Network Theory II: Stochastic Petri Nets, Chemical Reaction Networks and Feynman Diagrams

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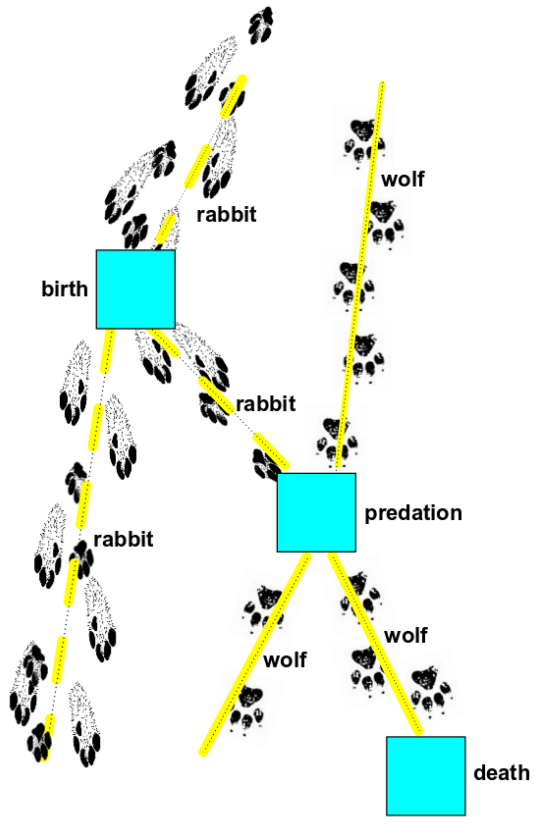
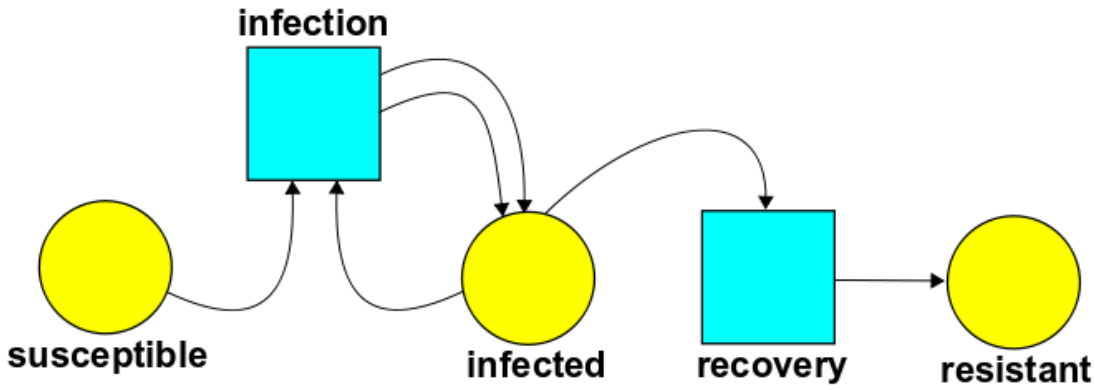


A **Petri net** is a way of drawing a finite set S of **species**, a finite set T of **transitions**, and maps $s, t\colon T \to \mathbb{N}^S$ saying how many times each species appears in the **source** (input) and **target** (output) of each transition:



In this famous example from epidemiology:

$S = \{\text{susceptible, resistant, infected}\}$ $\qquad$ $T = \{\text{infection, recovery}\}$

$s(\text{infection}) = \text{susceptible} + \text{infected}$ $\qquad$ $t(\text{infection}) = 2\ \text{infected}$

$s(\text{recovery}) = \text{infected}$ $\qquad$ $t(\text{recovery}) = \text{resistant}$

A Petri net is actually a way of *presenting a symmetric monoidal category:* one that is freely generated by some set S of objects and some set T of morphisms!

