ESI-MDPI-Submission-Stochastic Modeling and Simulation of Filament Aggregation in Alzheimer's Disease

December 2023

S1 Monte Carlo Simulation's Pseudo-Code

Algorithm S1 Monte Carlo Simulation

```
Require: rate_constants (list): The rate constants for the reactions.
Require: stoichiometry (list): The stoichiometry of the reactions. A 2D
    list where the i-th list contains the stoichiometric coefficients of the i-th
    reaction.
Require: initial_state (list): The initial numbers of molecules for each
    species.
Require: time_end (float): The simulation time end.
Require: num_simulations (int): The number of simulations to run.
num_species ← length(initial_state)
all_reactions_occurred ← []
all_reaction_times ← []
time_grid ← linspace(0, time_end, 1000)
states_interpolated ← zero array of shape (num_simulations,
    num_species, length(time_grid))
for i ← 0 to num_simulations - 1 do
    times, states, reactions_occurred, reaction_times ← GillespieAlgo-
    rithm(rate_constants, stoichiometry, initial_state, time_end)
    for j ← 0 to num_species - 1 do
        states_interp_func ← interpolate(time_grid, times, states[j])
        states_interpolated[i, j, :] ← states_interp_func
    end for
    all_reactions_occurred.append(reactions_occurred)
    all_reaction_times.append(reaction_times)
end for
avg_states ← mean of states_interpolated over axis 0
avg_std ← standard deviation of states_interpolated over axis 0
return time_grid, avg_states, avg_std, all_reactions_occurred,
    all_reaction_times
```

Algorithm S2 Gillespie Algorithm

Require: rate_constants (list): The rate constants for the reactions.
Require: stoichiometry (list): The stoichiometry of the reactions. A 2D list where the i-th list contains the stoichiometric coefficients of the i-th reaction.
Require: initial_state (list): The initial numbers of molecules for each species.
Require: time_end (float): The simulation time end.

```
num_reactions ← length(rate_constants)
num_species ← length(initial_state)
state ← copy(initial_state)
time ← 0
times ← [time]
states ← [copy(state)]
reactions_occurred ← []
reaction_times ← []
while time < time_end do
    propensities ← []
    for i ← 0 to num_reactions - 1 do
        propensity ← rate_constants[i]
        for j ← 0 to num_species - 1 do
            if stoichiometry[i][j] < 0 then
                propensity ← propensity × state[j]^|stoichiometry[i][j]|
            end if
        end for
        propensities.append(propensity)
    end for
    total_propensity ← sum(propensities)
    if total_propensity ≤ 0 then
        break
    end if
    time ← time + exponential_random_variable(total_propensity)
    reaction_index ← random_choice(range(num_reactions),
    weights=propensities, k=1)[0]
    for j ← 0 to num_species - 1 do
        state[j] ← state[j] + stoichiometry[reaction_index][j]
    end for
    times.append(time)
    states.append(copy(state))
    reactions_occurred.append(reaction_index)
    reaction_times.append(time)
end while
return times, transpose(states), reactions_occurred, reaction_times
```

S2 Reaction Kinetics Tables

The reaction kinetics table and their respective stochiometry are given below.

S2.1 Kinetics of Amyloid-beta aggregation

The table S1 only contains the kinetics of amyloid-beta aggregation and does not consider the fragmentation.

Table S1: Kinetics of Amyloid Beta Aggregations

Reaction	**Propensity Function**	**Reaction**	**Propensity Function**
$M_1 + M_1 = M_2$	$k_0 M_1 M_1$	$M_2 + M_2 + M_1 + M_1 = M_6$	$k_{10} M_2 M_2 M_1 M_1$
$M_1 + M_2 = M_3$	$k_1 M_1 M_2$	$M_1 + M_6 = M_7$	$k_{11} M_1 M_6$
$M_1 + M_3 = M_4$	$k_2 M_1 M_3$	$M_2 + M_5 = M_7$	$k_{12} M_2 M_5$
$M_2 + M_2 = M_4$	$k_3 M_2 M_2$	$M_3 + M_3 + M_1 = M_7$	$k_{13} M_3 M_3 M_1$
$M_1 + M_4 = M_5$	$k_4 M_1 M_4$	$M_3 + M_4 = M_7$	$k_{14} M_3 M_4$
$M_1 + M_2 + M_2 = M_5$	$k_5 M_1 M_2 M_2$	$M_1 + 3M_2 = M_7$	$k_{15} M_1 M_2 M_2 M_2$
$M_3 + M_3 = M_5$	$k_6 M_2 M_3$	$M_1 + M_7 = M_8$	$k_{16} M_1 M_7$
$M_1 + M_5 = M_6$	$k_7 M_1 M_5$	$M_2 + M_6 = M_8$	$k_{17} M_2 M_6$
$M_2 + M_4 = M_6$	$k_8 M_2 M_6$	$M_3 + M_5 = M_8$	$k_{18} M_3 M_5$
$M_3 + M_3 = M_6$	$k_9 M_3 M_3$	$M_4 + M_4 = M_8$	$k_{19} M_4 M_4$
$M_1 + M_2 + M_5 = M_8$	$k_{20} M_1 M_2 M_5$	$M_1 + M_3 + M_4 = M_8$	$k_{21} M_1 M_3 M_4$
$M_2 + M_2 + M_4 = M_8$	$k_{22} M_2 M_2 M_4$	$M_2 + M_3 + M_3 = M_8$	$k_{23} M_2 M_3 M_3$
$M_1 + M_1 + M_3 + M_3 = M_8$	$k_{24} M_1 M_1 M_3 M_3$	$4M_2 = M_8$	$k_{25} M_2 M_2 M_2 M_2$
$M_1 + M_1 + M_2 + M_4 = M_8$	$k_{26} M_1 M_1 M_2 M_4$		

S2.2 Kinetics of Amyloid-beta aggregation and fragmentation

The table S2 contains the kinetic of both aggregation and fragmentation reaction that could be possible.

