(b) Gillespie Algorithm:

for $k \xrightarrow{\lambda} \emptyset$ (k-particle annihilation reaction).

(a). Master equation.

combination in which the reaction occurs

number of possible combinations of the n particles for k particles to annihilate

$$\frac{\partial P}{\partial t}(n,t) = \lambda\Big[\underbrace{\binom{n+k}{k}P(n+k,t)}_{\text{gain term}} - \underbrace{\binom{n}{k}P(n,t)}_{\text{loss term}}\Big].$$

$$(n-k) \xleftarrow{\text{loss}} (n) \xleftarrow{\text{gain}} (n+k)$$

(b). We want to argue that this is equivalent to a biased random walk, with $q = 1 - r_n\, dt$ the probability of pausing and $p = r_n\, dt$ prob. of hopping k-steps, with $r_n = \lambda\binom{n}{k}$.

$$(n-k) \xleftarrow{p} (n) \circlearrowleft^{1-p}$$

Likewise:

$1-p$: prob. of "no reaction" (pause).

$$p = \underbrace{\underbrace{\lambda\binom{n}{k}}_{\text{total no. of reaction}}\,dt}_{\text{prob. of reaction}}$$ (for annihilation).

- For one of this to make sense, we need to have dt be sufficiently small. (otherwise more than one reaction can occur in a single time-step and our one-step model fails).

This isn't very efficient! (computationally).
- initially, we have lots of particles ⇒ "fast" reactions: $\binom{n}{k}$ is big;
- As n decreases, it will take progressively longer for a reaction to occur (on average), which means we'll have lots of "pauses" that are clogging our simulation, i.e. we're forced to generate many (pseudo-)random numbers that most likely will not advance the simulation. (By advance, I mean move towards $n=0$).

c) · Attempt:
· Prob. that it changes: $p = r_n\,dt$
· Prob. that it doesn't change: $q = 1 - r_n\,dt$.

· In this derivation, I assume that only one reaction occurs in τ $(\text{and } \tau + d\tau)$

What about after $\underline{\tau = A\,dt}$:

$$\cdot\ q_n(\tau) = \underbrace{q \cdot q \cdots q}_{A \text{ times}} = q^A = (1 - r_n\,dt)^A.$$

$$\cdot\ q_n(\tau + d\tau) = q^{A+1} = q \cdot q_n(\tau).$$

& $d\tau = dt$

This way: $\dfrac{q_n(\tau + d\tau) - q_n(\tau)}{d\tau} = q_n(\tau)\,\dfrac{q-1}{d\tau} \Rightarrow$

$$\Rightarrow \frac{dq_n(\tau)}{d\tau} = -q_n(\tau)\, r_n \cancel{\frac{dt}{d\tau}} \Rightarrow \frac{dq_n(\tau)}{d\tau} = -r_n\, q_n(\tau).$$ QED.

$\Rightarrow q_n(\tau) = q_n(0)\, e^{-r_n \tau} \Rightarrow$

$\Rightarrow q_n(\tau) = e^{-r_n \tau}$.

& $\tau = 0$: $q_n(0) = 1$

· Reasoning: at $\tau = 0$, then the number of reactions containing does not change! $\Rightarrow$
$\Rightarrow$ prob. of not changing: $1 = q_n(0)$.

· Now, for $p_n(\tau)$:

$\cdot\ p_n(\tau) = q^{A-1} \cdot p$

$\cdot\ p_n(\tau + d\tau) = q^A \cdot p$

· & $d\tau = dt$.

$$\Rightarrow \frac{p_n(\tau + d\tau) - p_n(\tau)}{d\tau} = q^{A-1} p \cdot \frac{q-1}{d\tau} \Rightarrow$$

$$\Rightarrow \frac{dp_n(\tau)}{d\tau} = -p_n(\tau)\, r_n \frac{dt}{d\tau} \Rightarrow \frac{dp_n(\tau)}{d\tau} = -r_n\, p_n(\tau)$$

$$\Rightarrow p_n(\tau) = p_n(0)\, e^{-r_n \tau}$$

· initial condition? $p_n(\tau = 0) = r_n$?

