Gillespie Algorithm

Leonhard Horstmeyer

June 9, 2017

A General Method for Numerically Simulating the Stochastic Time Evolution of Coupled Chemical Reactions

DANIEL T. GILLESPIE

Research Department, Naval Weapons Center, China Lake, California 93555

Received January 27, 1976; revised April 21, 1976

An exact method is presented for numerically calculating, within the framework of the stochastic formulation of chemical kinetics, the time evolution of any spatially homogeneous mixture of molecular species which interreact through a specified set of coupled chemical reaction channels. The method is a compact, computer-oriented, Monte Carlo simulation procedure. It should be particularly useful for modeling the transient behavior of well-mixed gas-phase systems in which many molecular species participate in many highly coupled chemical reactions. For "ordinary" chemical systems in which fluctuations and correlations play no significant role, the method stands as an alternative to the traditional procedure of numerically solving the deterministic reaction rate equations. For nonlinear systems near chemical instabilities, where fluctuations and correlations may invalidate the deterministic equations, the method constitutes an efficient way of numerically examining the predictions of the stochastic master equation. Although fully equivalent to the spatially homogeneous master equation, the numerical simulation algorithm presented here is more directly based on a newly defined entity called "the reaction probability density function." The purpose of this article is to describe

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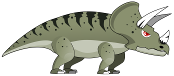
Species : 

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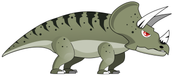
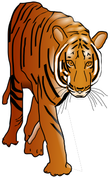
Species :  

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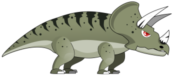
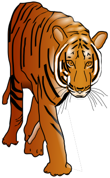
Species :   . . . 

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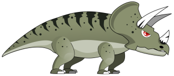
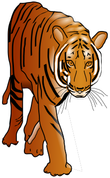
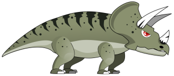
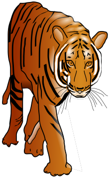
Species :   . . . 

Abundances :

Species

Species :   ... 

Abundances : N_1 N_2 ... N_S

Reactions

Reaction :

Reactions

Reaction :

Reactions

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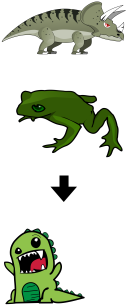

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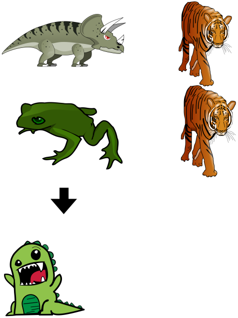

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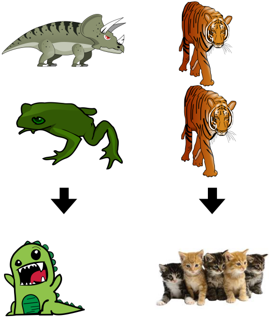

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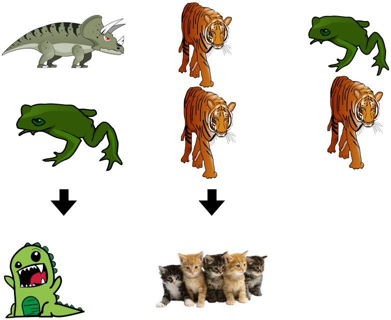

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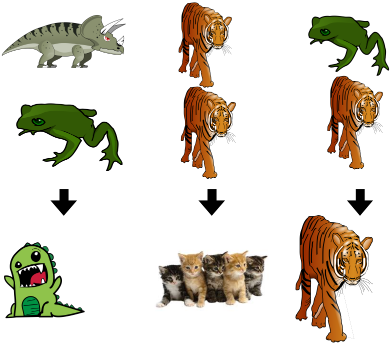

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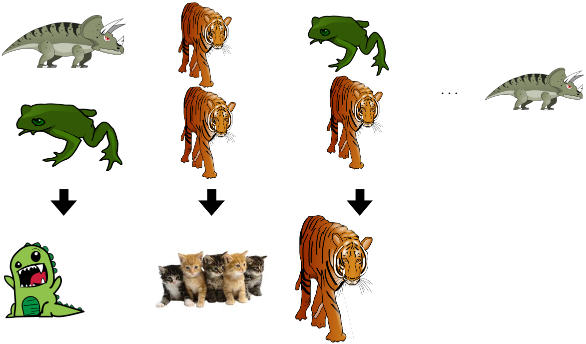

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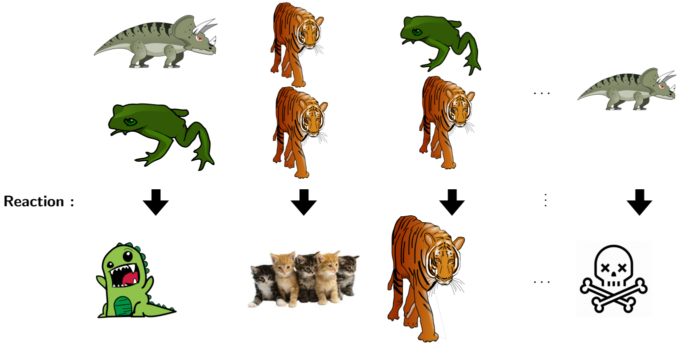

