Scientific Modeling with Categories

7/7/2025

James Fairbanks

$$\begin{tikzcd} G \arrow[r] \arrow[d] \arrow[dr, phantom, "\Downarrow\tau"] & A \arrow[d] \\ A \arrow[r] & S \end{tikzcd}$$

Spectrum of Scientific Computing Technology

Programs that have explicit representations of the model

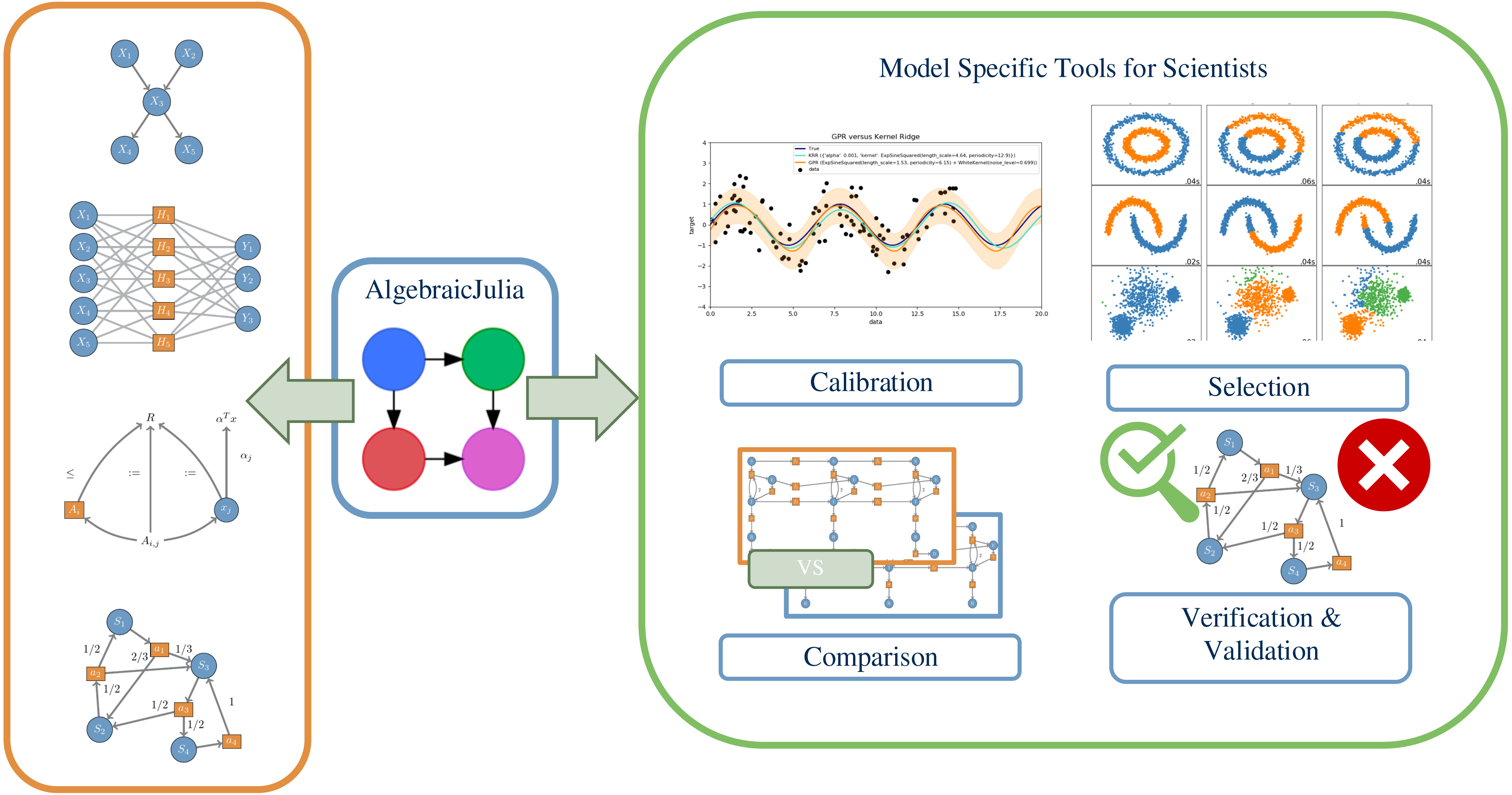
Arbitrary Code

Domain Specific Languages

Modeling Frameworks

Computer Algebra Systems

Vision: Model Aware Scientific Computing with Categories



Two Paths to Applying Category Theory to Scientific Computing

$$\begin{tikzcd}
P_{\mathsf{stratified}} \arrow[r, dashed] \arrow[d, dashed] \arrow[dr, phantom, "\lrcorner", very near start] & P_{\mathsf{strata}} \arrow[d] \\
P_{\mathsf{disease}} \arrow[r] & P_{\mathsf{infectious}}
\end{tikzcd}
\qquad
\begin{tikzcd}
\mathrm{Petri} \arrow[r, "kinetics"] \arrow[dr, "sim"'] & \mathrm{Dynam} \arrow[d, "rk"] \\
& \mathrm{DDS}
\end{tikzcd}$$

$$\begin{tikzcd}
\text{Math} \arrow[r, "\text{ACT}"] \arrow[d, "\text{formalization}"'] & \text{CT} \arrow[d, "\texttt{AlgebraicJulia}"] \\
\text{Logic} \arrow[r, "\texttt{Func. Prog.}"'] & \texttt{Code}
\end{tikzcd}$$

```julia
function stratify(disease::Petri, strata::Petri)
  stratified = pullback(disease, strata)
  return object(stratified)
end
function sim(P::Petri)
  prob = ODEProblem(kinetics(P))
  return solve(prob, (t₀,tₑ), alg=RungeKutta())
end
```

$$\frac{x : \sigma \in \Gamma}{\Gamma \vdash_D x : \sigma}$$

$$\frac{\Gamma \vdash_D e_0 : \tau \to \tau' \qquad \Gamma \vdash_D e_1 : \tau}{\Gamma \vdash_D e_0\ e_1 : \tau'}$$

$$\frac{\Gamma,\ x : \tau \vdash_D e : \tau'}{\Gamma \vdash_D \lambda\, x\,.\ e : \tau \to \tau'}$$

```haskell
rungekutta:: Float -> Float -> Float
f:: Float -> Float -> Float
scanl::(a -> a -> a) -> (a,a) -> List a -> List a
rungekutta (t, y) t' = (t', y + h*(k1 + 2.0*k2 + 2.0*k3 + k4)/6.0)
  where
  h = t' - t
  k1 = f t y
  k2 = f (t + 0.5*h) (y + 0.5*h*k1)
  k3 = f (t + 0.5*h) (y + 0.5*h*k2)
  k4 = f (t + 1.0*h) (y + 1.0*h*k3)

f t y = (t**2 - y**2)*sin(y)
scanl rungekutta (0, -1) [0.01, 0.03, 0.04, 0.06]
```

Operad Algebras of Dynamical Systems

Operad Algebra

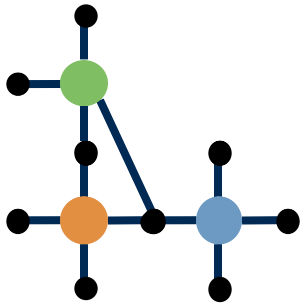
Compose and then Apply

=

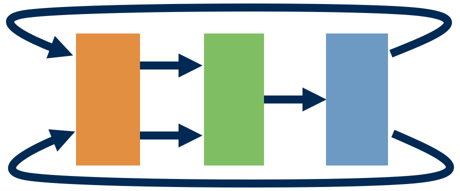
Apply and then Compose

- An Operad defines a *way of composing*
- Operads form a Category
- Functors from an Operad O to Set are *Operad Algebras or Algebras of O*
- *Dynam* ⊂ *Set* has sets of dynamical systems as objects
- Analogous to *Group Actions*

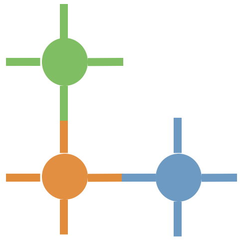
$$\mathcal{O} \xrightarrow{F} Set$$



$$\xrightarrow{\text{Resource Sharing}} Dynam$$



$$\xrightarrow{\text{Machines}} Dynam$$

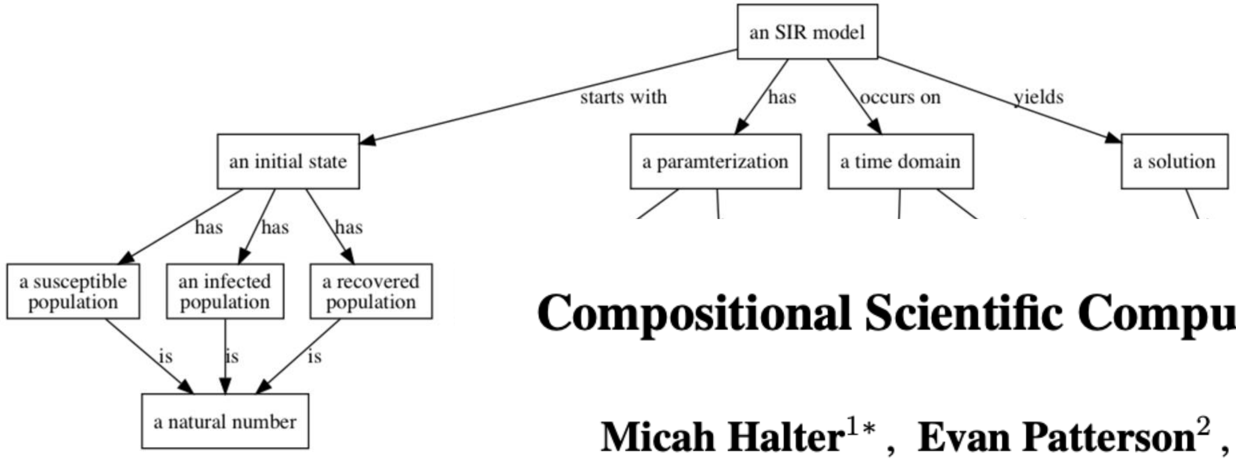


$$\xrightarrow{\text{Method of Lines}} Dynam$$

DARPA ASKE: Layers of Modeling

UF

1) Structural knowledge layer



3) Model semantics layer

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

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

Compositional Scientific Computing with Catlab and SemanticModels

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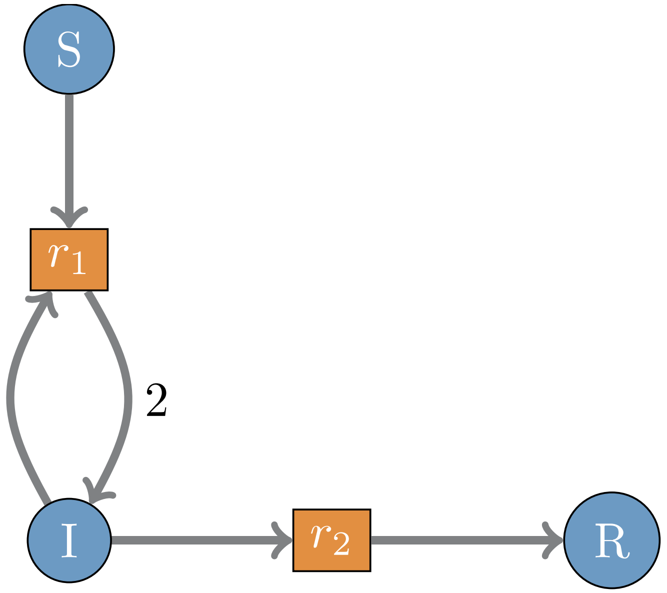
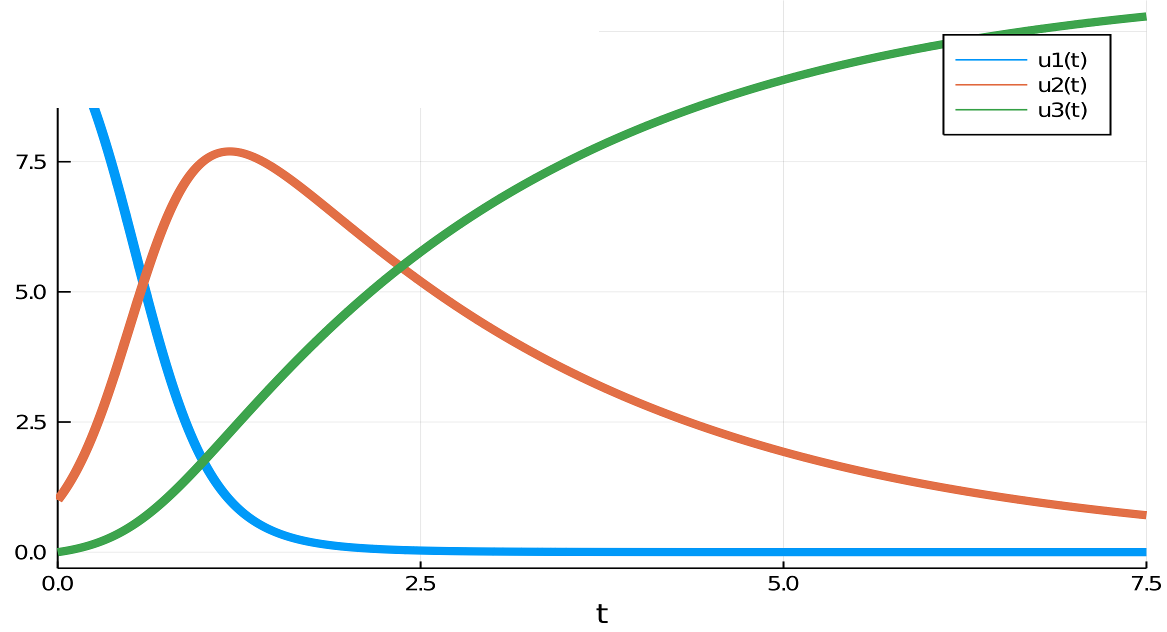
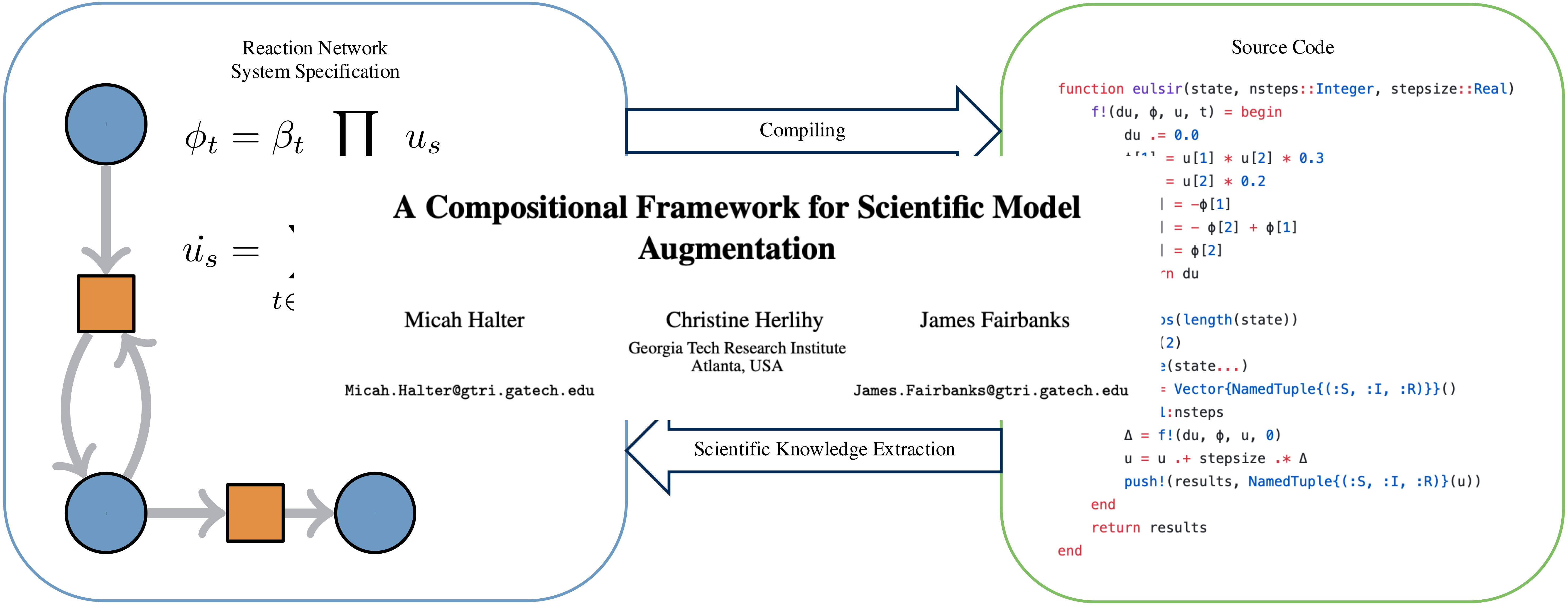
2) System



olution layer



DARPA ASKE: Scientific Knowledge Extraction

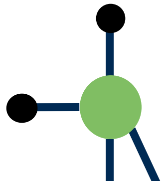


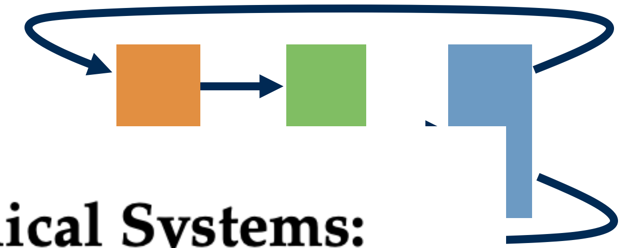
Extracting Knowledge from legacy simulators

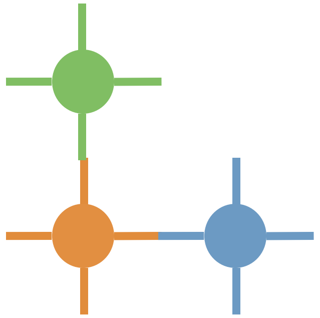
to accelerate adaptation and discovery

Landscape of Composition

Operads implement[…]
with ACSets







Operadic Modeling of Dynamical Systems: Mathematics and Computation

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Operad Algebras

ines

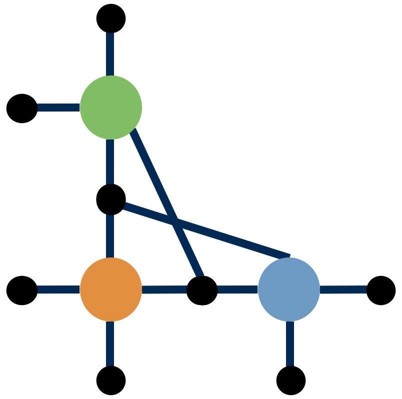
FDTD

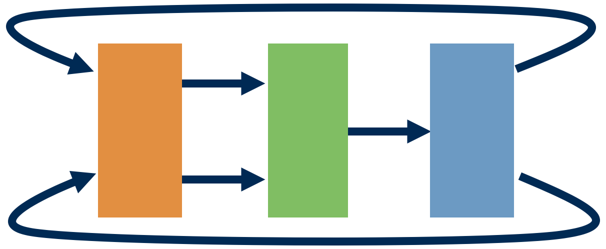
Dynamical Systems (ODEs)