Table S2: Kinetics of Amyloid Beta Aggregations and Fragmentation

Reaction	Propensity Function	Reaction	Propensity Function
$M_1 + M_1 = M_2$	$k_0M_1M_1$	$M_2 = 2M_1$	k_1M_2
$M_1 + M_2 = M_3$	$k_2M_1M_2$	$M_3 = M_1 + M_2$	k_3M_3
$M_1 + M_3 = M_4$	$k_4M_1M_3$	$M_4 = M_1 + M_3$	k_5M_4
$M_2 + M_2 = M_4$	$k_6M_2M_2$	$M_4 = 2M_2$	k_7M_4
$M_1 + M_4 = M_5$	$k_8M_1M_4$	$M_5 = M_1 + M_4$	k_9M_5
$M_1 + M_2 + M_2 = M_5$	$k_{10}M_1M_2M_2$	$M_5 = M_1 + 2M_2$	$k_{11}M_5$
$M_2 + M_3 = M_5$	$k_{12}M_2M_3$	$M_5 = M_2 + M_3$	$k_{13}M_5$
$M_1 + M_5 = M_6$	$k_{14}M_1M_5$	$M_6 = M_1 + M_5$	$k_{15}M_6$
$M_2 + M_4 = M_6$	$k_{16}M_2M_4$	$M_6 = M_2 + M_4$	$k_{17}M_6$
$M_3 + M_3 = M_6$	$k_{18}M_3M_3$	$M_6 = 2M_3$	$k_{19}M_6$
$M_2 + M_2 + M_1 + M_1 = M_6$	$k_{20}M_2M_2M_1M_1$	$M_6 = 2M_2 + 2M_1$	$k_{21}M_6$
$M_1 + M_6 = M_7$	$k_{22}M_1M_6$	$M_7 = M_1 + M_6$	$k_{23}M_7$
$M_2 + M_5 = M_7$	$k_{24}M_2M_5$	$M_7 = M_2 + M_5$	$k_{25}M_7$
$M_3 + M_3 + M_1 = M_7$	$k_{26}M_3M_3M_1$	$M_7 = 2M_3 + M_1$	$k_{27}M_7$
$M_3 + M_4 = M_7$	$k_{28}M_3M_4$	$M_7 = M_3 + M_4$	$k_{29}M_7$
$M_1 + 3M_2 = M_7$	$k_{30}M_1M_2M_2M_2$	$M_7 = M_1 + 3M_2$	$k_{31}M_7$
$M_1 + M_7 = M_8$	$k_{32}M_1M_7$	$M_8 = M_1 + M_7$	$k_{33}M_8$
$M_2 + M_6 = M_8$	$k_{34}M_2M_6$	$M_8 = M_2 + M_6$	$k_{35}M_8$
$M_3 + M_5 = M_8$	$k_{36}M_3M_5$	$M_8 = M_3 + M_5$	$k_{37}M_8$
$M_4 + M_4 = M_8$	$k_{38}M_4M_4$	$M_8 = 2M_4$	$k_{39}M_8$
$M_1 + M_2 + M_5 = M_8$	$k_{40}M_1M_2M_3$	$M_8 = M_1 + M_2 + M_5$	$k_{41}M_8$
$M_1 + M_3 + M_4 = M_8$	$k_{42}M_1M_3M_4$	$M_8 = M_1 + M_3 + M_4$	$k_{43}M_8$
$M_2 + M_2 + M_4 = M_8$	$k_{44}M_2M_2M_4$	$M_8 = 2M_2 + M_4$	$k_{45}M_8$
$M_2 + M_3 + M_3 = M_8$	$k_{46}M_2M_3M_3$	$M_8 = M_2 + 2M_3$	$k_{47}M_8$
$M_1 + M_1 + M_3 + M_3 = M_8$	$k_{48}M_1M_1M_3M_3$	$M_8 = 2M_1 + 2M_3$	$k_{49}M_8$
$4M_2 = M_8$	$k_{50}M_2M_2M_2M_2$	$M_8 = 4M_2$	$k_{51}M_8$
$M_1 + M_1 + M_2 + M_4 = M_8$	$k_{52}M_1M_1M_2M_4$	$M_8 = 2M_1 + M_2 + M_4$	$k_{53}M_8$

S2.3 Stochiometry matrix for aggregations with and without fragmentation

S2.3.1 Stochiometry without fragmentation

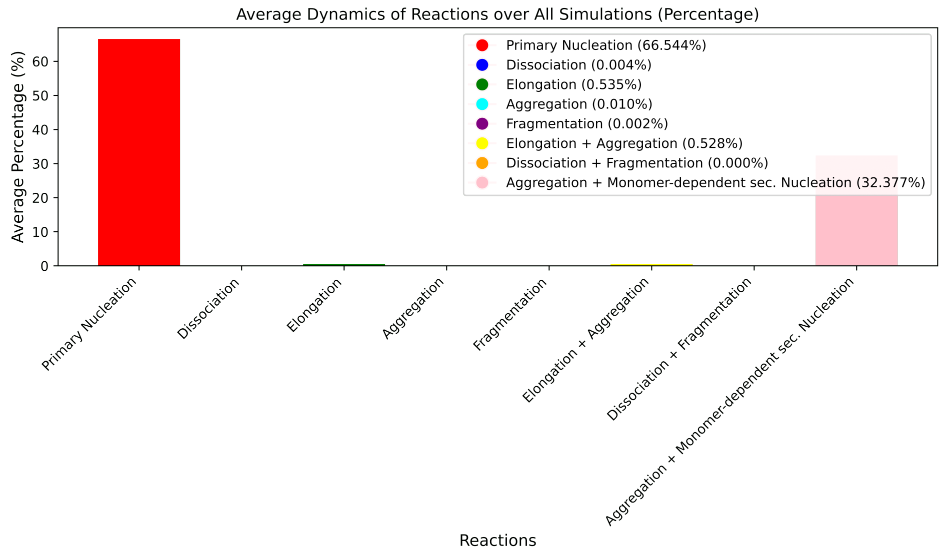
$$S_a = \begin{bmatrix}
-2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & -1 & 1 & 0 & 0 & 0 & 0 \\
0 & -2 & 0 & 1 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & -1 & 1 & 0 & 0 & 0 \\
-1 & -2 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & -1 & -1 & 0 & 1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\
0 & -1 & 0 & -1 & 0 & 1 & 0 & 0 \\
0 & 0 & -2 & 0 & 0 & 1 & 0 & 0 \\
-2 & -2 & 0 & 0 & 0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & -1 & 1 & 0 \\
0 & -1 & 0 & 0 & -1 & 0 & 1 & 0 \\
-1 & 0 & -2 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & -1 & -1 & 0 & 0 & 1 & 0 \\
-1 & -3 & 0 & 0 & 0 & 0 & 1 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\
0 & -1 & 0 & 0 & 0 & -1 & 0 & 1 \\
0 & 0 & -1 & 0 & -1 & 0 & 0 & 1 \\
0 & 0 & 0 & -2 & 0 & 0 & 0 & 1 \\
-1 & -1 & 0 & 0 & -1 & 0 & 0 & 1 \\
-1 & 0 & -1 & -1 & 0 & 0 & 0 & 1 \\
0 & -2 & 0 & -1 & 0 & 0 & 0 & 1 \\
0 & -1 & -2 & 0 & 0 & 0 & 0 & 1 \\
-2 & 0 & -2 & 0 & 0 & 0 & 0 & 1 \\
0 & -4 & 0 & 0 & 0 & 0 & 0 & 1 \\
-2 & -1 & 0 & -1 & 0 & 0 & 0 & 1
\end{bmatrix} \tag{S1}$$