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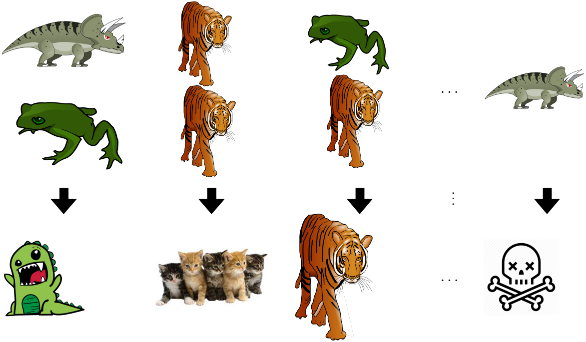
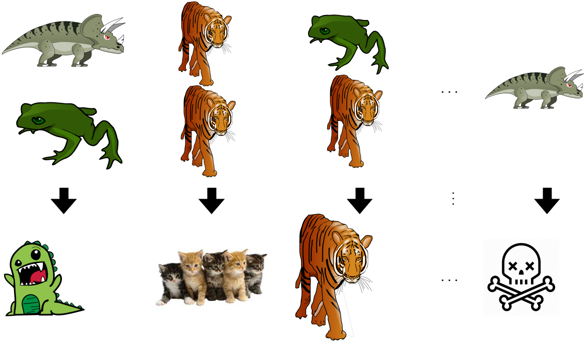


Reaction :

Number of Reactants: h_1

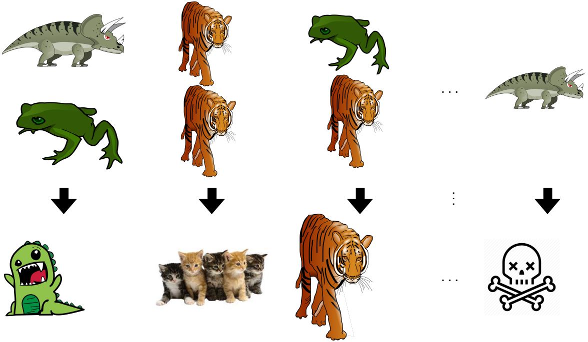
Reactions



Reaction :

Number of Reactants: $h_1 = N_1 \cdot N_S$ h_2

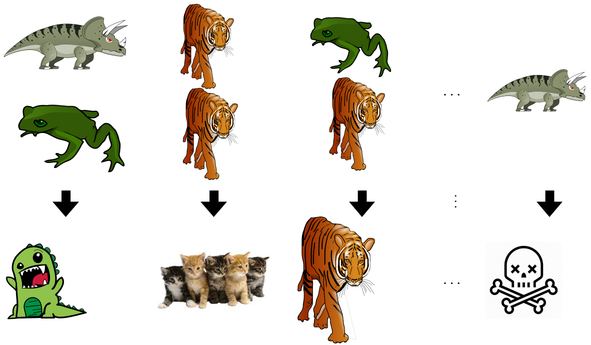
Reactions



Reaction :

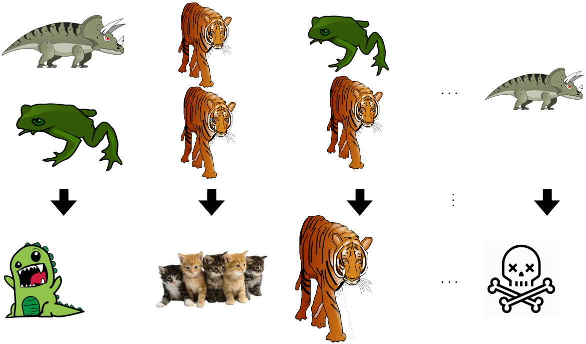
Number of Reactants: $h_1 = N_1 \cdot N_S$ $h_2 = N_2 \cdot (N_2 - 1)/2$ h_3

Reactions



Reaction :

Number of Reactants: $h_1 = N_1 \cdot N_S$ $\quad h_2 = N_2 \cdot (N_2 - 1)/2$ $\quad h_3 = N_2 \cdot N_S$ $\quad \ldots$ $\quad h_M$



Reaction :

Number of Reactants: $h_1 = N_1 \cdot N_S$ $h_2 = N_2 \cdot (N_2 - 1)/2$ $h_3 = N_2 \cdot N_S$ $\ldots$ $h_M = N_1$

Reactions

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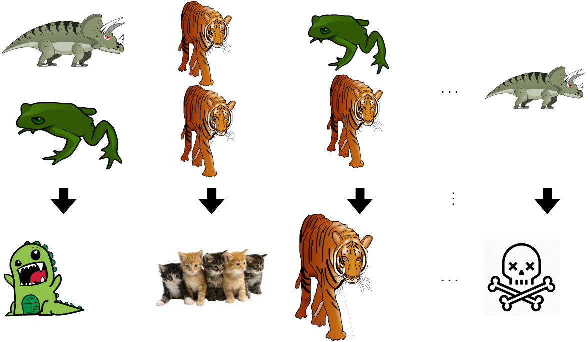

Number of Reactants:	$h_1 = N_1 \cdot N_S$	$h_2 = N_2 \cdot (N_2 - 1)/2$	$h_3 = N_2 \cdot N_S$	$\dots$	$h_M = N_1$
Reaction Rates:	c_1	c_2	c_3	$\dots$	c_M

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:				

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$			

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	Master Equation		

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'}; t)$		

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}} \mathbb{P}(\boldsymbol{N'}; t)$	$\prod_j N_j$	

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1,\ldots,N_S;t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N};t)=\sum_{\boldsymbol{N'}}W_{\boldsymbol{NN'}}\mathbb{P}(\boldsymbol{N'};t)$	$\mathbb{P}:\prod_j N_j\to[0,1]$	

Our Options

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Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{NN'}}\mathbb{P}(\boldsymbol{N'}; t)$	$\mathbb{P} : \prod_j N_j \rightarrow [0, 1]$	ODE solver

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Option 2:				

Our Options

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Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}} \mathbb{P}(\boldsymbol{N'}; t)$	$\mathbb{P} : \prod_j N_j \to [0, 1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N}; t\Big], \ldots, \mathbb{E}\Big[\frac{N_S}{N}; t\Big]$			

