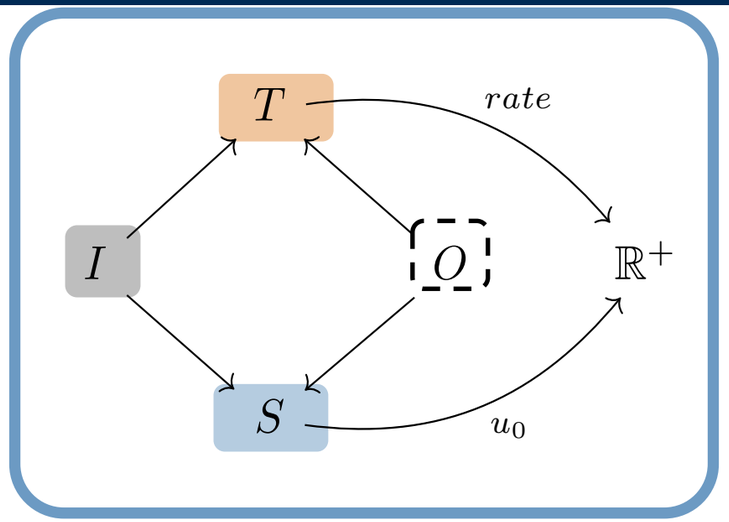
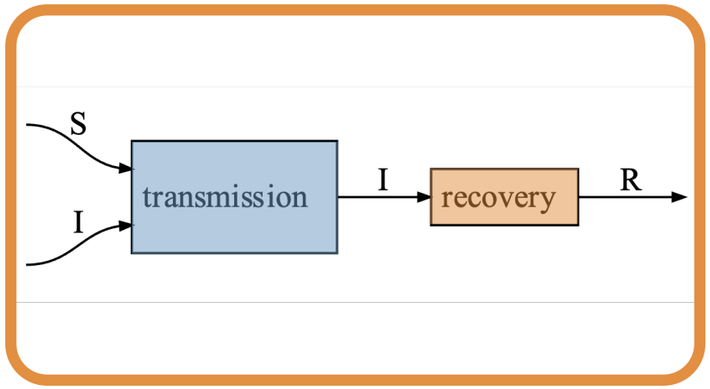
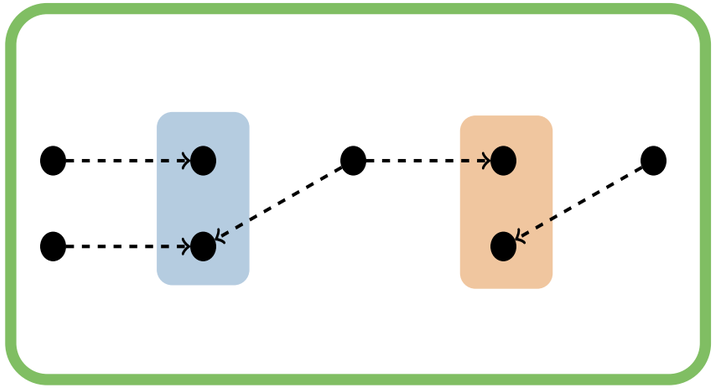


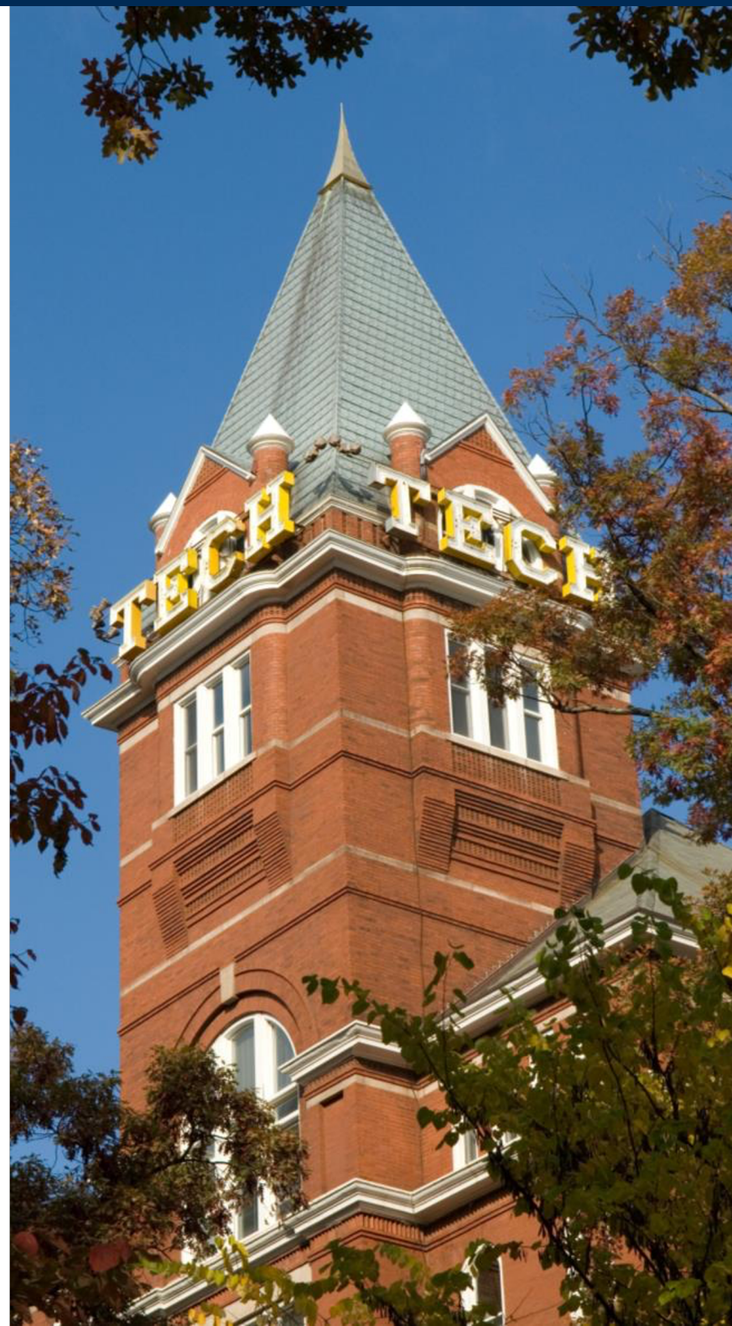




ACT Modeling with AlgebraicJulia and Catlab

Micah Halter
Evan Patterson
James Fairbanks
Georgia Tech Research Institute (GTRI)

7/8/2020



Spectrum of Scientific Computing Technology

Georgia Tech Research Institute

Programs that have *explicit* representations of the model

Arbitrary Code

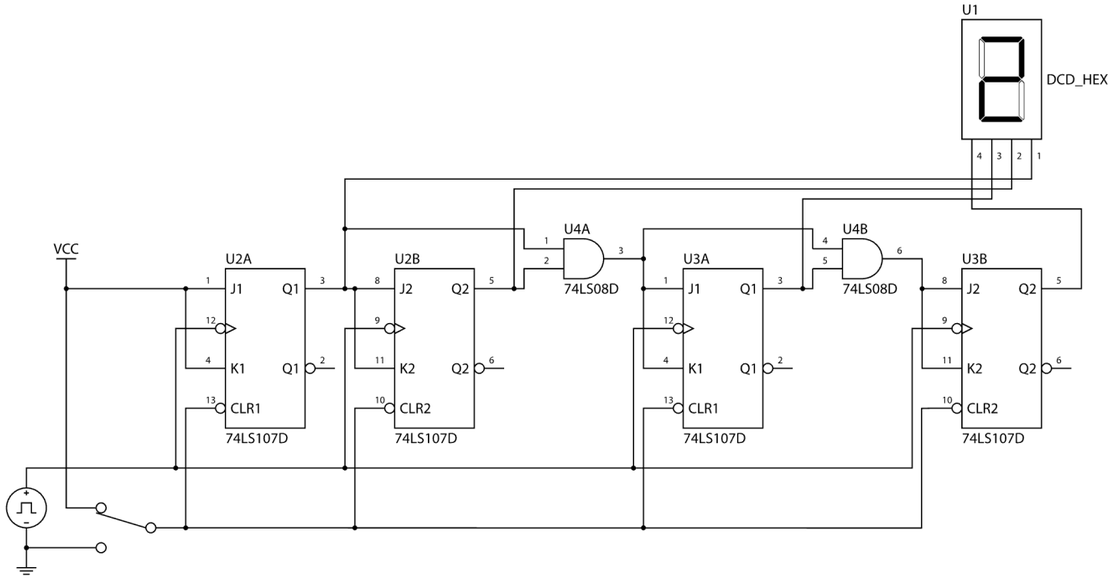
Domain Specific Languages

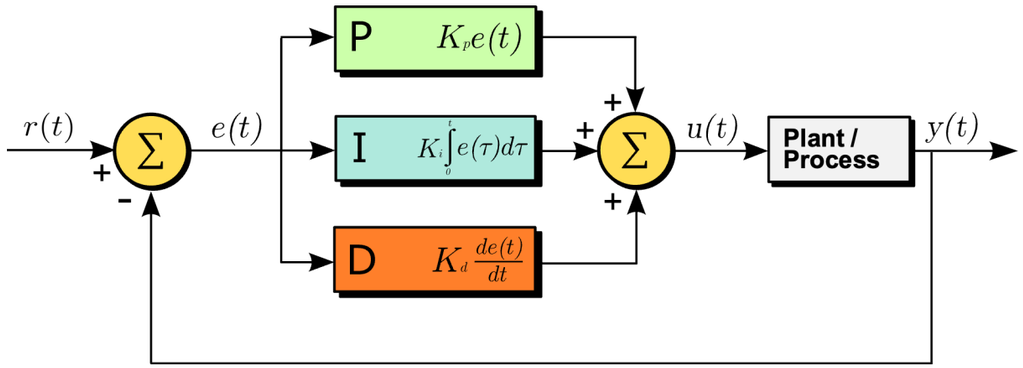
Modeling Frameworks

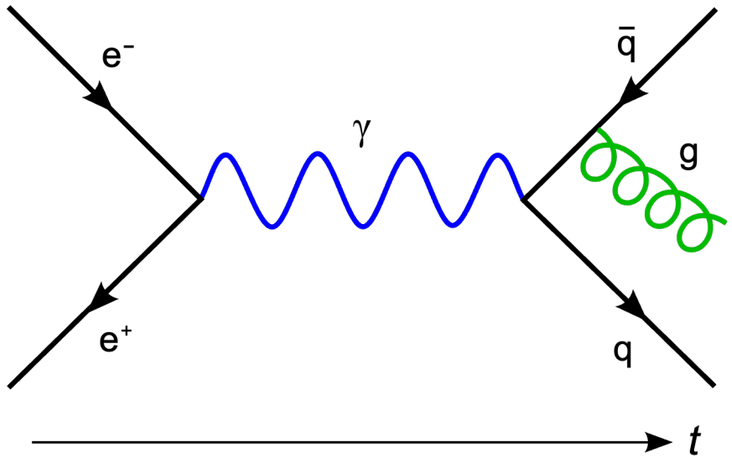
Computer Algebra Systems

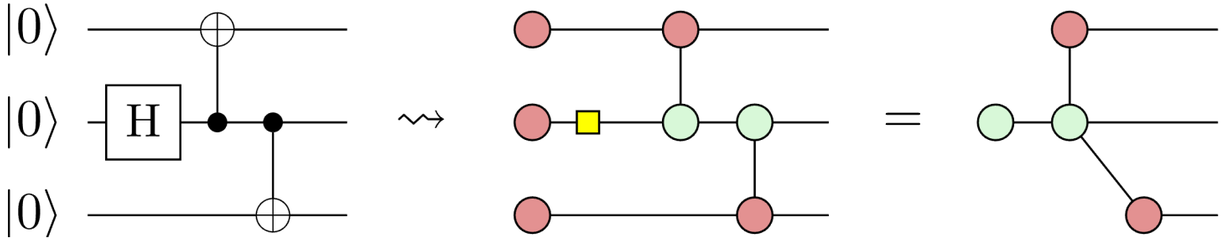
SymPy

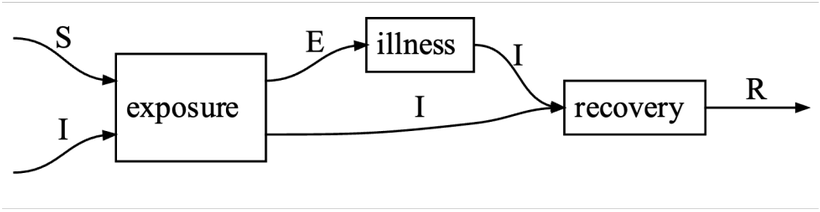
Formal Scientific Diagrams











Behavioral Approach to Modeling Systems

Georgia Tech Research Institute

$$Syntax \longrightarrow Semantics$$

Functional Programming

$$Programs \xrightarrow{F} Functions$$

$$\begin{tikzcd} S \arrow[r, "F"] \arrow[d, "prog"'] & A \arrow[d, "F(prog)"] \\ T \arrow[r, "F"] & B \end{tikzcd}$$