S2.3.2 Stochiometry with fragmentation

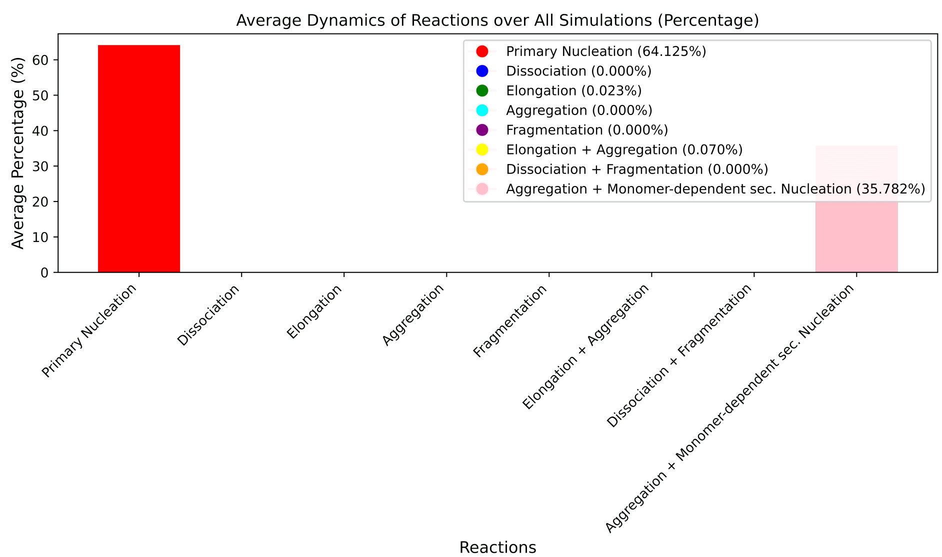
$$S_b = \begin{bmatrix}
-2.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
2.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
-1.00 & -1.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
1.00 & 1.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
-1.00 & 0.00 & -1.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
1.00 & 0.00 & 1.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & -2.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 2.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
-1.00 & 0.00 & 0.00 & -1.00 & 1.00 & 0.00 & 0.00 & 0.00 \\
1.00 & 0.00 & 0.00 & 1.00 & -1.00 & 0.00 & 0.00 & 0.00 \\
-1.00 & -2.00 & 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 \\
1.00 & 2.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 \\
0.00 & -1.00 & -1.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 1.00 & 1.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 \\
-1.00 & 0.00 & 0.00 & 0.00 & -1.00 & 1.00 & 0.00 & 0.00 \\
1.00 & 0.00 & 0.00 & 0.00 & 1.00 & -1.00 & 0.00 & 0.00 \\
0.00 & -1.00 & 0.00 & -1.00 & 0.00 & 1.00 & 0.00 & 0.00 \\
0.00 & 1.00 & 0.00 & 1.00 & 0.00 & -1.00 & 0.00 & 0.00 \\
0.00 & 0.00 & -2.00 & 0.00 & 0.00 & 1.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 2.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 \\
-2.00 & -2.00 & 0.00 & 0.00 & 0.00 & 1.00 & 0.00 & 0.00 \\
2.00 & 2.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 \\
-1.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 1.00 & 0.00 \\
1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 & -1.00 & 0.00 \\
0.00 & -1.00 & 0.00 & 0.00 & -1.00 & 0.00 & 1.00 & 0.00 \\
0.00 & 1.00 & 0.00 & 0.00 & 1.00 & 0.00 & -1.00 & 0.00 \\
-1.00 & 0.00 & -2.00 & 0.00 & 0.00 & 0.00 & 1.00 & 0.00 \\
1.00 & 0.00 & 2.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 \\
0.00 & 0.00 & -1.00 & -1.00 & 0.00 & 0.00 & 1.00 & 0.00 \\
0.00 & 0.00 & 1.00 & 1.00 & 0.00 & 0.00 & -1.00 & 0.00 \\
-1.00 & -3.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 & 0.00 \\
1.00 & 3.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 \\
-1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 1.00 \\
1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 & -1.00 \\
0.00 & -1.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & 1.00 \\
0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 1.00 & 0.00 & -1.00 \\
0.00 & 0.00 & -1.00 & 0.00 & -1.00 & 0.00 & 0.00 & 1.00 \\
0.00 & 0.00 & 1.00 & 0.00 & 1.00 & 0.00 & 0.00 & -1.00 \\
0.00 & 0.00 & 0.00 & -2.00 & 0.00 & 0.00 & 0.00 & 1.00 \\
0.00 & 0.00 & 0.00 & 2.00 & 0.00 & 0.00 & 0.00 & -1.00 \\
-1.00 & -1.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 & 1.00 \\
1.00 & 1.00 & 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & -1.00 \\
-1.00 & 0.00 & -1.00 & -1.00 & 0.00 & 0.00 & 0.00 & 1.00 \\
1.00 & 0.00 & 1.00 & 1.00 & 0.00 & 0.00 & 0.00 & -1.00 \\
0.00 & -2.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 1.00 \\
0.00 & 2.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & -1.00 \\
0.00 & -1.00 & -2.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 \\
0.00 & 1.00 & 2.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 \\
-2.00 & 0.00 & -2.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 \\
2.00 & 0.00 & 2.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 \\
0.00 & -4.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.00 \\
0.00 & 4.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 \\
-2.00 & -1.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 1.00 \\
2.00 & 1.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & -1.00
\end{bmatrix} \tag{S2}$$

