1.

By the symmetry of the system we can see that

$$A + B = N \quad \Rightarrow B = N - A$$

2.

$$\frac{\partial p_n}{\partial t} = P_{n-1}\underbrace{\Big(\overbrace{k_1 \underbrace{(N-n+1)}_{B=N-(n-1)}}^{\text{Reac. a)}} + \overbrace{\frac{k_2}{v}\underbrace{(n-1)}_{A}\underbrace{(N-n+1)}_{B}}^{\text{Reac. c)}} + \overbrace{\frac{k_3}{v^2}\underbrace{(n-1)}_{A}\underbrace{(n-2)}_{(A-1)}\underbrace{(N-n+1)}_{B}}^{\text{Reac. e)}}\Big)}_{\text{term 1}}$$

$$+ P_{n+1}\underbrace{\Big(\overbrace{k_1 \underbrace{(n+1)}_{A}}^{\text{Reac. b)}} + \overbrace{\frac{k_2}{v}\underbrace{(n+1)}_{A}\underbrace{(N-n-1)}_{B=N-(n+1)}}^{\text{Reac. d)}} + \overbrace{\frac{k_3}{v^2}\underbrace{(n+1)}_{A}\underbrace{(N-n-1)}_{B}\underbrace{(N-n-2)}_{B-1}}^{\text{Reac. f)}}\Big)}_{\text{term 2}}$$

$$\underbrace{- P_n\Big(k_1 N + 2\frac{k_2}{v} n (N-n) + \frac{k_3}{v^2} n \cancel{N} (N-n)(N-2)\Big)}_{\text{term 3}}$$

Rename reactions as follow.

a) $B \xrightarrow{k_1} A$, c) $A + B \xrightarrow{k_2} 2A$, e) $2A + B \xrightarrow{k_3} 3A$

b) $A \xrightarrow{k_1} B$, d) $A + B \xrightarrow{k_2} 2B$, f) $A + 2B \xrightarrow{k_3} 3B$

$$P_n(t+dt) = \overset{*_1}{P_n}(t)(1 - \text{prob. SomethingHappens}) + \overset{*_2}{P_{n+1}}(t)\,(\text{propensity func.}) + \overset{*_3}{P_{n-1}}(t)\,(\text{propens. func.})$$

$*_1$ we are in the correct state ~~and~~ so nothing happens.

$*_2$ we have n+1 molecules of A. so we loose one (Reac b), d), f))

$*_3$ we have n-1 molecules of A. so we get one. (Reac. a), c), e))

$$P_n(t+dt) = P_n(t)\,(1-\text{term}_3) + \text{term}_1\,dt + \text{term}_2\,dt$$

$$\frac{P_n(t+dt)-P_n(t)}{dt} = -P_n\,\text{term}3 + \text{term}1 + \text{term}2.$$

For term3 we have the propensity function of any reaction occurs:

$$\overbrace{k_1(N-n)}^{\text{Reac. a)}} + \overbrace{k_1 n}^{\text{Reac. b)}} + \overbrace{\frac{k_2}{v}N(N-n)}^{\text{Reac. c)}} + \overbrace{\frac{k_2}{v}N(N-n)}^{\text{Reac. d)}} + \overbrace{\frac{k_3}{v^2}n(n-1)(N-n)}^{\text{Reac. e)}} + \overbrace{k_3 n(N-n)(N-n-1)}^{\text{Reac. f}}$$

$$= k_1 N + 2\frac{k_2}{v}N(N-n) + \frac{k_3}{v^2}n(N-n)(n-1+N-n-1) =$$

$$k_1 N + 2\frac{k_2}{v}N(N-n) + \frac{k_3}{v^2}n(N-n)(N-2) = \underline{\text{term}_3}$$

3. $M := \langle n \rangle$ (not)

$$\frac{\partial M}{\partial t} = \frac{\partial \sum_n P_n\cdot n}{\partial t} = \sum_{n=0}^{\infty} n P_{n-1}\left(k_1(N-n+1) + \frac{k_2}{v}(n-1)(N-n+1) + \frac{k_3}{v^2}(n-1)(n-2)(N-n+1)\right)$$

$$+\sum_{n=0}^{\infty} n P_{n+1}\left(k_1(n+1) + \frac{k_2}{v}(n+1)(N-n-1) + \frac{k_3}{v^2}(n+1)(N-n-1)(N-n-2)\right)$$

$$-\sum_{n=0}^{\infty} n P_n\left(k_1 N + 2\frac{k_2}{v}n(N-n) + \frac{k_3}{v^2}n(N-n)(N-2)\right). \quad = *$$