I'm not sure about this...

· Used in the Gillespie Algorithm.

$F(\tau) = 1 - e^{-r_n \tau}$

$\Rightarrow F(\tau) = x$, $x \in \text{Uniform}(0,1)$

$\Rightarrow \boxed{\tau = -\dfrac{\ln(1-x)}{r_n}}$.

d) Computational implementation of the Gillespie Algorithm.

$p_n(\tau) = r_n\, e^{-r_n \tau} \Rightarrow p_n[A_n \tau]$? $p_n(\tau_n) - r_n \tau \Rightarrow$

$\Rightarrow p_n(\dots)\, r_n \tau$

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Mean - field description
(needed for comparison with the experimental results).

$$\frac{\partial P(n,t)}{\partial t} = \frac{\lambda}{k!}\left[\underbrace{\frac{(n+k)!}{n!}}_{(n+k)\cdots(n+1)}\cdot P(n+k,t) - \underbrace{\frac{n!}{(n-k)!}}_{n(n-1)\cdots(n-k+1)} P(n,t)\right]$$

Multiply by n and $\sum_n$

$$\Rightarrow \frac{\partial \langle n(t)\rangle}{\partial t} = \frac{\lambda}{k!}\left[\sum_{\boxed{n'=k}}^{\infty} n'(n'-1)\cdots(n'-k)\,P(n',t) - \sum_{n=0}^{\infty} n^2(n-1)\cdots(n-k+1)\,P(n,t)\right] \Rightarrow$$

$\boxed{n+k \to n'}$

$n'=k$, can start at 0 since these extra initial terms don't contribute to the sum.

$k=3$

$$\Rightarrow \frac{\partial \langle n(t)\rangle}{\partial t} = \frac{\lambda}{k!}\sum_{n=0}^{\infty}\left[n(n-1)(n-2)(n-3)P(n,t) - n^2(n-1)(n-2)P(n,t)\right]$$

$$\Rightarrow \frac{\partial \langle n(t)\rangle}{\partial t} = \frac{\lambda}{3!}\left[\langle n(n-1)(n-2)(n-3)\rangle - \langle n^2(n-1)(n-2)\rangle\right].$$

$\Rightarrow$ ... After some algebra ... $\Rightarrow$ Here, I assume no correlation, i.e. $\langle n^3\rangle \approx \langle n\rangle^3$ and $\langle n^2\rangle \approx \langle n\rangle^2$.

$$\Rightarrow \frac{\partial \langle n(t)\rangle}{\partial t} = \frac{\lambda \cdot 3}{3!}\left(-\langle n\rangle^3 + 3\langle n\rangle^2 - 2\langle n\rangle\right) \Rightarrow$$

- if $\langle n\rangle \gg 1$: $\langle n\rangle^3$ dominates the RHS.

$$\Rightarrow \frac{\partial \langle n(t)\rangle}{\partial t} = -\frac{\lambda}{2}\cdot\langle n\rangle^3 \Rightarrow$$

$$\Rightarrow \frac{\partial \langle n(t)\rangle}{\langle n\rangle^3} = -\frac{\lambda}{\cancel{2}}\,\partial t \Rightarrow -\frac{1}{\cancel{2}\langle n(t)\rangle^2} = -\frac{\lambda}{\cancel{2}}t + C \Rightarrow$$

$$\Rightarrow \langle n(t)\rangle = \frac{1}{\sqrt{\lambda t - C}}.$$

$$\langle n(t=0)\rangle = n_0 \Rightarrow -C = \frac{1}{n_0^2} \Rightarrow \boxed{\langle n(t)\rangle = \frac{1}{\sqrt{n_0^{-2} + \lambda t}}}$$