S3 Referenced Analysis and Ablation

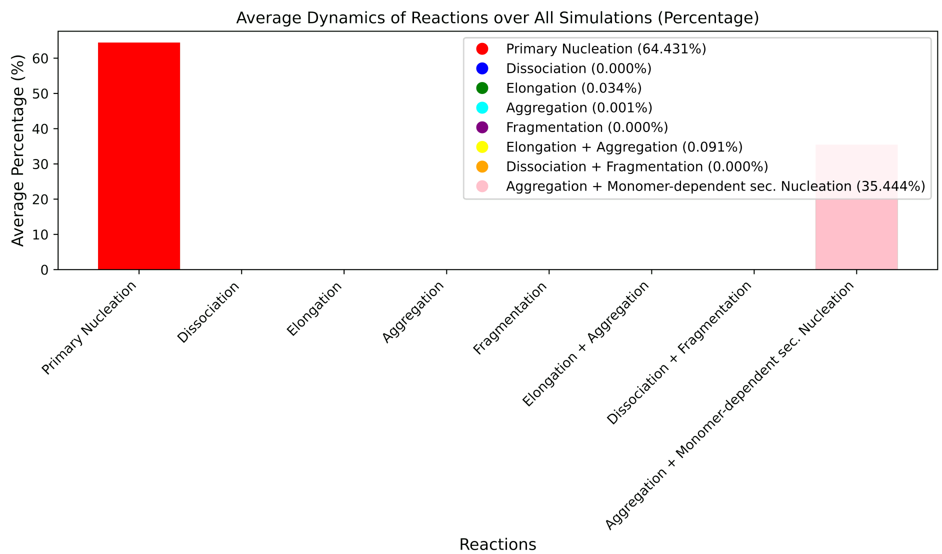
S3.1 Categorical Dynamics of Different Events



(a) The Average Reaction Dynamics Corresponding to Figure 6 of Manuscript, with $M_1 = 10000$ and $M_2, \ldots, M_8 = 1$



(b) The Average Reaction Dynamics Corresponding to Figure 7 of Manuscript, with $M_1 = 10000$ and $M_2, \ldots, M_8 = 100$

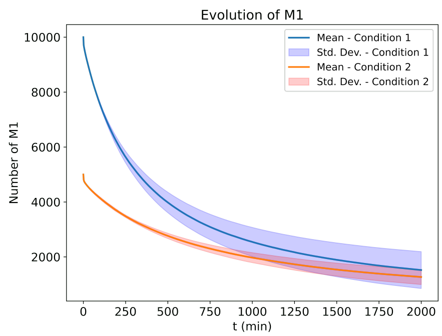


(c) The Average Reaction Dynamics with and Random Switching. Constants with $M_1 = 10000$ and $M_2, \ldots, M_8 = 100$ and fixed constants $k_0 = 0.0000001$, e.g $k_1, \ldots, k_{26} = 0.0000000002$ and $k_{27}, \ldots k_{53} = 0.0000000002/2$.

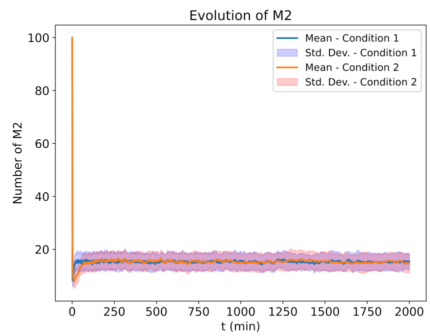
Figure S2: The Evolution of Amyloid beta aggregations and fragmentation events and their occurrence dynamics with different initial conditions and reaction rates

S4 Aggregation of Filaments with Fixed Constant Rates

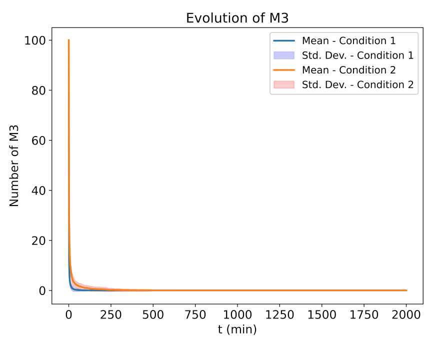
In this section, we show how changing initial conditions affect the final convergence when we use fixed constant for all the events.



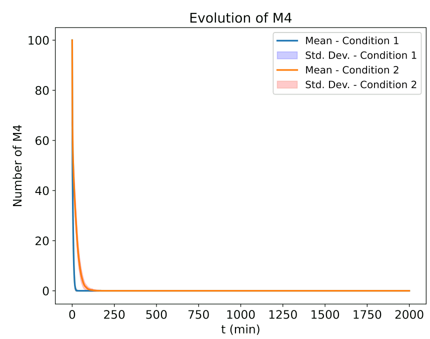
(a) The Evolution of Free Monomers (Free Proteins)



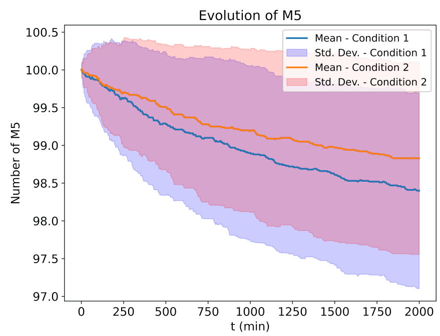
(b) The Evolution of Filament of length 2