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{NN'}}\mathbb{P}(\boldsymbol{N'}; t)$	$\mathbb{P} : \prod_j N_j \to [0, 1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N}; t\Big], \ldots, \mathbb{E}\Big[\frac{N_S}{N}; t\Big]$	Mean Field Equations		

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Option 2:	$\mathbb{E}\Big[\frac{N_1}{N}; t\Big], \ldots, \mathbb{E}\Big[\frac{N_S}{N}; t\Big]$	Mean Field Equations	$[0, 1]^S$	

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \dots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}} \mathbb{P}(\boldsymbol{N'}; t)$	$\mathbb{P} : \prod_j N_j \to [0, 1]$	ODE solver
Option 2:	$\mathbb{E}\left[\frac{N_1}{N}; t\right], \dots, \mathbb{E}\left[\frac{N_S}{N}; t\right]$	Mean Field Equations	$\cancel{[0, 1]^S}$	

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'}; t)$	$\mathbb{P} : \prod_j N_j \to [0, 1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N}; t\Big], \ldots, \mathbb{E}\Big[\frac{N_S}{N}; t\Big]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'}; t)$	$\mathbb{P} : \prod_j N_j \rightarrow [0, 1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N}; t\Big], \ldots, \mathbb{E}\Big[\frac{N_S}{N}; t\Big]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver

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Option 2:	$\mathbb{E}\left[\frac{N_1}{N}; t\right], \ldots, \mathbb{E}\left[\frac{N_S}{N}; t\right]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
Option 3:	$N_1(t), \ldots, N_S(t)$			

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1,\ldots,N_S;t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N};t)=\sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'};t)$	$\mathbb{P}:\prod_j N_j \to [0,1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N};t\Big],\ldots,\mathbb{E}\Big[\frac{N_S}{N};t\Big]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
		Fix Δt.		
Option 3:	$N_1(t),\ldots,N_S(t)$			

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'}; t)$	$\mathbb{P} : \prod_j N_j \rightarrow [0, 1]$	ODE solver
Option 2:	$\mathbb{E}\left[\frac{N_1}{N}; t\right], \ldots, \mathbb{E}\left[\frac{N_S}{N}; t\right]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
Option 3:	$N_1(t), \ldots, N_S(t)$	Fix Δt. Consider all reactions $R_\mu : \boldsymbol{N} \rightarrow \boldsymbol{N'}$		

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}} \mathbb{P}(\boldsymbol{N'}; t)$	$\mathbb{P} : \prod_j N_j \to [0, 1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N}; t\Big], \ldots, \mathbb{E}\Big[\frac{N_S}{N}; t\Big]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
Option 3:	$N_1(t), \ldots, N_S(t)$	Fix Δt. Consider all reactions $R_\mu : \boldsymbol{N} \to \boldsymbol{N'}$ Approximate $\mathbb{P}\big(\boldsymbol{N'}; t + \Delta t \big\| \boldsymbol{N}; t\big)$		

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1,\ldots,N_S;t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N};t)=\sum_{\boldsymbol{N'}}W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'};t)$	$\mathbb{P}:\prod_j N_j \to [0,1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N};t\Big],\ldots,\mathbb{E}\Big[\frac{N_S}{N};t\Big]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
Option 3:	$N_1(t),\ldots,N_S(t)$	Fix Δt. Consider all reactions $R_\mu:\boldsymbol{N}\to\boldsymbol{N'}$ Approximate $\mathbb{P}\big(\boldsymbol{N'};t+\Delta t\big\vert\boldsymbol{N};t\big)$ by *rate* $\cdot\Delta t$ and update.		

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N};t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{NN'}}\mathbb{P}(\boldsymbol{N'};t)$	$\mathbb{P} : \prod_j N_j \rightarrow [0,1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N};t\Big], \ldots, \mathbb{E}\Big[\frac{N_S}{N};t\Big]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
Option 3:	$N_1(t), \ldots, N_S(t)$	Fix Δt. Consider all reactions $R_\mu : \boldsymbol{N} \rightarrow \boldsymbol{N'}$ Approximate $\mathbb{P}\big(\boldsymbol{N'}; t + \Delta t \big\vert \boldsymbol{N}; t\big)$ by *rate* $\cdot \Delta t$ and update.	Collect enough runs to make the result statistically meaningful	

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1,\ldots,N_S;t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N};t)=\sum_{\boldsymbol{N'}}W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'};t)$	$\mathbb{P}:\prod_j N_j\rightarrow[0,1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N};t\Big],\ldots,\mathbb{E}\Big[\frac{N_S}{N};t\Big]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
Option 3:	$N_1(t),\ldots,N_S(t)$	Fix Δt. Consider all reactions $R_\mu:\boldsymbol{N}\rightarrow\boldsymbol{N'}$ Approximate $\mathbb{P}\big(\boldsymbol{N'};t+\Delta t\big\vert\boldsymbol{N};t\big)$ by *rate* $\cdot\Delta t$ and update.	Collect enough runs to make the result statistically meaningful	Simply Monte Carlo for $\big[0,\mathbb{P}\big(\boldsymbol{N'}\vert\boldsymbol{N}\big)\big]$ consecutively.