— $n-1=k$ — $n+1=k$

$n=k+1$ $n=k-1$

$n=0 \Rightarrow k=-1$ $n=0 \Rightarrow k=1$

$$* = \sum_{k=0}^{\infty}(k+1)P_k\Big(k_1(N-(k+1)+1) + \frac{k_2}{v}((k+1)-1)(N-(k+1)+1) +$$

(term is 0 if $k=-1$)

$$\frac{k_3}{v^2}((k+1)-1)((k+1)-2)(N-(k+1)+1)\Big)$$

$$+\sum_{k=0}^{\infty}(k-1)P_k\Big(k_1(k-1+1) + \frac{k_2}{v}(k-1+1)(N-(k-1)-1) + \frac{k_3}{v^2}((k-1)+1)$$

($k=1$ vanishes)

$$(N-(k-1)-1)(N-(k-1)-2).$$

$$-\sum_{k=0}^{\infty}kP_k\left(k_1 N + 2\frac{k_2}{v^2}k(N-k) + \frac{k_3}{v^2}k(N-k)(N-2)\right)$$

$$= \sum_{k=0}^{\infty} \left[(k+1) P_k \left(k_1 (N-k)\right) + \frac{k_2}{v} k(N-k) + \frac{k_3}{v^2} k(k-1)(N-k)\right)$$

$$+ \sum_{k=0}^{\infty} \left((k-1) P_k \left(k_1 k + \frac{k_2}{v} k (N-k) + \frac{k_3}{v^2} (k(N-k)(N-k-1)\right)\right)$$

$$- \sum_{k=0}^{\infty} \left[k P_k \left(k_1 N + \frac{2k_2}{v} k(N-k) + \frac{k_3}{v^2} k (N-k)(N-2)\right)\right)$$

$$= \underbrace{\sum_{k=0}^{\infty} P_k\, k_1 \left((k+1)(N-k) + (k-1)k - kN\right)}_{\text{part 1}} + \underbrace{\sum_{k=0}^{\infty} P_k \frac{k_2}{v} k(N-k) \underbrace{(k+1+k-1-2k)}_{0}}_{0}$$

$$+ \underbrace{\sum_{k=0}^{\infty} P_k \frac{k_3}{v^2} \left((k+1)k(k-1)(N-k) - k^2(N-k)(N-2)\right. \left. + k(N-k)(N-k-1)(k-1)\right)}_{\text{part 2.}}$$

part 1: $= \sum_{k=0}^{\infty} P_k k_1 (kN - k^2 + N - k + k^2 - k - kN) =$

$$\sum_{k=0}^{\infty} P_k k_1 (N-2k) = k_1 (N - 2\langle n \rangle)$$

part 2:

$$= \sum_{k=0}^{\infty} P_k \frac{k_3}{v^2} \left(k(k-1)(k+1)(N-k) + (k-1)k(N-k)(N-k-1) - k^2(N-k)(N-2)\right) =$$

$$\sum_{k=0}^{\infty} P_k \frac{k_3}{v^2} \left(k(k^2-1)(N-k) + k(N-k)(k-1)(N-k-1) - k^2(N-k)(N-2)\right) =$$

$$\sum_{k=0}^{\infty} P_k \frac{k_3}{v^2} \left(k^2 - 1 + Nk - k^2 - k - N + k + 1 - Nk + 2k\right) =$$

$$\sum_{k=0}^{\infty} P_k \frac{k_3}{v^2} \left(k(N-k)(2k-N)\right) = \sum_{k=0}^{\infty} P_k \frac{k_3}{v^2} (Nk - k^2)(2k - N) =$$

$$\sum_{k=0}^{\infty} P_k \frac{k_3}{v^2} (2Nk^2 - N^2 k - 2k^3 + k^2 N) = \sum_{k=0}^{\infty} P_k \frac{k_3}{v^2} (3Nk^2 - 2k^3 - N^2 k)$$

$$= 3N\langle n^2 \rangle - N^2 \langle n \rangle - 2\langle n^3 \rangle \quad \Rightarrow \frac{\partial \langle n \rangle}{\partial t} = k_1 (N - 2\langle n \rangle) + \frac{k_3}{v^2} (3N\langle n^2 \rangle - N^2 \langle n \rangle - 2\langle n^3 \rangle) \checkmark$$