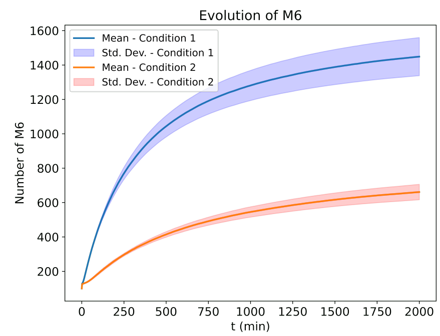
(c) The Evolution of Filament of length 3



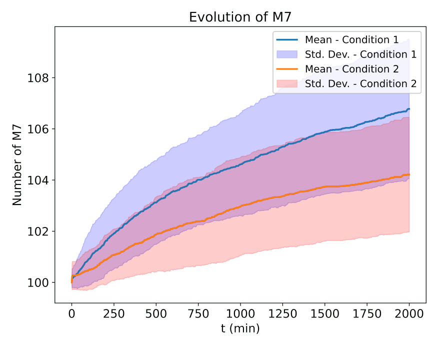
(d) The Evolution of Filament of length 4



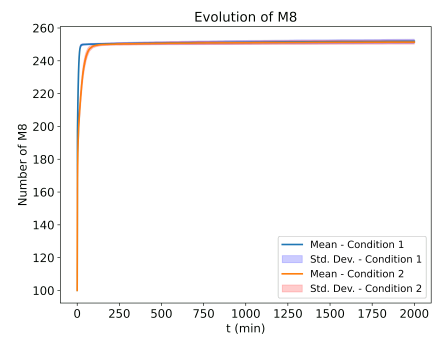
(e) The Evolution of Filament of length 5



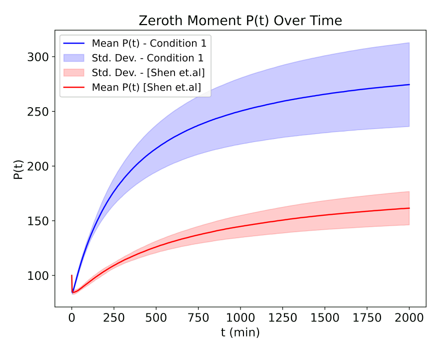
(f) The Evolution of Filament of length 6



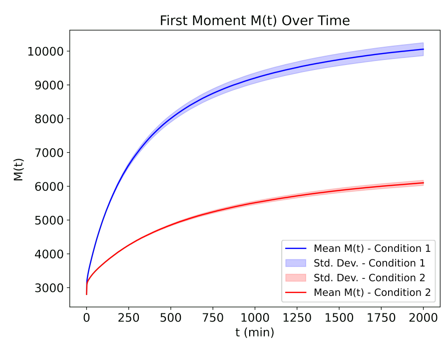
(g) The Evolution of Filament of length 7



(h) The Evolution of Filament of length 8

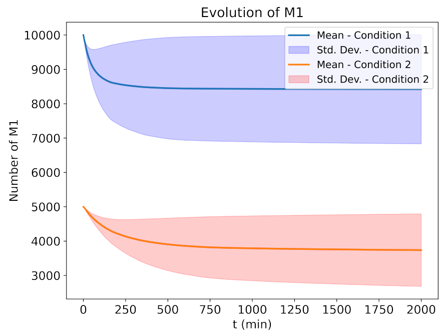


(i) The Evolution of Zeroth Moment P(t)

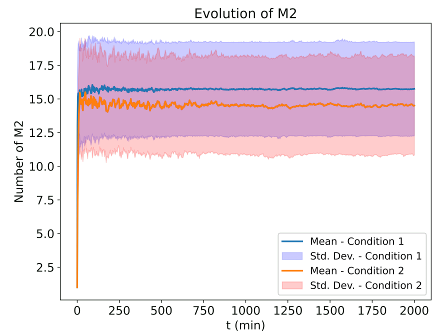


(j) The Evolution of First Moment M(t)

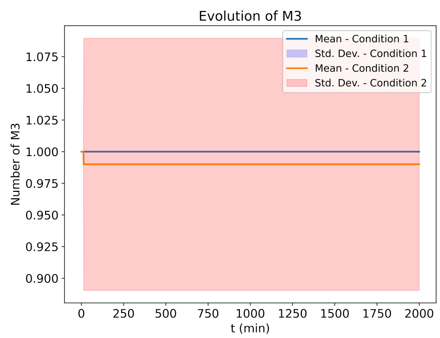
Figure S3: The Evolution of Amyloid beta aggregations when the rate con-stants are fixed, the Condition 1 with initial population of free proteins $M_1 = 10000$ and the Condition 2 with initial population of free proteins $M_1 = 5000$. The initial condition for each population except M_1 is same, 100, 100, 100, 100, 100, 100, 100 for $M_2, M_3, \ldots, M_8$ respectively. The start-ing reaction rate $k_0 = 0.0000001$, whereas $k_1, k_2, \ldots, k_{26} = 0.0000000002$.



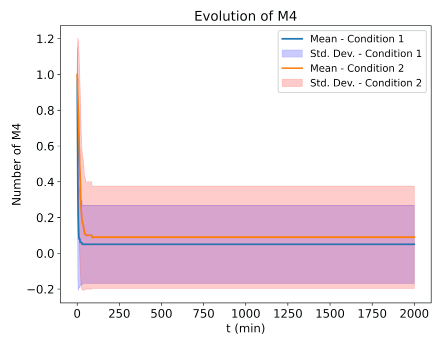
(a) The Evolution of Free Monomers (Free Proteins)



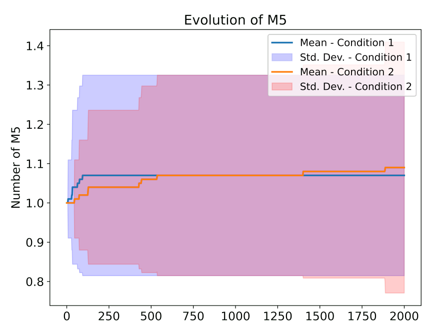
(b) The Evolution of Filament of length 2