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1, \ldots, N_S; t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N}; t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'}; t)$	$\mathbb{P} : \prod_j N_j \rightarrow [0, 1]$	ODE solver
Option 2:	$\mathbb{E}\left[\frac{N_1}{N}; t\right], \ldots, \mathbb{E}\left[\frac{N_S}{N}; t\right]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
Option 3:	$N_1(t), \ldots, N_S(t)$	Fix Δt. Consider all reactions $R_\mu : \boldsymbol{N} \rightarrow \boldsymbol{N'}$ Approximate $\mathbb{P}\big(\boldsymbol{N'}; t + \Delta t \big\vert \boldsymbol{N}; t\big)$ by *rate* $\cdot \Delta t$ and update.	Collect enough runs to make the result statistically meaningful	Simply Monte Carlo for $\big[0, \mathbb{P}\big(\boldsymbol{N'} \vert \boldsymbol{N}\big)\big]$ consecutively.
Option 4: **(Gillespie)**				

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1,\ldots,N_S;t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N};t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'};t)$	$\mathbb{P} : \prod_j N_j \rightarrow [0,1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N};t\Big],\ldots,\mathbb{E}\Big[\frac{N_S}{N};t\Big]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
Option 3:	$N_1(t),\ldots,N_S(t)$	Fix Δt. Consider all reactions $R_\mu : \boldsymbol{N} \rightarrow \boldsymbol{N'}$ Approximate $\mathbb{P}\big(\boldsymbol{N'};t+\Delta t\big\vert\boldsymbol{N};t\big)$ by *rate* $\cdot\Delta t$ and update.	Collect enough runs to make the result statistically meaningful	Simply Monte Carlo for $\big[0,\mathbb{P}\big(\boldsymbol{N'}\vert\boldsymbol{N}\big)\big]$ consecutively.
Option 4: **(Gillespie)**	$N_1(t),\ldots,N_S(t)$			

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1,\ldots,N_S;t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N};t)=\sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'};t)$	$\mathbb{P}:\prod_j N_j \rightarrow [0,1]$	ODE solver
Option 2:	$\mathbb{E}\left[\frac{N_1}{N};t\right],\ldots,\mathbb{E}\left[\frac{N_S}{N};t\right]$	Mean Field Equations	$\cancel{[0,1]^S}$ $\quad\Delta_{S-1}$	ODE solver
Option 3:	$N_1(t),\ldots,N_S(t)$	Fix Δt. Consider all reactions $R_\mu : \boldsymbol{N}\rightarrow\boldsymbol{N'}$ Approximate $\mathbb{P}\big(\boldsymbol{N'};t+\Delta t\big\vert\boldsymbol{N};t\big)$ by *rate* $\cdot\Delta t$ and update.	Collect enough runs to make the result statistically meaningful	Simply Monte Carlo for $\big[0,\mathbb{P}(\boldsymbol{N'}\vert\boldsymbol{N})\big]$ consecutively.
Option 4: **(Gillespie)**	$N_1(t),\ldots,N_S(t)$	sample the stochastic path by drawing the time of the next event τ and the type of event μ from the relevant distribution		

Our Options

	Qantity of interest	Evolution	Size of the Problem	Solution Method
Option 1:	$\mathbb{P}\Big(N_1,\ldots,N_S;t\Big)$	$\frac{\partial}{\partial t}\mathbb{P}(\boldsymbol{N};t) = \sum_{\boldsymbol{N'}} W_{\boldsymbol{N}\boldsymbol{N'}}\mathbb{P}(\boldsymbol{N'};t)$	$\mathbb{P} : \prod_j N_j \to [0,1]$	ODE solver
Option 2:	$\mathbb{E}\Big[\frac{N_1}{N};t\Big],\ldots,\mathbb{E}\Big[\frac{N_S}{N};t\Big]$	Mean Field Equations	$\cancel{[0,1]^S}$ Δ_{S-1}	ODE solver
Option 3:	$N_1(t),\ldots,N_S(t)$	Fix Δt. Consider all reactions $R_\mu : \boldsymbol{N} \to \boldsymbol{N'}$ Approximate $\mathbb{P}\big(\boldsymbol{N'};t+\Delta t\big\vert\boldsymbol{N};t\big)$ by *rate* $\cdot\Delta t$ and update.	Collect enough runs to make the result statistically meaningful	Simply Monte Carlo for $\big[0,\mathbb{P}\big(\boldsymbol{N'}\vert\boldsymbol{N}\big)\big]$ consecutively.
Option 4: **(Gillespie)**	$N_1(t),\ldots,N_S(t)$	sample the stochastic path by drawing the time of the next event τ and the type of event μ from the relevant distribution $P_t(\tau,\mu)$	Again, collect sufficiently many runs	

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Option 3:	$N_1(t),\dots,N_S(t)$	Fix Δt. Consider all reactions $R_\mu : \boldsymbol{N} \to \boldsymbol{N'}$ Approximate $\mathbb{P}\left(\boldsymbol{N'};t+\Delta t \middle| \boldsymbol{N};t\right)$ by *rate* $\cdot \Delta t$ and update.	Collect enough runs to make the result statistically meaningful	Simply Monte Carlo for $\left[0,\mathbb{P}\left(\boldsymbol{N'}\middle|\boldsymbol{N}\right)\right]$ consecutively.
Option 4: (Gillespie)	$N_1(t),\dots,N_S(t)$	sample the stochastic path by drawing the time of the next event τ and the type of event μ from the relevant distribution $P_t(\tau,\mu)$	Again, collect sufficiently many runs	Monte Carlo to sample $P_t(\tau,\mu)$

$P_t(\tau, \mu)$ - Derivation

Question

Suppose we have evolved the dynamics up to time t and the population is currently $\boldsymbol{N}(t) = (N_1, \ldots, N_S)$.

$P_t(\tau, \mu)$ - Derivation

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Answer

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What is the probability that the next reaction will take place after τ time units (i.e. at $t + \tau$) and will be of type μ?

Answer

$P_t(\tau, \mu) = h_\mu c_\mu \cdot \mathrm{e}^{-\sum_\nu h_\nu c_\nu \tau}$

Reaction ν happens during Δt

$$h_\nu c_\nu \cdot \Delta t$$

.

$P_t(\tau, \mu)$ - Derivation

Reaction ν doesn't happen during Δt

$$1 - h_\nu c_\nu \cdot \Delta t$$

.

$P_t(\tau, \mu)$ - Derivation

No reaction happens during Δt

$$\prod_\nu (\; 1 - \; h_\nu c_\nu \cdot \Delta t \;)$$

.

