Supplementary materials

Stochastic simulation algorithm of beta-amyloid aggregation in Alzheimer Disease

Network Modeling and Simulation course report

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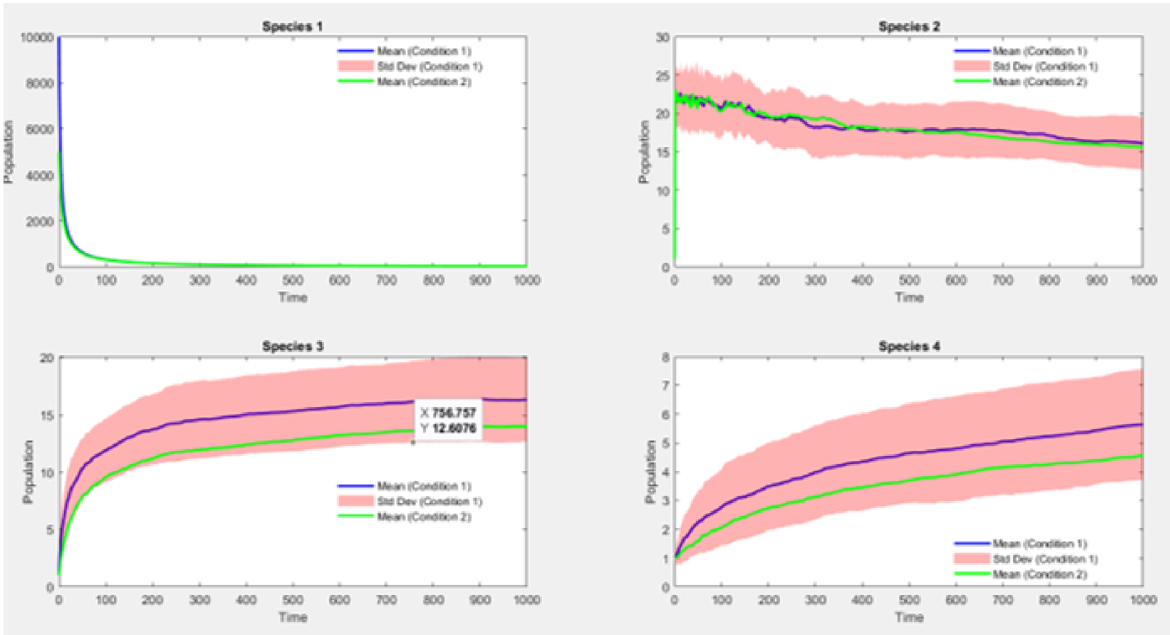

Figure 1: The evolution of amyloid beta aggregations for M1, M2, M3 and M4. Rate constants ($k_0 \neq \ldots \neq k_{53}$), $k_0 = 0.00001$, $k_2 = k_0/2, \ldots$.Condition 1 $M1 = 10000$ and Condition 2 $M2 = 5000$, and the other populations $M2, \ldots, M8 = 1$

