Gillespie Algorithm:

- Consider N molecular types that undergo M reactions, governed by reaction rates r_i $(i = 1, \ldots, M)$

- Want to stochastically simulate the number of molecules of each type, $C_j(t)$, as a function of time t.

- Idea: one of the M reactions will occur randomly and take a time dt. The number of molecules change according to this reaction and the time elapsed goes from $t \to t+dt$

- For a chemical reaction the distribution of reaction times follows

$$P(\tau) = re^{-rt}\, d\tau$$

- Want to randomly sample times from this distribution: generate a random number $u \in [0, 1)$ then

$$\tau = -\frac{1}{r} \ln(u) \qquad (1)$$

Algorithm:

Do $i = 1, N_{steps}$ ← some large #

① generate M τ_i from M random numbers using Eqn(1)

② Reaction with smallest τ_i occurs $= \tau_i^*$

③ update particle #'s based on the reaction in ②

④ update time: $t = t + \tau_i^*$

⑤ output: $t, \{C_i(t)\}$

end do