If we have n molecular species and M reactions, the master equation is

$$\frac{d}{dt}p(x,t) = \sum_j \left[p(x - V_j, t)a_j - p(x,t)a_j\right]$$

$$a_j(x(t)) = c_k(\#A(t))(\#B(t))$$
$$c_j = \frac{k_j}{N_A \cdot \text{volume}}$$
$$X(t) = [\#A(t)\#B(t)\#C(t)]^T$$

Derivation of the Gillespie algorithm

Let $p_0(\tau|x,t)$ be the probability that no reaction occurs in the time interval $[t, t+\tau]$ given that the state of your system is currently $X(t) = x$.

Prob [no reaction occurs in $[t, t+\tau+\Delta\tau]$]

Prob [no reaction occurs in $[t, t+\tau]$] $\times$ Prob[no reaction in $[t+\tau, t+\tau+\Delta\tau]$] $= p_0(\tau|x,t)\left(1 - \sum_{j=1}^M a_j\Delta\tau\right)$

$$p_0(\tau + \Delta\tau|x,t) = p_0(\tau|x,t)\left(1 - \sum_{j=1}^M a_j\Delta\tau\right)$$
$$p_0(\tau+\Delta\tau|x,t) - p_0(\tau|x,t) = -\left(\sum a_j\Delta\tau\right)p_0(\tau|x,t)$$
$$\frac{d}{d\tau}p_0(\tau|x,t) = -\left(\sum a_j\Delta\tau\right)p_0(\tau|x,t)$$
$$\frac{d}{d\tau}p_0(\tau|x,t) = -a_{sum}p_0(\tau|x,t)$$

The solution is

$$p(\tau|x,t) = exp(-a_{sum}\tau)$$

Let $p(\tau, j|x,t)\Delta\tau$ be the probability (given that $X(t) = x$) that the next reaction

1. will be the j^{th} reaction
2. will occur in the time interval $[t+\tau, t+\tau+\Delta\tau]$

$$p(\tau, j|x,t) = p_0(\tau|x,t)a_j\Delta\tau = exp(-a_{sum}\tau)a_j\Delta\tau$$
$$p(\tau, j|x,t) = exp(-a_{sum}\tau)a_j$$

This formula is what we want.

$$p(\tau, j|x,t) = \frac{a_j}{a_{sum}} \cdot a_{sum}exp(-a_{sum}\tau)$$

The Gillespie Algorithm (for real this time)

1. Evaluate $a_k(X(t))$ for all k
2. Draw two independent uniform random numbers R_1 and R_2 from (0, 1)
3. Set j to be the smallest number such that $\sum_{k=1}^j a_k > R_1 a_{sum}$
4. forget about it...we'll cover it next time