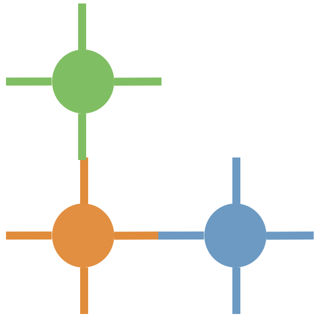
$$\begin{bmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \dot{u}_3 \end{bmatrix} = f\left(\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}\right)$$

Application Achievement: Solving ODEs and PDEs

Languages for Hierarchical System Descriptions







Variable Sharing (Biology)

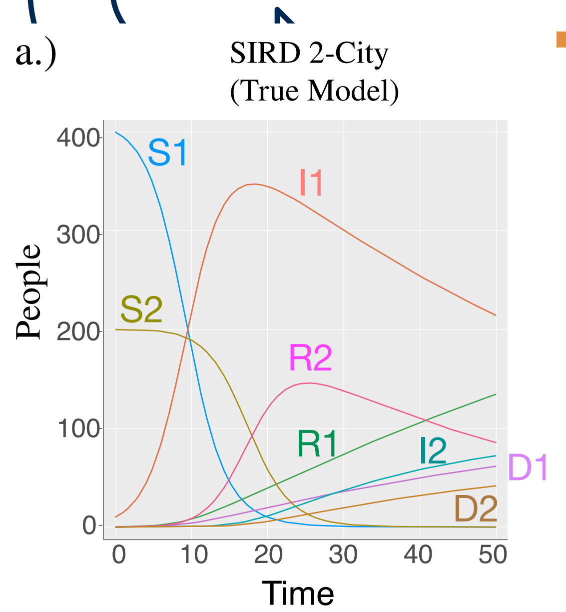
Signal Flow (Electronics / Controls)

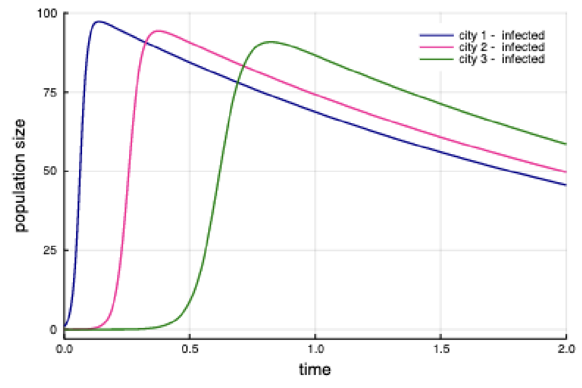
FEM/Stencils (Physics)

Mathematical Interpreters

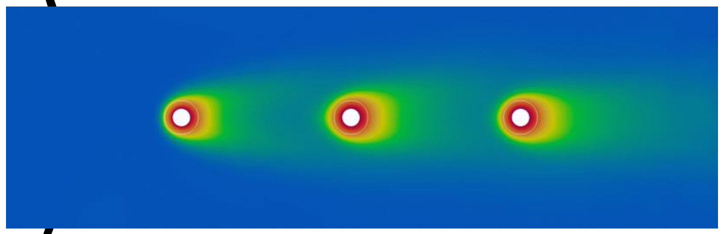
Common Dynamical Systems Se

Support simulation with existing



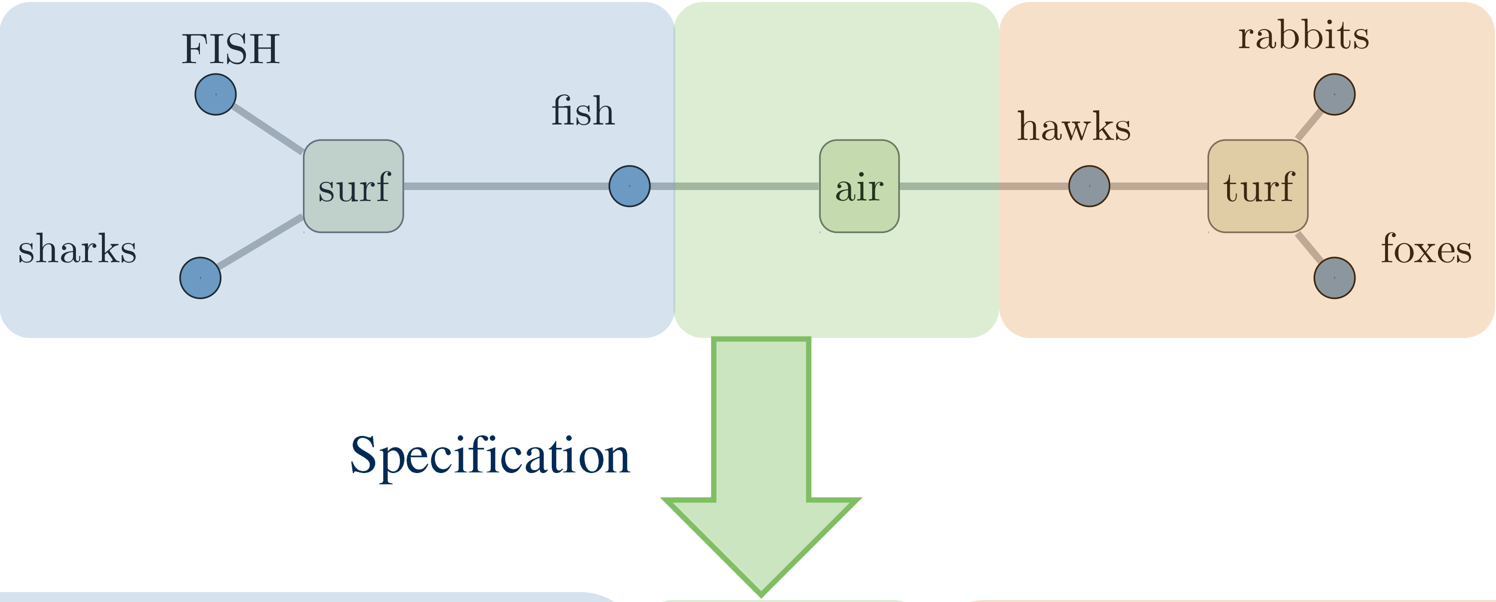


(a)

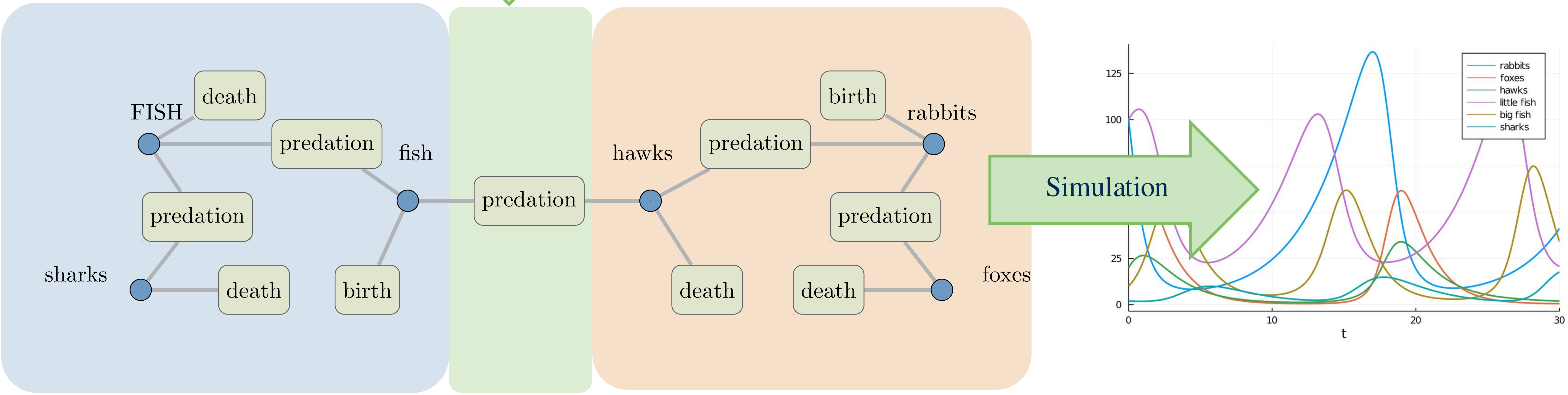


Operadic Modeling of Dynamical Systems: Mathematics and Computation, S. Libkind, A. Baas, E. Patterson, J. Fairbanks, *Applied Category Theory* Proceedings 2021

Hierarchy is a Fundamental Tool for Understanding



Can we combine denotational semantics and network science to understand hierarchical structures in complex systems?

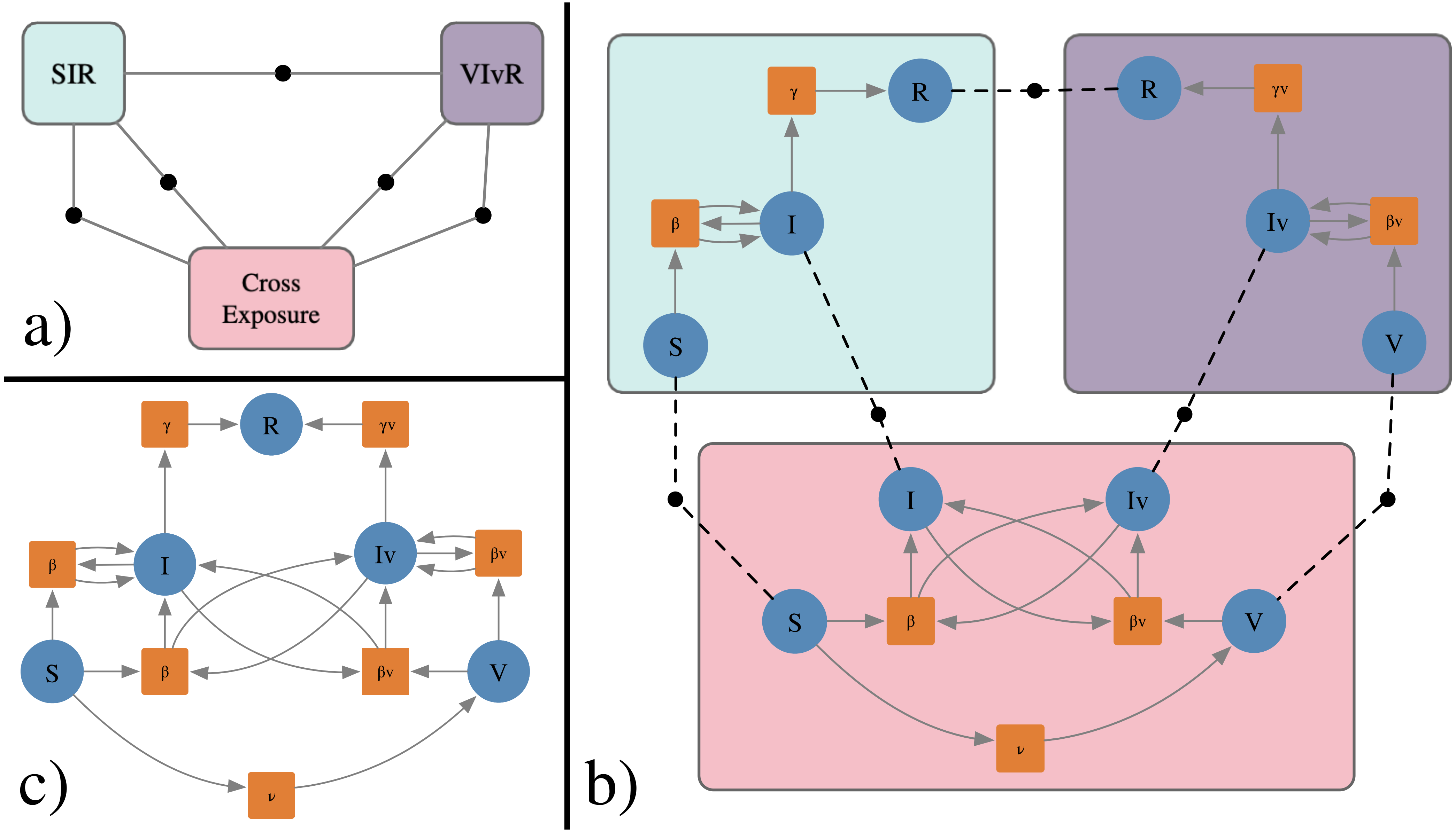


Composing Compartmental Models with UWDs

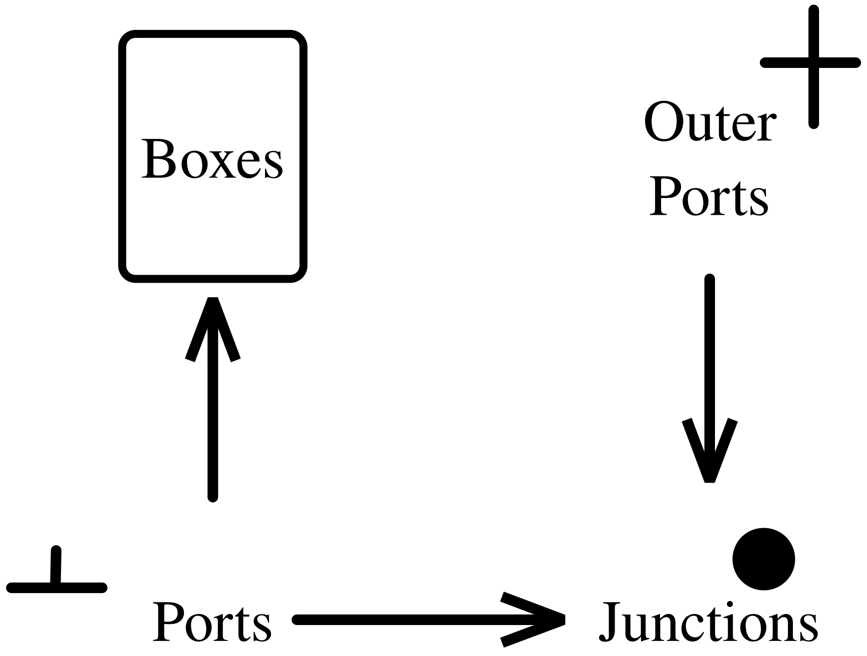
a) Pattern of shared variables between subsystems

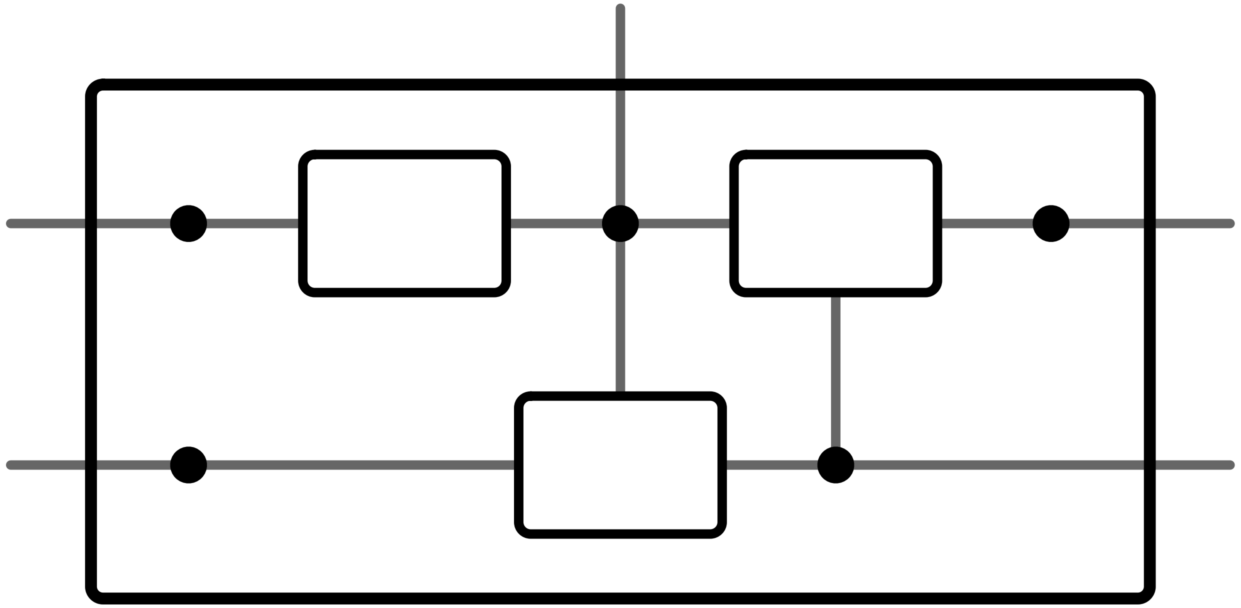
b) The component subsystems

c) The composite system



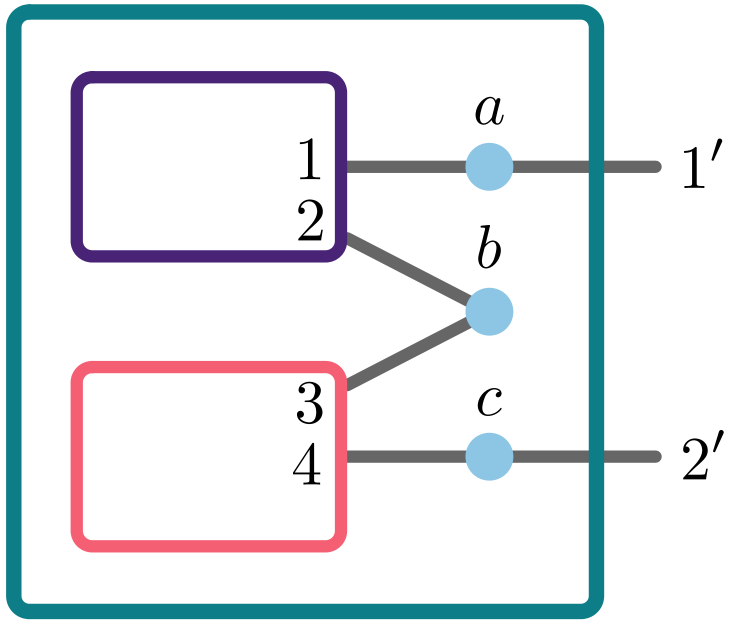
Undirected Wiring Diagrams

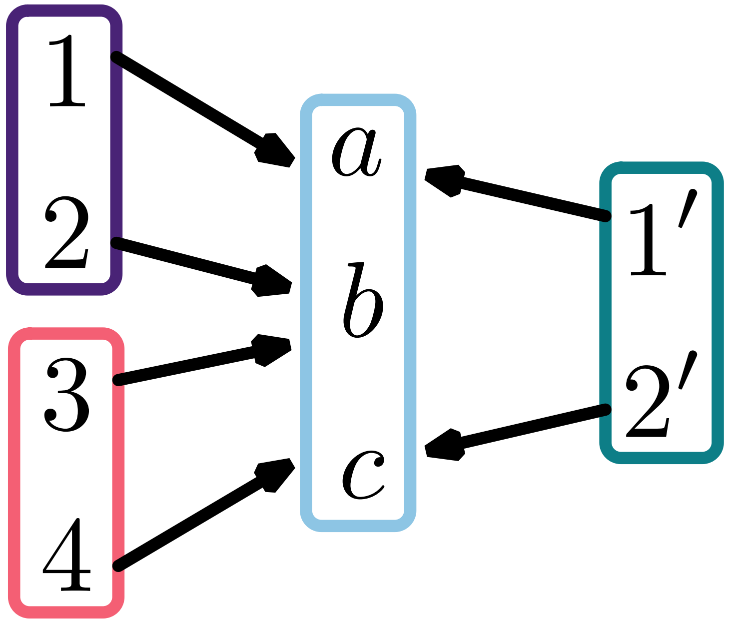




- UWDs provide a syntax for systems that compose without orientation
- No distinction between inputs vs outputs just interfaces