Behavioral Semantics

$$Designs \xrightarrow{F} Behaviors$$

$$\begin{tikzcd} Input \arrow[r, "F"] \arrow[d, "sys"'] & V \arrow[d, "F(sys)"] \\ Output \arrow[r, "F"] & U \end{tikzcd}$$

Three Layers of GAT Based Modeling

Georgia Tech Research Institute

Theory

$$A, B, C$$

$$a : A, b : B, c : C$$

$$a \otimes b \cdot c$$

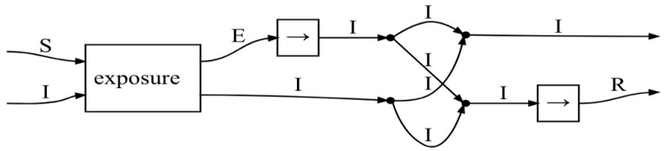
$$(a \otimes b) \cdot (c \otimes d) = (a \cdot c) \otimes (b \cdot d)$$

Syntax

Formula Notation

$$seir = expo \cdot (f_{E,I} \otimes id_I) \cdot \nabla_I \cdot \Delta_I \cdot (id_I \otimes f_{I,R})$$

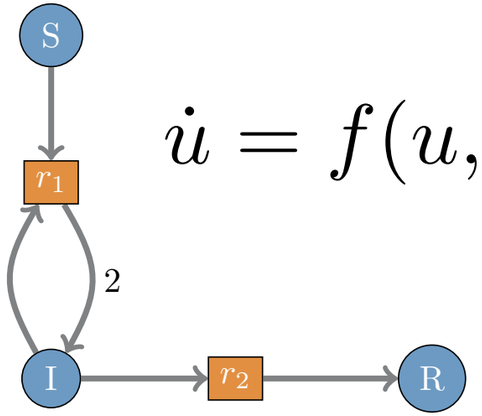
Wiring Diagram



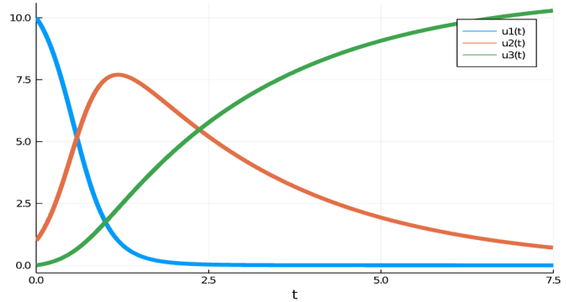
Embedded Domain Specific Language

```
d = @program Disease (s::S, e::E, i::I) begin
    e1, i1 = exposure{S,I,E}(s,i)
    i2 = spontaneous{E,I}(e1)
    e = [e, e1]
    e_out = spontaneous{E,E}(e)
    i1 = [i1, i2]
    r = spontaneous{I,R}(i1)
    s_out = spontaneous{S,S}(s)
    return s_out, e_out, spontaneous{I,I}(i1)
end
```

Instance



$$\dot{u} = f(u, t)$$



AlgebraicJulia

FinOrd: the Category of Natural Numbers

Georgia Tech Research Institute

```
@theory Category(Ob,Hom) begin
Ob::TYPE
Hom(dom::Ob,codom::Ob)::TYPE

id(A::Ob)::(A → A)
compose(f::(A → B), g::(B → C))::(A → C)
⊣ (A::Ob, B::Ob, C::Ob)
end
```

```
@instance Category(FinOrd, FinOrdMap) begin
dom(f::FinOrdMap) = FinOrd(f.dom)
codom(f::FinOrdMap) = FinOrd(f.codom)

id(A::FinOrd) = FinOrdFunction(identity, A, A)

function compose(f::FinOrdMap, g::FinOrdMap)
@assert codom(f) == dom(g)
FinOrdFunction(compose(f.func,g.func), dom(f), codom(g))
end
end
```

```
struct FinOrd n:: Int end

struct FinOrdFunc <: FinOrdMa
func::Function
dom::Int
codom::Int
end

(f::FinOrdFunc)(x) = f.func(x

struct FinOrdVec <: FinOrdMap
func::Vector{Int}
codom::Int
end

(f::FinOrdVec)(x) = f.func[x]
```

Categorical Algebra as a Programming Paradigm

Georgia Tech Research Institute

Initial Object

$$0 \longrightarrow A$$

```
initial(::Type{FinOrd}) = FinOrd(0)
```

Coproducts

$$\begin{tikzcd} & B \arrow[d, "i_2"] \\ A \arrow[r, "i_1"] & A \sqcup B \end{tikzcd}$$

```
function coproduct(A::FinOrd, B::FinOrd)
m, n = A.n, B.n
ι1 = FinOrdMap(1:m, m, m+n)
ι2 = FinOrdMap(m+1:m+n, n, m+n)
Cospan(ι1, ι2)
end
```

Coequalizers

$$E \xleftarrow{u} A \leftleftarrows B$$

Pushout of f, g,
$u = coequalizer(f \cdot i_1, g \cdot i_2)$

$$\begin{tikzcd} A & & \\ & X \sqcup Y \arrow[ul, "u"] & Y \arrow[l, "i_2"'] \arrow[uul, bend right] \\ & X \arrow[u, "i_1"] \arrow[uul, bend left] & Z \arrow[l, "f"] \arrow[u, "g"'] \end{tikzcd}$$

```
function pushout(span::Span{<:FinOrdMap,<:FinOrdMap})
f, g = left(span), right(span)
coprod = coproduct(codom(f), codom(g))
ι1, ι2 = left(coprod), right(coprod)
coeq = coequalizer(f·ι1, g·ι2)
Cospan(ι1·coeq, ι2·coeq)
end
```

Non-Functional Programming with ACT

Coequalizers

$$E \xleftarrow{u} A \leftleftarrows B$$

```
function coequalizer(f::FinOrdMap, g::FinOrdMap)
@assert dom(f) == dom(g) && codom(f) == codom(g)
m, n = dom(f).n, codom(f).n
sets = IntDisjointSets(n)
for i in 1:m
union!(sets, f(i), g(i))
end
h = [ find_root(sets, i) for i in 1:n ]
roots = unique!(sort(h))
FinOrdMap([ searchsortedfirst(roots, r)
for r in h],
length(roots))
end
```

Mutation!

Application: Simulating a Petri Net as ODEs

Georgia Tech Research Institute

Novel coronavirus 2019-nCoV: early estimation of epidemiological parameters and epidemic predictions
Version 2. Updated 27 Jan 2020

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Impact of international travel and border control measures on the global spread of the novel 2019 coronavirus outbreak

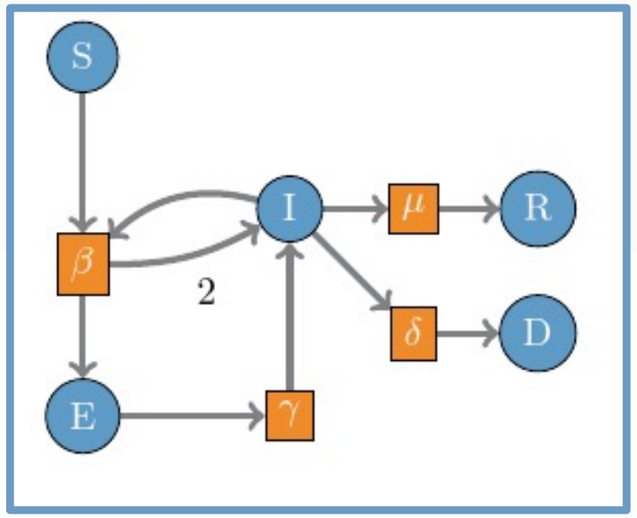
Chad R. Wells[a], Pratha Sah[a], Seyed M. Moghadas[b], Abhishek Pandey[a], Affan Shoukat[a], Yaning Wang[c], Zheng Wang[d], Lauren A. Meyers[e,f], Burton H. Singer[g,1], and Alison P. Galvani[a]

[a]Center for Infectious Disease Modeling and Analysis, Yale School of Public Health, New Haven, CT 06520; [b]Agent-Based Modelling Laboratory, York University, Toronto, ON M3J 1P3, Canada; [c]State Key Laboratory of Mycology, Institute of Microbiology, Chinese Academy of Sciences, 100101 Beijing, China; [d]Department of Biostatistics, Yale School of Public Health, New Haven, CT 06510; [e]Department of Integrative Biology, The University of Texas at Austin, Austin, TX 78712; [f]Santa Fe Institute, Santa Fe, NM 87501; and [g]Emerging Pathogens Institute, University of Florida, Gainesville, FL 32610

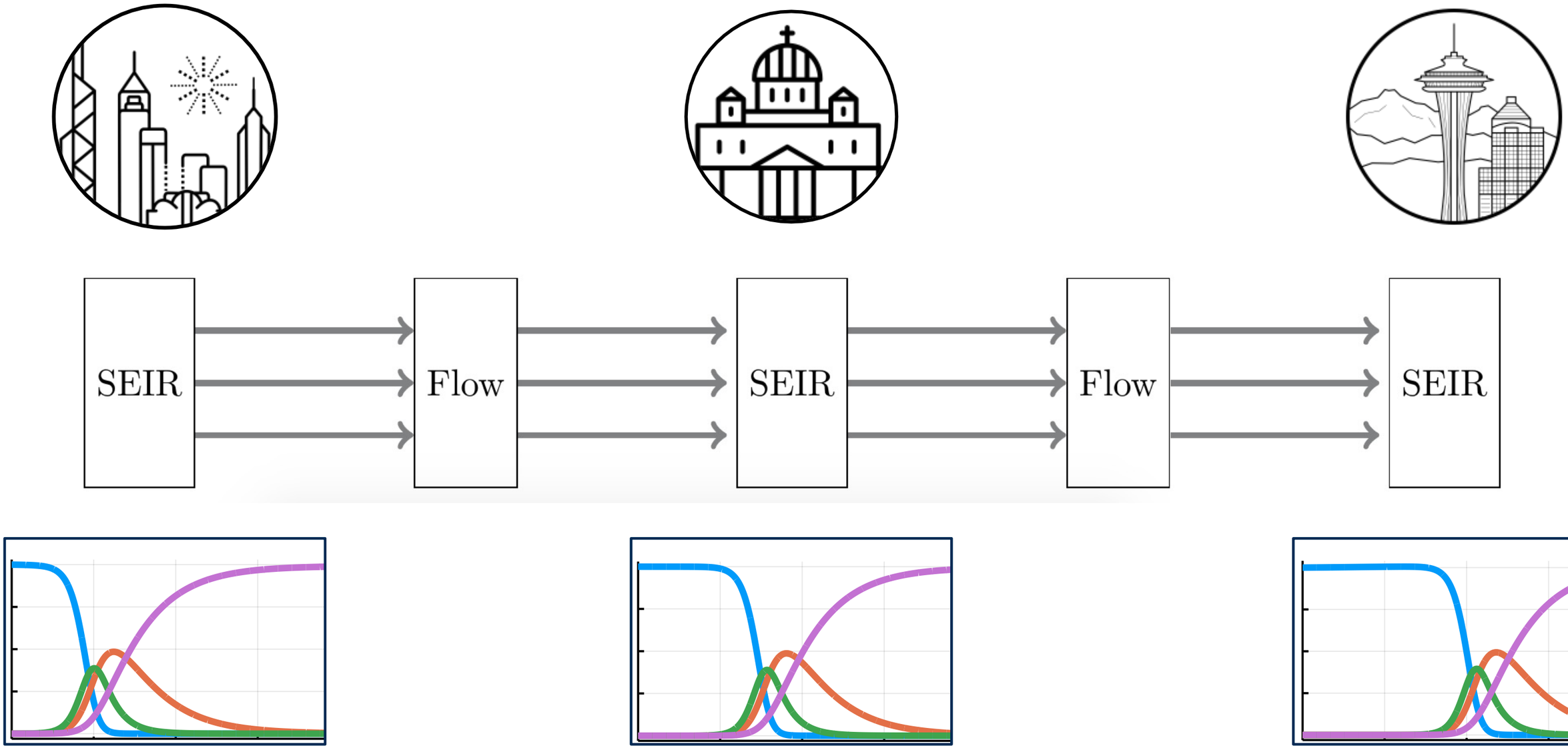
Contributed by Burton H. Singer, February 27, 2020 (sent for review February 12, 2020; reviewed by Yoav Keynan and Heman Shakeri)

Solve the initial value problem for $\dot{u} = f(u, t)$

```
f(u, p) = begin
    for (i, t) in enumerate(reactions)
        reagents = t[1]
        products = t[2]
        ϕ = p[i]*prod(u[reagents])
        du[reagents] .-= ϕ
        du[products] .+= ϕ
    end
    return du
end
```



Epidemiology Modeling Framework



Basic SIR model

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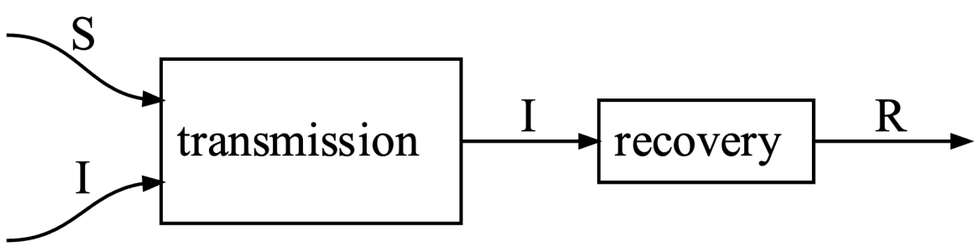
```
sir = transmission · recovery
```