Expanding in Δt

$$\prod_\nu (\ 1 - \ h_\nu c_\nu \cdot \Delta t\ ) = (1 - \sum_\nu h_\nu c_\nu \cdot \Delta t)$$

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$$\prod_\nu (1- h_\nu c_\nu \cdot \Delta t) = (1 - \sum_\nu h_\nu c_\nu \cdot \Delta t) \quad +\mathcal{O}\left(\Delta t^2\right)$$

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$$\prod_\nu (1 - h_\nu c_\nu \cdot \Delta t) = (1 - \sum_\nu h_\nu c_\nu \cdot \Delta t) \quad + \mathcal{O}\big(\Delta t^2\big)$$

No reaction occurs during $\tau = K \cdot \Delta t$

$$(1 - \sum_\nu h_\nu c_\nu \cdot \Delta t)^K$$

.

$P_t(\tau, \mu)$ - Derivation

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$$(1 - \sum_\nu h_\nu c_\nu \cdot \ \tfrac{\tau}{K} \ )^K$$

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Taking the limit $K \to \infty$

$$\lim_{K \to \infty} \ (1 - \sum_\nu h_\nu c_\nu \cdot \ \tfrac{\tau}{K} \ )^K = \mathsf{e}^{-\tau \sum_\nu h_\nu c_\nu}$$

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no reaction during τ, but μ happens during $[\tau, \tau + \Delta\tau]$

$$(h_\mu \quad c_\mu \cdot \Delta\tau) \cdot \mathrm{e}^{-\tau \sum_\nu h_\nu \quad c_\nu}$$

$P_t(\tau, \mu)$ - Derivation

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no reaction during $[t, t+\tau]$, but μ happens in $[t+\tau, t+\tau+\Delta\tau]$

$$(h_\mu(t) c_\mu \cdot \Delta\tau) \cdot \mathrm{e}^{-\tau \sum_\nu h_\nu(t) c_\nu}$$

$P_t(\tau, \mu)$ - Derivation

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Drawing from $P_t(\tau, \mu)$ - The Monte Carlo Step

Another Question

How can we sample from $P_t(\tau, \mu)$

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How can we sample from $P_t(\tau, \mu) = a_\mu \mathrm{e}^{-\boldsymbol{a}\tau}$
Where $a_\mu = h_\mu c_\mu$ and $\boldsymbol{a} = \sum_\nu a_\nu$.

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$\Rightarrow$ only 2 one dim'l distributions

Drawing from $P_t(\tau, \mu)$ - The Monte Carlo Step

$$P(\tau) = \boldsymbol{a}\mathrm{e}^{-\boldsymbol{a}\tau}$$

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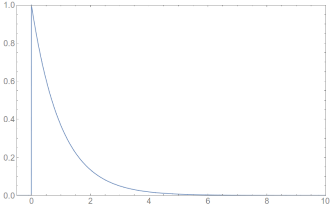

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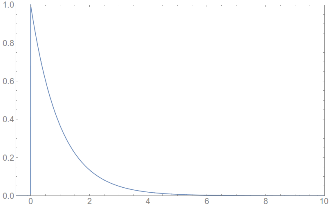

$$F(\tau) = 1 - \mathrm{e}^{-\boldsymbol{a}\tau}$$

Drawing from $P_t(\tau, \mu)$ - The Monte Carlo Step

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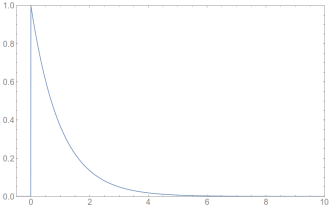

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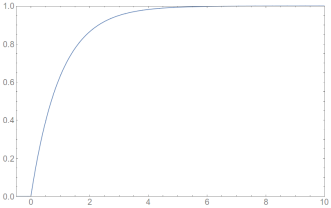

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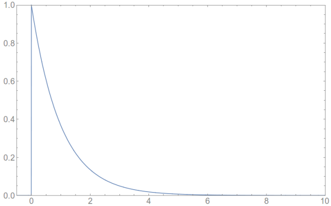

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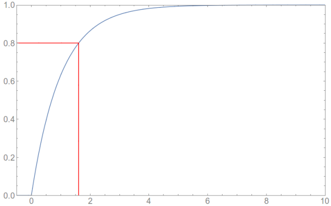

Drawing from $P_t(\tau, \mu)$ - The Monte Carlo Step

Answer for $P(\tau)$

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Generate a random number $r = rand()$

Drawing from $P_t(\tau, \mu)$ - The Monte Carlo Step

Answer for $P(\tau)$

Generate a random number $r = rand()$
Solve $r = F(\tau)$

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So $\tau = -\frac{1}{a}\log(1-r)$

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Generate a random number $s = rand()$
Invert $s = F(\mu|\tau) = \sum_{\nu=1}^{\mu} \frac{a_\nu}{\boldsymbol{a}}$

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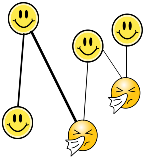
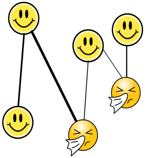
Find μ such that
$\sum_{\nu=1}^{\mu-1} \frac{a_\nu}{\boldsymbol{a}} < s \leq \sum_{\nu=1}^{\mu} \frac{a_\nu}{\boldsymbol{a}}$

What's the Story for Networks



$\boldsymbol{x} = (x_i)\,,\ \boldsymbol{A} = (A_{ij})$

What's the Story for Networks



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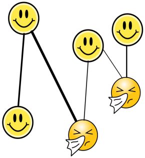
Reaction :

What's the Story for Networks



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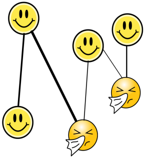