Undirected Wiring Diagrams





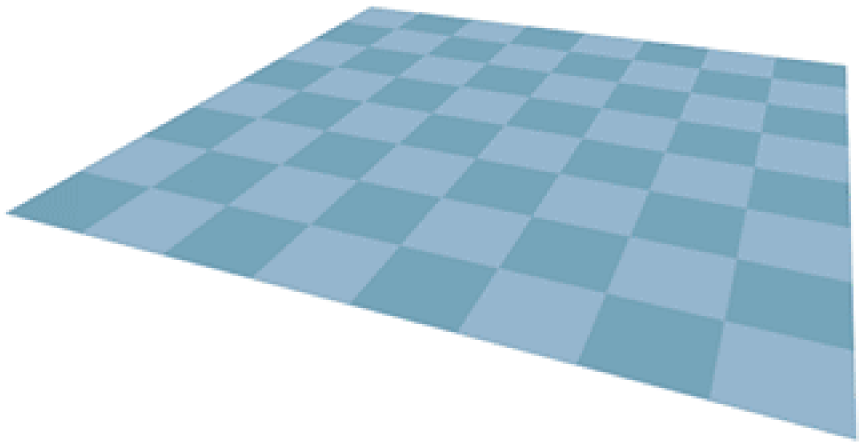
- UWDs provide a syntax for systems that compose without orientation
- No distinction between inputs vs outputs just interfaces

Colimits build large objects by gluing

- The torus is a colimit by gluing the edges together with coequalizers
- Coequalizers are a standard form of merging parts of an object together with an equivalence relation

$$\begin{tikzcd} {[0,1]} \arrow[r, shift left, "top"] \arrow[r, shift right, "bottom"'] & {[0,1]^2} \arrow[r, "K"] & {[0,1] \times S_1} \end{tikzcd}$$

$$\begin{tikzcd} S_1 \arrow[r, shift left, "left"] \arrow[r, shift right, "right"'] & {[0,1] \times S_1} \arrow[r] & \mathbb{T} = S_1 \times S_1 \end{tikzcd}$$

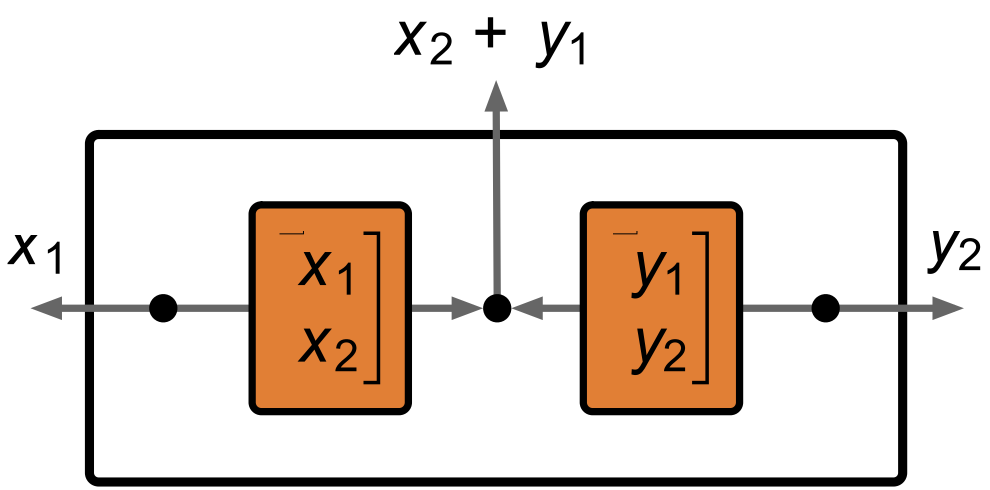


https://upload.wikimedia.org/wikipedia/commons/6/60/Torus_from_rectangle.gif

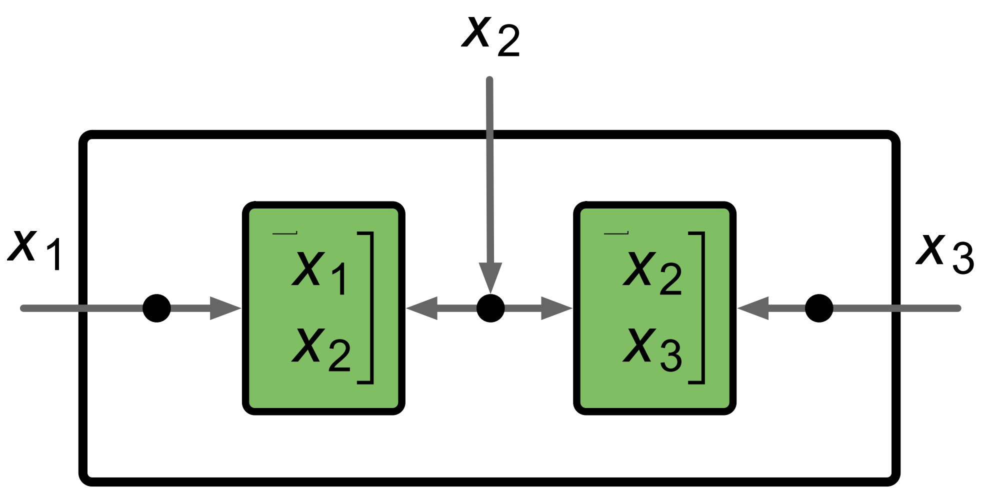
Information Flow For Composite Systems

- The simplest notion of system on n variables is just vectors
- We combine systems with linear maps that merge/share information

A.



B.

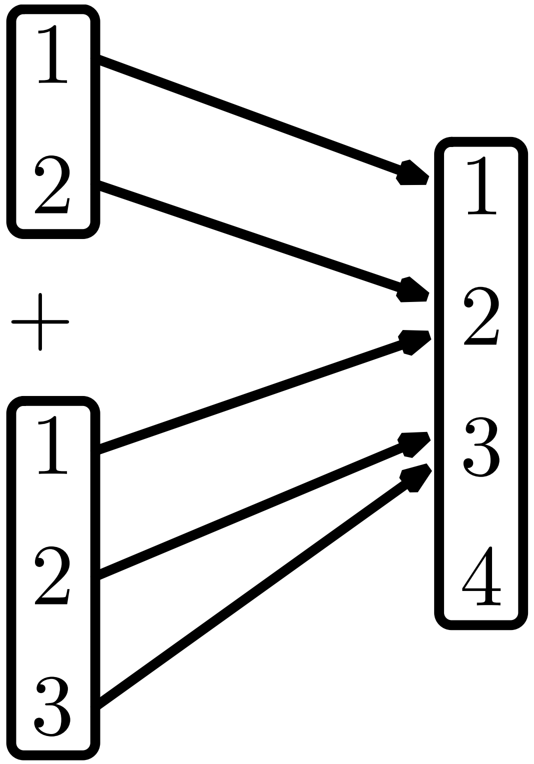


$$\Phi_{\leftarrow}\left((x_1, x_2), (y_1, y_2)\right) = (x_1, x_2 + y_1, y_2) \qquad \Phi^{\leftarrow}(x_1, x_2, x_3) = \left((x_1, x_2), (x_2, x_3)\right)$$

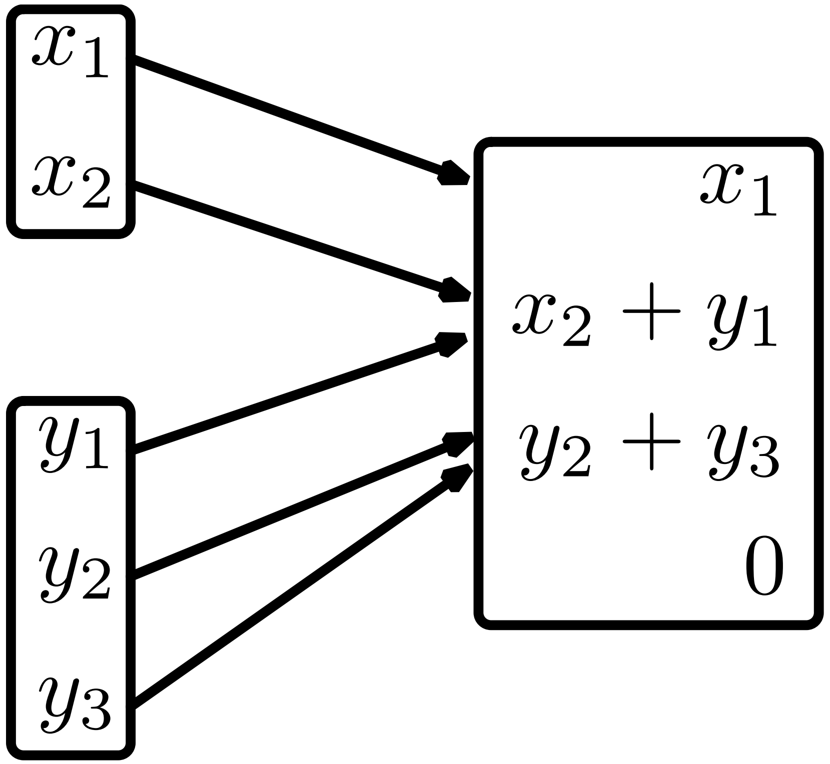
$$M(\Phi_{\leftarrow}) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad M(\Phi^{\leftarrow}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = M(\Phi_{\leftarrow})^T$$

Information Flow For Composite Systems

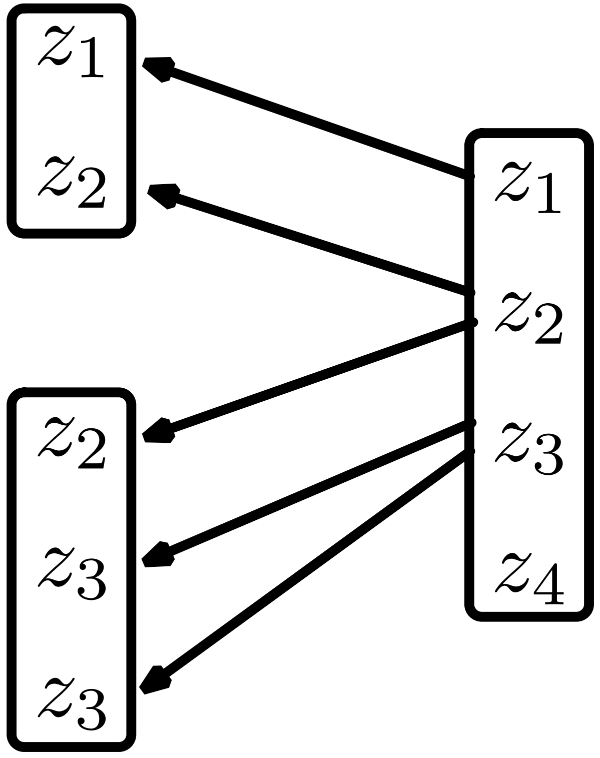
- The simplest notion of system on n variables is just vectors
- We combine systems with linear maps that merge/share information



$\phi\colon [2] + [3] \to [4]$



$\phi_*(x, y)\colon \mathbb{R}^2 \times \mathbb{R}^3 \to \mathbb{R}^4$



$\phi^*(z)\colon \mathbb{R}^4 \to \mathbb{R}^2 \times \mathbb{R}^3$

Composing Dynamical Systems

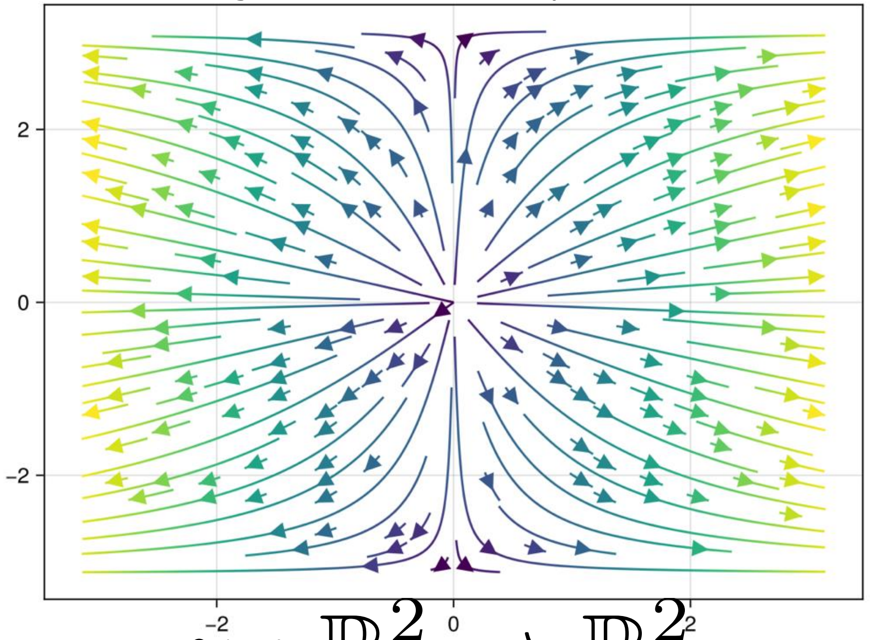
Example 2.12 (Composing Dynamical Systems). There is a finset algebra $\mathsf{Dynam}\colon (\mathbf{FinSet}, +) \to (\mathbf{Set}, \times)$ given by the following maps:

- On objects, Dynam takes a finite set N to the set of smooth maps $\{\upsilon\colon \mathbb{R}^N \to \mathbb{R}^N\}$.
- Given a morphism $\phi\colon N \to M$ in $\mathbf{FinSet}$, $\mathsf{Dynam}(\phi)\colon \mathsf{Dynam}(N) \to \mathsf{Dynam}(M)$ is defined by the function $\upsilon \mapsto \phi_* \circ \upsilon \circ \phi^*$.
- Given finite sets N and M, the product comparison $\varphi_{N,M}\colon \mathsf{Dynam}(N) \times \mathsf{Dynam}(M) \to \mathsf{Dynam}(N+M)$ is given by the function
$$(\upsilon, \rho) \mapsto \iota_{N*} \circ \upsilon \circ \iota_N^* + \iota_{M*} \circ \rho \circ \iota_M^*, \tag{25}$$
where $\iota_N\colon N \to N + M$ and $\iota_M\colon M \to N + M$ are the natural inclusions.
- The unit comparison $\varphi_0\colon \{*\} \to \mathsf{Dynam}(\emptyset)$ is uniquely determined because the set of maps $\{\mathbb{R}^0 \to \mathbb{R}^0\}$ is a singleton.

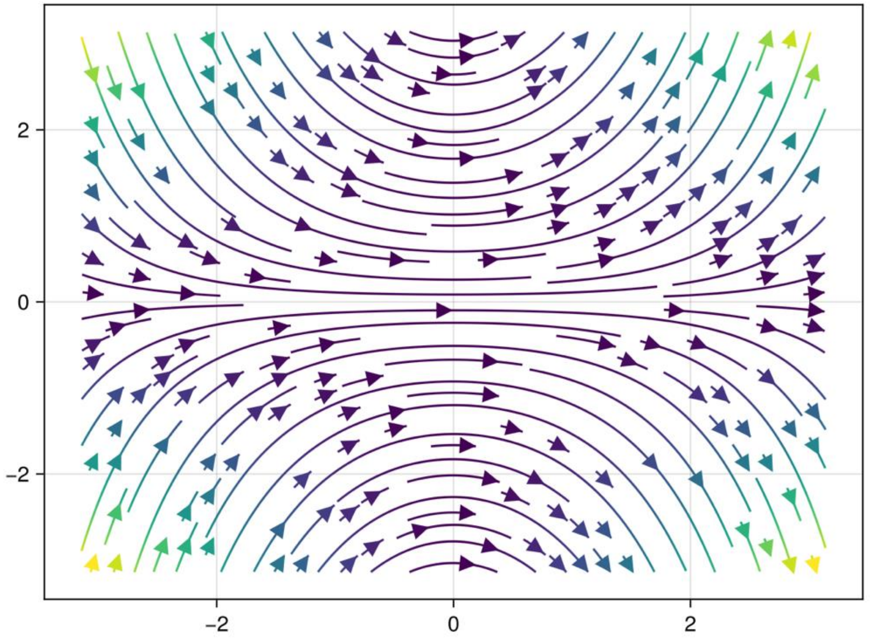
- Share variables by copying their values
- Compose tangent vectors by adding them