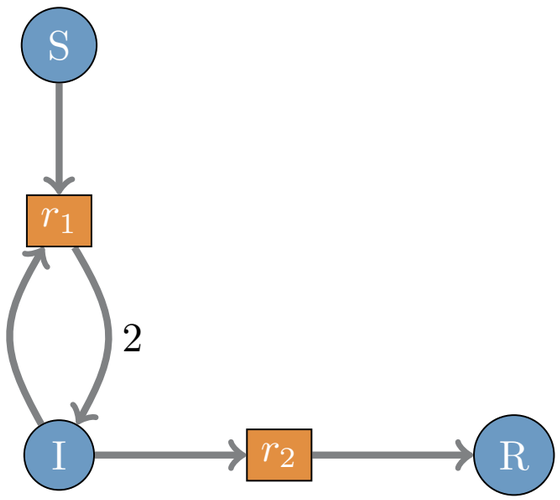

```
f = vectorfield(sirᵈ)
```

$$\dot{u}_1 = -r_1 u_1 u_2$$

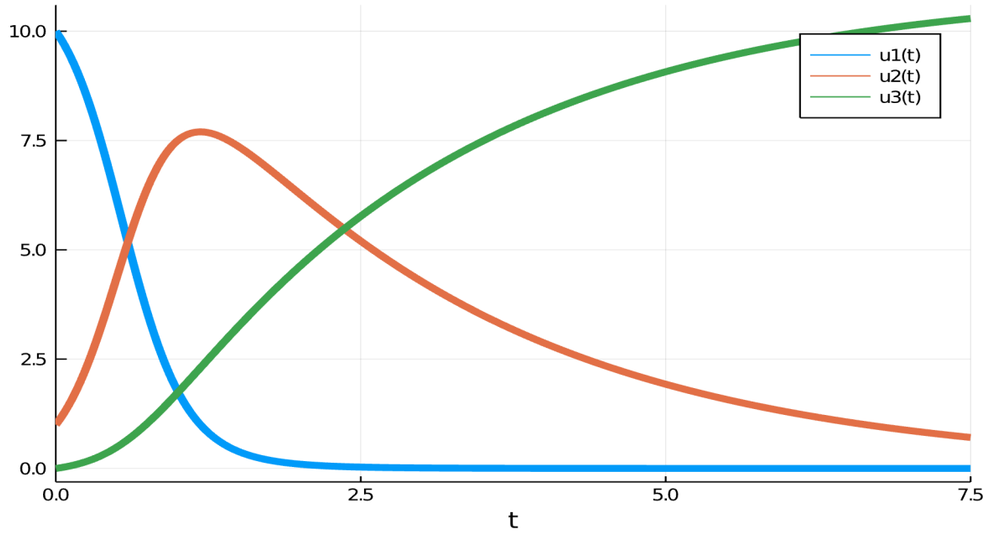
$$\dot{u}_2 = r_1 u_1 u_2 - r_3 u_2$$

$$\dot{u}_3 = r_3 u_2$$

```
sirᵈ = decoration(F(sir))
```



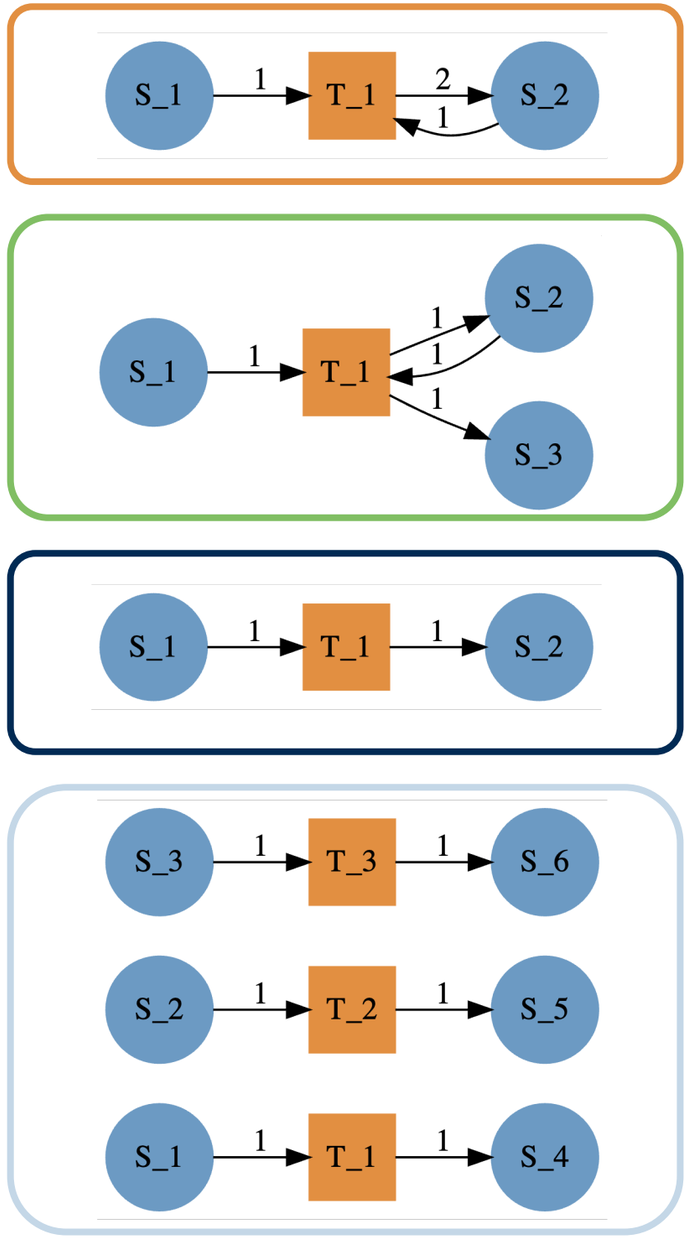

```
sol = solve(f, u₀, r, (t₀, t₁))
```



Epidemiology Modeling

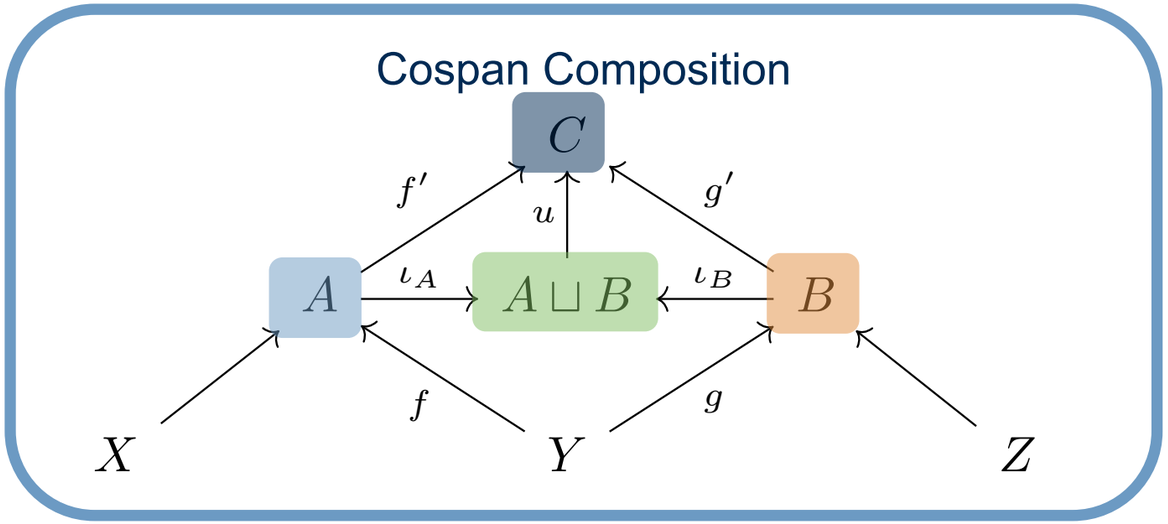
```
@present Epidemiology(FreeBiproductCategory) beg:
S::Ob
E::Ob
I::Ob
R::Ob
D::Ob
transmission::Hom(S⊗I, I)
exposure::Hom(S⊗I, E⊗I)
illness::Hom(E,I)
recovery::Hom(I,R)
death::Hom(I,D)
travel::Hom(S⊗E⊗I,S⊗E⊗I)
end
```