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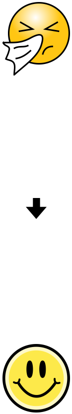

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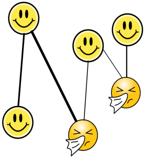

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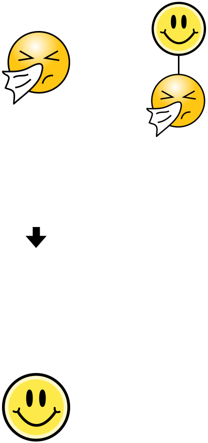

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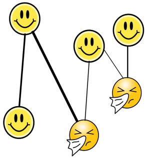

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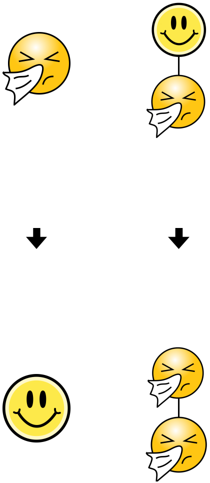

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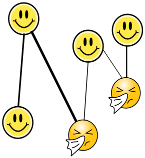

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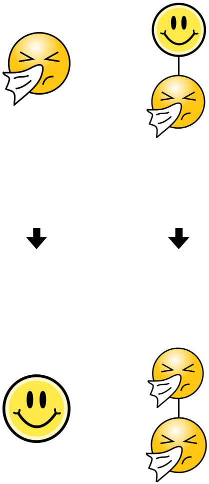
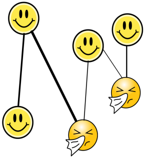


Number of Reactants: h_1

What's the Story for Networks



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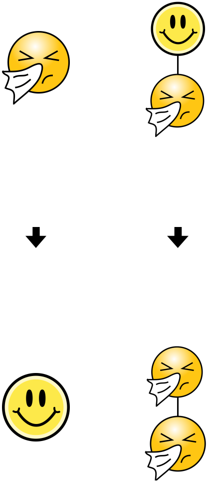
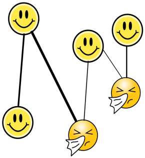


Number of Reactants: $h_1 = N_I$

What's the Story for Networks



$\boldsymbol{x} = (x_i)\,,\ \boldsymbol{A} = (A_{ij})$

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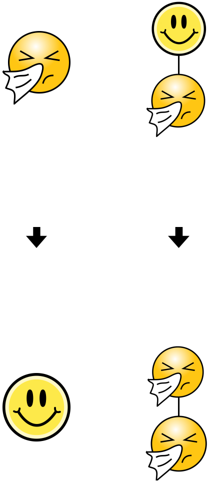
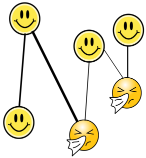


Number of Reactants: $h_1 = N_I = \sum_i x_i$

What's the Story for Networks



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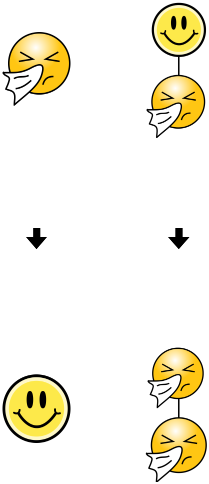

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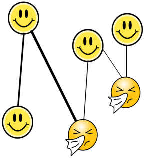

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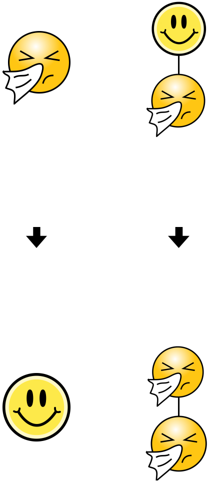
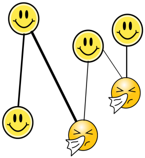


Number of Reactants: $h_1 = N_I$ h_2

What's the Story for Networks



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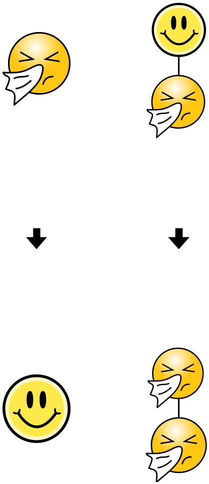
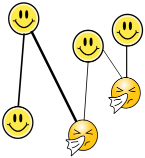


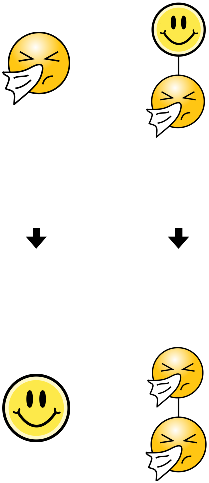
Number of Reactants: $h_1 = N_I$ $h_2 = N_{SI}$

What's the Story for Networks



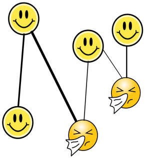
$\boldsymbol{x} = (x_i)\,,\ \boldsymbol{A} = (A_{ij})$

Reaction :



Number of Reactants: $h_1 = N_I$ $\quad h_2 = N_{SI} = \sum_{ij}(1 - x_i)A_{ij}x_j$

What's the Story for Networks



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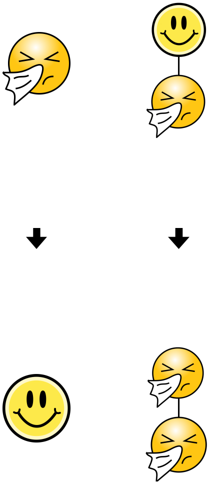

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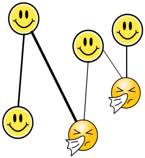