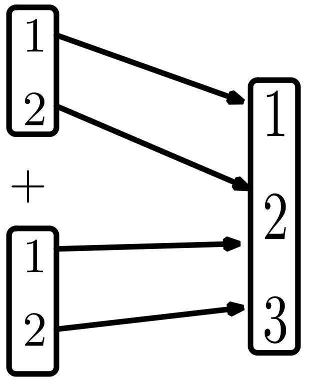
Superposition in Composite Systems

$v : \mathbb{R}^2 \to \mathbb{R}^2$

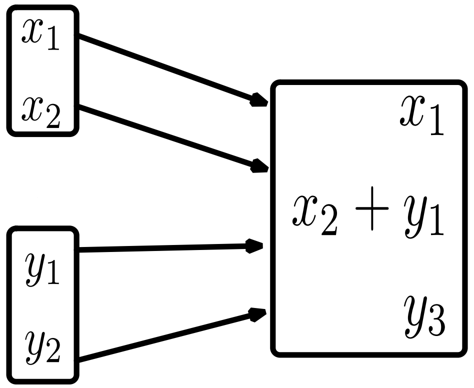


$u : \mathbb{R}^2 \to \mathbb{R}^2$

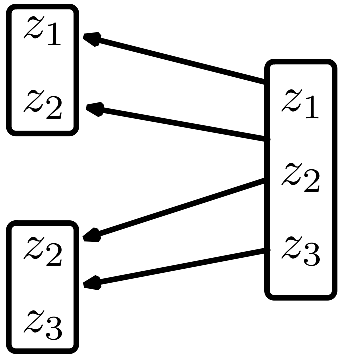




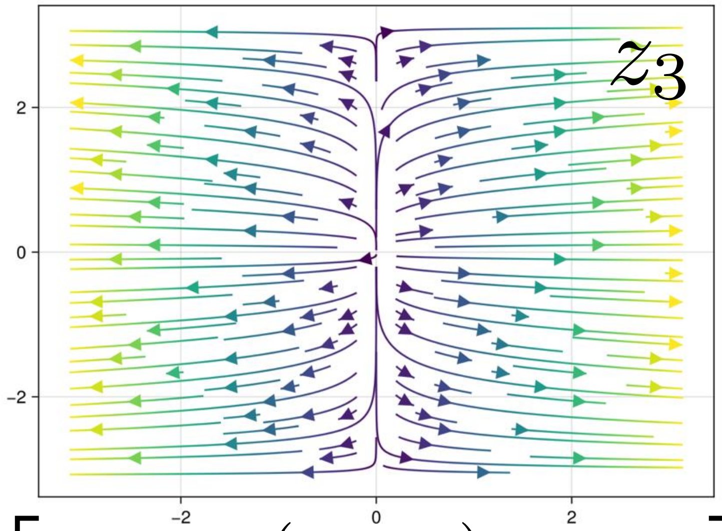
$\phi\colon [2] + [2] \to [3]$



$\phi_*(x, y)\colon \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}^3$

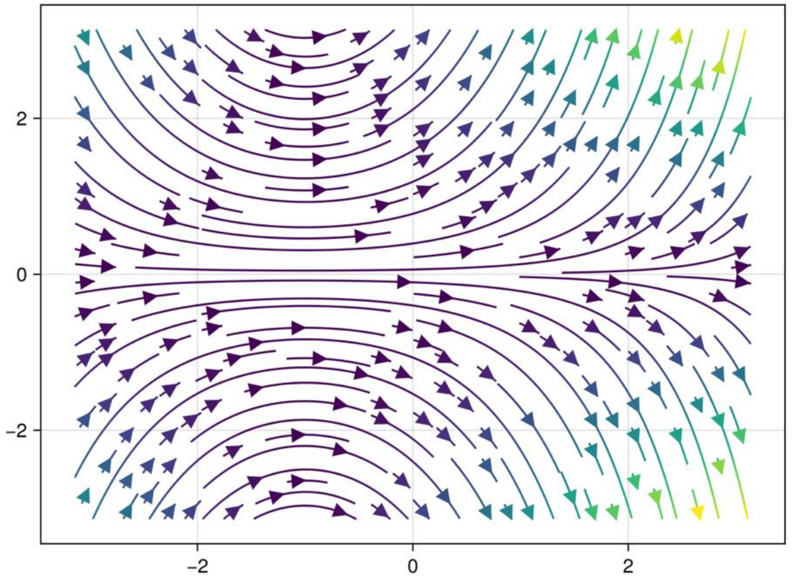


$\phi^*(z)\colon \mathbb{R}^3 \to \mathbb{R}^2 \times \mathbb{R}^2$



$z_3 = 3$

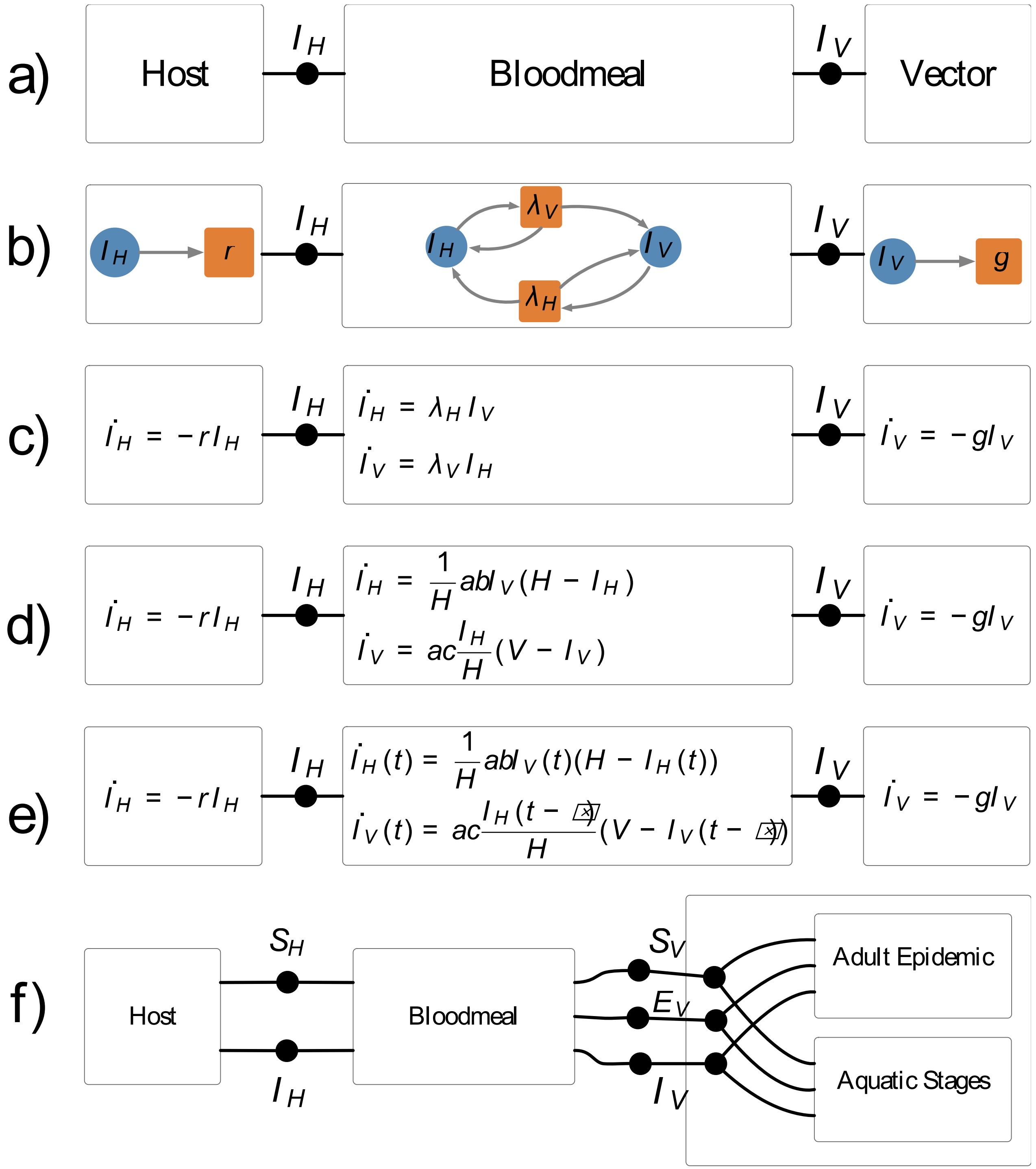
$z_1 = 3$



$$\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} \mapsto \begin{bmatrix} v(z_1, z_2)_1 \\ v(z_1, z_2)_2 + u(z_2, z_3)_1 \\ u(z_2, z_3)_2 \end{bmatrix}$$

Composing Compartmental Models with UWDs

- Easy to build complex models
- Subsystems can be modified independently
- CT gives rigorous language to compare models
- Easy to compare many models to the same data for quality of fit



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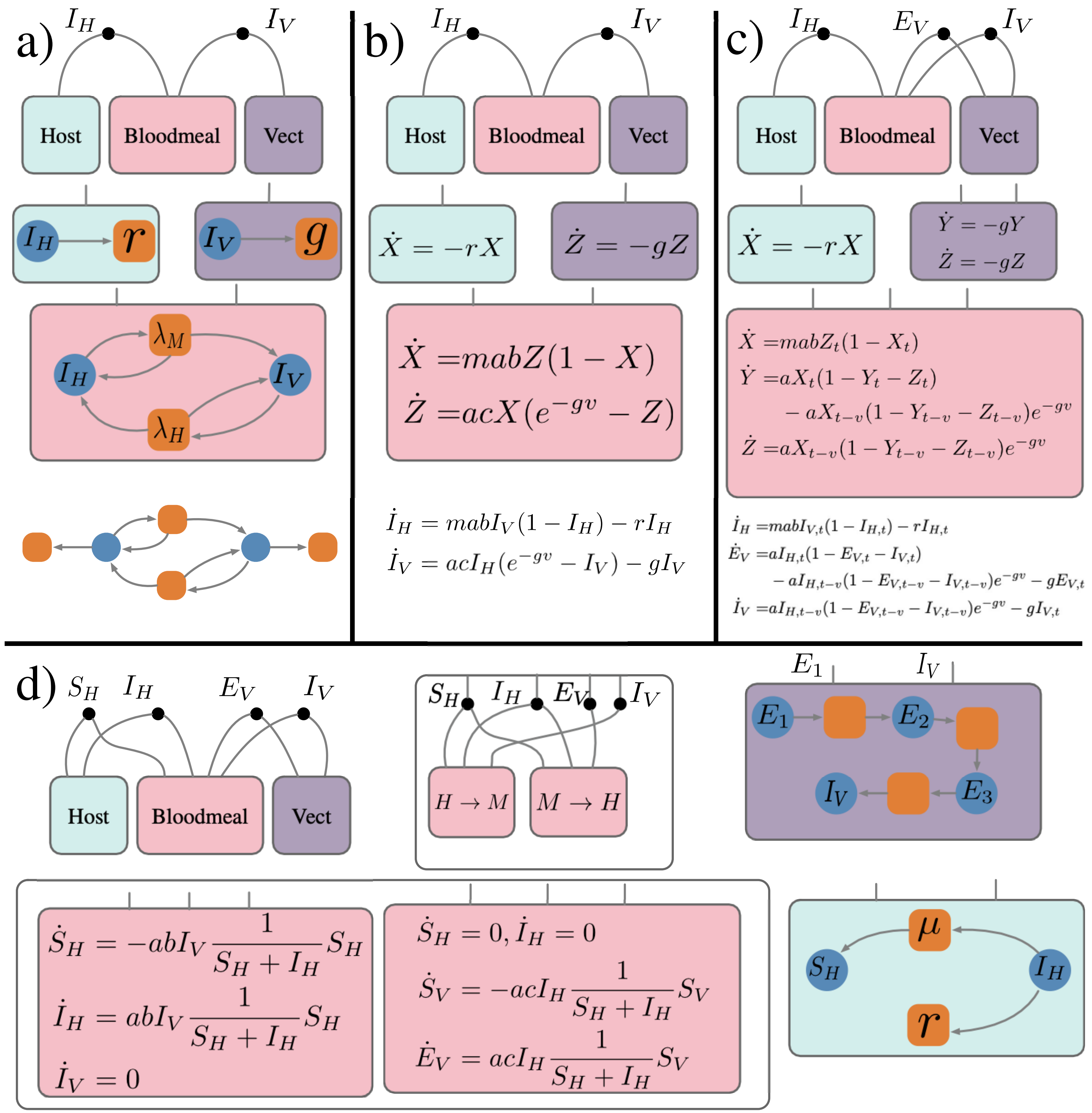

Euler's Method is Functorial

For each fixed step size h, Euler's method

$$x_{k+1} = x_k + hf(x)$$

is a functor for UWD composition of dynamical systems

Operadic Modeling of Dynamical Systems: Mathematics and Computation

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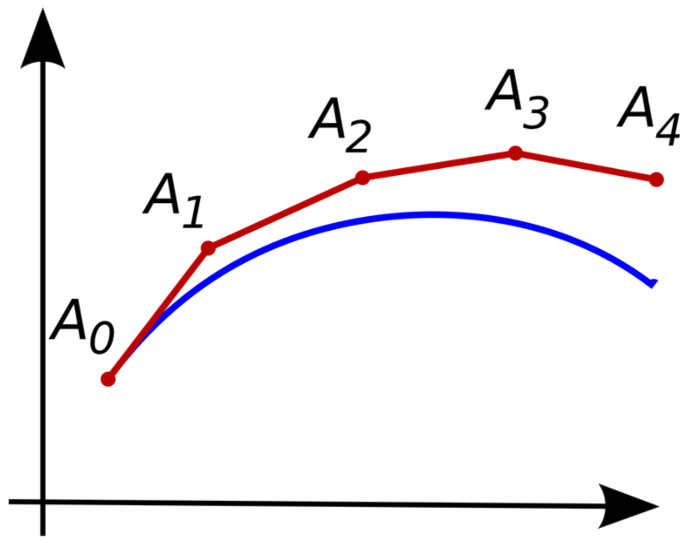
https://arxiv.org/pdf/2105.12282v2.pdf

Composing dynamical systems then discretizing in time

is

Discretizing the composite system



Slice Categories

- Maps f:X to R are data over a space
- Given f:X to R and g:Y to R you can ask about maps y:X to Y that preserve f,g

$$\forall x \quad f(x) = g(y(x))$$

$$\begin{tikzcd} X \arrow[rr, "y"] \arrow[dr, "f"'] & & Y \arrow[dl, "g"] \\ & \mathbb{R} & \end{tikzcd}$$

- Objects in the slice are "typed object"
- Morphisms are commuting triangles (right)

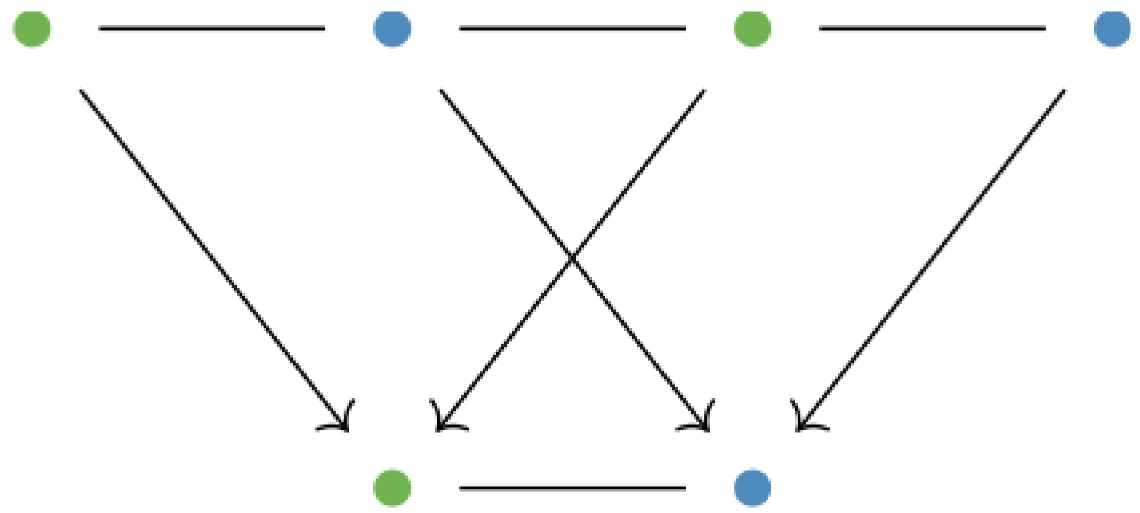
$$\begin{tikzcd} X \arrow[r, "y"] \arrow[dr, "f"'] & Y \arrow[r, "z"] \arrow[d, "g"] & Z \arrow[dl, "h"] \\ & \mathbb{R} & \end{tikzcd}$$