$$Epi \xrightarrow{\quad F \quad} Petri$$



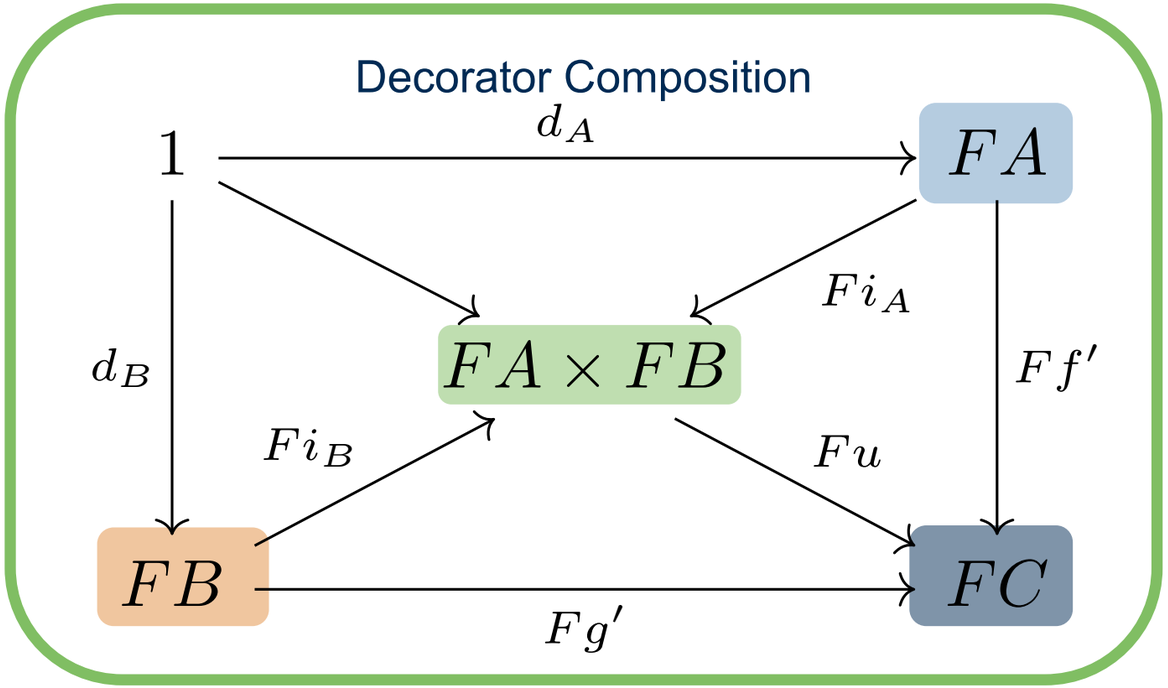
Computing Decorated Cospans

Georgia Tech Research Institute



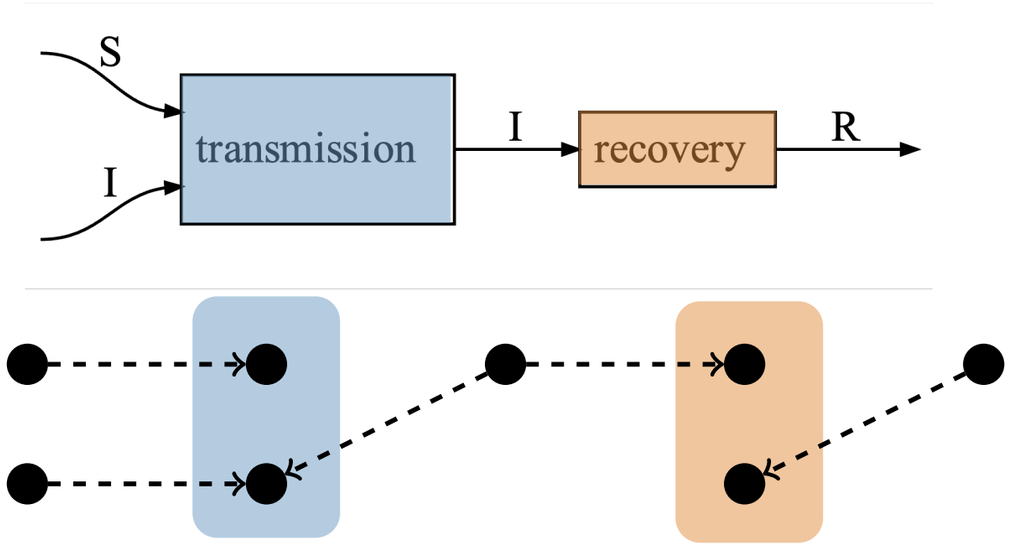
$$Epi \xrightarrow{F} Petri$$

$$FA \sqcup FB \xrightarrow{L} F(A \sqcup B)$$

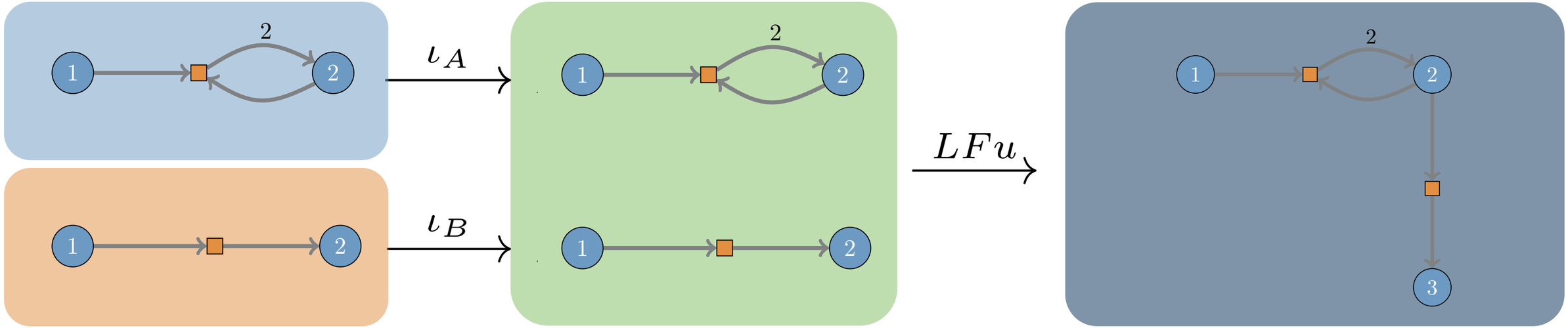



```
compose(p::PetriCospan, q::PetriCospan) = begin
u, f', g' = pushout(f,g)
F = functor(decorator(p))
L = laxator(decorator(p))
dc = F(u)(L(decoration(p), decoration(q)))
return PetriCospan(Cospan(f', g'), decorator(p), dc)
end
```

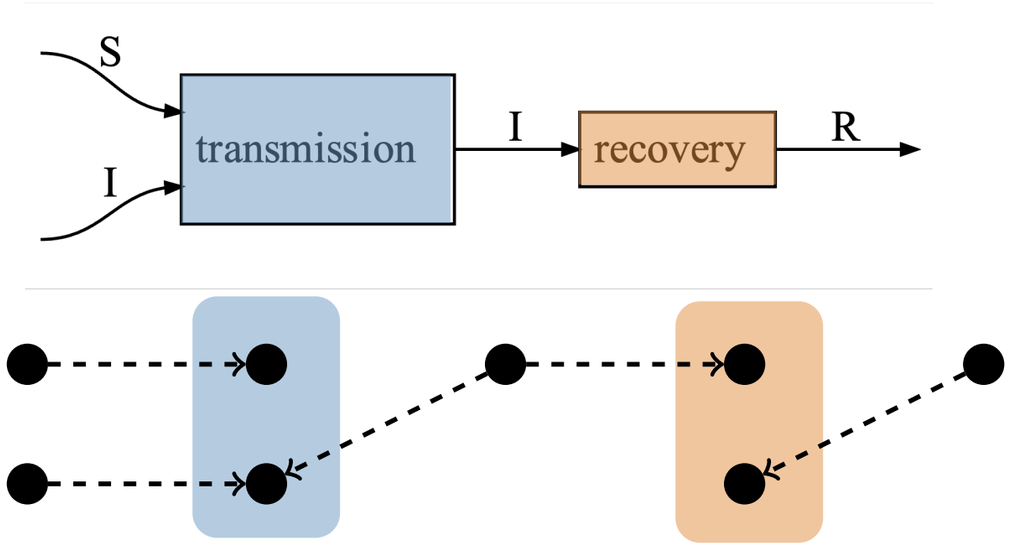
Petri Net Decorated Cospan Composition

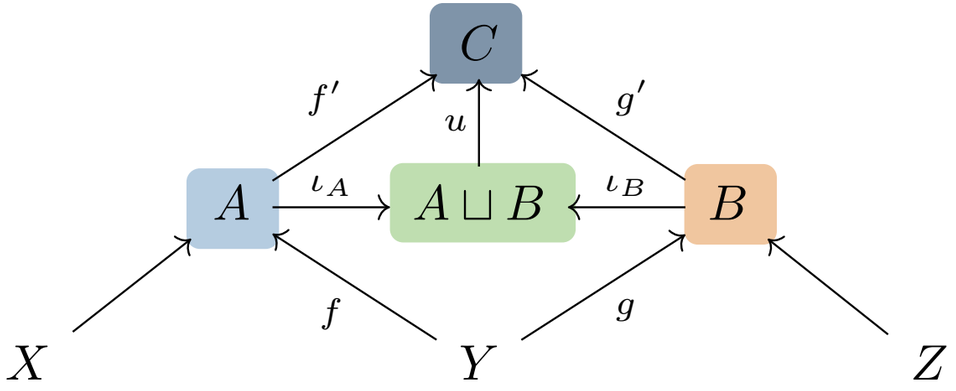


$$\begin{tikzcd}
 & & C & & \\
 & A \arrow[ur, "f'"] \arrow[r, "\iota_A"] & A \sqcup B \arrow[u, "u"] & B \arrow[ul, "g'"'] \arrow[l, "\iota_B"'] & \\
X \arrow[ur] & & Y \arrow[ul, "f"] \arrow[ur, "g"'] & & Z \arrow[ul]
\end{tikzcd}$$



Resource Sharing to Assign Kinetics





$$\begin{aligned}\dot{u}_1 &= -r_1 u_1 u_2\\ \dot{u}_2 &= r_1 u_1 u_2\end{aligned} \xrightarrow{\iota_A} \begin{aligned}\dot{u}_1 &= -r_1 u_1 u_2\\ \dot{u}_2 &= r_1 u_1 u_2\\ \dot{u}_3 &= -r_3 u_2\\ \dot{u}_4 &= r_3 u_2\end{aligned}$$

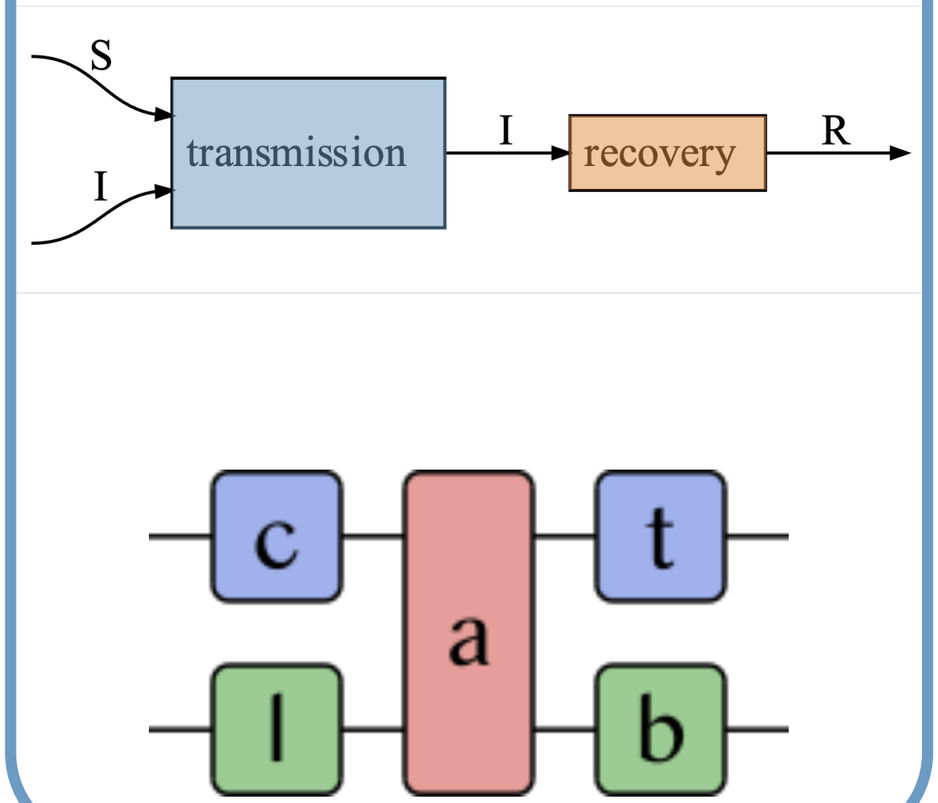
$$\begin{aligned}\dot{u}_1 &= -r_3 u_2\\ \dot{u}_2 &= r_3 u_2\end{aligned} \xrightarrow{\iota_B}$$

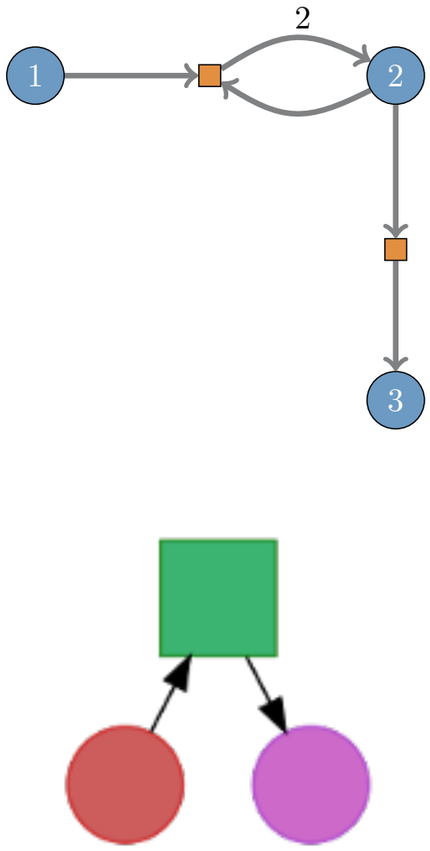
$$\xrightarrow{LFu} \begin{aligned}\dot{u}_1 &= -r_1 u_1 u_2\\ \dot{u}_2 &= r_1 u_1 u_2 - r_3 u_2\\ \dot{u}_3 &= r_3 u_2\end{aligned}$$