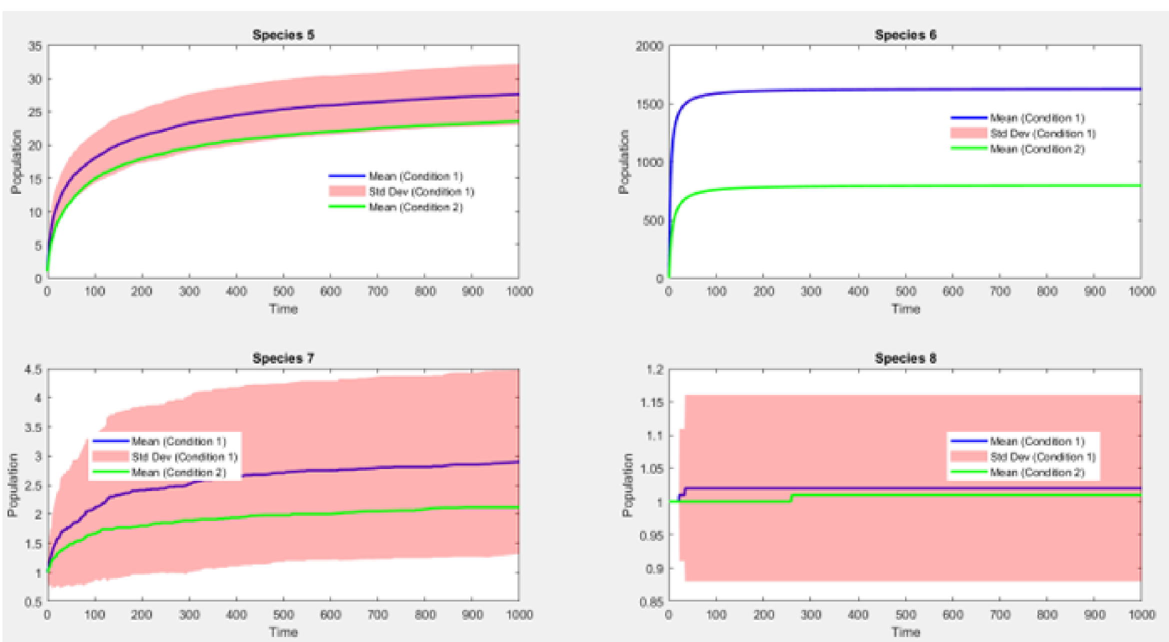

Figure 2: The evolution of amyloid beta aggregations for M5, M6, M7 and M8. Rate constants ($k_0 \neq \ldots \neq k_{53}$), $k_0 = 0.00001$, $k_2 = k_0/2, \ldots$.Condition 1 $M1 = 10000$ and Condition 2 $M2 = 5000$, and the other populations $M2, \ldots, M8 = 1$

Function Name	Calls	Total Time (s)	Self Time* (s)	Total Time Plot (dark band = self time)
modelwithoutfragmentation	1	46.602	0.637	
MonteCarloSimulation	2	44.515	0.071	
GillespieAlgorithm	200	44.329	25.212	
randsample	754845	16.146	4.692	
RandStream.RandStream>RandStream.getGlobalStream	754845	5.958	0.829	
RandStream.RandStream>localGetSetGlobalStream	754845	5.128	5.128	
histcounts	754845	3.172	2.195	
exprnd	754845	2.970	2.970	
RandStream.rand	754845	2.325	2.325	

Figure 3: Profiling of the Monte Carlo-Gillespie algorithm using aggregation.

Function Name	Calls	Total Time (s)	Self Time* (s)	Total Time Plot (dark band = self time)
modelwithoutfragmentation	1	46.948	0.709	
MonteCarloSimulation	2	44.814	0.070	
NextReactionMethod	200	44.629	25.033	
randsample	754906	16.584	4.894	
RandStream.RandStream>RandStream.getGlobalStream	754906	6.060	0.839	
RandStream.RandStream>localGetSetGlobalStream	754906	5.221	5.221	
histcounts	754906	3.292	2.273	
exprnd	754906	3.012	3.012	
RandStream.rand	754906	2.337	2.337	

Figure 4: Profiling of the FRM algorithm using aggregation.