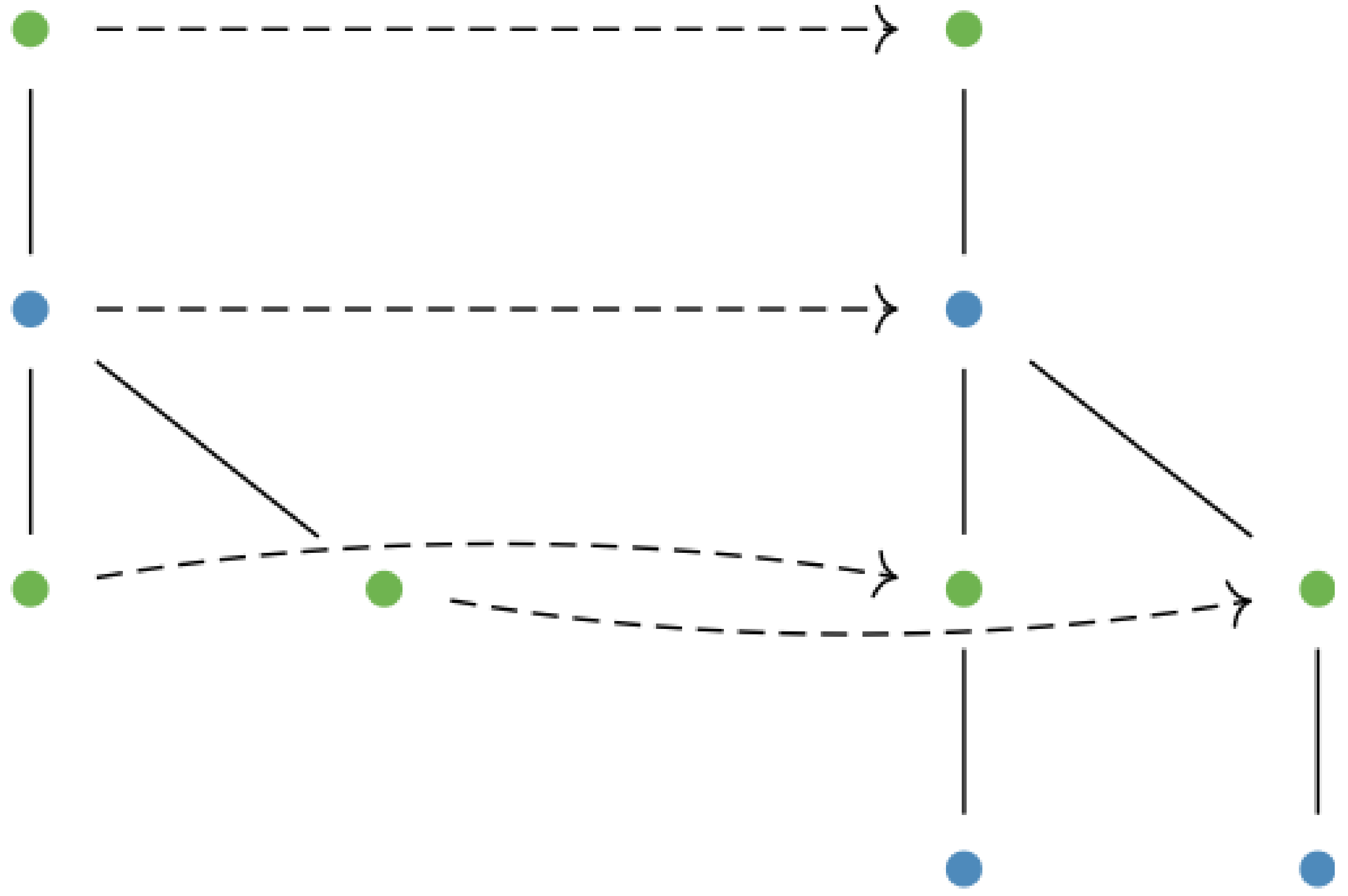
$$f(x) = g(y(x)) \quad h(z(y)) = g(y)$$

$$\implies h(z(y(x))) = f(x)$$

Slice Categories

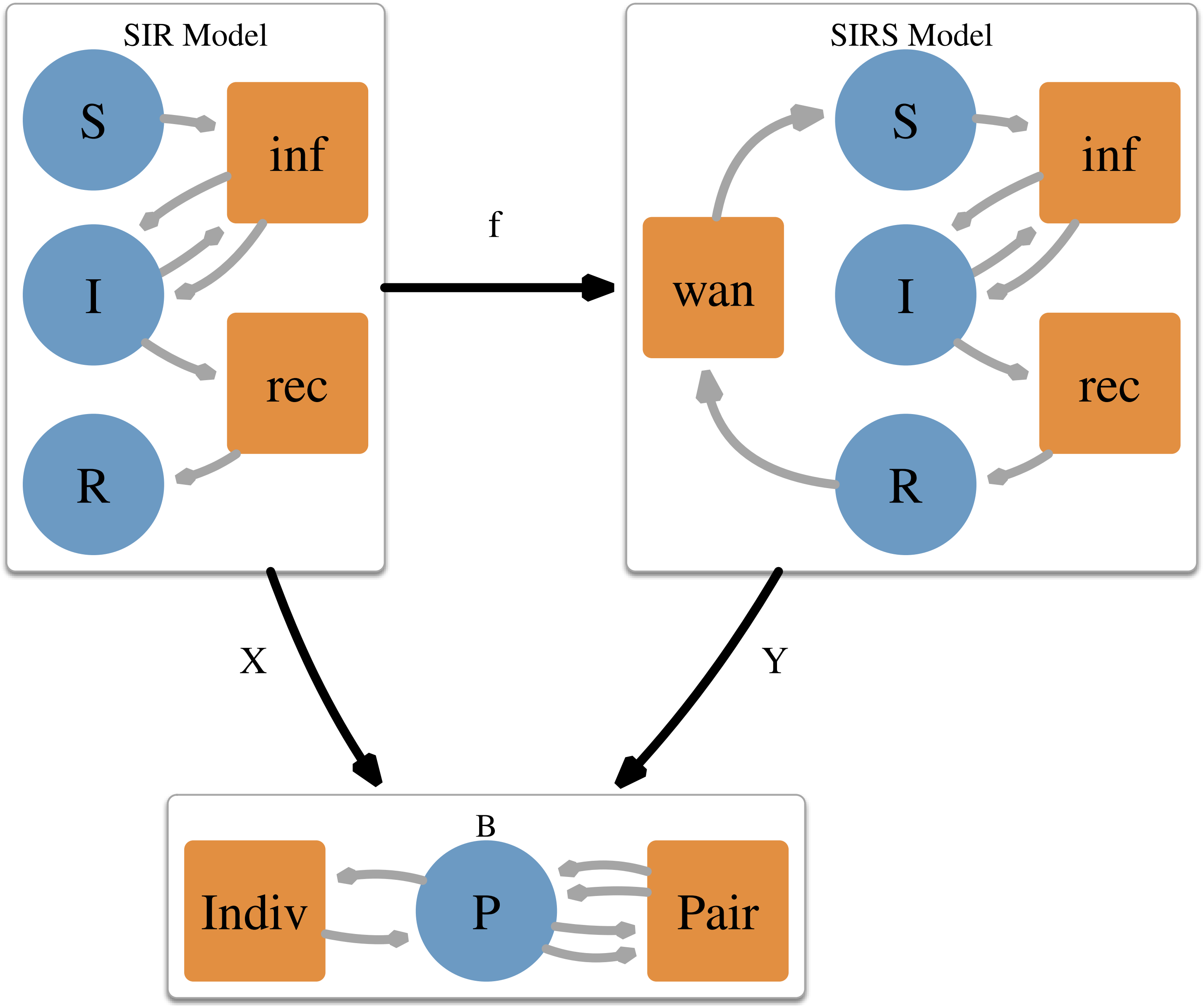
- The new objects are maps into a fixed object called the base point
- The new maps are maps in the original category that preserve the maps into the base point
- We use color coding to represent the map into the base point



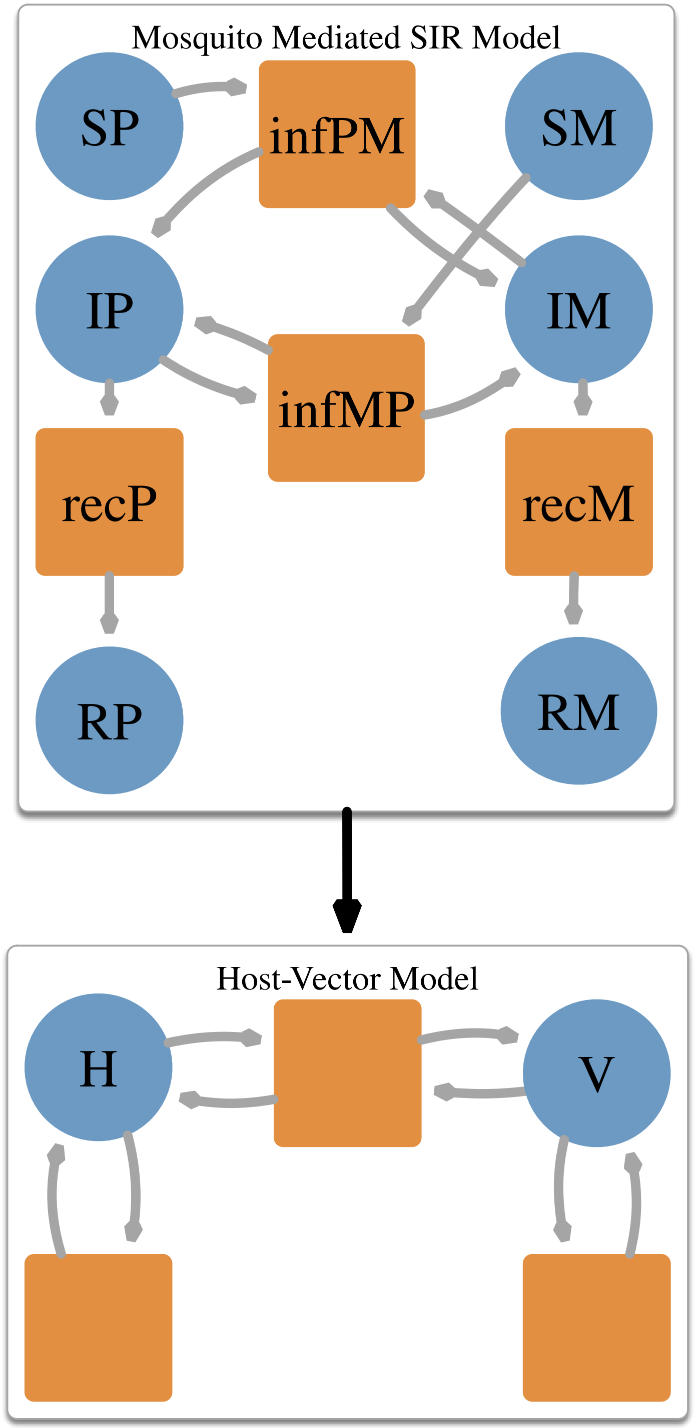


Epi = Petri/B

- Define a category of epidemiological models as Petri nets where each reaction has either 1 input 1 output or 2 inputs and 2 outputs.
- These models conserve population and have only binary effects
- Objects in the slice are "typed reaction networks"
- Morphisms are commuting triangles (right)

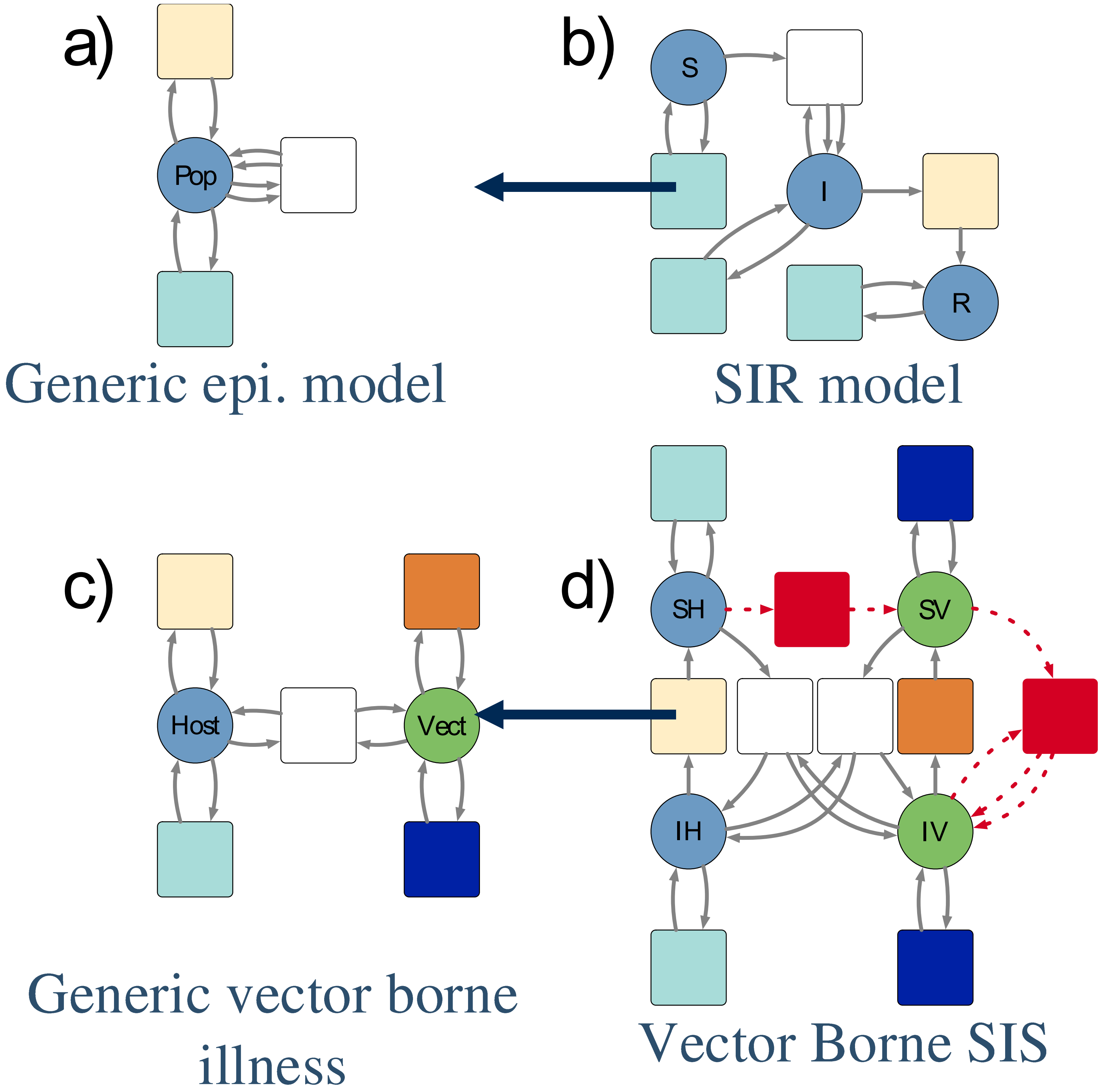


Formalizing Scientific Knowledge as Types



- We can statically prove that any model in this slice satisfies both a conservation of hosts and conservation of vectors
- No process is allowed to convert people into mosquitos
- Model morphisms must preserve types (hosts to hosts and vectors to vectors)

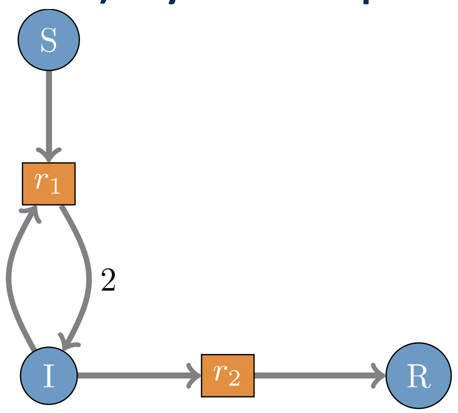
Formalizing Scientific Knowledge as Rules



- An Algebraic Framework for Structured Epidemic Modeling, S. Libkind, A. Baas, M. Halter, E. Patterson, and J. Fairbanks, *The Royal Society Phil. Trans. A*
- We can statically prove that any model following the rules satisfies both a conservation of hosts/vectors law
- No process is allowed to convert people into mosquitos (red processes forbidden)
- Supports “conceptual inheritance” for these scientific types
- Modeling operations must respect the Host-Vector distinction
- Basis for automating model stratification (take SEIR dynamics over 5 age groups and 15 cities arranged in a transit network)
- Successful composition/stratification implies conceptual validity as a scientific model