Functorial Modeling Pipeline

Georgia Tech Research Institute

$$Epi \xrightarrow{F} Petri \xrightarrow{K} Dynam$$





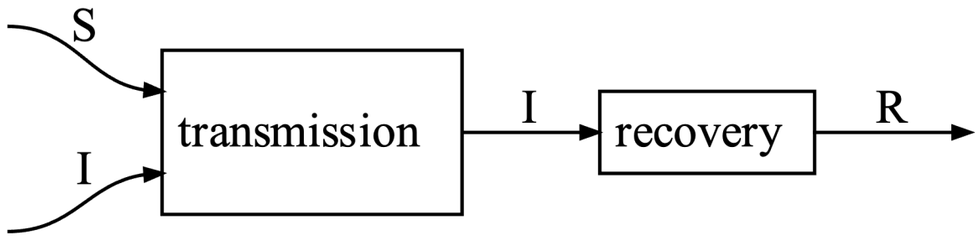
$$\dot{u}_1 = -r_1 u_1 u_2$$

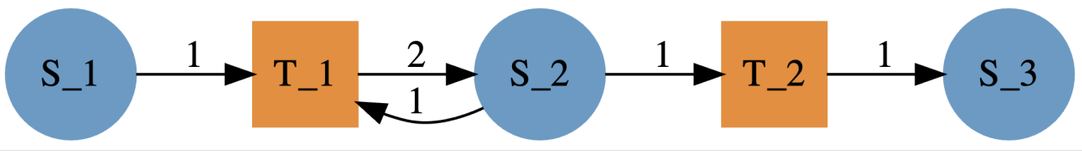
$$\dot{u}_2 = r_1 u_1 u_2 - r_3 u_2$$

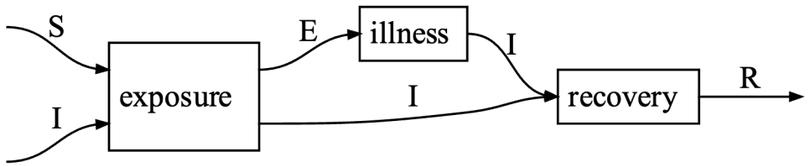
$$\dot{u}_3 = r_3 u_2$$

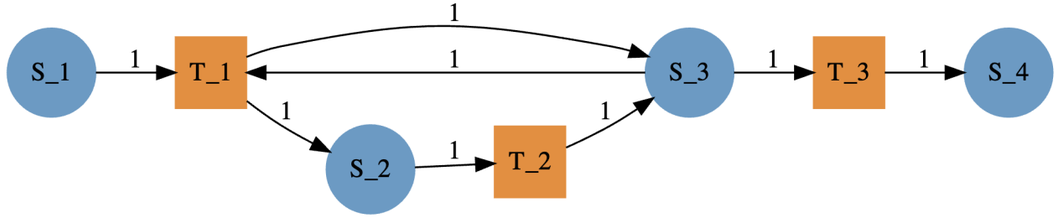
EpiModels: SIR, SEIR, SEIRD with Travel

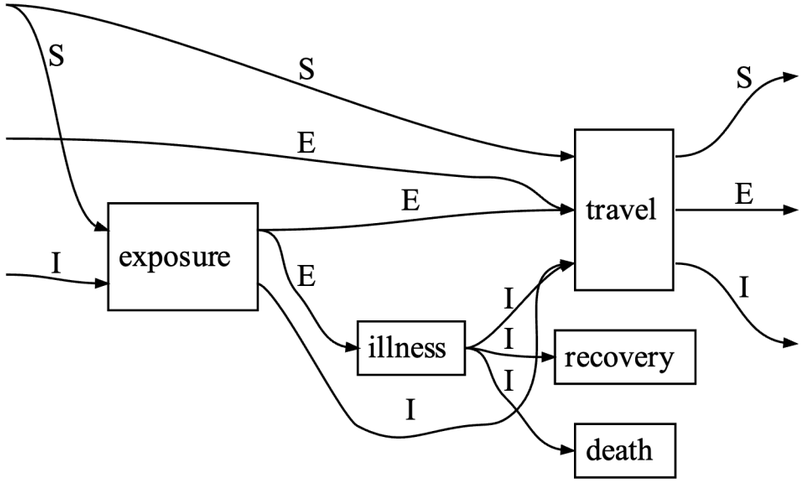
$$Epi \xrightarrow{F} Petri$$

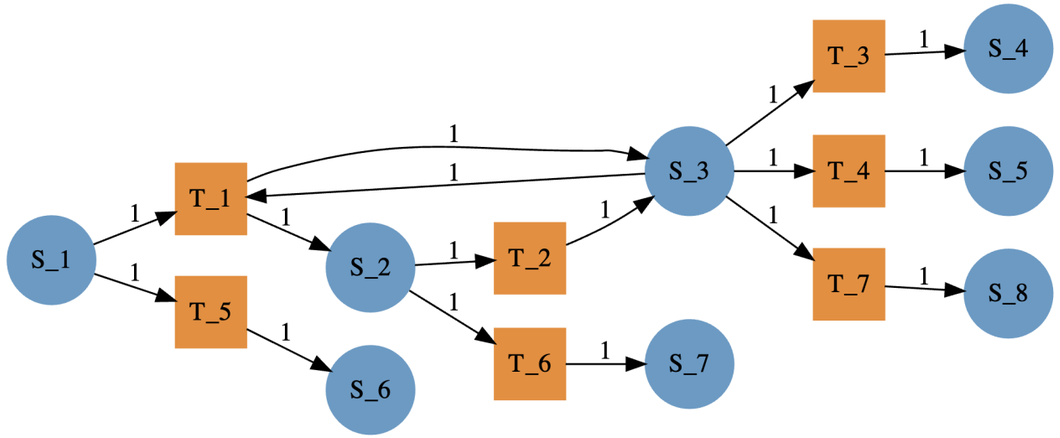








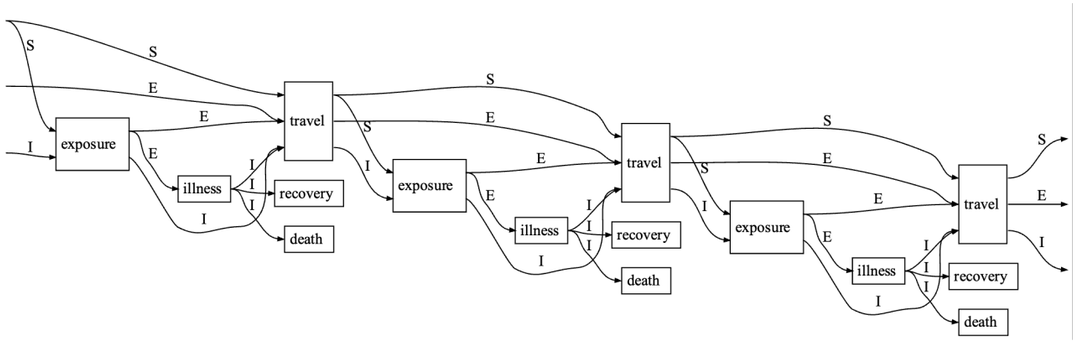


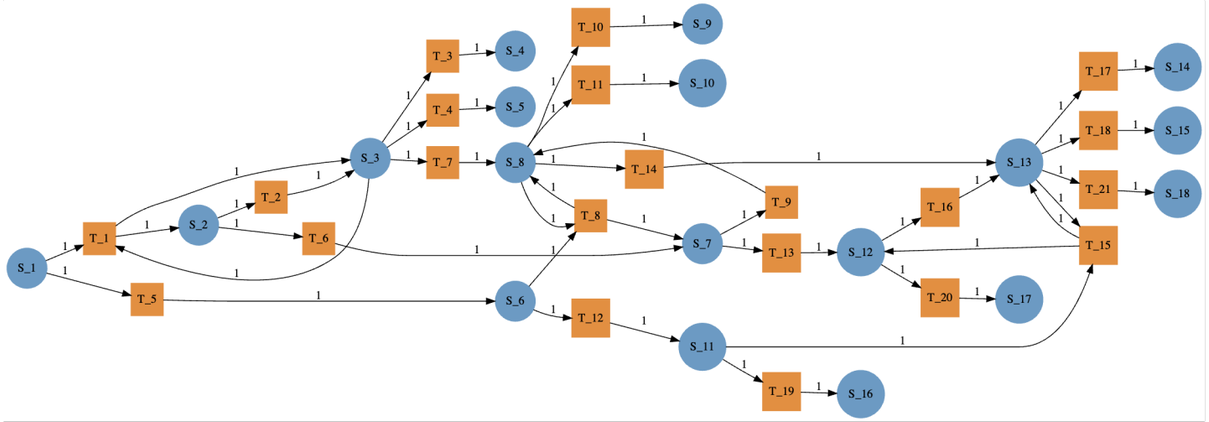


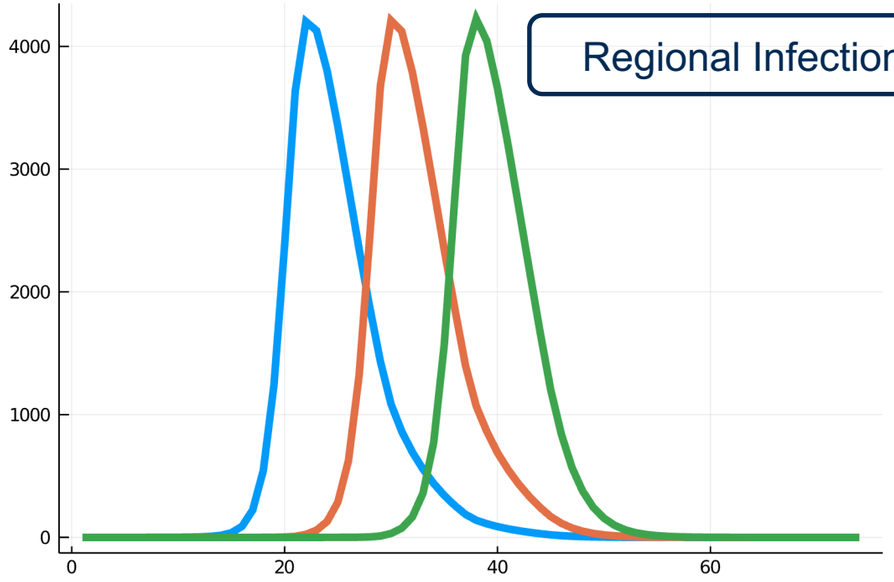
Superposition of Regions Yield Multi-peaks

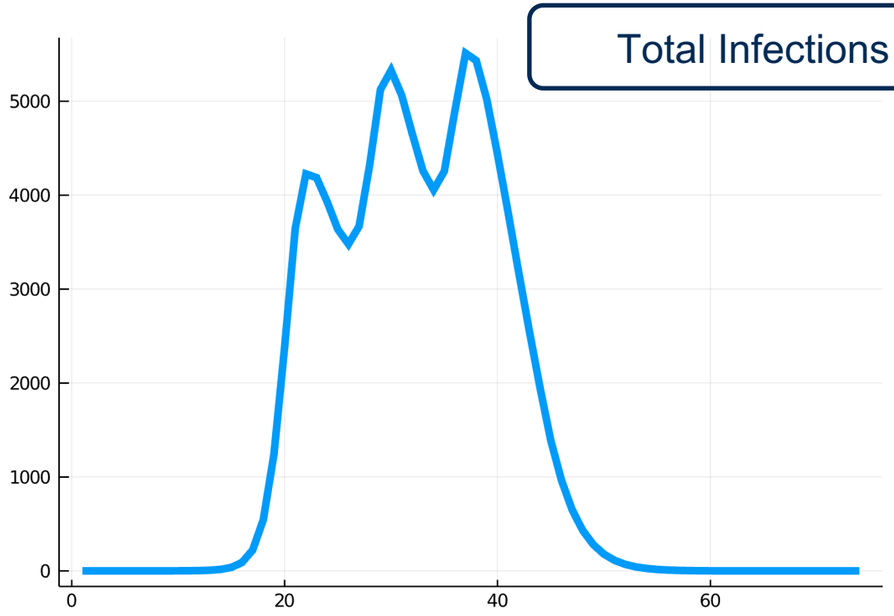
Georgia Tech Research Institute

```
seird_city = @program Epidemiology (s::S, e::E, i::I) begin
e2, i2 = exposure(s, i)
i3 = illness(e2)
d = death(i3)
r = recovery(i3)
return travel(s, [e, e2], [i2, i3])
end

^(f,n::Int) = fold(compose, repeat(f,n))
seird_3 = seird_city^3
```