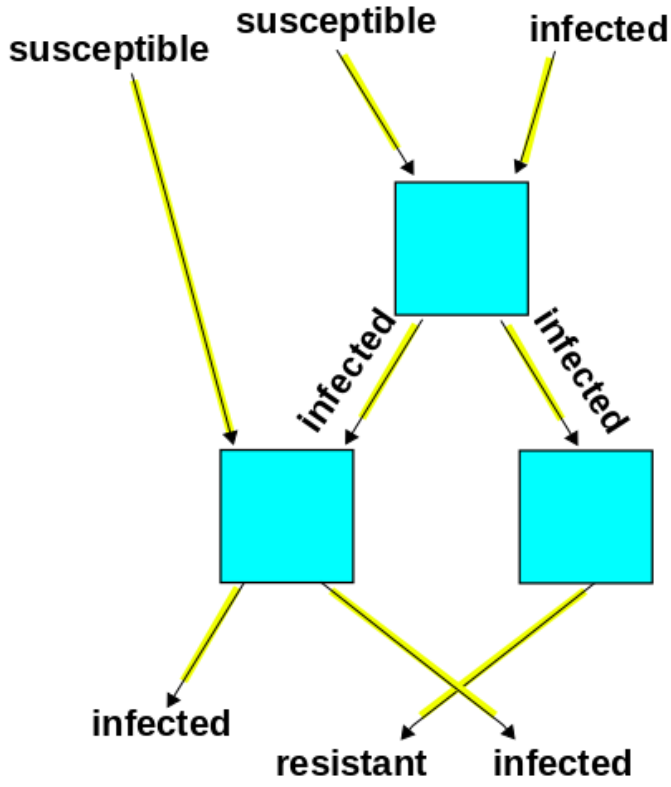
In our example the generating morphisms are:

$$\text{infection: susceptible} + \text{infected} \to \text{infected} + \text{infected}$$

$$\text{recovery: infected} \to \text{resistant}$$

where we write the tensor product as $+$.

Any morphism in the resulting symmetric monoidal category can be drawn as a 'Feynman diagram':



In particle physics we can compute the *amplitude* for any process to occur as a sum over Feynman diagrams. Here we can compute the *probability* for any process to occur.

To do this, we use an unorthodox analogy between quantum mechanics and probability theory, where we treat probabilities as analogous to amplitudes.

Jacob Biamonte and I have a book on this, free online:

- *A Course on Quantum Techniques for Stochastic Mechanics*.

Stochastic mechanics is a way to borrow math from quantum mechanics and apply it to stochastic processes.

Suppose we have a system with n possibilities:

$$X = \{1, \ldots, n\}$$

In quantum theory we consider **quantum states**:

$$\psi \colon X \to \mathbb{C}$$

with

$$\sum_{i \in X} |\psi_i|^2 = 1$$

In probability theory we consider **stochastic states**:

$$\psi \colon X \to \mathbb{R}$$

with

$$\sum_{i \in X} \psi_i = 1 \quad \text{and} \quad \psi_i \geq 0$$

An operator $U\colon \mathbb{C}^n \to \mathbb{C}^n$ that sends quantum states to quantum states is called **unitary**.

An operator $U\colon \mathbb{R}^n \to \mathbb{R}^n$ that sends stochastic states to stochastic states is called **stochastic**.

Concretely, U is stochastic iff

$$\sum_i U_{ij} = 1 \ \text{ and } \ U_{ij} \geq 0$$

An operator $H\colon \mathbb{C}^n \to \mathbb{C}^n$ for which $\exp(-itH)$ is unitary for all $t \in \mathbb{R}$ is called **self-adjoint**.

An operator $H\colon \mathbb{R}^n \to \mathbb{R}^n$ for which $\exp(tH)$ is stochastic for all $t \in [0, \infty)$ is called **infinitesimal stochastic**.

Concretely, H is infinitesimal stochastic iff

$$\sum_i H_{ij} = 0 \;\text{ and }\; H_{ij} \geq 0 \text{ if } i \neq j$$

If H is self-adjoint, we can describe time evolution of quantum states using **Schrödinger's equation**:

$$\frac{d}{dt}\psi(t) = -iH\psi(t)$$

If H is infinitesimal stochastic, we can describe time evolultion of stochastic states using the **master equation**:

$$\frac{d}{dt}\psi(t) = H\psi(t)$$

Unitary operators have unitary inverses; stochastic operators rarely have stochastic inverses! So, we only evolve forwards in time in stochastic physics.

Suppose we have a Petri net:

$$T \overset{s}{\underset{t}{\rightrightarrows}} \mathbb{N}^S$$

Chemists call an element of $\mathbb{N}^S$ a **complex**: it says how many items of each species we have. For example, if

$$S = \{\text{susceptible, resistant, infected}\}$$

then

$$3 \text{ susceptible} + 2 \text{ resistant} + 5 \text{ infected} \in \mathbb{N}^S$$

We call the space of functions $\psi \colon \mathbb{N}^S \to \mathbb{R}$ the **stochastic Fock space**.