Automated Model Exploration for Epidemics

1) System specification



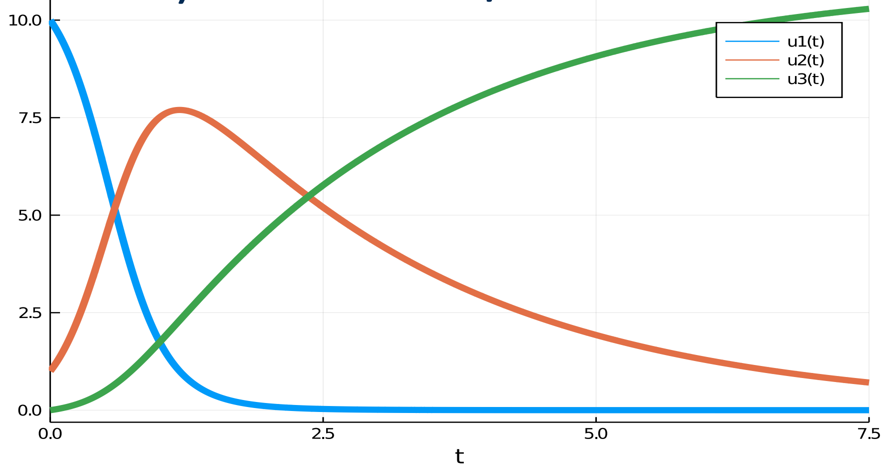
2) Model semantics

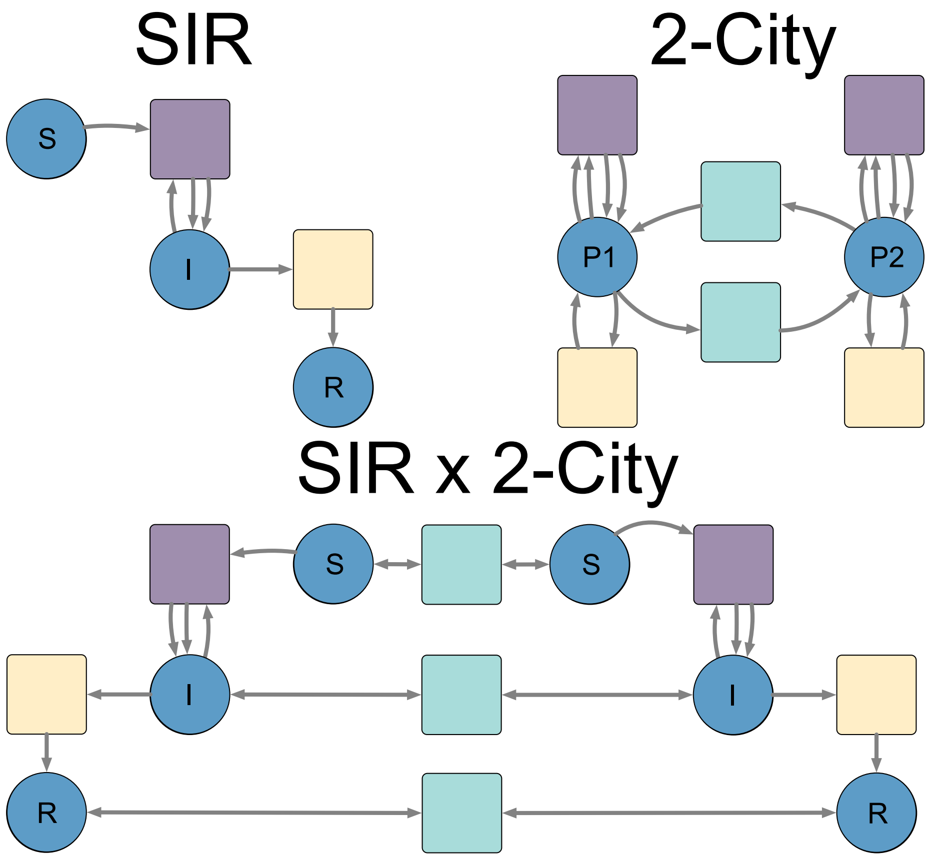
$$\dot{u}_1 = -r_1 u_1 u_2$$

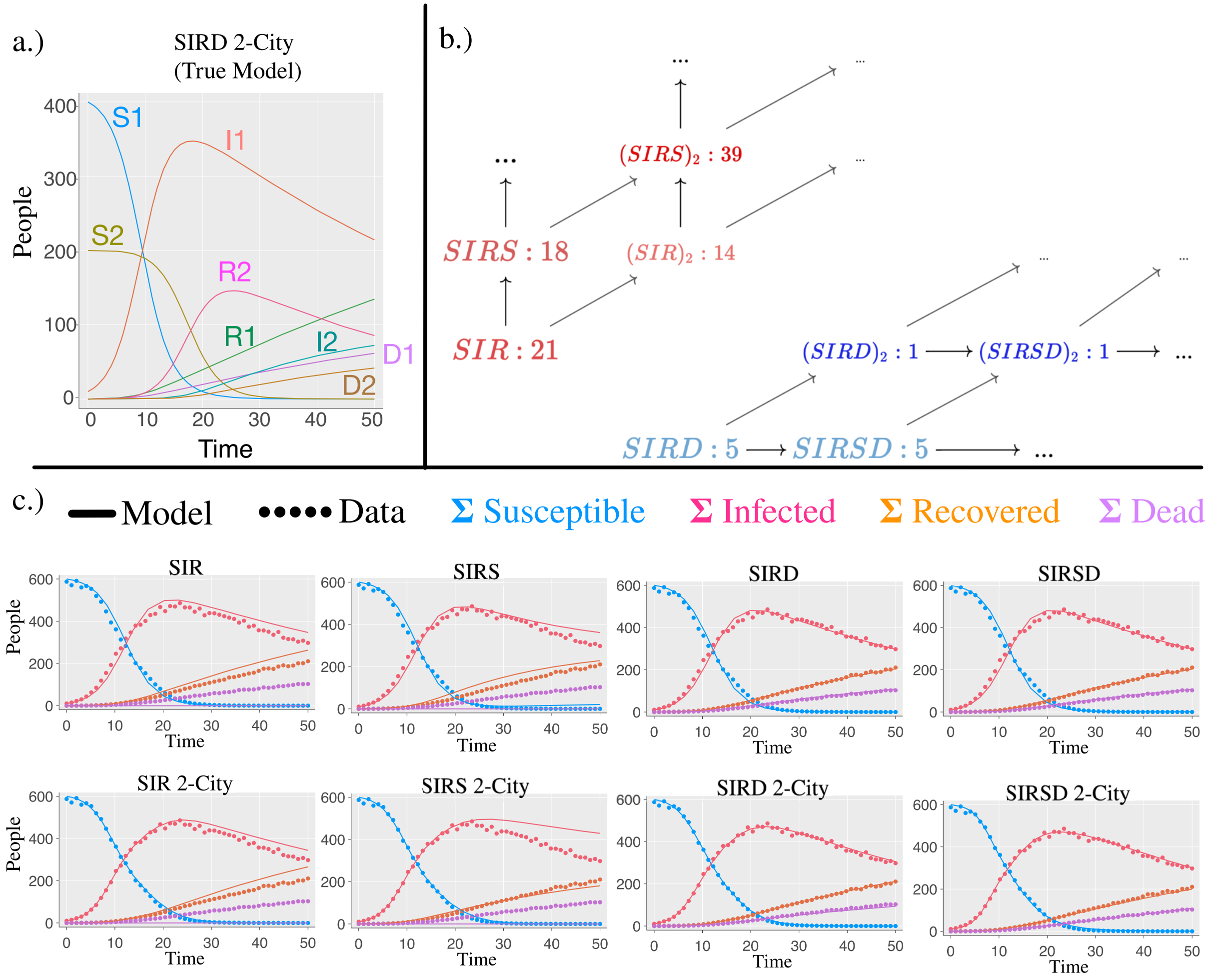
$$\dot{u}_2 = r_1 u_1 u_2 - r_3 u_2$$

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

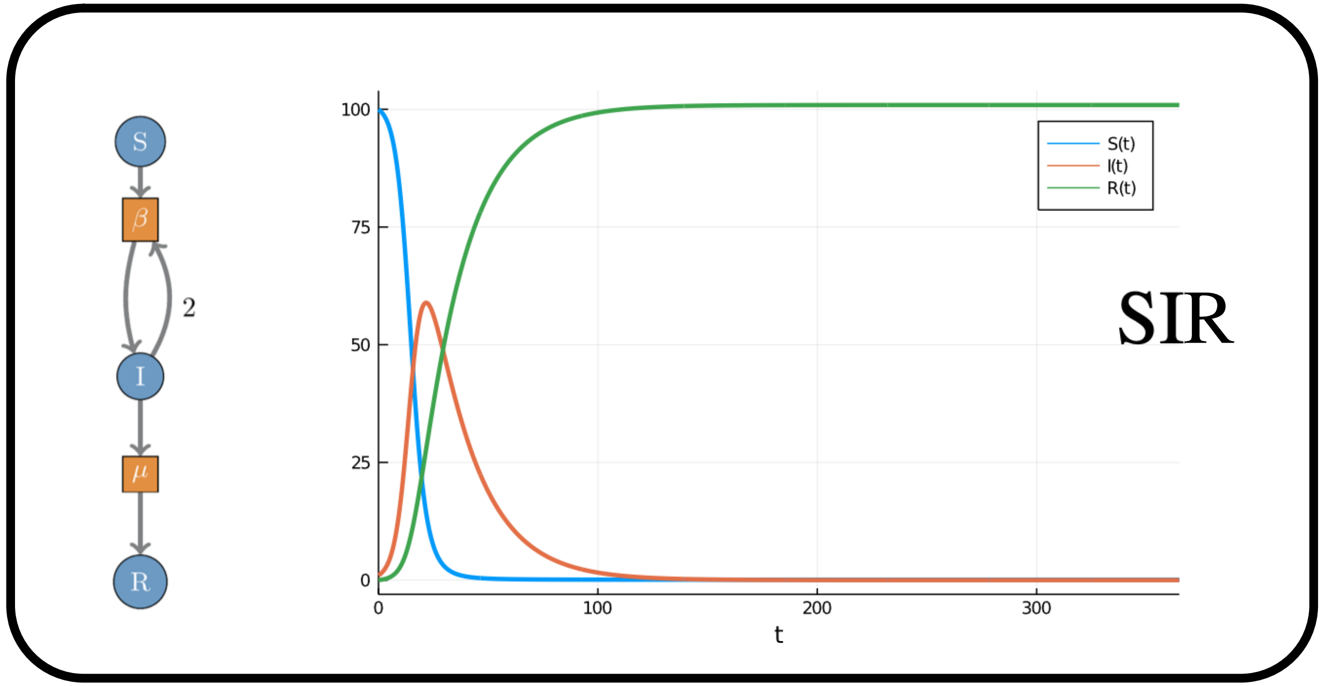
3) Simulation/solution

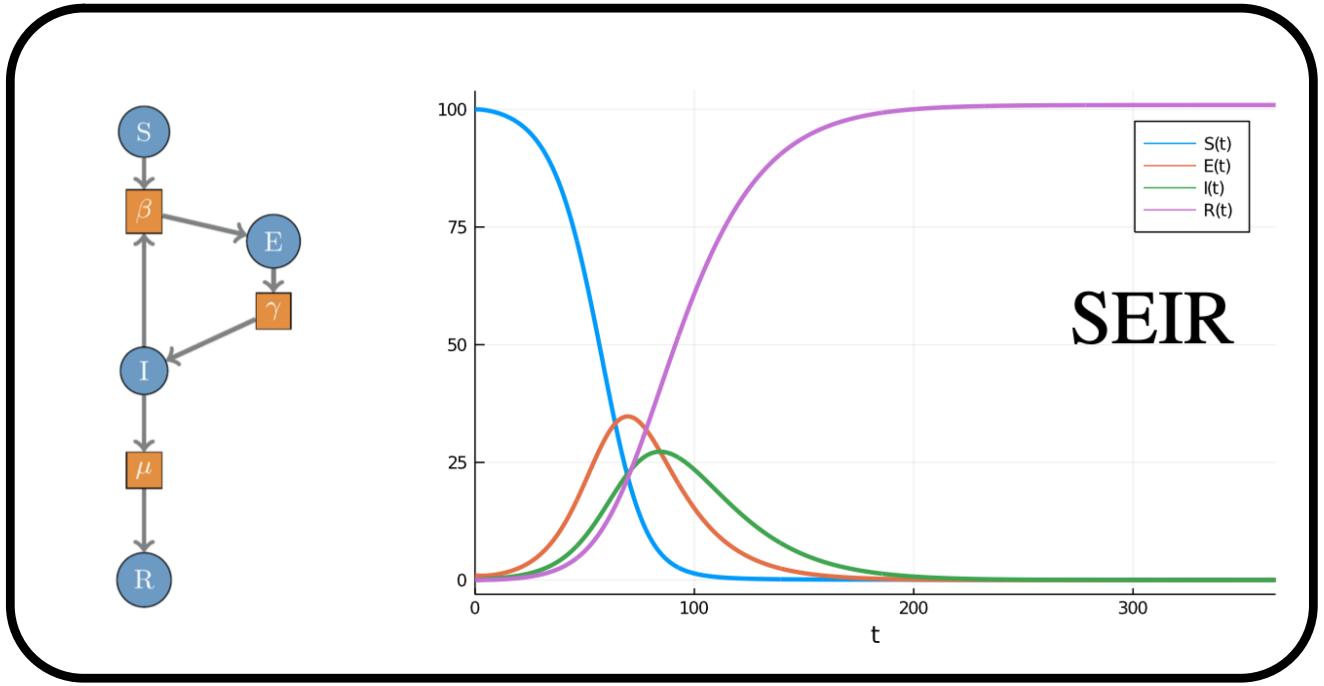


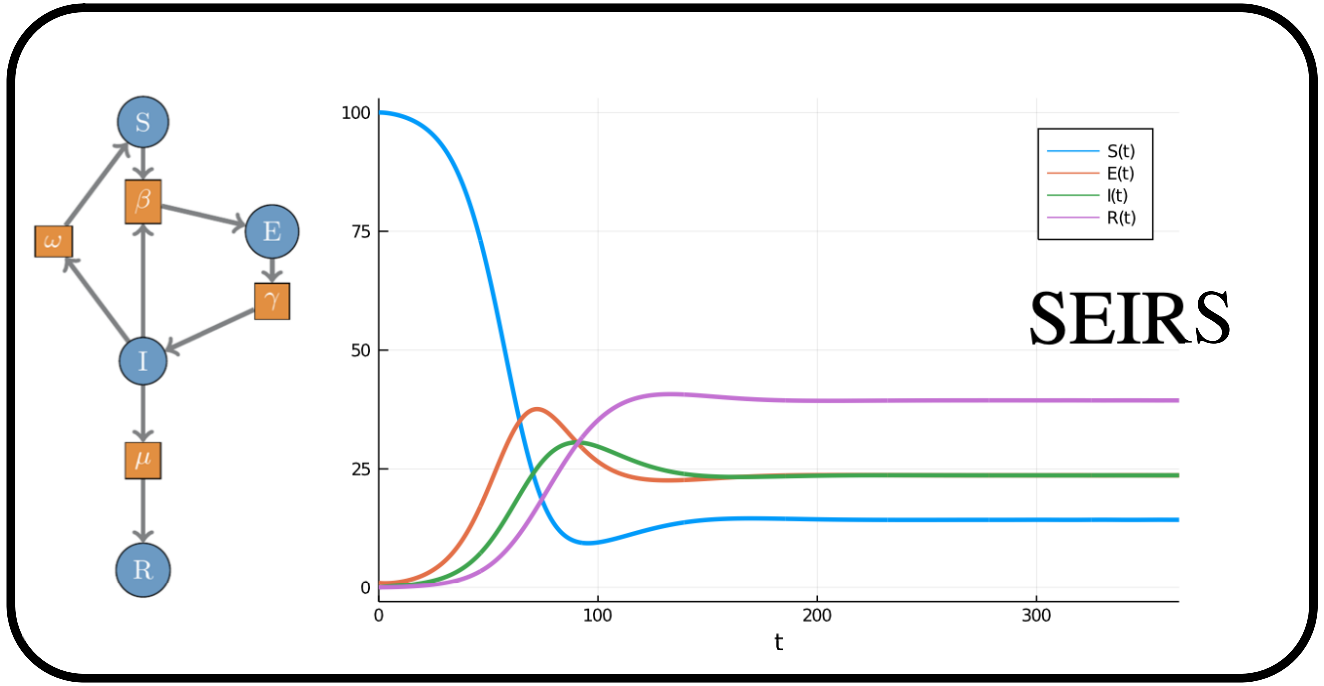


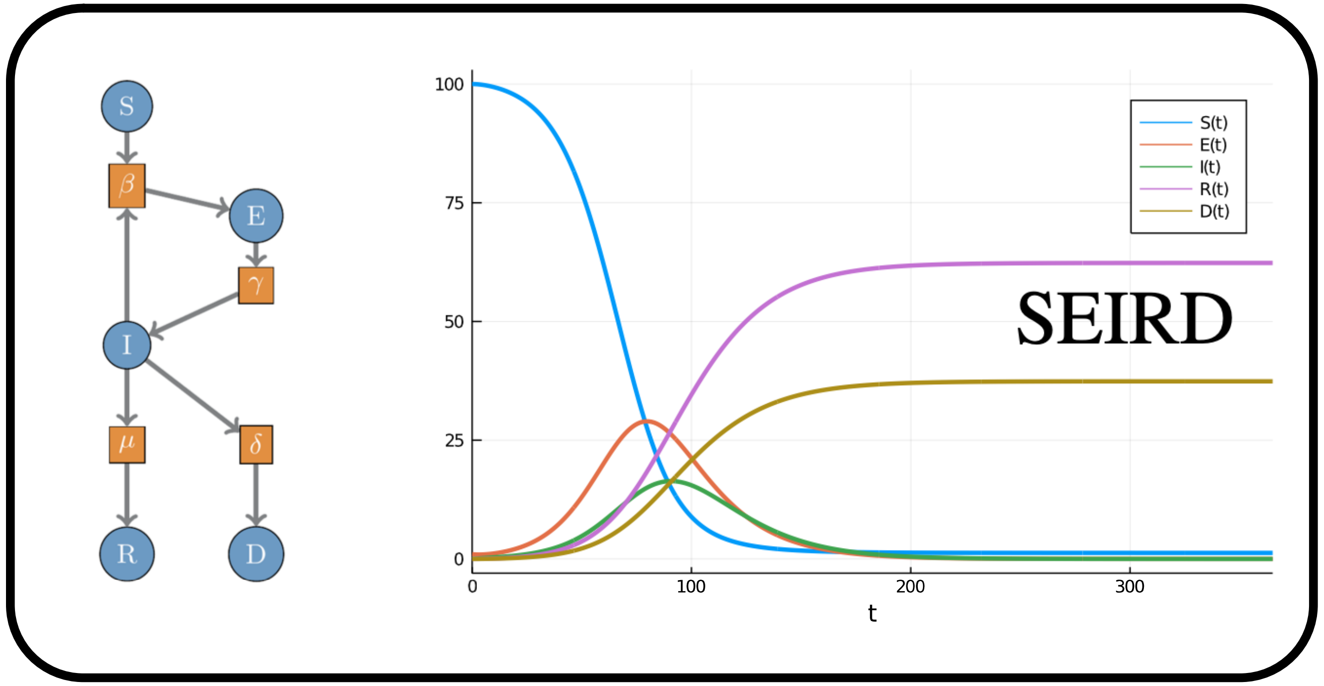


Model Spaces for Comparison and Selection









Composing Equations is Hard

SIR Model

$$\frac{dS}{dt} = -\beta \frac{SI}{N}$$
$$\frac{dI}{dt} = \beta \frac{SI}{N} - \gamma I.$$
$$\frac{dR}{dt} = \gamma I$$

Flux Transport Model

$$\frac{dN_i}{dt} = -\sum_{j=1}^{K} f_{i,j} N_i + \sum_{j=1}^{K} f_{j,i} N_j,$$

$$\frac{dS_i}{dt} = -\beta_i \frac{S_i I_i}{N_i} - \sum_{j=1}^{K} f_{i,j} S_i + \sum_{j=1}^{K} f_{j,i} S_j$$

$$\frac{dI_i}{dt} = \beta_i \frac{S_i I_i}{N_i} - \gamma I_i - \sum_{j=1}^{K} f_{i,j} I_i + \sum_{j=1}^{K} f_{j,i} I_j.$$

$$\frac{dR_i}{dt} = \gamma I_i - \sum_{j=1}^{K} f_{i,j} R_i + \sum_{j=1}^{K} f_{j,i} R_j$$

Composite Model

Composing Equations is Hard

SIR Model

$$\frac{dS}{dt} = -\beta\frac{SI}{N}$$
$$\frac{dI}{dt} = \beta\frac{SI}{N} - \gamma I.$$
$$\frac{dR}{dt} = \gamma I$$

Simple Trip Transport Model

$$\frac{dN_{i,i}}{dt} = -\sum_{j=1}^{K}\phi_{i,j}N_{i,i} + \sum_{j=1}^{K}\tau_{i,j}N_{i,j}.$$
$$\frac{dN_{i,j}}{dt} = -\tau_{i,j}N_{i,j} + \phi_{i,j}N_{i,i}$$

$$\frac{dS_{i,i}}{dt} = -\beta_i\frac{S_{i,i}\sum_{k=1}^{K}I_{k,i}}{\sum_{k=1}^{K}N_{k,i}} - \sum_{k=1}^{K}\phi_{i,k}S_{i,i} + \sum_{k=1}^{K}\tau_{i,k}S_{i,k}$$
$$\frac{dS_{i,j}}{dt} = -\beta_j\frac{S_{i,j}\sum_{k=1}^{K}I_{k,j}}{\sum_{k=1}^{K}N_{k,j}} + \phi_{i,j}S_{i,i} - \tau_{i,j}S_{i,j}$$
$$\frac{dI_{i,i}}{dt} = \beta_i\frac{S_{i,i}\sum_{k=1}^{K}I_{k,i}}{\sum_{k=1}^{K}N_{k,i}} - \gamma I_{i,i} - \sum_{k=1}^{K}\phi_{i,k}I_{i,i} + \sum_{k=1}^{K}\tau_{i,k}I_{i,k}.$$
$$\frac{dI_{i,j}}{dt} = \beta_j\frac{S_{i,j}\sum_{k=1}^{K}I_{k,j}}{\sum_{k=1}^{K}N_{k,j}} - \gamma I_{i,j} + \phi_{i,j}I_{i,i} - \tau_{i,j}I_{i,j}$$
$$\frac{dR_{i,i}}{dt} = \gamma I_{i,i} - \sum_{k=1}^{K}\phi_{i,k}R_{i,i} + \sum_{k=1}^{K}\tau_{i,k}R_{i,k}$$
$$\frac{dR_{i,j}}{dt} = \gamma I_{i,j} + \phi_{i,j}R_{i,i} - \tau_{i,j}I_{i,j}$$