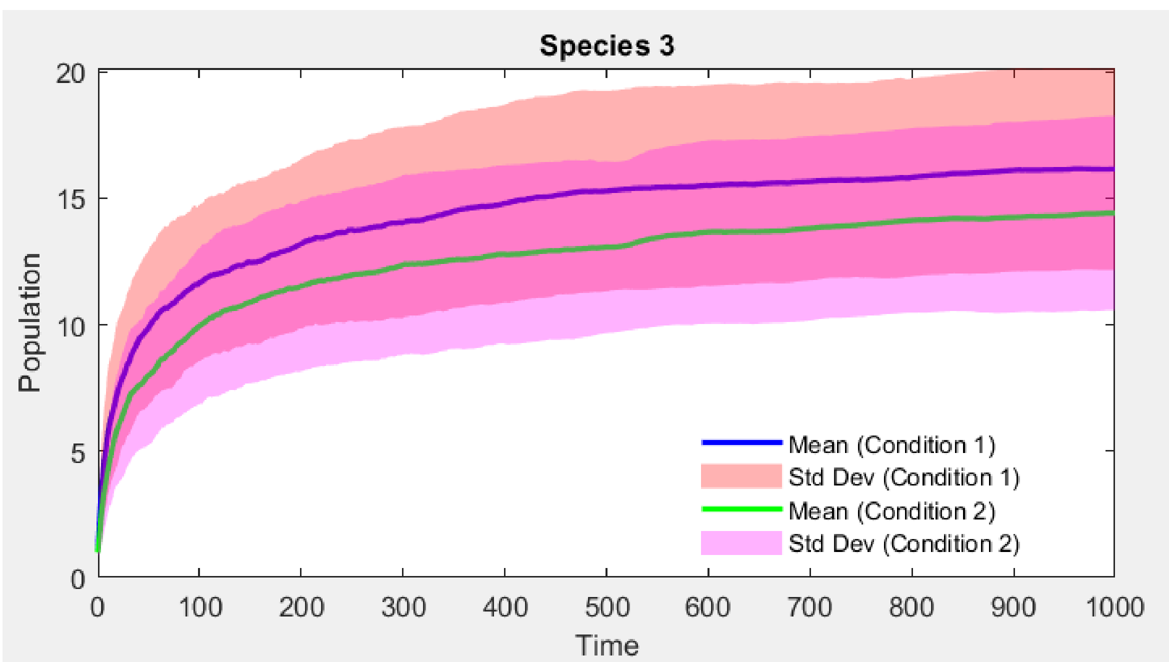

Figure 5: The evolution of amyloid beta aggregations and fragmentation for M3. Rate constants $(k_0 \neq \ldots \neq k_{53})$, $k_0 = 0.00001$, $k_2 = k_0/2, \ldots$.Condition 1 $M1 = 10000$ and Condition 2 $M2 = 5000$, and the other populations $M2, \ldots, M8 = 1$

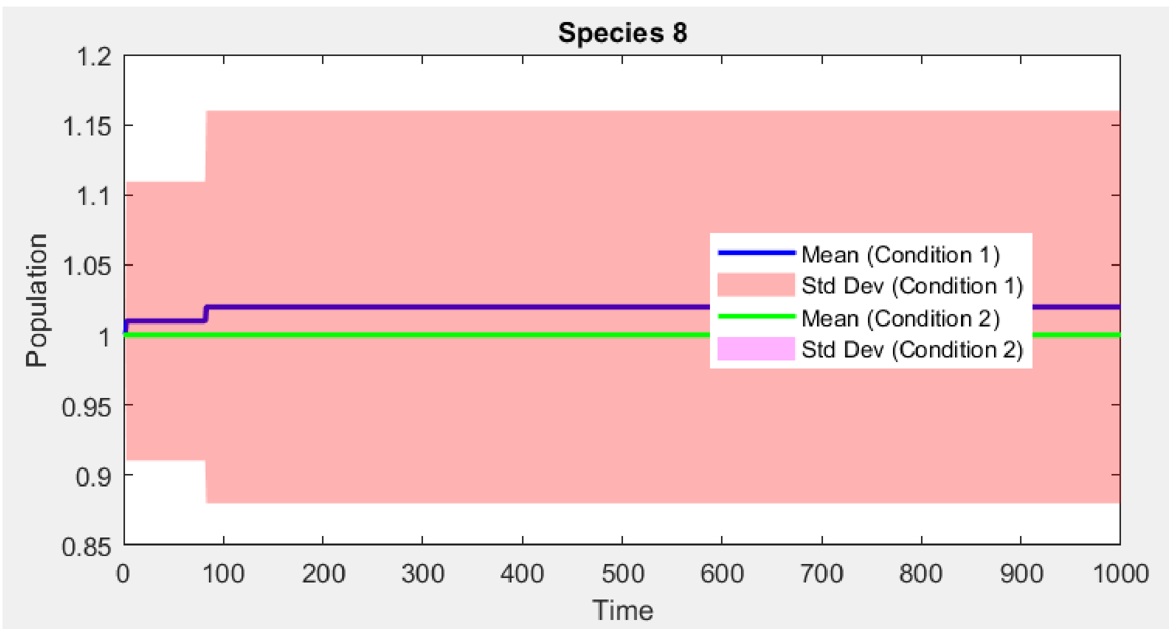

Figure 6: he evolution of amyloid beta aggregations and fragmentation for M3. Rate constants ($k_0 \neq \ldots \neq k_{53}$), $k_0 = 0.00001$, $k_2 = k_0/2, \ldots$.Condition 1 $M1 = 10000$ and Condition 2 $M2 = 5000$, and the other populations $M2, \ldots, M8 = 1$

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

Figure 7: Stechiomatrix without 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}$$

Figure 8: Stechiomatrix with fragmentation