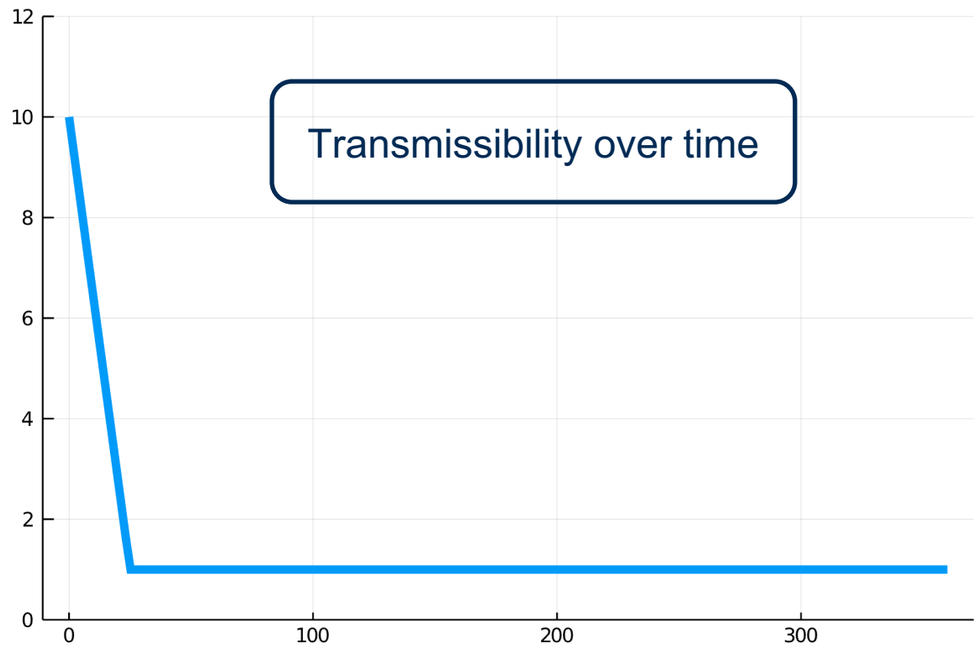


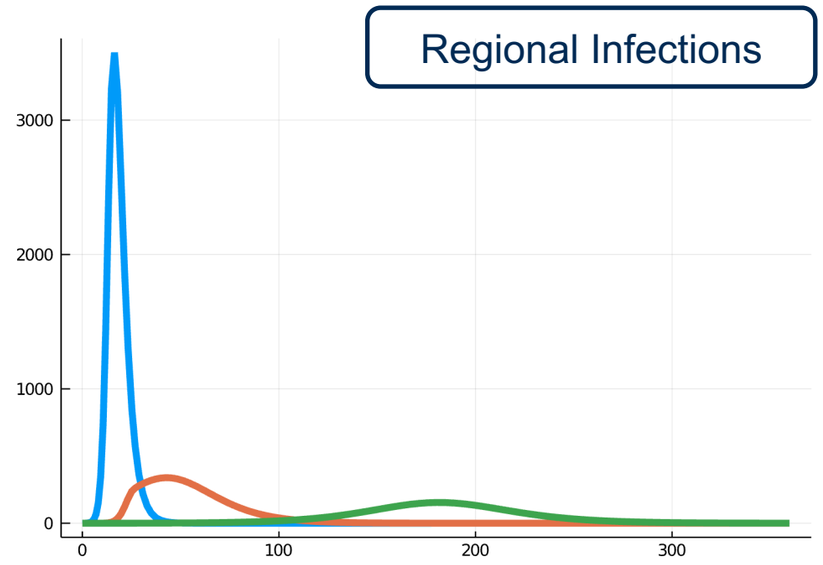


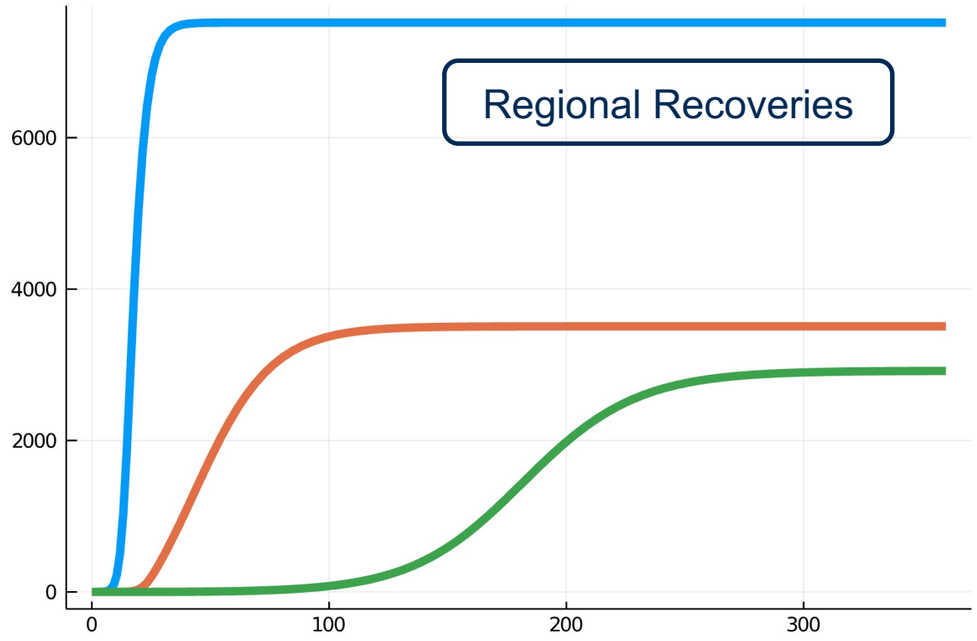


Flattening the Curve

Assuming this mitigation strategy, Region 3 “flattens the curve”



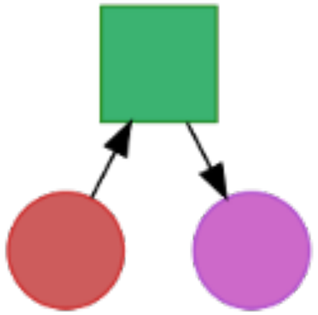




AlgebraicJulia Ecosystem

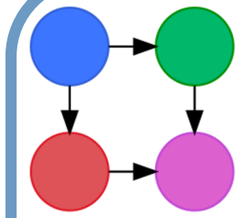
Georgia Tech Research Institute

Petri.jl

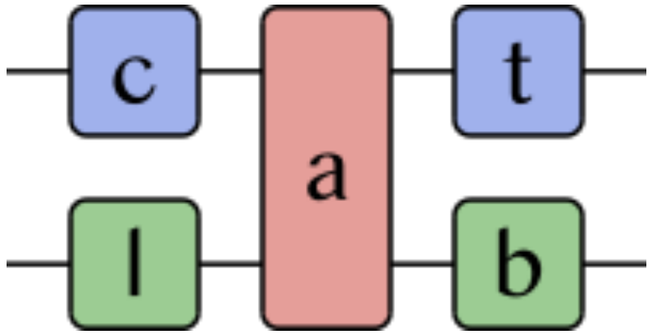


DiffEq.jl

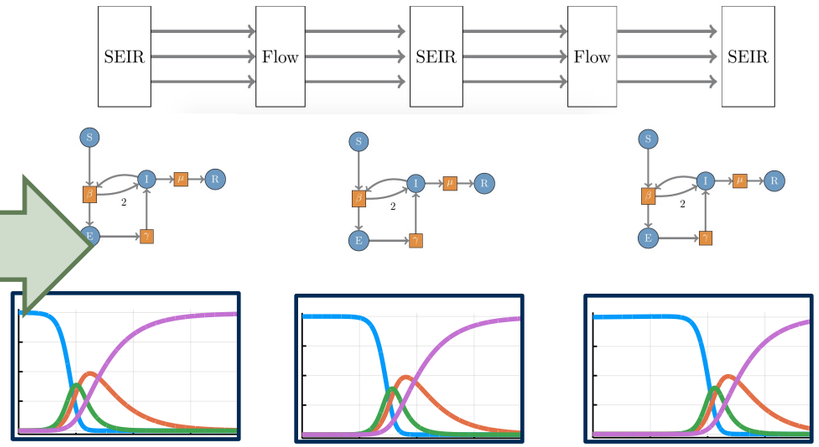
AlgebraicJulia

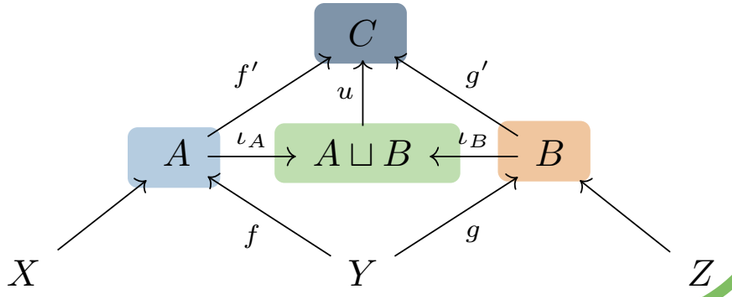


A, B, C	Types
$a : A, b : B, c : C$	Terms
$a \otimes b \cdot c$	Term Constructors
$(a \otimes b) \cdot (c \otimes d) = (a \cdot c) \otimes (b \cdot d)$	Axioms



Solvers exploiting hierarchical structure

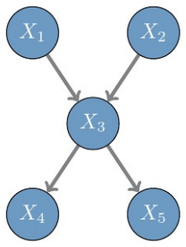




Modeling Frameworks use Graphs + Math

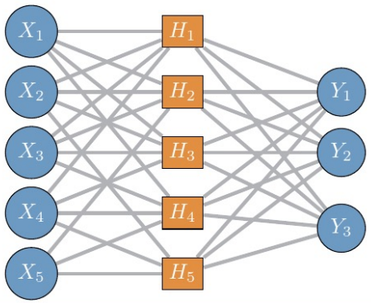
Georgia Tech Research Institute

Bayesian Network



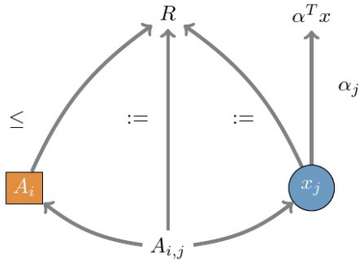
$P(X_4, X_5 \mid X_3)P(X_3 \mid X1, X_2)$

Neural Network



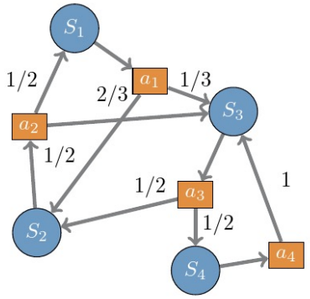
$\min \sum_i \ell_\theta(y, x)$

Optimization Problems



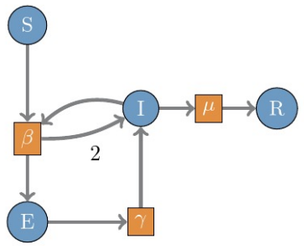
$\min_x \alpha^T x$ s.t. $Ax < b$

Markov Decision Process



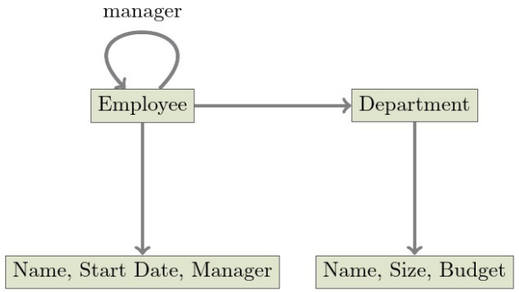
Construct $\pi : State \rightarrow Action$ maximizing $E[R]$

Petri Net



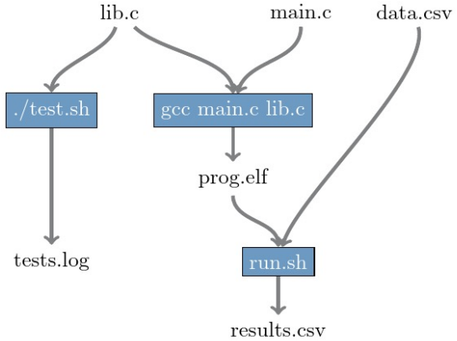
Law of Mass Action: $\dot{u} = f(u, t)$

Databases



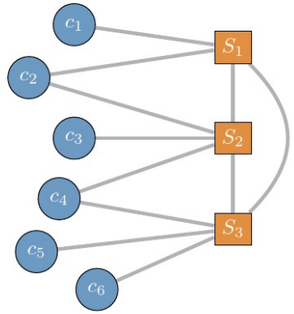
Relational Algebra

Dependency Graph



Scheduling and Compilation

Computer Network

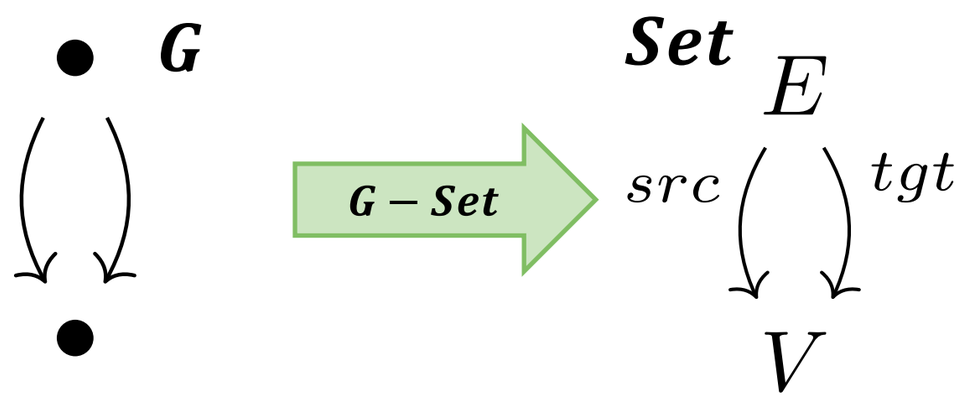


Bandwith, Latency, Routing

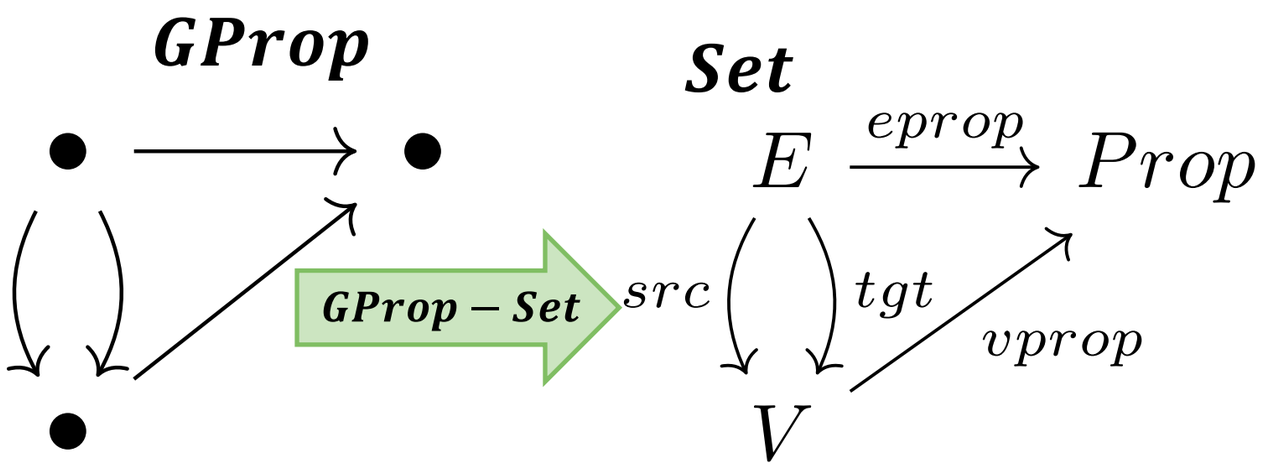
$\mathcal{C}$-Sets: Categorical Data Structures