4.
$$\frac{d\langle n\rangle}{dt} = k_1 (N - 2\langle n\rangle) + \frac{k_3}{v^2} (3N \langle n\rangle^2 - N^2 - 2\langle n\rangle^3)$$

5. For steady state set $\frac{\partial \langle n\rangle}{\partial t} = 0$

$$0 = k_1 (N - 2\langle n\rangle) + \frac{k_3}{v^2} (3N\langle n\rangle^2 - N^2\langle n\rangle - 2\langle n\rangle^3)$$

$$0 = k_1 N - 2k_1\langle n\rangle + \frac{3k_3}{v^2} N\langle n\rangle^2 - 2\frac{k_3}{v^2}\langle n\rangle^3 - \frac{k_3}{v^2} N^2 \langle n\rangle$$

$$-\frac{2k_3}{v^2}\langle n\rangle^3 + \frac{3k_3}{v^2} N\langle n\rangle^2 - \left(2k_1 + \frac{k_3}{v^2} N^2\right)\langle n\rangle + k_1 N = 0$$

rename: $r_1 = k_1$, $r_2 = k_2/v$, $r_3 = \frac{k_3}{v^2}$, $x = \langle n\rangle$

and fix: $N = 50$

by the symmetry of the system we can see that 25 is a steady state

$$-2r_3x^3 + 150r_3x^2 - (2r_1 + r_3 \cdot 50^2) \cdot 50^2 x^2 + 50 r_1 = 0$$

$$
\begin{array}{llll}
-2r_3x^3 & +150r_3x^2 - (2r_1 + r_3 \cdot 50^2) x & + 50r_1 & \quad \underline{|x - 25} \\
+2r_3x^3 & -50r_3x^2 & & \quad -2r_3x^2 + 100xr_3 - 2r_1 \\
\hline
/ & 100r_3x^2 - (2r_1 + r_3 \cdot 50^2) & + 50r_1 & \\
 & -100r_3x^2 + 2500\,xr_3 & & \\
\hline
 & / \quad -2r_1x & +50r_1 & \\
 & \quad\;\; 2r_1x & -50r_1 & \\
\hline
 & & / &
\end{array}
$$

$A_1 = 25$ is a steady state

The equation can be written as:

$$(x - 25)\underbrace{(-2r_3x^2 + 100x\, r_3 - 2r_1)}_{\text{Solve this eq.}} = 0$$

$$x = \frac{-100r_3 \pm \sqrt{100^2 r_3^2 - 4(-2r_3)(-2r_1)}}{2(-2r_3)} \; ; \quad \begin{cases} x = 13,82 & (r_1 = 2.5,\ r_3 = 0.005) \\ x = 36.18 \end{cases}$$

CW

We have real solutions if:

$$100^2 r_3^2 - 16 r_3 r_1 \geq 0$$

$$100^2 r_3^2 - 16 r_3 r_1 = 0 \Rightarrow r_3 (100^2 - 16 r_1) = 0 \quad \begin{cases} r_1 = 0 \\ r_3 = \frac{16 r_1}{100^2} \end{cases}$$

$$\begin{array}{ccccc} + & & - & & + \\ \hline & 0 & & \frac{16r_1}{100^2} & \end{array}$$

$$\Rightarrow r_3 \geq \frac{16 r_1}{100^2} \; *$$

Steady states:

$$\underline{A_1 = 25, \quad A_2 = 13.82, \quad A_3 = 36.18}$$

- Stability analysis:

$$-\frac{2k_3}{v^2} \langle n \rangle^3 + \frac{3k_3}{v^2} N \langle n \rangle^2 - \left(2k_1 + \frac{k_3}{v^2} N^2\right) \langle n \rangle + k_1 N = 0$$

$$N = 50, \quad k_1 = 2.5, \quad \frac{k_2}{v} = 2, \quad \frac{k_3}{v^2} = 0.05$$

$$-2(0.005)\langle n \rangle^3 + 3 \cdot 0.005 \cdot 50 \langle n \rangle^2 - (2 \cdot 2.5 + 0.005 \cdot 50^2)\langle n \rangle + 2.5 \cdot 50 = 0$$

$$f(\langle n \rangle) := -0.01 \langle n \rangle^3 + 0.75 \langle n \rangle^2 - (17.5)\langle n \rangle + 125 = 0$$

$$\frac{\partial f}{\partial \langle n \rangle} = -3\,0.01 \langle n \rangle^2 + 2 \cdot 0.75 \langle n \rangle - 17.5 = -0.03 \langle n \rangle^2 + 1.5 \langle n \rangle - 17.5$$