Composite Model

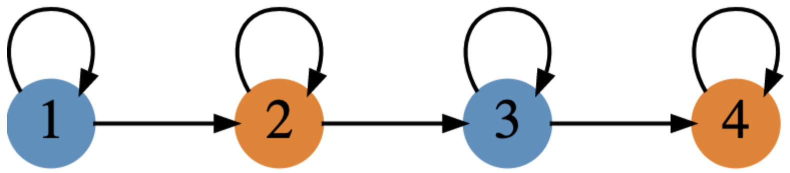
Example: Colored Graphs

Colored Graphs

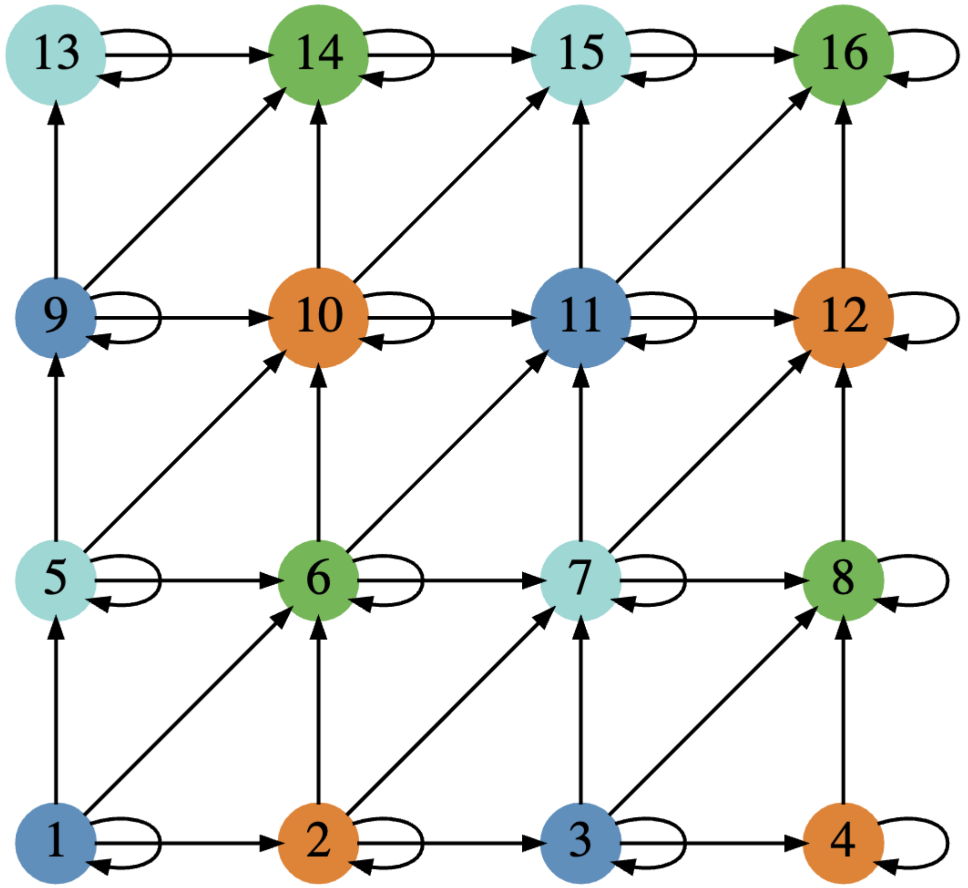
$$G = (V, E \subseteq V \times V, \phi\colon V \to K)$$

$$E \underset{tgt}{\overset{src}{\rightrightarrows}} V \xrightarrow{color} K$$

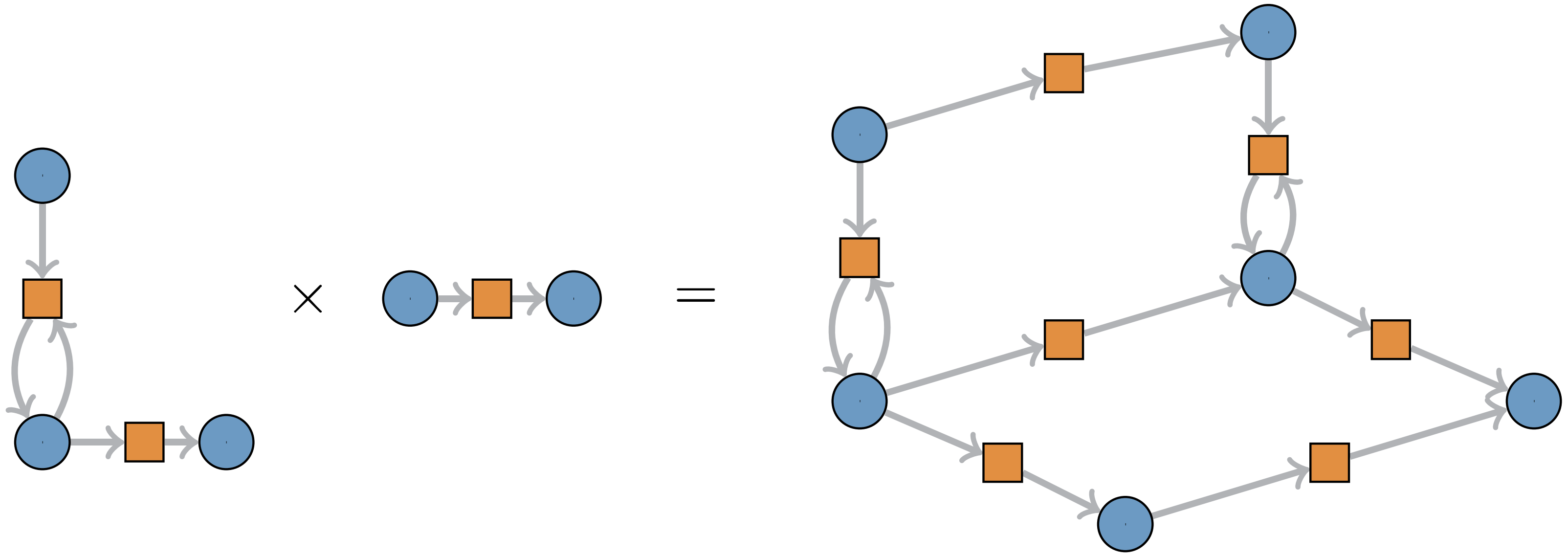
```julia
rp4 = @acset ColoredGraph begin
    V = 4
    E = 7
    K = 2
    src = [1,2,3,1,2,3,4]
    tgt = [2,3,4,1,2,3,4]
    color = [1,2,1,2]
end

draw(rp4)
```



$rp4 \times rp4$



Model Transformation in Rxn-Set

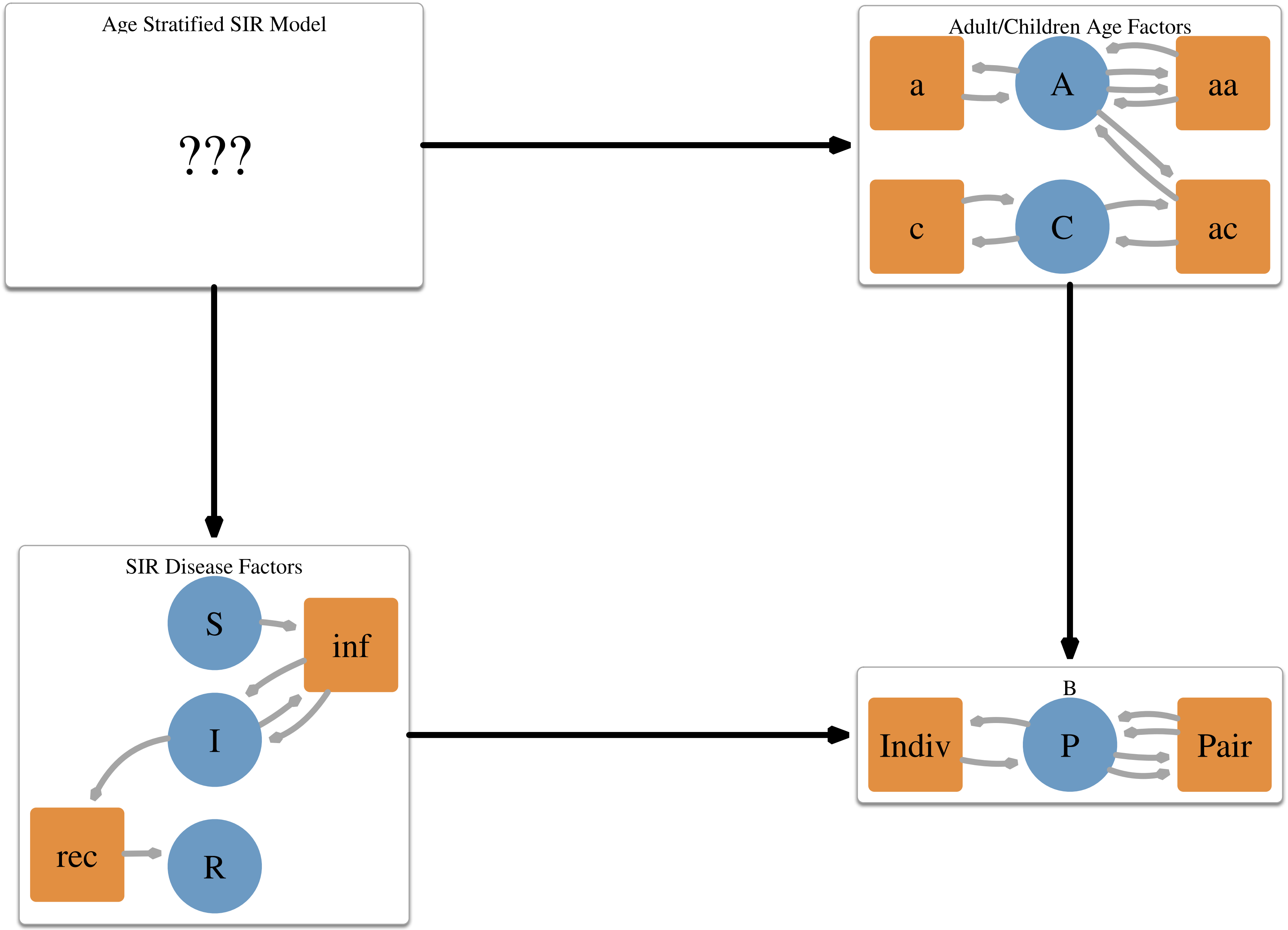


$$\dot{u} = \begin{bmatrix} -\beta_1 u_1 u_2 - \beta_3 u_1 \\ \beta_1 u_1 u_2 - \beta_3 u_2 - \beta_4 u_2 \\ \beta_2 u_2 - \beta_6 u_3 \\ -\beta_1 u_4 u_5 + \beta_3 u_4 \\ \beta_1 u_4 u_5 - \beta_3 u_5 + \beta_4 u_2 \\ \beta_2 u_5 + \beta_6 u_3 \end{bmatrix}$$

- Simple operations on the compartmental model is a complex operation on the differential equations
- Above: $SIR \times AB$ has two regions undergoing SIR with a flow $A \rightarrow B$

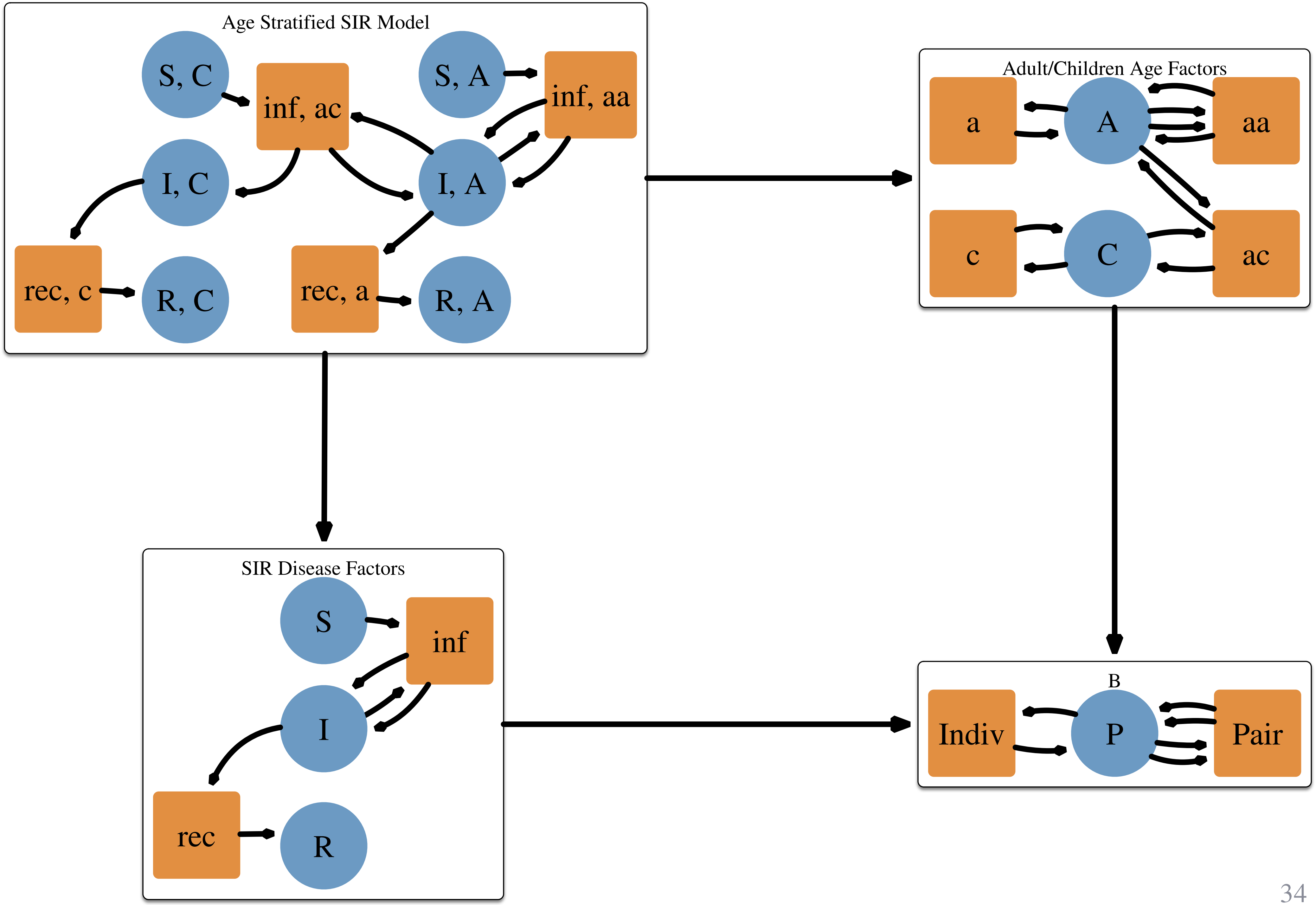
Model Stratification by Universal Property

What is the unique model that factors into SIR disease factors and Adult/Children Age Factors, such that any other model with those factors factors through our model?

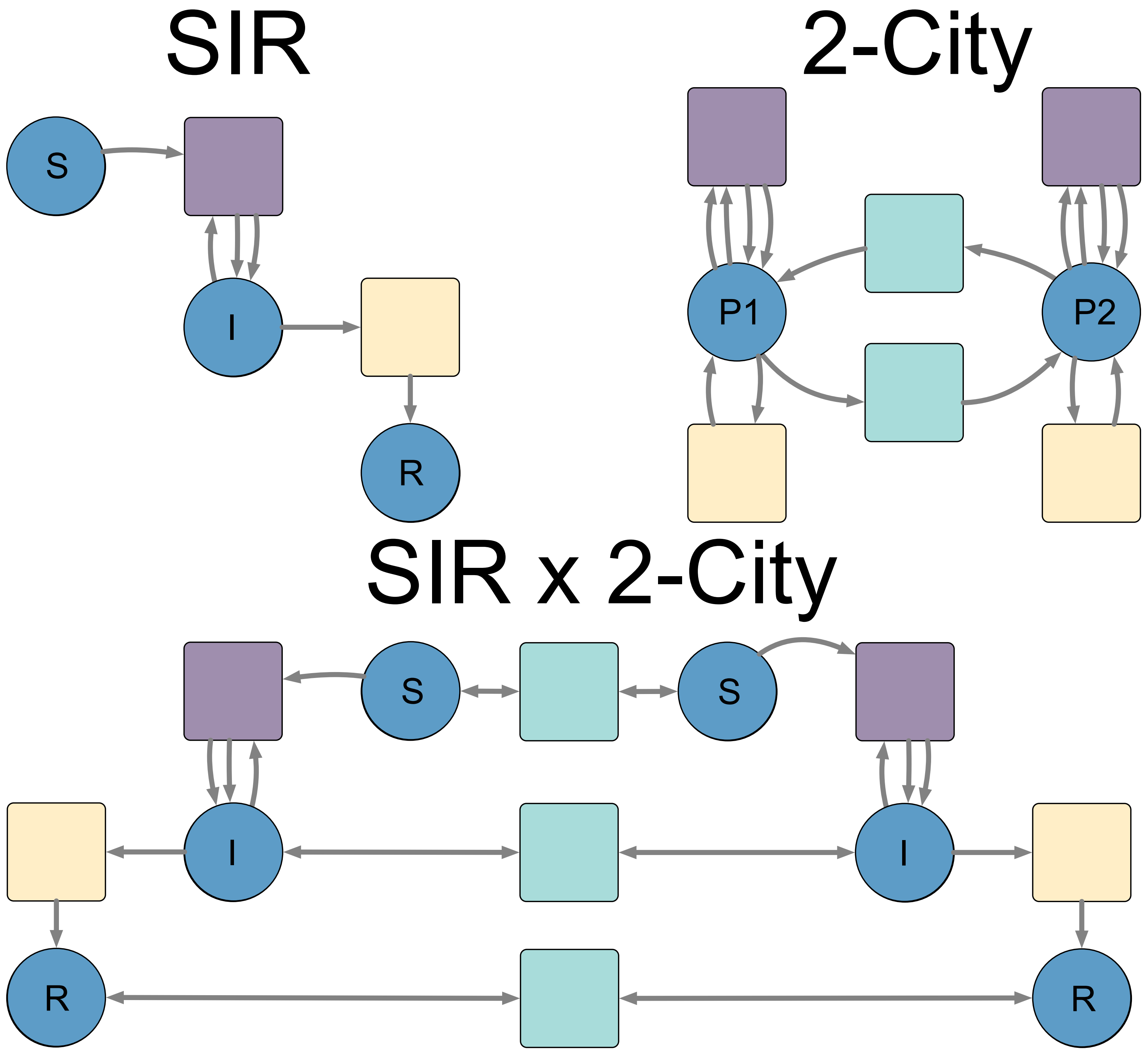


Model Stratification with Pullbacks!

- Pullbacks let you specify model stratification, a basic pattern of compositional modeling in Epidemiology
- Defining this operation on models without using its universal mapping property (UMP) would be ad hoc.
- UMPs imply properties of model constructions, ie. stratification is an associative, commutative (up to isomorphism) binary operation.