Georgia Tech Research Institute

Logically extending a data structure with ACT principles

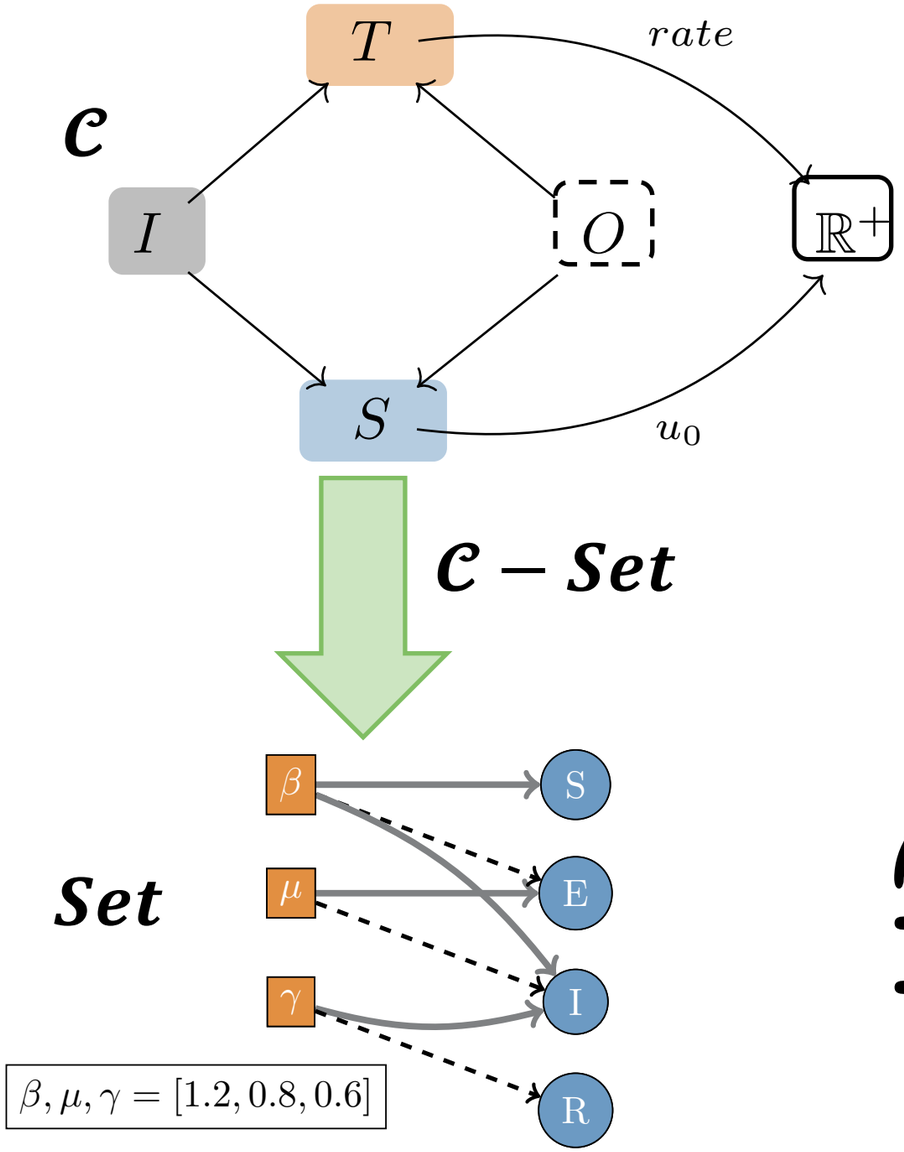



```
@present TheoryGraph(FreeCategory) begin
V::Ob
E::Ob
src::Hom(E,V)
tgt::Hom(E,V)
end
Graph = CSetType(TheoryGraph)
```



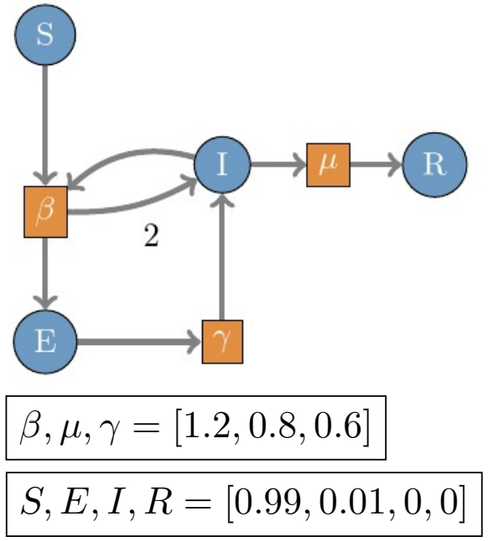

```
@present TheoryPropertyGraph <: TheoryGraph begin
Prop::Ob

vprops::Hom(V,Prop)
eprops::Hom(E,Prop)
end

PropertyGraph = CSetType(TheoryPropertyGraph)
```

$\mathcal{C}$-Sets: Categorical Data Structures

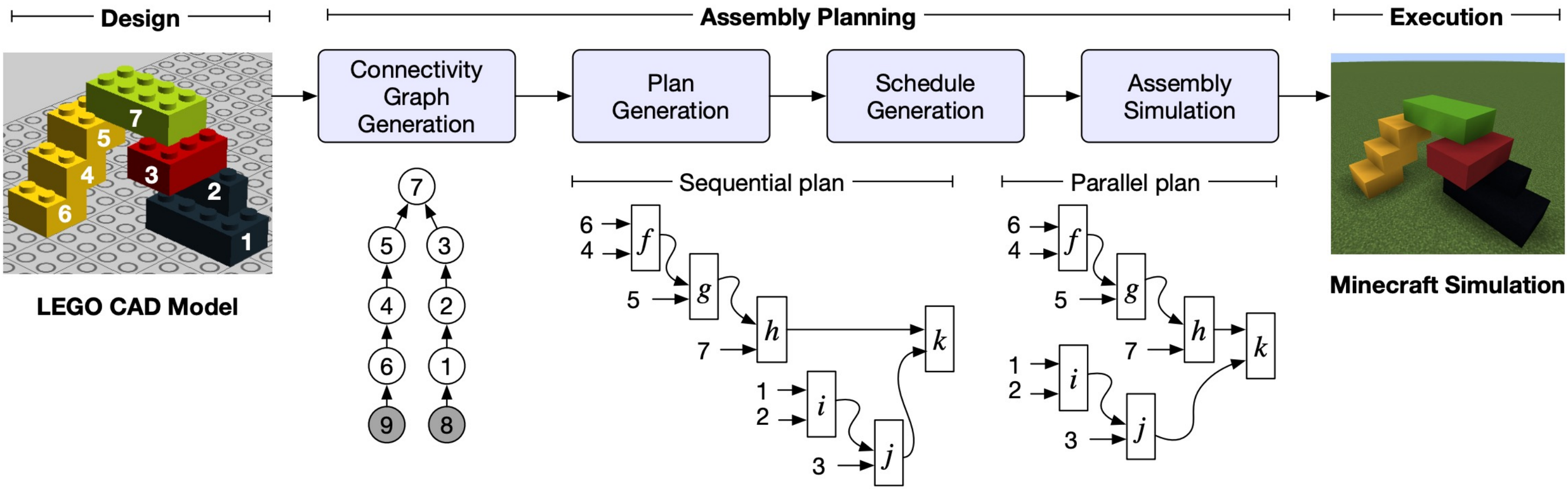


- The data structure is a directed graph
- Instances are Sets with Functions
- Provides compositional framework for structured data
- Mathematically Elegant

$\cong$



Compositional Planning

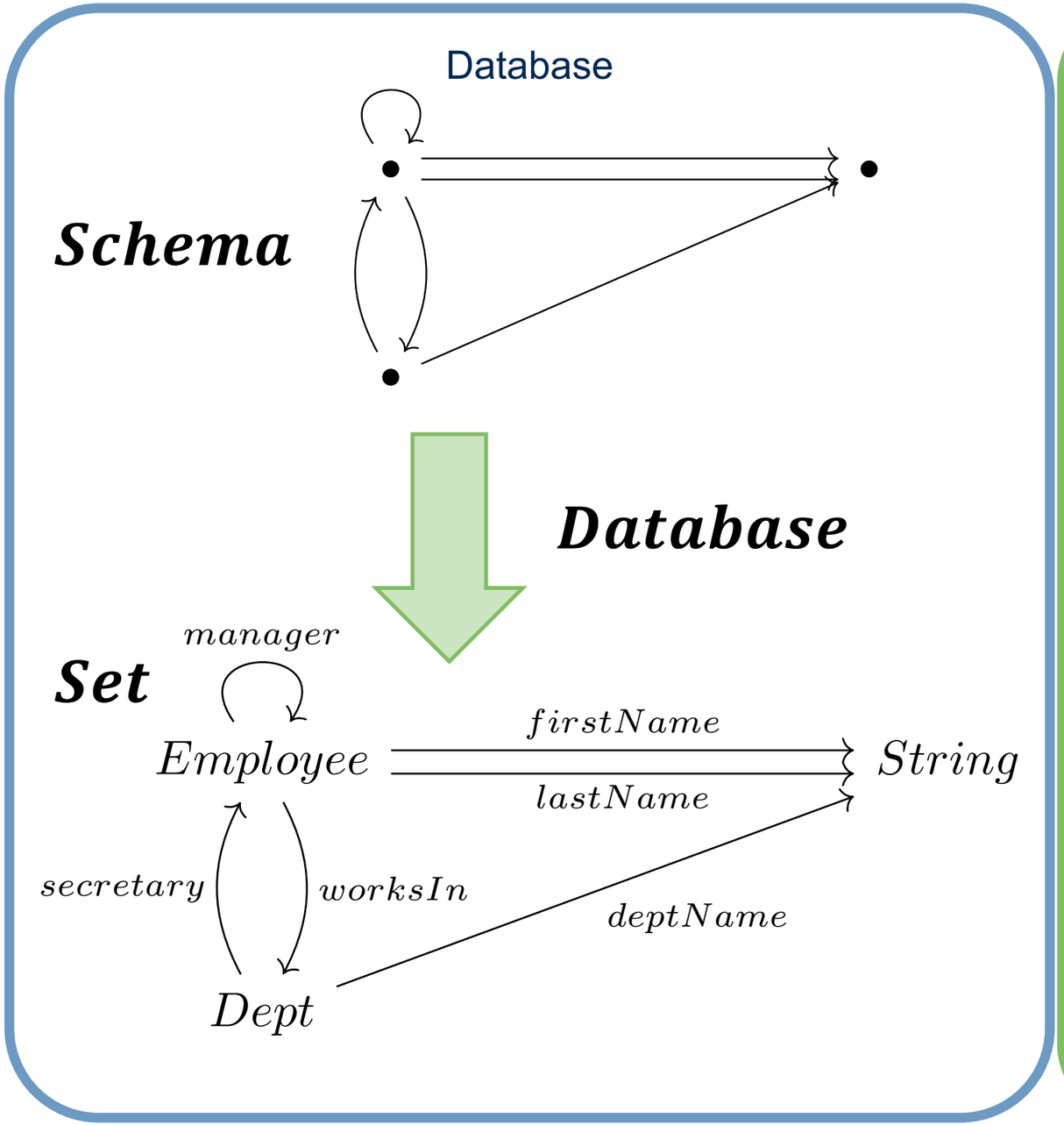


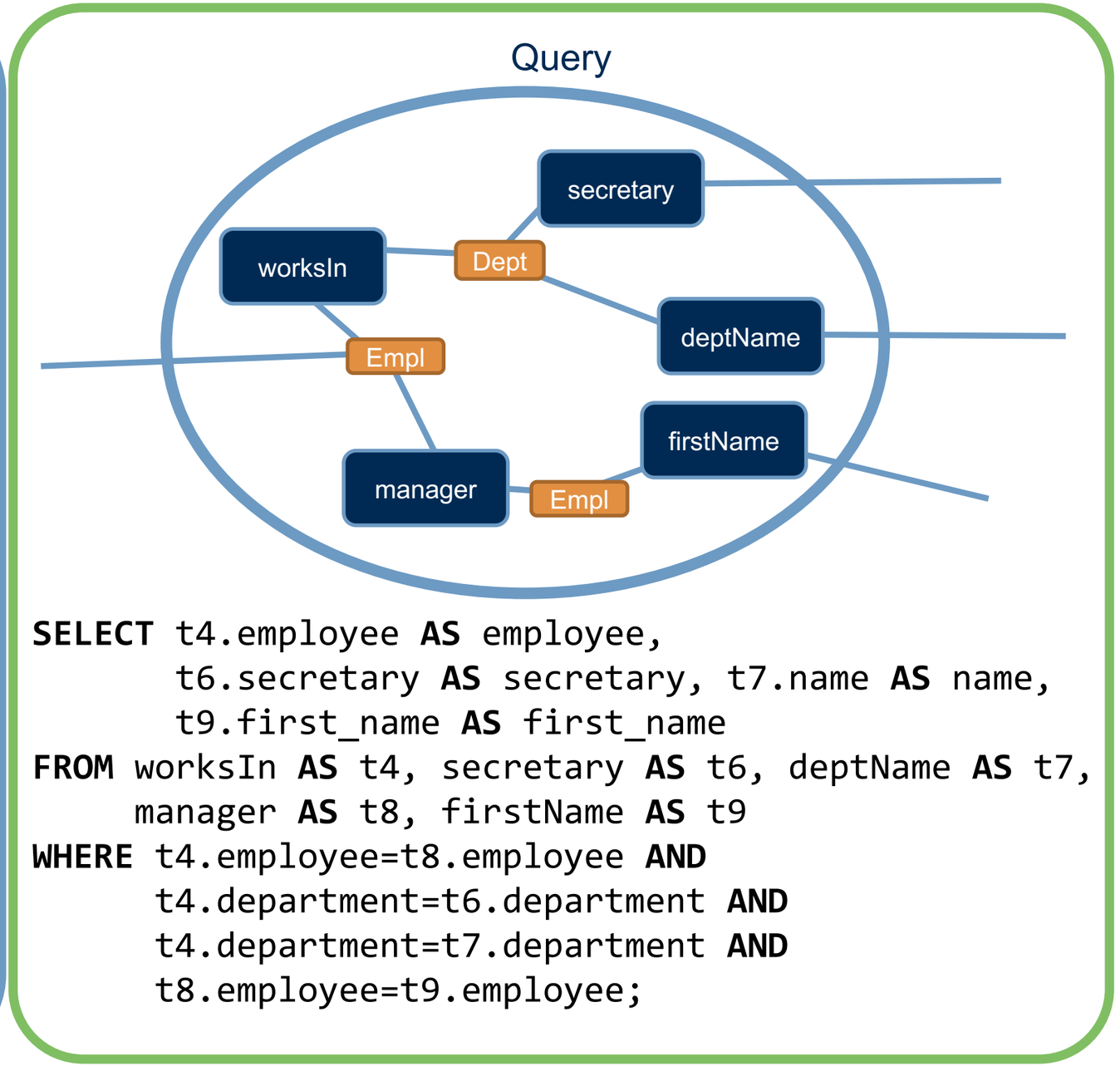
Automatic parallelization and optimization of construction plans

