Compositional modelling of open reaction networks

Blake S. Pollard
Department of Physics and Astronomy
University of California, Riverside

John C. Baez
Department of Mathematics
University of California, Riverside
and
Centre for Quantum Technologies
National University of Singapore
A reaction network with rates \((S, T, s, t, r)\) consists of:

- a finite set \(S\) of species,
- a finite set \(T\) of transitions,
- functions \(s, t : T \rightarrow \mathbb{N}^S\) assigning source and target complexes, and
- a function \(r : T \rightarrow (0, \infty)\), assigning rates to each transition.
Open reaction networks

Open reaction networks are generalizations of reaction networks in which certain species are labelled as **input** and **output** species.

\[ R: X \rightarrow Y \]
Black-boxing open reaction networks

RxNet → Dynam → Rel
The category of open reaction networks

**Definition**

An **open reaction network** \( R: X \rightarrow Y \) consists of a cospan of finite sets

\[
\begin{array}{ccc}
S & \rightarrow & \leftarrow & S \\
\uparrow & i & & o & \downarrow \\
X & & & Y \\
\end{array}
\]

together with a reaction network \( R = (S, T, s, t, r) \) on \( S \).

**Theorem (Baez, P.)**

There is a category \( \text{RxNet} \) whose objects are finite sets and whose morphisms are isomorphism classes of open reaction networks.
Reaction networks as decorations

\[ F: (\text{FinSet}, +) \rightarrow (\text{Set}, \times) \]

\[ F(S) = \{ \text{all reaction networks on } S \} \]

\[ f: S \rightarrow S' \]

\[ F(f): F(S) \quad \rightarrow \quad F(S') \]

\[ (S, T, s, t, r) \quad \mapsto \quad (S', T, f^*(s), f^*(t), r) \]

\[ f^*(s(\tau))(\sigma') = \sum_{\{\sigma|f(\sigma)=\sigma'\}} s(\tau)(\sigma) \]
Reaction networks as decorations

\[ F : (\text{FinSet}, +) \to (\text{Set}, \times) \]

\[ F(S) = \{\text{all reaction networks on } S\} \]

\[ \Phi_{S, S'} : F(S) \times F(S') \to F(S + S') \]

\[ (S, T, s, t, r) \times (S', T', s', t', r') \mapsto (S + S', T + T', s + s', t + t', [r, r']) \]

\[ s + s', t + t' : T + T' \to \mathbb{N}^{S + S'} \]

\[ [r, r'] : T + T' \to (0, \infty) \]
Composition of open reaction networks

\[ R: X \rightarrow Y \]
Composition of open reaction networks

\[ R' : Y \rightarrow Z \]
Composition of open reaction networks

To compose $R: X \rightarrow Y$ and $R': Y \rightarrow Z$ we first combine them
Composition of open reaction networks

Then, we identify any species which are in the image of the same point in $Y$

This gives a new open reaction network $RR' : X \rightarrow Z$. 
The rate equation

A reaction network with rates specifies a set of coupled, non-linear differential equations called its **rate equation**:

\[
\begin{align*}
\frac{dA(t)}{dt} &= -r(\alpha)A(t)B(t) \\
\frac{dB(t)}{dt} &= -r(\alpha)A(t)B(t) \\
\frac{dC(t)}{dt} &= 2r(\alpha)A(t)B(t)
\end{align*}
\]
The rate equation

Given a reaction network with rates \( R = (S, T, s, t, r) \), with species set \( S = \{1, 2, \ldots, |S|\} \), let us denote a vector of concentrations of each species by \( c = (c_1, c_2, \ldots, c_{|S|}) \in \mathbb{R}^S \). Concentrations are non-negative.

Introducing the notation

\[
c^s(\tau) = \prod_{\sigma \in S} c^{s\sigma}(\tau),
\]

we can write the rate equation of a general reaction network obeying mass-action kinetics as

\[
\frac{dc}{dt} = \sum_{\tau \in T} r(\tau) \left( t(\tau) - s(\tau) \right) c^s(\tau).
\]
The rate equation

Given a reaction network $R = (S, T, s, t, r)$, we can define a vector field

$$v(c) = \sum_{\tau \in T} r(\tau) \left( t(\tau) - s(\tau) \right) c^{s(\tau)}$$

generating the time evolution of the concentrations $c \in \mathbb{R}^S$ via

$$\frac{dc}{dt} = v(c).$$

For mass-action kinetics, the vector field $v : \mathbb{R}^S \to \mathbb{R}^S$ is polynomial in the concentrations.
A category of open dynamical systems

**Definition**

An open dynamical system \( D : X \rightarrow Y \) on \( S \) consists of a cospan of finite sets

\[ \begin{align*}
    & S \\
  \downarrow & i \ar & \downarrow & o \\
  & X \ar & & Y
\end{align*} \]

together with an algebraic vector field \( v \) on \( \mathbb{R}^S \).