- Subs $\langle n \rangle = 25$ in $\frac{\partial f}{\partial \langle n \rangle}$: $-0.03(25)^2 + 1.5 \cdot 25 - 17.5 = 1.25 > 0$

  $\Rightarrow A_1 = 25$ <u>unestable</u>

- Subs $\langle n \rangle = 13.82$, in $\frac{\partial f}{\partial \langle n \rangle}$: $-0.03(13.82)^2 + 1.5 \cdot 13.82 - 17.5 = -2.5 < 0$

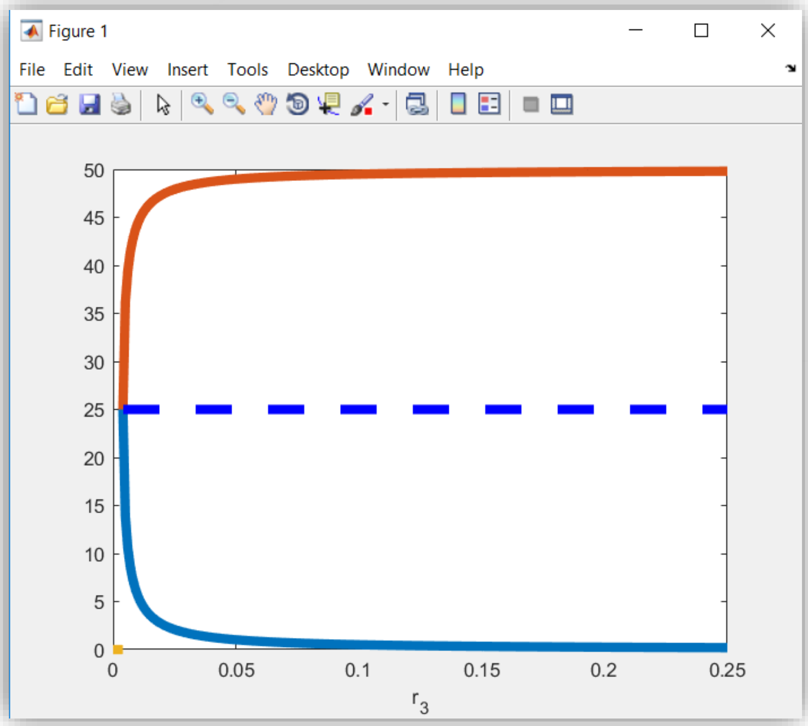
  $A_2 = 13.82$ <u>stable</u>

- Subs $\langle n \rangle = 36.2$ in $\frac{\partial f}{\partial \langle n \rangle}$: $-0.03(36.2)^2 + 1.5 \cdot 36.2 - 17.5 = -2.51 < 0$

  $A_3 = 36.18$ <u>stable</u>

6.

We can see a pitchfork bifurcation as the parameter r_3 passes the value $\frac{16 r_1}{100^2} = \frac{16 \cdot 25}{100^2} = 0.004$ from * in question 5.



7.

With the deterministic description of the system, we found that the deterministic ODEs do not provide an exact description of the mean behaviour of the system. Moreover, with second-order (or higher-order) reactions, we do not obtain a closed evolution equation for the mean, we need to use moment closure to obtain an aproximate set of equation.

In paraddition, in systems with many favourable steady states SSA gives results which cannot be obtained from the deterministic model.