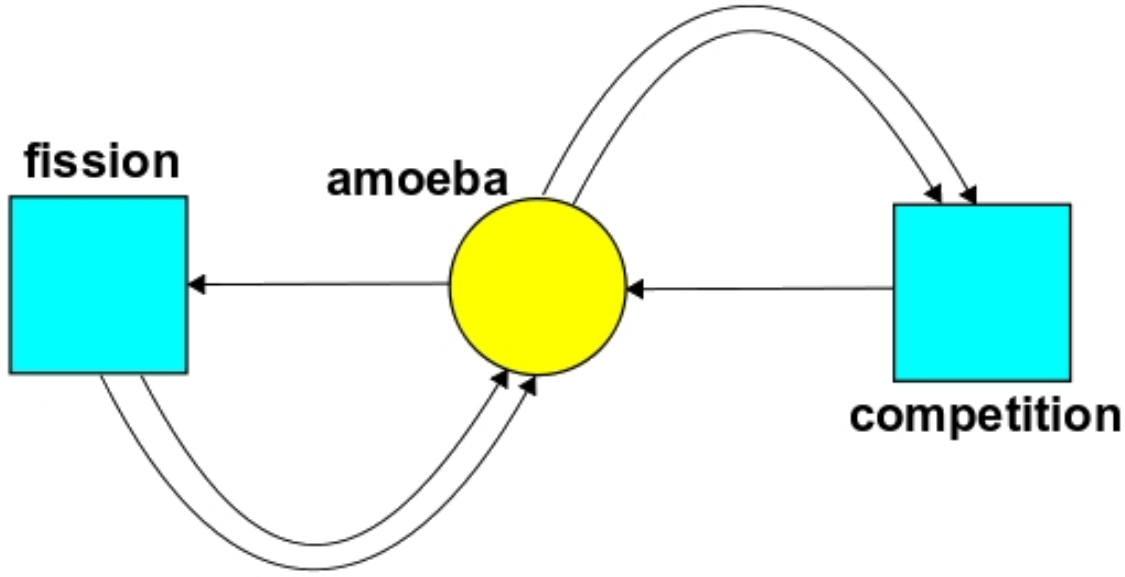
If ψ is a stochastic state and $\kappa \in \mathbb{N}^S$ is a complex, $\psi_\kappa \in [0,1]$ is the probability that we have exactly κ_i items of the ith species.

If we choose a **rate constant** $r(\tau) > 0$ for each transition $\tau \in T$ of our Petri net, we can define a **Hamiltonian** H on the stochastic Fock space. Then the master equation

$$\frac{d}{dt}\psi(t) = H\psi(t)$$

describes how stochastic states evolve in time.

Let's see how to define the Hamiltonian in this example:



Here we have just one species and two transitions:

fission: amoeba $\to$ 2 amoeba

competition: 2 amoeba $\to$ amoeba

Suppose ψ_n is the probability of having n amoebas. We can summarize this information in a power series:

$$\Psi(z) = \sum_{n=0}^{\infty} \psi_n z^n$$

The creation operator $a^\dagger$ creates an amoeba:

$$a^\dagger \Psi = z\Psi$$

The annihilation operator a destroys one:

$$a\Psi = \frac{d}{dz}\Psi$$

We have $az^n = nz^{n-1}$ since there are n amoebas to choose from.

We're used to

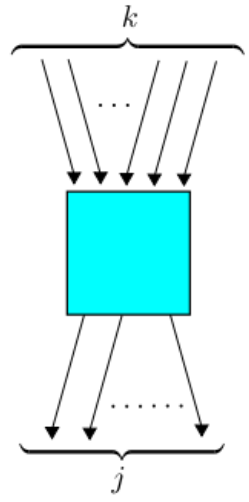
$$aa^\dagger - a^\dagger a = 1$$

for indistinguishable bosons. Can this be right for classical objects if we use probabilities instead of amplitudes?

Yes! There's one more way to create an amoeba and then kill one, than to kill one and then create one.

But let's try some examples.