(Master, Patterson, Yousfi & Canedo, 2020)

Generating SQL Queries from *BiCatRel*

Georgia Tech Research Institute






```
SELECT t4.employee AS employee,
       t6.secretary AS secretary, t7.name AS name,
       t9.first_name AS first_name
FROM worksIn AS t4, secretary AS t6, deptName AS t7,
     manager AS t8, firstName AS t9
WHERE t4.employee=t8.employee AND
      t4.department=t6.department AND
      t4.department=t7.department AND
      t8.employee=t9.employee;
```

Three Layers of GAT Based Modeling

Georgia Tech Research Institute

Theory

$$A, B, C$$

$$a : A, b : B, c : C$$

$$a \otimes b \cdot c$$

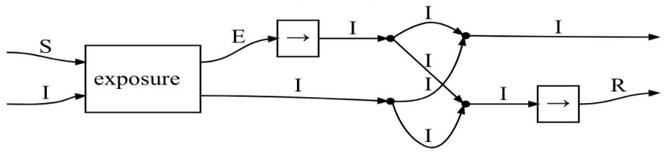
$$(a \otimes b) \cdot (c \otimes d) = (a \cdot c) \otimes (b \cdot d)$$

Syntax

Formula Notation

$$seir = expo \cdot (f_{E,I} \otimes id_I) \cdot \nabla_I \cdot \Delta_I \cdot (id_I \otimes f_{I,R})$$

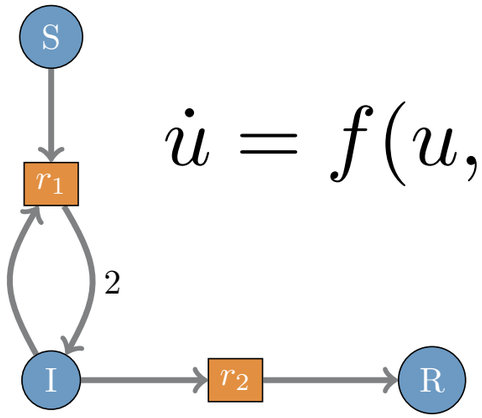
Wiring Diagram



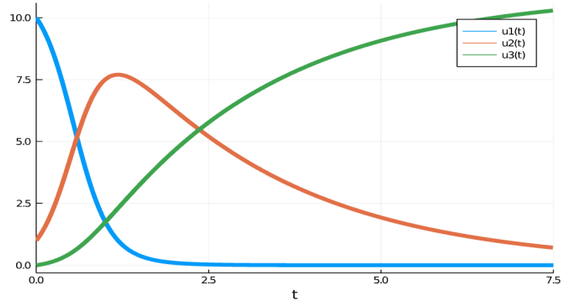
Embedded Domain Specific Language

```
d = @program Disease (s::S, e::E, i::I) begin
    e1, i1 = exposure{S,I,E}(s,i)
    i2 = spontaneous{E,I}(e1)
    e = [e, e1]
    e_out = spontaneous{E,E}(e)
    i1 = [i1, i2]
    r = spontaneous{I,R}(i1)
    s_out = spontaneous{S,S}(s)
    return s_out, e_out, spontaneous{I,I}(i1)
end
```

Instance



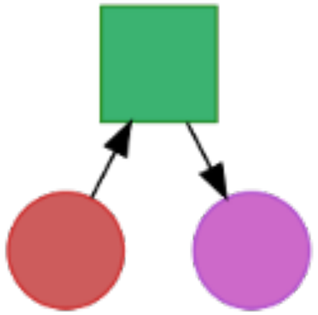
$$\dot{u} = f(u, t)$$



AlgebraicJulia Ecosystem

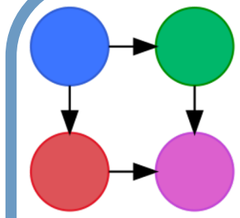
Georgia Tech Research Institute

Petri.jl



DiffEq.jl

AlgebraicJulia



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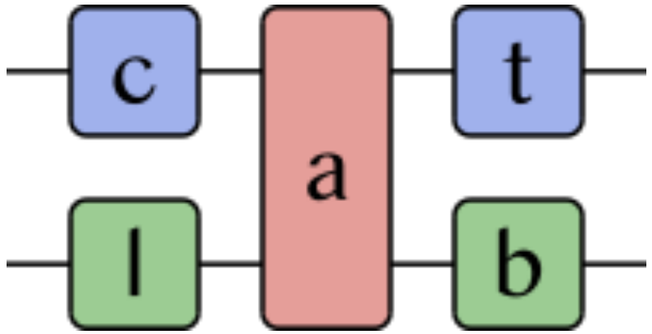
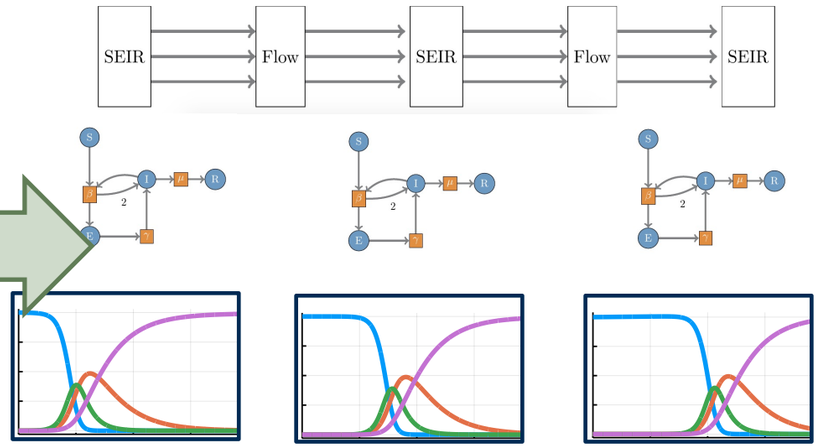
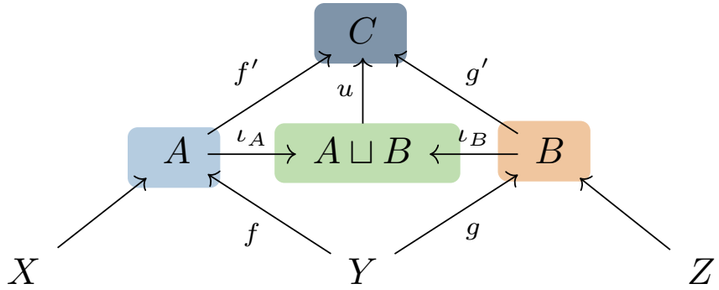


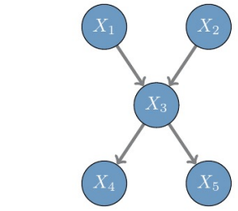
Solvers exploiting hierarchical structure

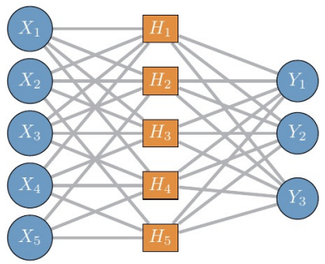


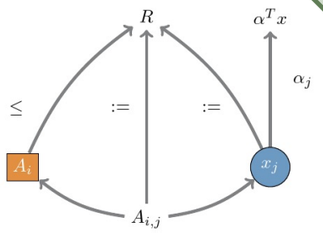


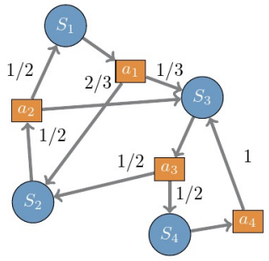
Model Aware Scientific Computing Vision

Georgia Tech Research Institute

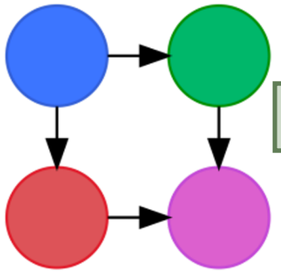




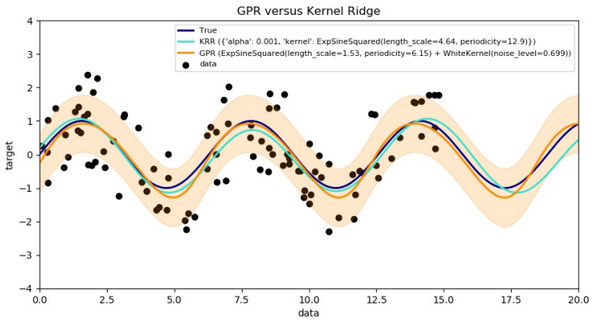


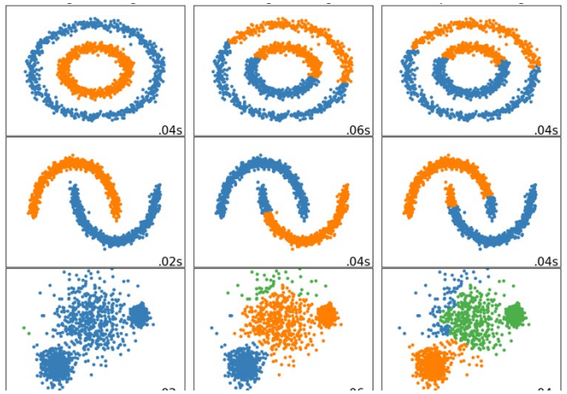


AlgebraicJulia



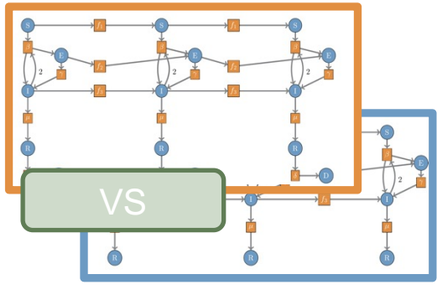
Model Specific Tools for Scientists



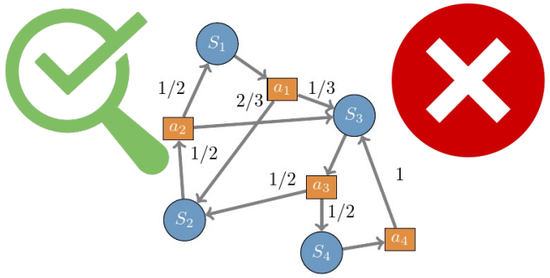


Calibration

Selection



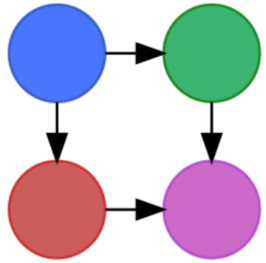
Comparison



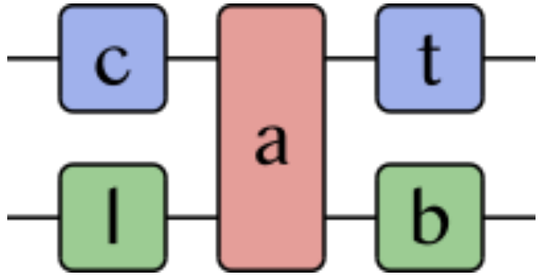
Verification & Validation

AlgebraicJulia Team

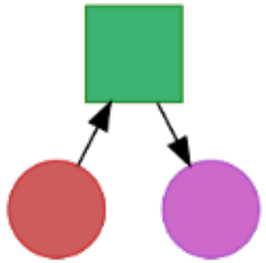
Georgia Tech Research Institute



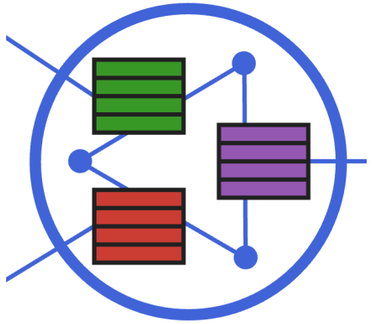
AlgebraicJulia



Catlab.jl



Petri.jl



AlgebraicRelations.jl

Evan Patterson

Micah Halter

Sophie Libkind

Andrew Baas