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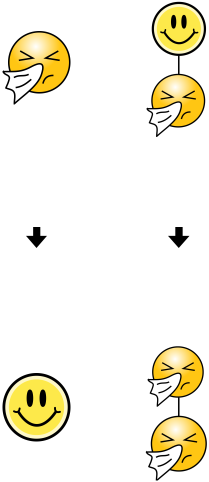

Number of Reactants:	$h_1 = N_I$	$h_2 = N_{SI}$
Reaction Rates:	r	λ

Implementation - Initialisation

```
% Initialise Network
N=100;
Edges=200;
x=randi([0,1],1,N);
A=newERG(N,Edges);
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h=[N_I,N_SI];
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recovery=1;
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% Initialise Rates
recovery=1;
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% Initialise Times
t=0;
tmax=300;
Nt=1000;
times=t:(tmax-t)/Nt:tmax;
i=0;
```

Implementation - Iteration

```
while t<tmax
    a_mu=h.*c; %vector of reaction rates
    a=sum(a_mu); %sum of all a_mu
    mu=1+(a_mu(1)<rand()*a);
    tau=-log(rand())/a;
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    if mu==1
        inf=find(x); % find all infected nodes
        k=randi(length(inf)); % pick an infected node
        x(k)=0; % recover that node
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    elseif mu==2
        SI=(A & (x')*ones(1,N)==0 & ones(N,1)*x); % SI-links
        [ro,co]=find(SI);
        k=randi(length(ro));
        x(ro(k))=1;
    end
```

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    h=[N_I,N_SI];
    t=t+tau;  % update time
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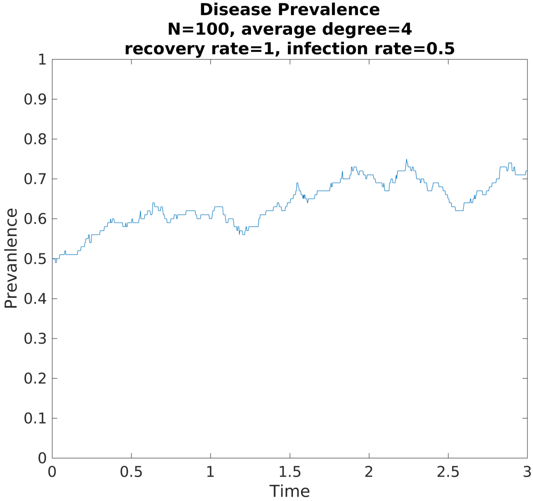
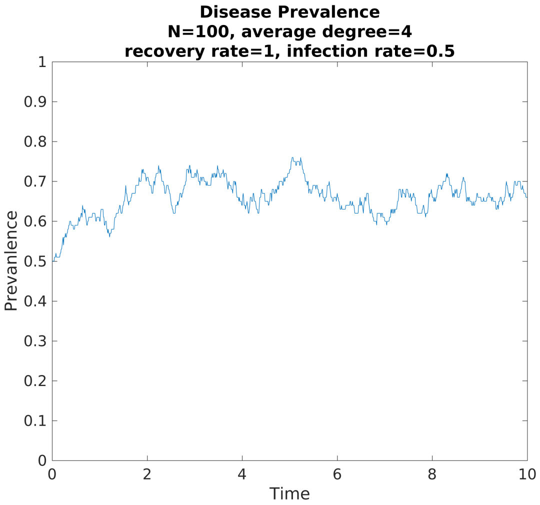
    h=[N_I,N_SI];
    t=t+tau;  % update time
```