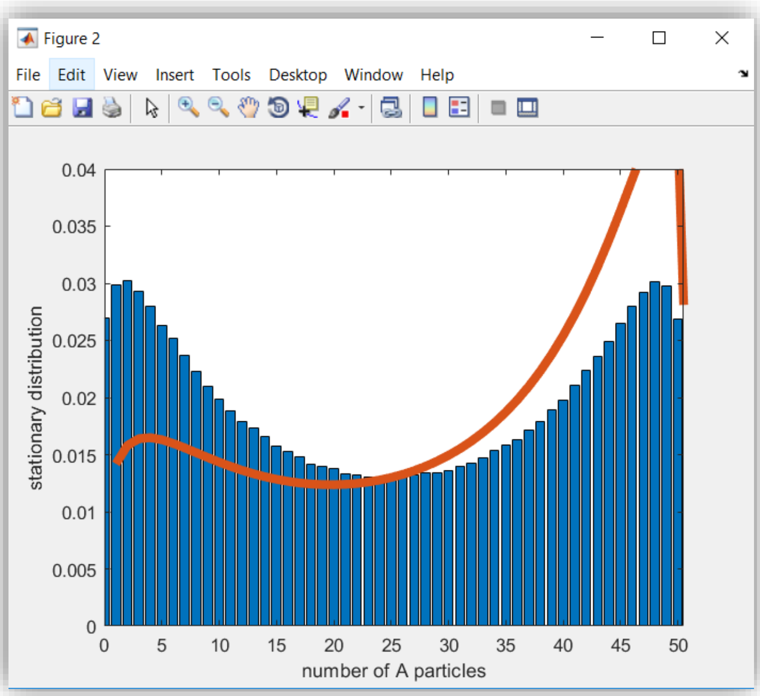
4
cw.

The random switching between stable states is missed by the deterministic description of the system.

8

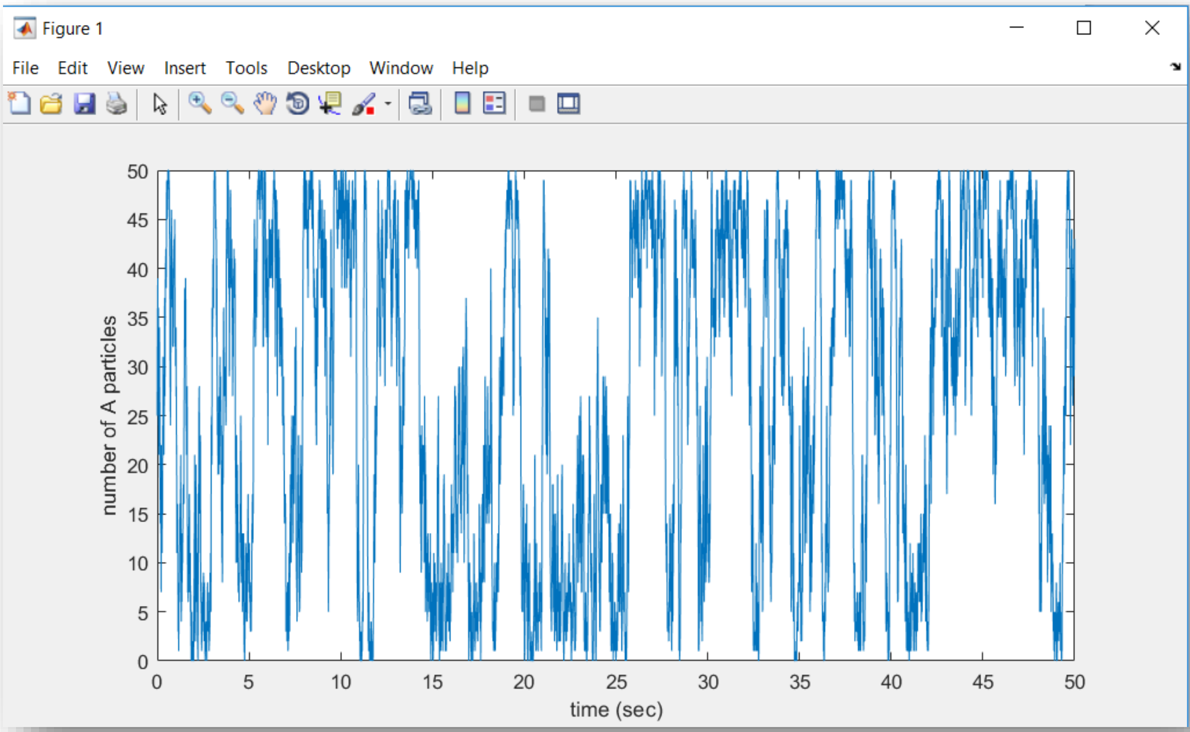
mean switching time = 0.4169

9.



The analytically derived stationary probability distribution does not fit very well with the histogram but I computed it as follows:

10



As we can see in the figure, the number of A particles changes dramatically between 0 and 50.

If we consider the figure in question 6 and we realise that k3onu2 = 0.005, we see the huge bifurcation between the two values 0 and 50 of A, fact which explains this figure.

11.

If we change the parameter k3onu2 to 0.003, the two stable states A_2 and A_3 disappear, because of the result from question 5.