**Theorem (Baez, P.)**

There is a category \( \text{Dynam} \) where objects are finite sets and morphisms are isomorphism classes of open dynamical systems.
Decorating with algebraic vector fields

\[ D: (\text{FinSet}, +) \to (\text{Set}, \times) \]

\[ D(S) = \{ v: \mathbb{R}^S \to \mathbb{R}^S | \text{v is algebraic} \} \]

\[ f: S \to S' \]

\[ D(f): D(S) \to D(S') \]

\[ v \mapsto f_* \circ v \circ f^* \]

\[ f^*(c')(\sigma) = (c' \circ f)(\sigma) \quad f_*(v)(\sigma') = \sum_{\{\sigma | f(\sigma) = \sigma'\}} v(\sigma) \]
The gray-boxing functor

**Theorem (Baez, P.)**

There is a functor $\Box : \text{RxNet} \to \text{Dynam}$ sending an open reaction network to its corresponding open dynamical system.
The gray-boxing functor

\((R : X \rightarrow Y)\)

\[v_A = -r(\alpha)A(t)B(t)\]

\[v_B = -r(\alpha)A(t)B(t)\]

\[v_C = 2r(\alpha)A(t)B(t)\]
The gray-boxing functor

\[(R': Y \rightarrow Z)\]

\[v_D = -r(\beta)D(t)\]

\[v_E = r(\beta)D(t)\]

\[v_F = r(\beta)D(t)\]
The gray-boxing functor

\[(R: X \rightarrow Y)(R': Y \rightarrow Z)\]

\[v_A = -r(\alpha)AB\]
\[v_B = -r(\alpha)AB\]
\[v_C = 2r(\alpha)AB\]
\[v_D = -r(\beta)D\]
\[v_E = r(\beta)D\]
\[v_F = r(\beta)D\]
The gray-boxing functor

\((R: X \to Y) \circ (R': Y \to Z)\)

\[
\begin{align*}
v_A &= -r(\alpha)AB \\
v_B &= -r(\alpha)AB \\
v_C + v_D &= 2r(\alpha)AB - r(\beta)D \text{ and } C = D \\
v_E &= r(\beta)D \\
v_F &= r(\beta)D
\end{align*}
\]
The gray-boxing functor

\( (RR' : X \to Z) \)

\[
\begin{align*}
  v_A &= -r(\alpha)AB \\
  v_B &= -r(\alpha)AB \\
  v_C &= 2r(\alpha)AB - r(\beta)C \\
  v_E &= r(\beta)C \\
  v_F &= r(\beta)C
\end{align*}
\]
The gray-boxing functor

\[ \square : \text{RxNet} \to \text{Dynam} \]

\[ \theta_S : F(S) \to D(S) \]

\[ F(S) \xrightarrow{F(f)} F(S') \]

\[ \theta_S \downarrow \quad \quad \theta_{S'} \downarrow \]

\[ D(S) \xrightarrow{D(f)} D(S') \]

\[ f : S \to S' \]

\[ R = (S, T, s, t, r) \quad R' = (S', T, f_*(s), f_*(t), r) \]

\[ D(f)(v^R) = v^{R'} \]

\[ f_* \circ v^R \circ f_* = v^{R'} \]

\[ v^{R'}(c') = \sum_{\tau \in T} r(\tau)(f_*(t)(\tau) - f_*(s)(\tau)) c' f_*(s)(\tau) \]
The calculation

\[ C'f_*(s)(\tau) = \prod_{\sigma' \in S'} C'_{\sigma'} f_*(s)(\tau)(\sigma') \]

\[ = \prod_{\sigma' \in S'} C'_{\sigma'} \sum_{\{\sigma : f(\sigma) = \sigma'\}} s(\tau)(\sigma) \]

\[ = \prod_{\sigma' \in S'} \prod_{\{\sigma : f(\sigma) = \sigma'\}} C'_{\sigma'} s(\tau)(\sigma) \]

\[ = \prod_{\sigma \in S} C'_f(\sigma) s(\tau)(\sigma) \]

\[ = \prod_{\sigma \in S} f^*(c')_\sigma s(\tau)(\sigma) \]

\[ = f^*(c')^s(\tau). \]
And then!

\[ \nu^{R'}(c') = \sum_{\tau \in T} r(\tau)(f_*(t)(\tau) - f_*(s)(\tau)) f^*(c')^{s(\tau)} \]

= \( f_*(\nu^R(f^*(c'))) \).

So \( \nu^{R'} = f_* \circ \nu^R \circ f^* \) as desired.
Recap

RxNet → Dynam → Rel
Open Markov processes

RxNet $\rightarrow$ Dynam $\rightarrow$ Rel

Mark
Thank you!

For more:

- John C. Baez and Blake S. Pollard, *A compositional framework for reaction networks*, *Reviews in Mathematical Physics*.
- Blake S. Pollard, *Open Markov processes: A compositional perspective on non-equilibrium steady states in biology*, *Entropy*.