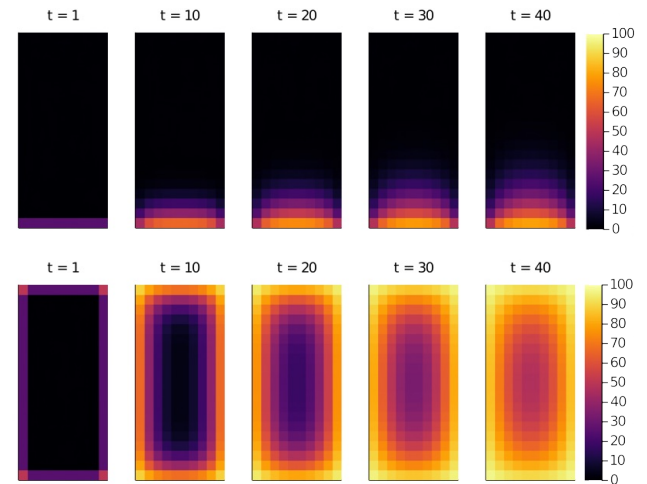
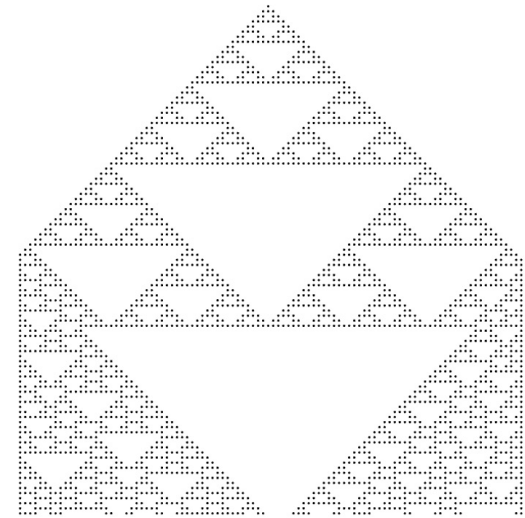
- Functorial euler's method: proofs and implementation

III. Conclusion - contributions

directed
Composition



- a new operad of circular port graphs



III. Conclusion - Future work

- "abstractions informed by implementation"
- implementing abstractions coming from
Higher category theory
- general theory of operads defined by \mathcal{E} -sets

THANK YOU!

Evan
Patterson



Brendan
Fong



Maia Gatlin



Andrew
Baas



Jesus
Arias



Sophie
Libkind



John Baez

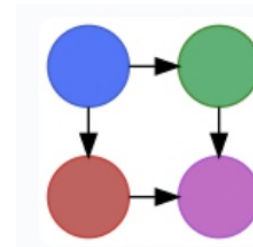
David
Spivak



Owen
Lynch



James
Fairbanks



AlgebraicJulia

<https://www.algebraicjulia.org>

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