Discussion of the Monte Carlo Simulation Method

This Monte Carlo simulation method is based on the algorithm developed by Shah et al. (1976) for structured models. The system is comprised of $N(t)$ cells at time t where the age of the i^{th} cell is τ_i and the identity of its state is s_i. Then, this i^{th} cell could make a discrete state transition from its current state, s_i, to the j^{th} state at the rate, $\Gamma_{s_i,j}(\tau_i)$, which depends on the cell's age. In this setting, the age of a cell is the amount of time that has passed since some "key" event during its lifetime such as a discrete state transition.

So, the probability that the i^{th} cell transitions to the j^{th} state nearly exactly after a time-period of length τ passes with no transition, the quiescent interval, after which the transition occurs during the infinitesimal interval τ to $\tau + d\tau$ is

$$P(\tau + d\tau) = P(\tau)\left[1 - \Gamma_{s_i,j}(\tau_i + \tau + d\tau)d\tau\right].$$

When all N cells and all J possible transition are considered, the probability that ANY cell makes ANY of transition during the period $(\tau, \tau + d\tau)$ is

$$P(\tau + d\tau) = P(\tau)\left[1 - \sum_{i=1}^{N(t)}\sum_{j=1}^{J}\Gamma_{s_i,j}(\tau_i + \tau + dt)d\tau\right].$$

Rearranging, dividing by $d\tau$, letting $d\tau \to 0$, and solving the resulting differential equation gives an exponential distribution for the quiescent interval

$$P(\tau) = \exp\left[-\sum_{i=1}^{N(t)}\sum_{j=1}^{J}\int_0^{\tau}\Gamma_{s_i,j}(\tau_i + \tau')d\tau'\right].$$

The cumulative distribution for the quiescent interval is thus

$$F(\tau) = 1 - \exp\left[-\sum_{i=1}^{N(t)}\sum_{j=1}^{J}\int_0^{\tau}\Gamma_{s_i,j}(\tau_i + \tau')d\tau'\right].$$

The Monte Carlo routine consists of randomly selecting a quiescent interval, T, from the cumulative distribution using a uniform random variable, R, by iterative solving

$$-\ln(1 - R) = \sum_{i=1}^{N(t)}\sum_{j=1}^{J}\int_0^{T}\Gamma_{s_i,j}(\tau_i + \tau')d\tau'$$

And then choosing a cell and transition where the probability of the i^{th} cell transitioning to the j^{th} state is

$$\frac{\Gamma_{s_i,j}(\tau_i + T)}{\sum_{i=1}^{N(t)} \sum_{j=1}^{J} \Gamma_{s_i,j}(\tau_i + T)}.$$

Once the cell transition has been selected, the age of all cells can be updated, the appropriate cell transition is made, and the process begins again by selecting a new quiescent interval based on the updated ages.

Reference:

Shah BH, Borwanker JD, and Ramkrishna D. "Monte Carlo simulation of microbial population growth," *Mathematical Biosciences*, **31:** 1-23, 1976.