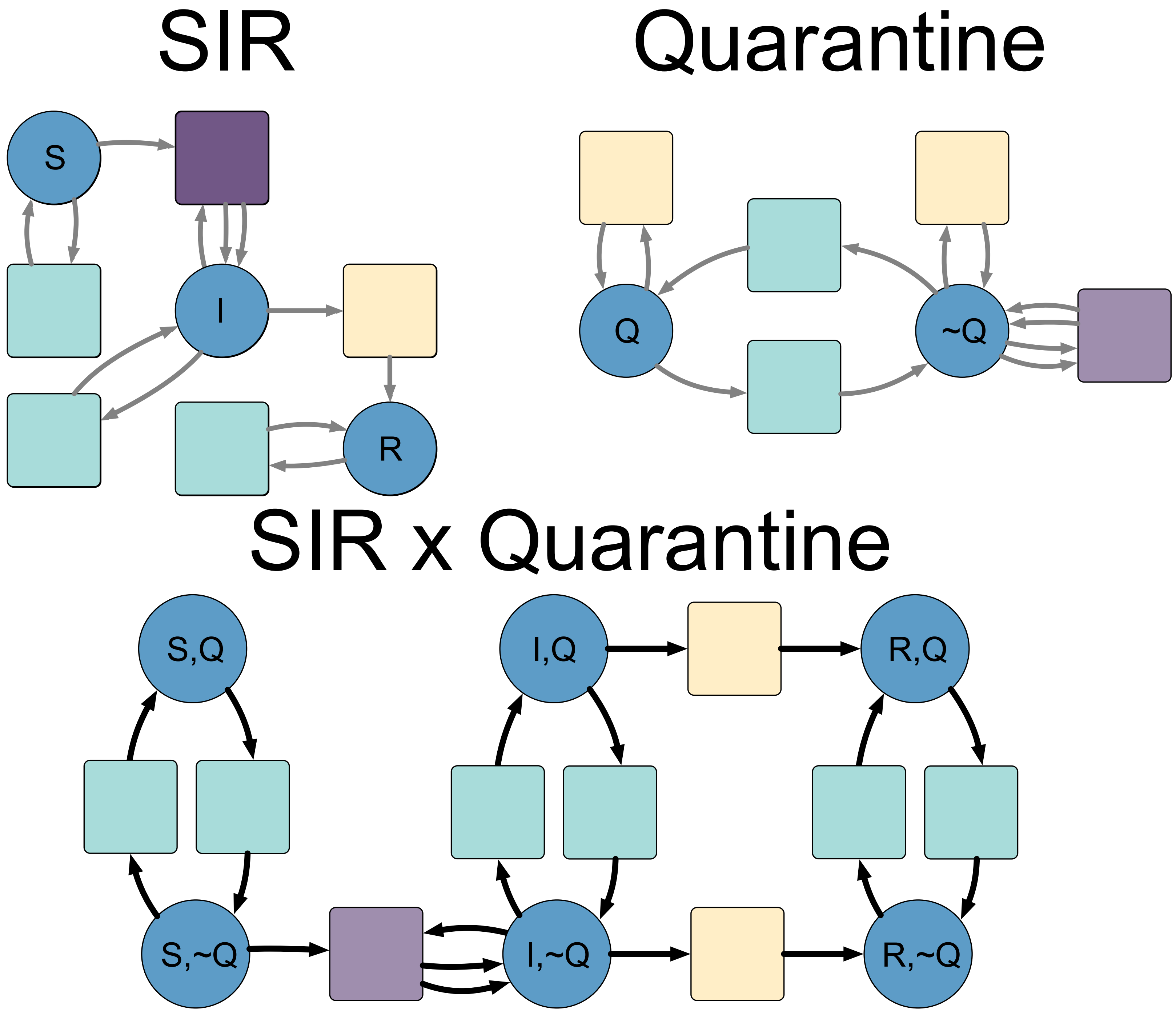


Spatial Models with Disease x Transport



- Models Migration or Commuting of Populations
- People travel between cities
- Can only infect people in the same city

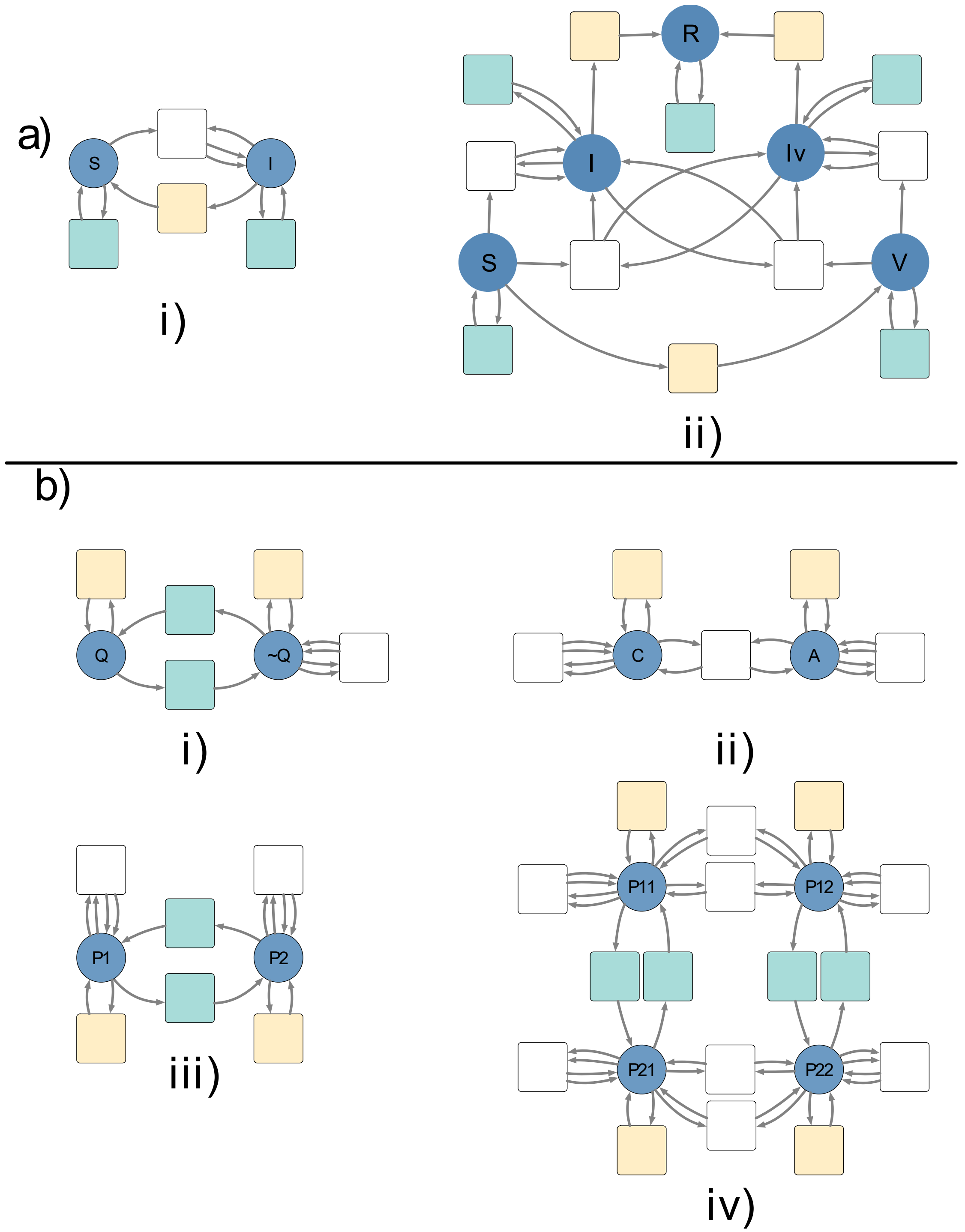
Example of adding Quarantine to SIR



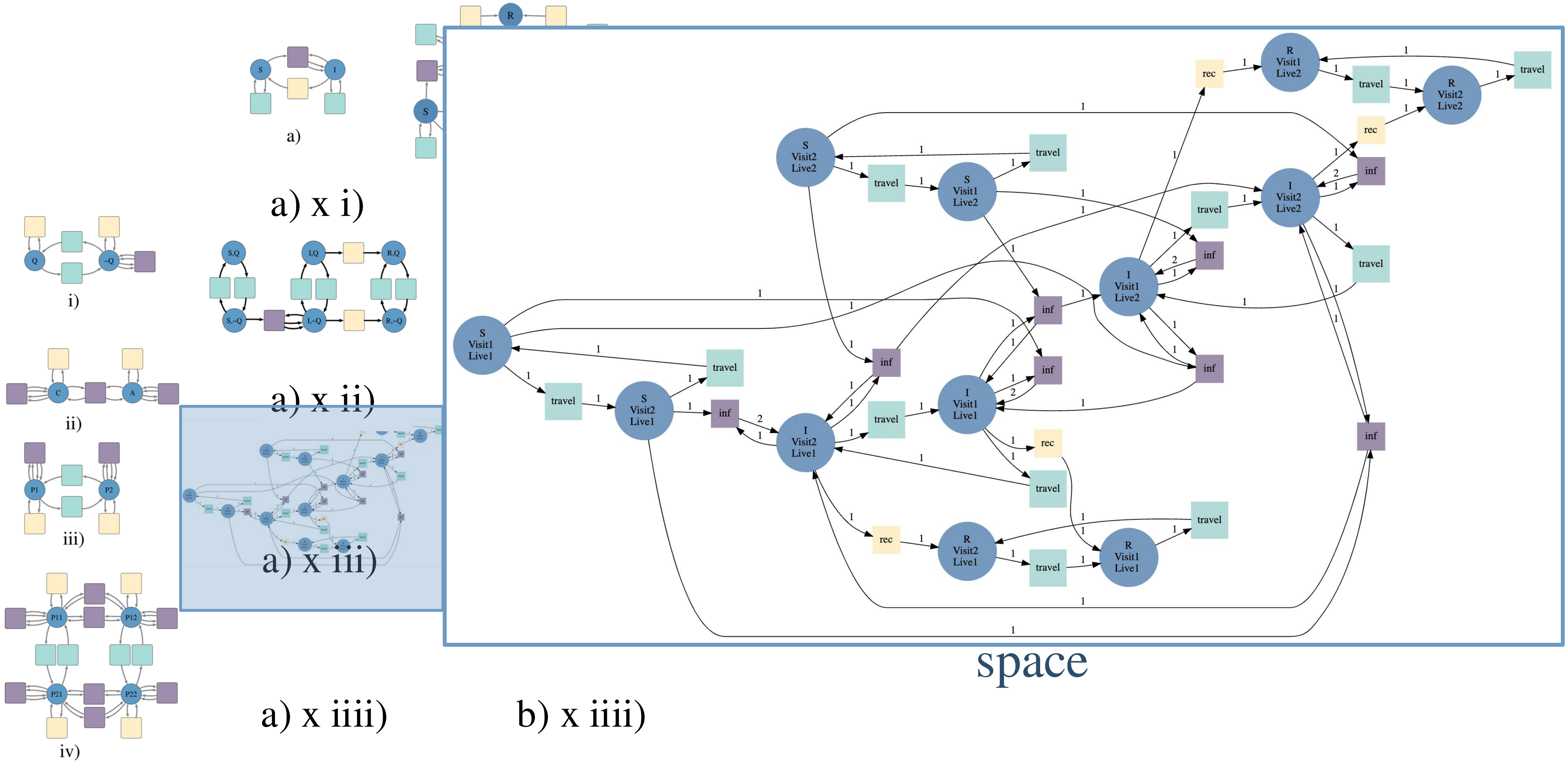
- Each pair a x b gives a new model.
- We can easily generate new models for scientists
- What is this space of all possible products?

Stratifying Compartmental Models with Pullbacks

- Choose a disease model (a)
- Choose a stratification scheme (b)
- AlgebraicJulia computes the (b)-stratified version of model (a)
- Benefits
  - Easy to build complex models
  - Factors can be modified independently
  - CT gives rigorous language to articulate structural model comparisons
- Easy to compare many models to the same data for testing assumptions about disease or demographic dynamics

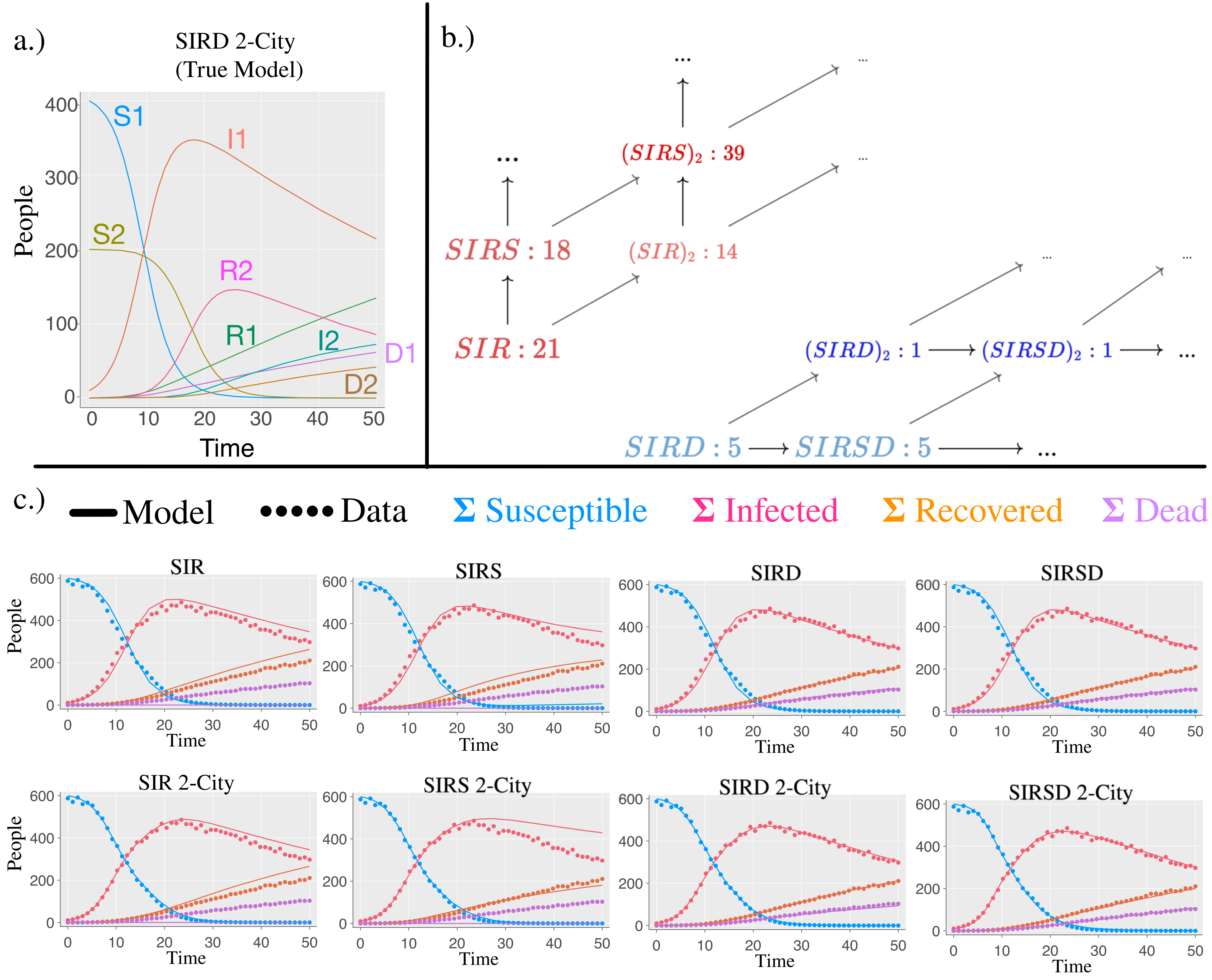


Defining Spaces of Models



Automated Model Selection

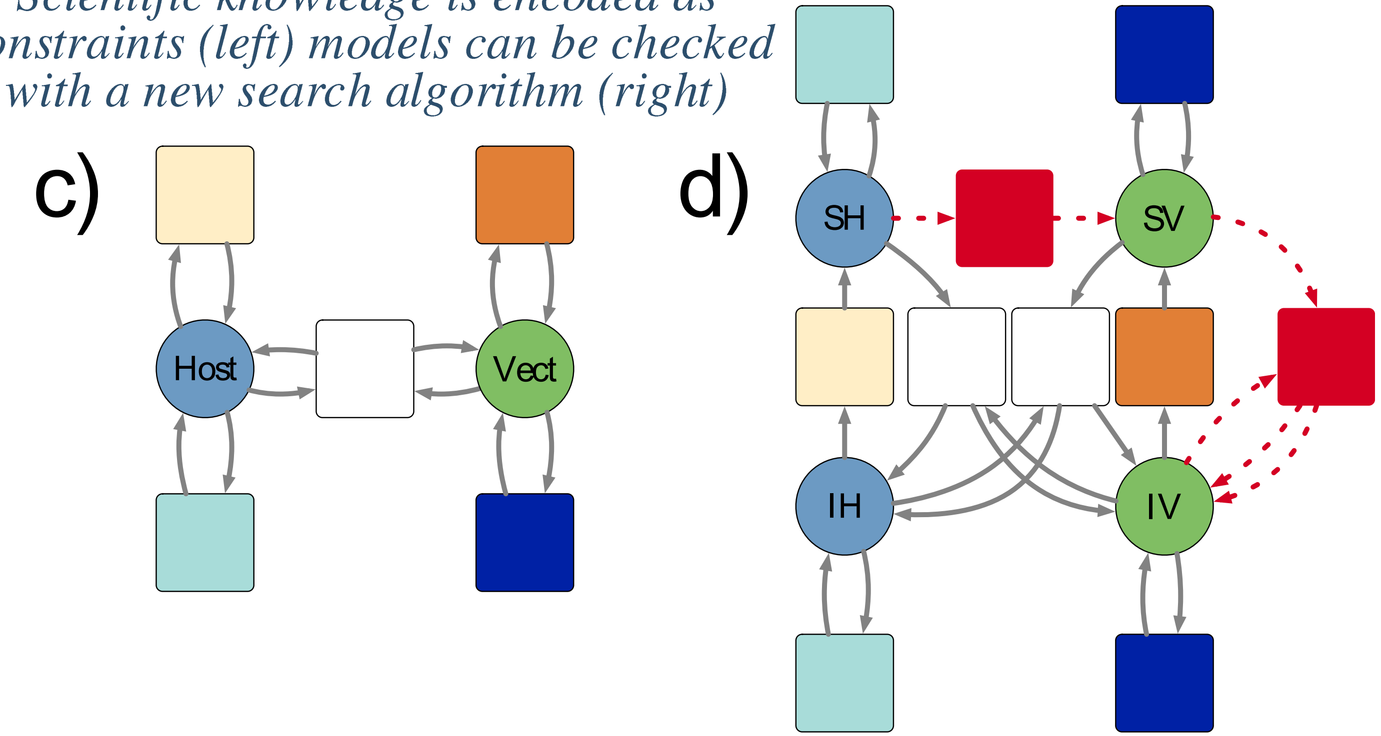
a) Trajectory of true phenomena
b) Space of considered models color coded by RMSE
c) Trajectories of best fit models compared to observed noisy sample from a)



Automating Model V&V and Selection

- Automated V&V uses the math of type theory to capture scientific theories as constraints on valid models, verification reduces to checking the constraints are satisfied. Efficient algorithm with a novel CSP solver.
- These types (shown as colors) are used again for compositional model construction to automate model comparison
- *[1] The Royal Society Phil. Trans. A*
- Automated model selection required the definition of Model Spaces which allows tools from topology and geometry to be applied to the space of governing equations
- Addresses Model Augmentation and Multi-perspective Modeling goals from proposal
- *[2] Applied Category Theory Proceedings 2022*

Scientific knowledge is encoded as constraints (left) models can be checked with a new search algorithm (right)



Model spaces represent possible assumptions about the world. All models can be checked efficiently for fitness for purpose