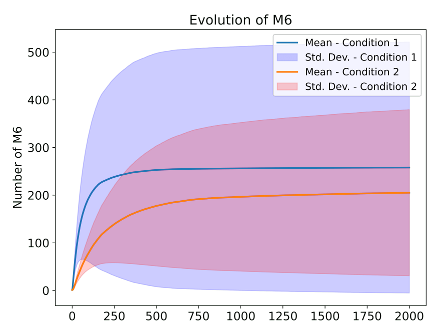
(c) The Evolution of Filament of length 3



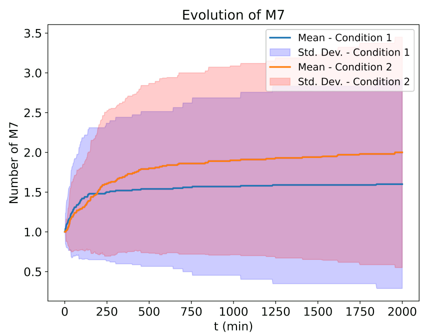
(d) The Evolution of Filament of length 4



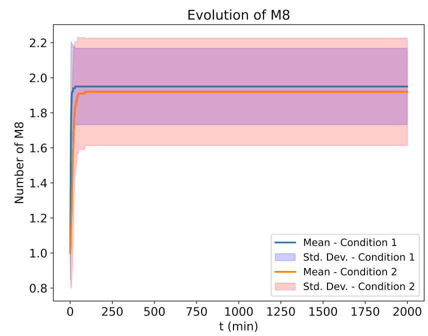
(e) The Evolution of Filament of length 5



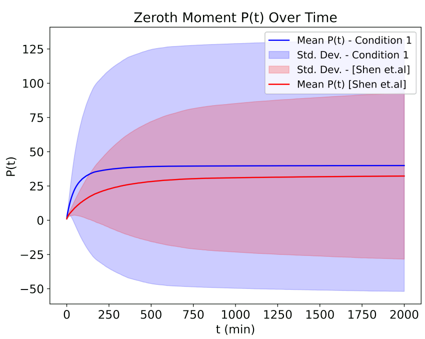
(f) The Evolution of Filament of length 6



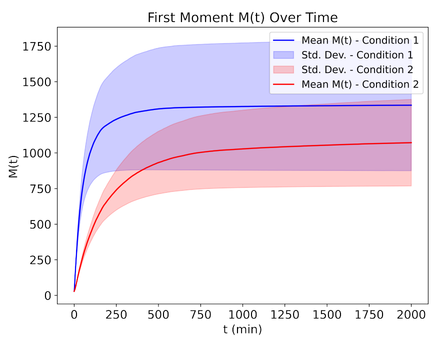
(g) The Evolution of Filament of length 7



(h) The Evolution of Filament of length 8

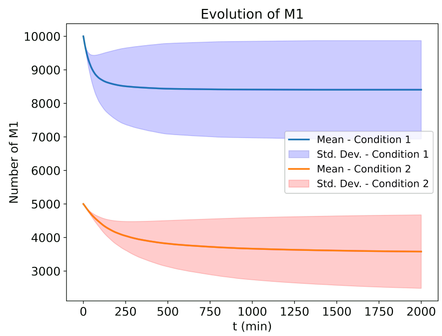


(i) The Evolution of Zeroth Moment P(t)

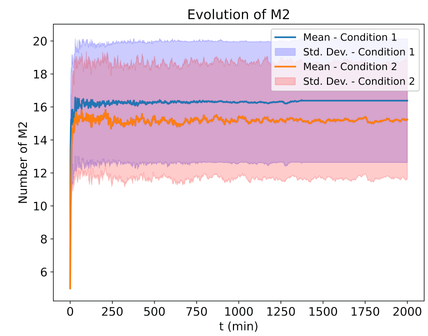


(j) The Evolution of First Moment M(t)

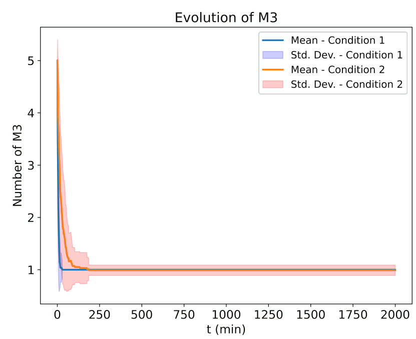
Figure S4: The Evolution of Amyloid beta aggregations when the rate con-stants are fixed, the Condition 1 with initial population of free proteins $M_1 = 10000$ and the Condition 2 with initial population of free proteins $M_1 = 5000$. The initial condition for each population except M_1 is same, 1, 1, 1, 1, 1, 1, 1 for $M_2, M_3, \ldots, M_8$ respectively. The starting reaction rate $k_0 = 0.0000001$, whereas $k_1, k_2, \ldots, k_{26} = 0.0000000002$.



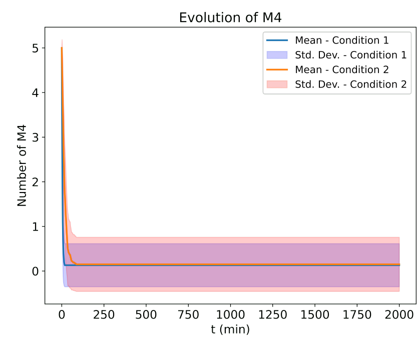
(a) The Evolution of Free Monomers (Free Proteins)



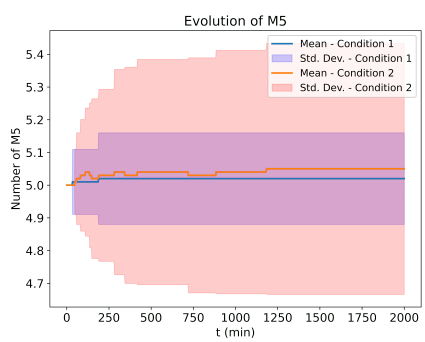
(b) The Evolution of Filament of length 2



