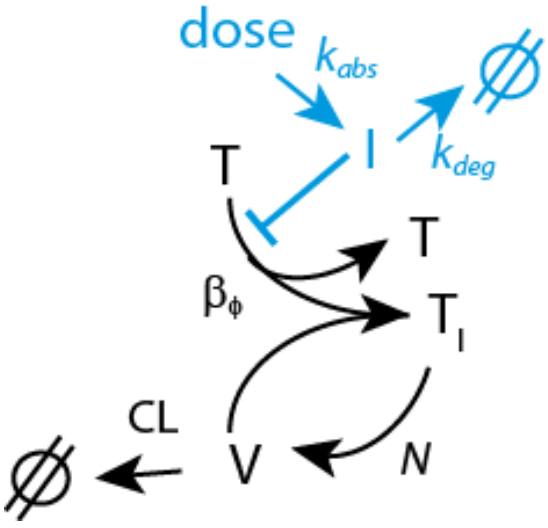
Tasks---Topic XY---Extrande

Tasks:

(1) Implement the Gillespie algorithm for the model of viral infection below (below with V0 = 1, T = 1000, β_Φ = 1/1000, CL = 10, N = 1000). Stop simulations if V(t) exceeds 5000. And count in how many simulations this occurs. This is your proxy for the probability of infection.

(2) Extend the model by including a competitive I modifying the infection reaction $\beta(t) = \beta_\Phi$ *(IC50/[I + IC50]), where IC50 is a constant. Here, 'dose' refers to the dose of the inhibitor, which is increased every 24h by an impulse ($dose_{t+} = dose_{t-} + \Delta$ dose). Analyse how the time steps in the SSA change as you increase Δ dose.



(3) Implement the extrande algorithm by considering an ODE for the dynamics of the inhibitor fast reactions (large Δ dose, highlighted in blue).

(4) Deduce suitable upper bounds for the time-dependent propensities

Article: M. Voliotis et al. Stochastic Simulation of Biomolecular Networks in Dynamic Environments (2016) PLoS Comput Biol.12(6): e1004923.

Review article:
(a) D.T. Gillespie Stochastic Simulation of Chemical Kinetics (2007) Annu. Rev. Phys. Chem.. 58:35–55;
(b) J. Pahle Biochemical simulations: stochastic, approximate stochastic and hybrid approaches (2009) BRIEFINGS IN BIOINFORMATICS. 10 (1). 53-64