```
    ind=find(times<=t,1,'last'); % index of the recorded events.
    if ind>i; rho(i+1:ind)=N_I/N;  end   % record rho
    i=ind; %update the new index.
end
```

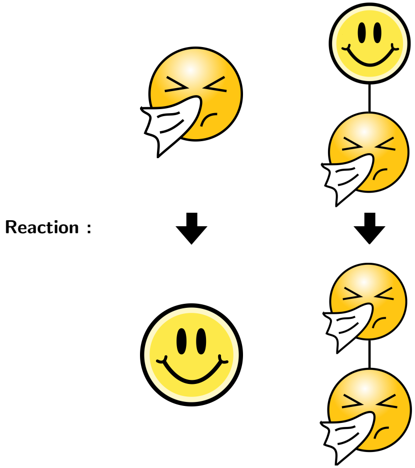
Implementation - Sample Path I



Implementation - Sample Path II



But How about Adaptive Networks?



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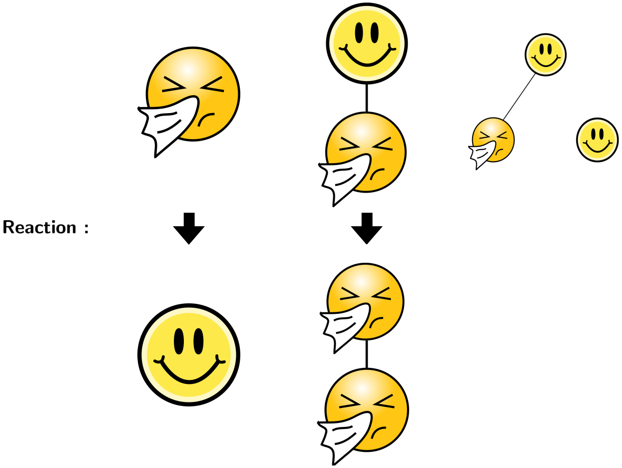

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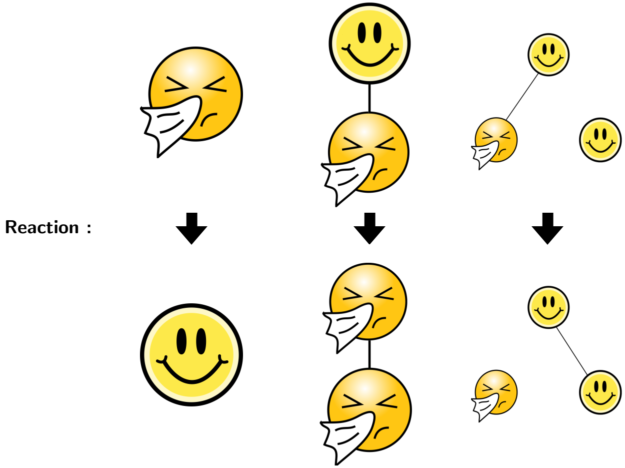

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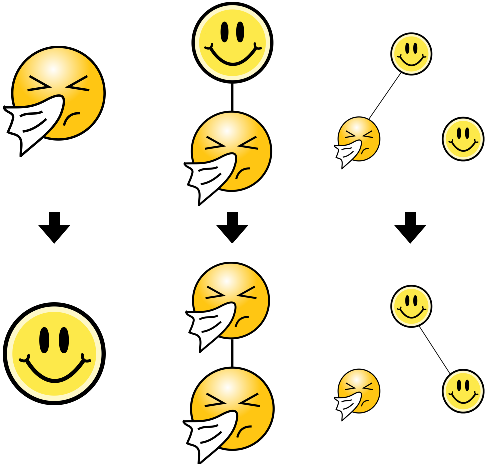

Reaction :

Number of Reactants: $h_1 = N_I$ $h_2 = N_{SI}$ $h_3 = N_{SI}$

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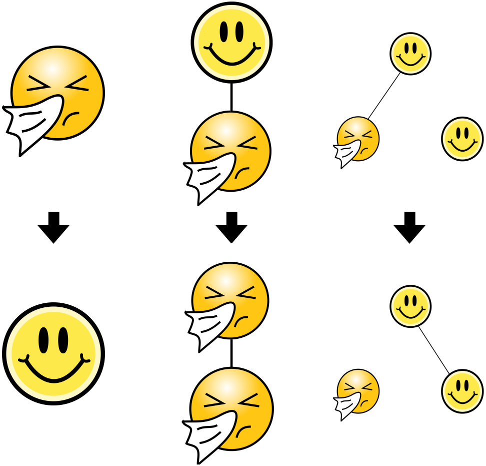

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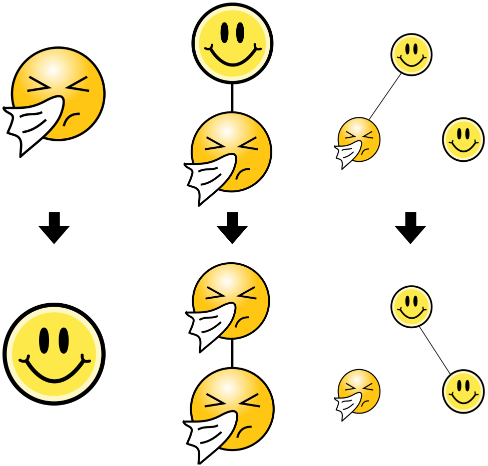

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Number of Reactants:	$h_1 = N_I$	$h_2 = N_{SI}$	$h_3 = N^{*}_{SI}$
Reaction Rates:	r	λ	

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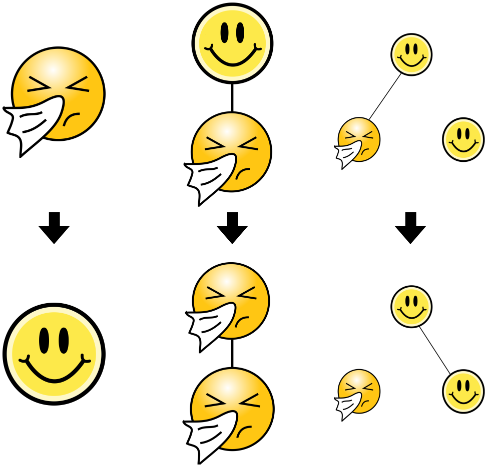

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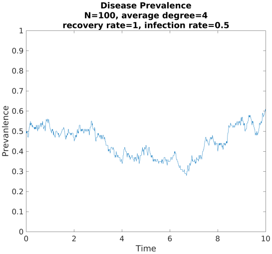
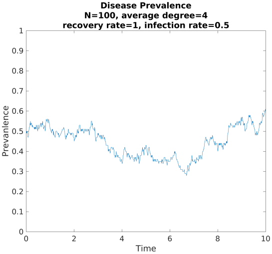
Implementation - Sample Path II



⟵ No rewiring

Implementation - Sample Path II



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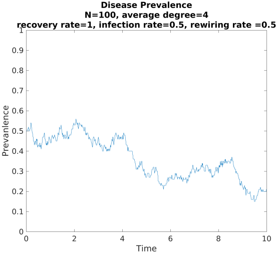
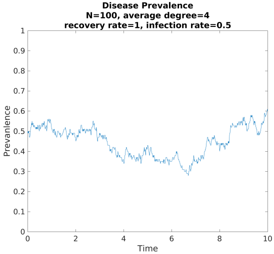


rewiring rate $= 0.5$.

Implementation - Sample Path II



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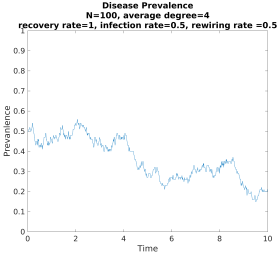

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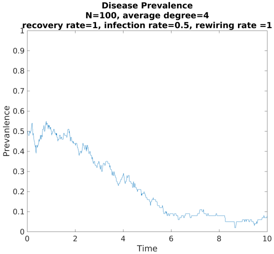

rewiring rate $= 1$.

Thank you

Every thing can be found on github.

https://github.com/leomarlo/TalkOnGillespieAlgorithm