We would like a Hamiltonian for a process that destroys k amoebas and creates j of them:



The obvious guess is $a^{\dagger j} a^k$. But this is not infinitesimal stochastic! The right answer has a 'correction term':

$$a^{\dagger j} a^k - a^{\dagger k} a^k$$

$H = a^\dagger - 1$ describes the random 'creation' of amoebas. The master equation

$$\frac{d}{dt}\Psi(t) = H\Psi(t)$$

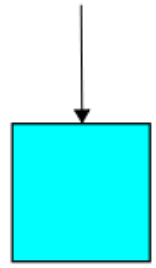
has this solution:

$$\Psi(t) = e^{t(z-1)}\Psi(0)$$

If we start with the 'vacuum state' $\Psi(0) = 1$, where there are no amoebas, at time t we have

$$\Psi(t) = \frac{e^{tz}}{e^t} = e^{-t}\sum_n \frac{t^n}{n!}z^n$$

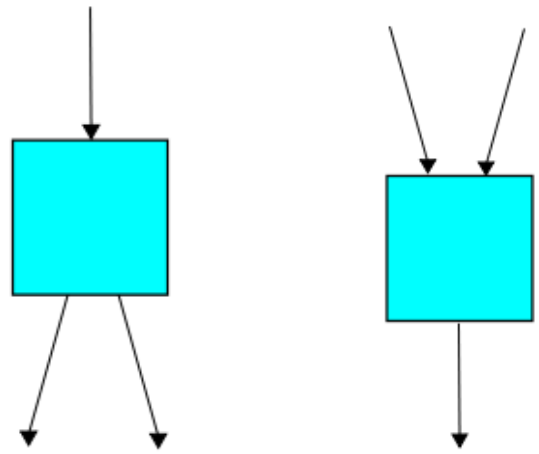
so the probability of having n amoebas is $e^{-t}\frac{t^n}{n!}$. This is just what we expect: a Poisson process.



$H = a - a^\dagger a$ describes the random 'annihilation' of amoebas.

Using this Hamiltonian, the master equation predicts that *the expected number of amoebas decays exponentially*. Again, this is just right.

The Petri net we care about has two transitions: *fission* and *competition*:



So, if these have rate constants α and β, we get

$$H = \alpha(a^{\dagger 2}a - a^{\dagger}a) \quad + \quad \beta(a^{\dagger}a^2 - a^{\dagger 2}a^2)$$

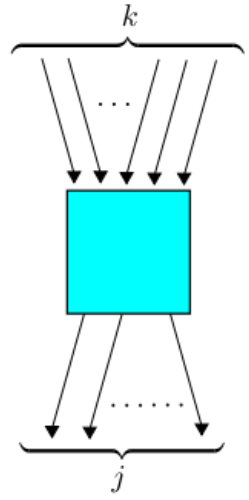
Here we can show that in the 'classical limit' where ψ_n is very sharply peaked near some very large number, the expected number of amoebas:

$$\langle N(t) \rangle = \sum_n n \, \psi_n(t)$$

obeys the logistic equation:

$$\frac{d}{dt} \langle N(t) \rangle = \alpha \langle N(t) \rangle - \beta \langle N(t) \rangle^2$$