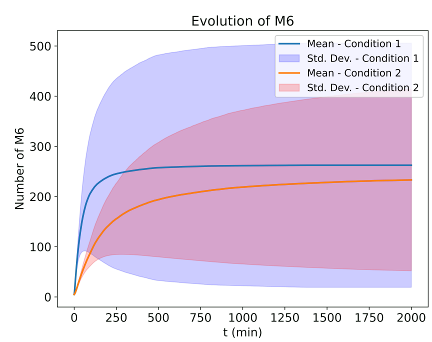
(c) The Evolution of Filament of length 3



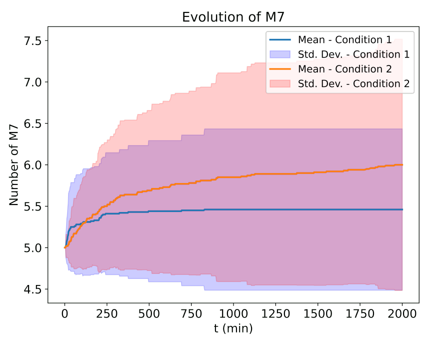
(d) The Evolution of Filament of length 4



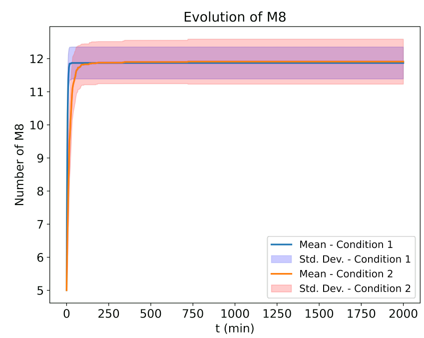
(e) The Evolution of Filament of length 5



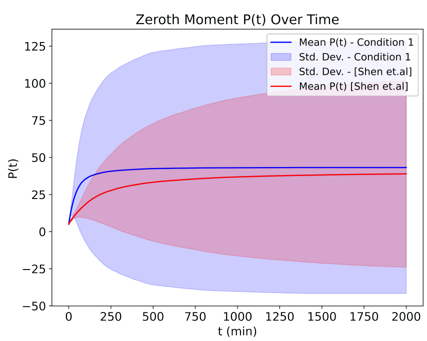
(f) The Evolution of Filament of length 6



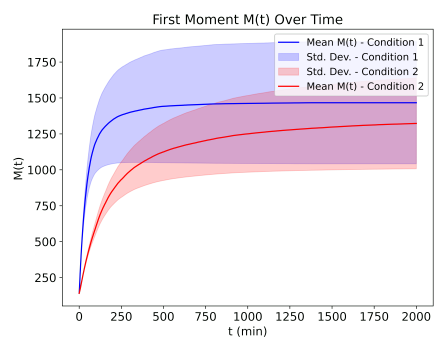
(g) The Evolution of Filament of length 7



(h) The Evolution of Filament of length 8

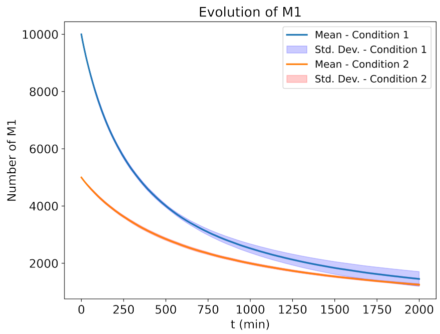


(i) The Evolution of Zeroth Moment P(t)

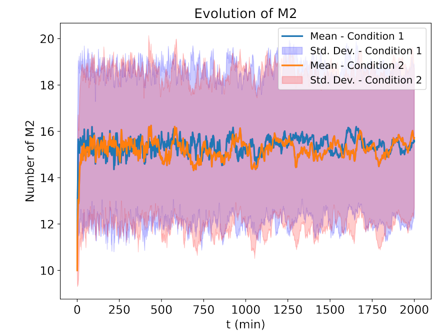


(j) The Evolution of First Moment M(t)

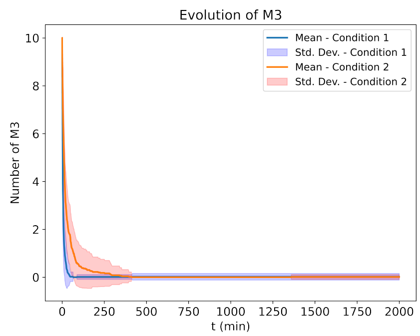
Figure S5: The Evolution of Amyloid beta aggregations when the rate con-stants are fixed, the Condition 1 with initial population of free proteins $M_1 = 10000$ and the Condition 2 with initial population of free proteins $M_1 = 5000$. The initial condition for each population except M_1 is same, 5, 5, 5, 5, 5, 5, 5 for M_2, M_3, . . . , M_8 respectively. The starting reaction rate $k_0 = 0.0000001$, whereas $k_1, k_2, \ldots, k_{26} = 0.0000000002$.



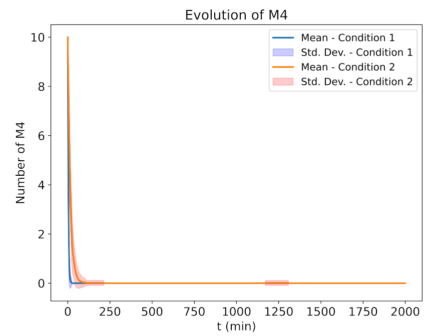
(a) The Evolution of Free Monomers (Free Proteins)



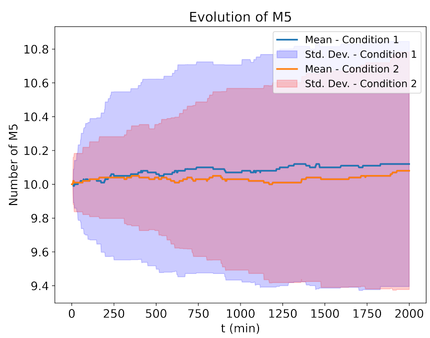
(b) The Evolution of Filament of length 2



