Integral ODE model of reaction:

$$\frac{d[A_f]}{dt} = 2k_1[G_f][A_f] - \frac{k_p[A]}{[A]+K_m}$$
$$\frac{d[G_f]}{dt} = V_{in} - k_1[G_f][A_f]$$
$$[G_f] = \frac{\int_\Omega G_p(x)dx}{Vol(\Omega)}, \Omega \subset \mathbb{R}^n$$
$$[A_f] = \frac{\int_\Omega A_p(x)dx}{Vol(\Omega)}, \Omega \subset \mathbb{R}^n$$
$$V_{in}(t) = \int_{\delta\Omega} V_p(x,t)dx, \delta\Omega - \text{boundary of } \Omega$$

Problem.

What are generic solution for $A_p(x)$ and $G_p(x)$?

Model.

RD model

Our model based on the graph sequence whose elements are so called flow graphs. The main property of these graphs is that all of them have the same set of vertices V

Suppose G is directed graph that have N vertices. Some of the vertices are connected with oriented edges (also called arrows). Arrow between two vertices is associated with material flow between them.

Details.

Vertex can be one of types:

- input gate which is modelled as some (some) periodical function;
- output gate which is also some time and environment function;
- diffuse input/output gates are stochastic processes;
- transitive gates which are connections between edges;
- source gate which is special kind of input gate where materials are generated

The type of vertex depends on material. The same vertex can be an input gate for one material and can work as output gate for another material.

There are many methods to model material flow on the edge. We use stochastic particle transfer and diffuse model.

Materials are modelled as sets of particles that we call abstract "molecules". Every partial model have a set of different molecules *types*.

Some types of molecules can react. Reaction is just a (probabilistic) rule which describes conditions when one type of molecule(s) becomes another type.