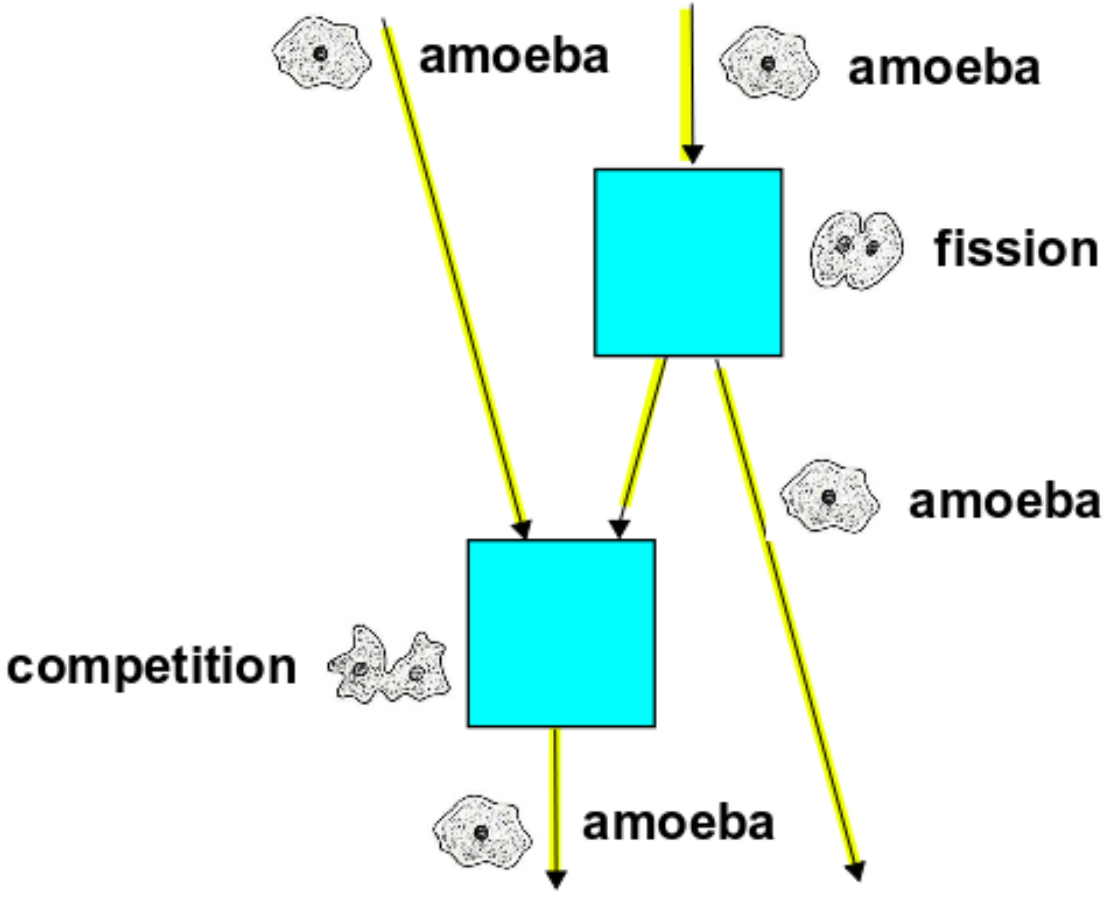
In fact, for *any* Hamiltonian that is a linear combination of terms like this:



$$a^{\dagger j} a^k - a^{\dagger k} a^k$$

it is easy to write a differential equation describing how the expected number of particles $\langle N(t) \rangle$ changes with time in the classical limit. This is called the 'rate equation'.

Moreover, we can always express the time evolution operator $\exp(tH)$ as a sum over Feynman diagrams:



All this easily generalizes to Petri nets with more than one species.

In some ways stochastic mechanics works *better* than quantum mechanics! It might seem hard to find a stationary state

$$H\Psi = 0$$

for our Hamiltonian

$$H = \alpha({a^\dagger}^2 a - a^\dagger a) \;\; + \;\; \beta(a^\dagger a^2 - {a^\dagger}^2 a^2)$$

describing amoeba fission and competition. But we can do it using the Anderson–Craciun–Kurtz theorem.

First, find a stationary solution of the rate equation:

$$\frac{d}{dt}\langle N(t)\rangle = \alpha\langle N(t)\rangle - \beta\langle N(t)\rangle^2$$

In our case this easy:

$$\alpha\langle N(t)\rangle - \beta\langle N(t)\rangle^2 = 0$$

$$\langle N(t)\rangle = \alpha/\beta$$

Then form the 'coherent state' where the expected number of amoebas takes this value:

$$\Psi = \frac{e^{(\alpha/\beta)z}}{e^{\alpha/\beta}} = \frac{1}{e^{\alpha/\beta}} \sum_{n=0}^{\infty} \frac{(\alpha/\beta)^n}{n!} z^n$$

The Anderson–Craciun–Kurtz theorem implies $H\Psi = 0$!

Anderson, Craciun and Kurtz are chemists.

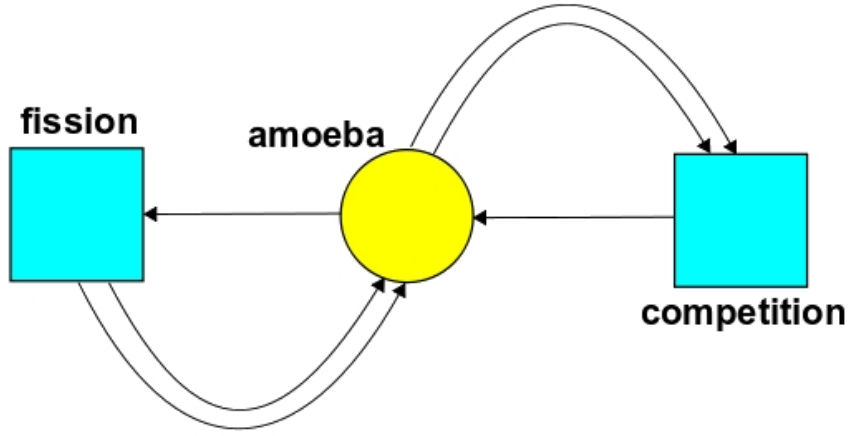
So, instead of Petri nets they use an equivalent formalism, 'reaction networks'. Here we take our Petri net:

$$T \underset{t}{\overset{s}{\rightrightarrows}} \mathbb{N}^S$$

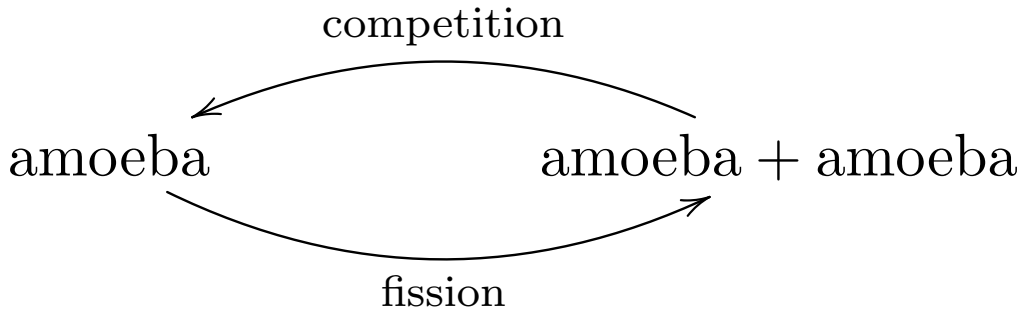
and draw a directed graph with:

- transitions $\tau \in T$ as edges,
- complexes in the image of s or t as vertices.

For example, this Petri net:



corresponds to this reaction network:



The Anderson–Craciun–Kurtz theorem, together with the 'deficiency zero theorem', says that:

- there exist nonzero equilibrium solutions of the rate equation

and

- every such equilibrium solution gives a coherent state Ψ in the stochastic Fock space obeying $H\Psi = 0$

if the reaction network is 'weakly reversible' and has 'deficiency zero'.

A reaction network is **weakly reversible** if for any edge (that is, transition):

$$\kappa \xrightarrow{\tau} \kappa'$$

there is a directed path of edges going back:

$$\kappa' \xrightarrow{\tau_0} \kappa_1 \xrightarrow{\tau_1} \cdots\cdots \xrightarrow{\tau_{n-1}} \kappa_n \xrightarrow{\tau_n} \kappa$$

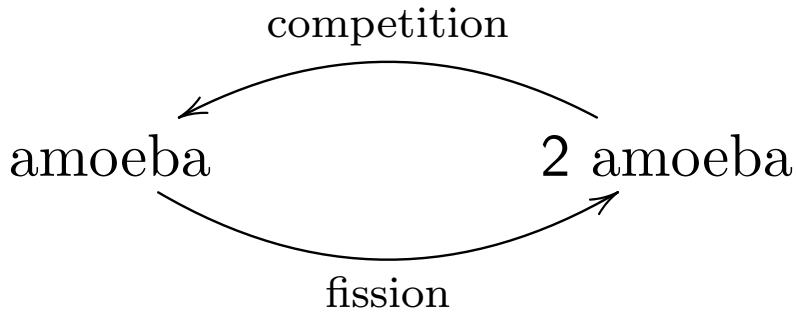
The **deficiency** of a reaction network is:

- its number of connected components (as a graph)
- *minus* its number of vertices
- *plus* the dimension of the subspace spanned by vectors

$$t(\tau) - s(\tau) \in \mathbb{N}^S \subseteq \mathbb{R}^S$$

where τ ranges over all transitions in T.

For example, this reaction network is weakly reversible:



It has:

- 1 connected component,
- 2 vertices,
- and the dimension of the subspace spanned by vectors

  2 amoeba - amoeba, amoeba - 2 amoeba

  is 1.

Thus its deficiency is $1 - 2 + 1 = 0$, and the theorems apply!

In summary:

1. We are seeing chemists prove highly nontrivial theorems about stochastic processes described by free symmetric monoidal categories where the generating morphisms are assigned 'rate constants'!
2. These results have applications not just in chemistry but also population biology, epidemiology and evolutionary game theory.
3. The mathematical context for this requires generalizing Feynman diagrams from quantum mechanics to stochastic mechanics. So: applied category theory of a new kind!