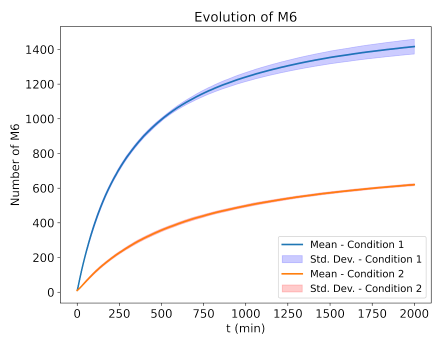
(c) The Evolution of Filament of length 3



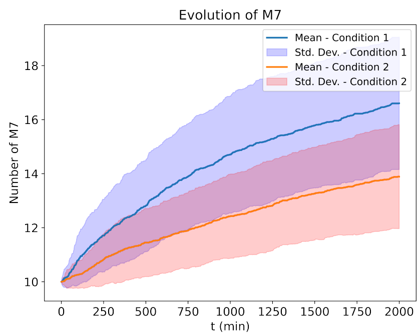
(d) The Evolution of Filament of length 4



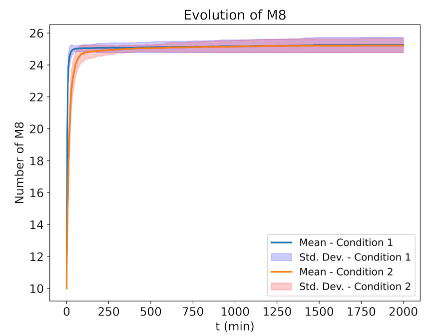
(e) The Evolution of Filament of length 5



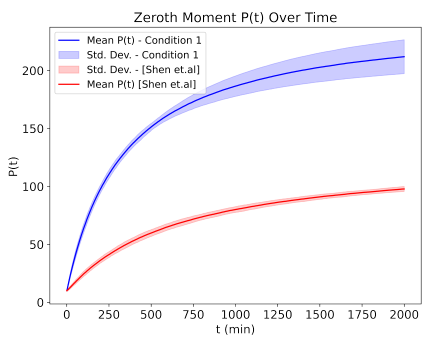
(f) The Evolution of Filament of length 6



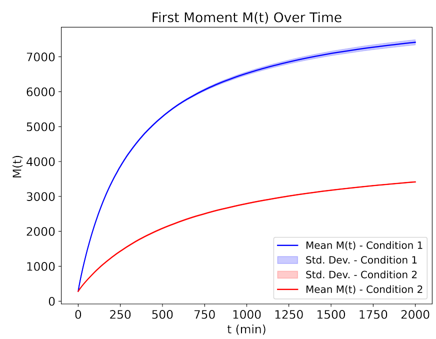
(g) The Evolution of Filament of length 7



(h) The Evolution of Filament of length 8



(i) The Evolution of Zeroth Moment P(t)



(j) The Evolution of First Moment M(t)

Figure S6: The Evolution of Amyloid beta aggregations when the rate con-stants are fixed, the Condition 1 with initial population of free proteins $M_1 = 10000$ and the Condition 2 with initial population of free proteins $M_1 = 5000$. The initial condition for each population except M_1 is same, 10, 10, 10, 10, 10, 10, 10 for $M_2, M_3, \ldots, M_8$ respectively. The starting reac-tion rate $k_0 = 0.0000001$, whereas $k_1, k_2, \ldots, k_{26} = 0.0000000002$.

In Figure S3, S4, S5 and S6, we can notice that there is a difference in how the amyloid beta aggregates when we keep the initial population of $M_2, \ldots, M_8$, 100 and 1. In latter case, overall population of filaments were less. What we can notice from Figure S4, S5, S6 is that until the initial population were less than 10, the convergence was similar, but once we make them 10, the convergence is comparable with that of the case in Figure S3.

This gives an interesting perspective in the initial population and final convergence.

S4.1 Comparison With Other Studies

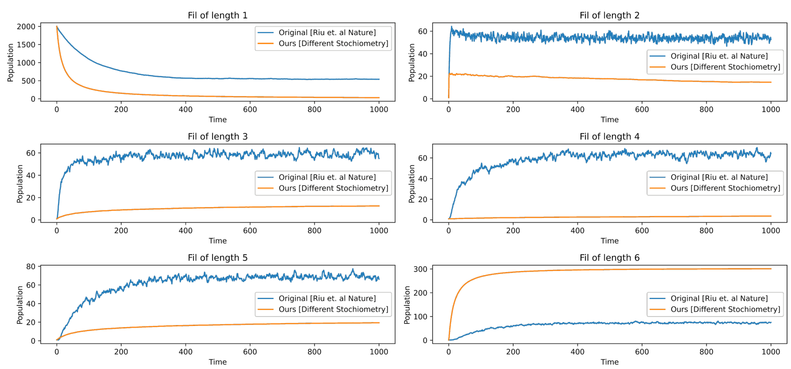


Figure S7: The evolution of different length of filaments, one in the configura-tion of Riu Et. al and the other in our configuration with our stochiometry matrix and the probability used are random, the M_0 is 2000 and time end is 1000 seconds.

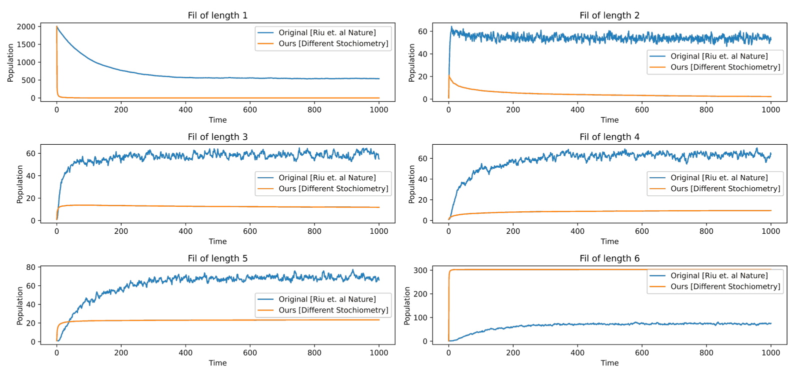


Figure S8: The evolution of different length of filaments, one in the configura-tion of Riu Et. al and the other in our configuration with our stochiometry matrix and the probability used are equal and fixed, the M_0 is 2000 and time end is 1000 seconds.