Stochastic Simulation Algorithm (Gillespie Algorithm)

Due to the complexity of solving the CME analytically for the Probabilistic Pharmacokinetic Two-Compartment System, we employ the Gillespie Stochastic Simulation Algorithm (SSA) to simulate the system numerically. The key steps are:

1. **Initialization:**
    - Set initial molecule counts $n_1(0) = D$ (initial drug dose) and $n_2(0) = 0$.
    - Initialize time $t = 0$.
2. **Iteration:**
    - Calculate propensities:
        - $a_1 = k_2 n_1$
        - $a_2 = k_1 n_2$
    - Compute total propensity:
        - $a_0 = a_1 + a_2$
    - Generate two random numbers:
        - $r_1, r_2 \sim \text{Uniform}(0,1)$
    - Determine time to next reaction:
        - $\Delta t = -\frac{\ln(r_1)}{a_0}$
    - Update time:
        - $t = t + \Delta t$
    - Decide which reaction occurs:
        - If $r_2 a_0 < a_1$, transfer from heart to lung:
            - $n_1 \rightarrow n_1 - 1$
            - $n_2 \rightarrow n_2 + 1$
        - Else, transfer from lung to heart:
            - $n_1 \rightarrow n_1 + 1$
            - $n_2 \rightarrow n_2 - 1$
    - Record the new state and time.
    - Repeat until the maximum simulation time is reached.