The MATLAB files:

- *a9cle.m* is a code to simulate the Chemical Langevin Equation for a simple model of enzymes modification.

1- The reactions model for self-modifying enzymes is the following:

$$\mathrm{E} + \mathrm{E} \xrightarrow{k_1} \mathrm{E}_2 \xrightarrow{k_2} E^*E \xrightarrow{k_3} E_2^* \xrightarrow{k_4} \mathrm{E} + \mathrm{E} \tag{1}$$

Here we have four types of reactions. If we start with N_E^0 molecules of of E, the state vector in the chemical master equation will have

$$\begin{pmatrix} 4 + \frac{N_E^0}{2} - 1 \\ \frac{N_E^0}{2} \end{pmatrix} = \frac{4 + \frac{N_E^0}{2} - 1!}{\frac{N_E^0}{2}!\,(4-1)!}$$

$$= \frac{(\frac{N_E^0}{2}+3)(\frac{N_E^0}{2}+2)(\frac{N_E^0}{2}+1)}{3!} \tag{2}$$

different number of compositions. It comes from the fact that the number of ways to sample k elements from a set of n elements allowing for duplicates (i.e., with replacement) but disregarding different orderings is:

$$\begin{pmatrix} n+k-1 \\ k \end{pmatrix} = \frac{n+k-1!}{k!\,n-1!}$$

2- Figure 1 shows the concentration of E_2^* as a function of time for two different volumes. It shows that the fluctuations in the concentration of E_2^* depends on the volume of the cell and it is bigger for the smaller volume.

For the two considered volumes, I obtained different values for the mean and the variance of concentration of E_2^*.

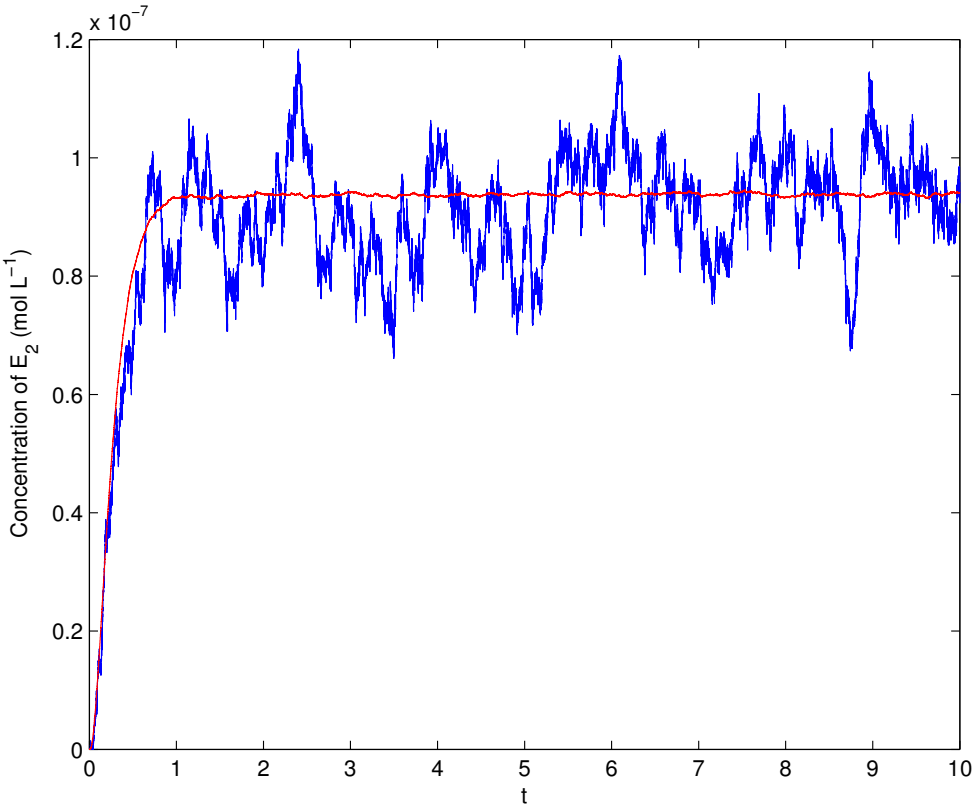

Figure 1: Concentration of E_2^* vs. time. The red color is for the volume of $10^{-12}L$ and the blue is for the volume of $10^{-15}L$. The initial concentration of E is $1\mu molL^{-1}$. The value of rate constants are: $k_1 = 10^6 Lmol^{-1}L^{-1}, k_2 = 10s^{-1}, k_3 = 100s^{-1}, k_4 = 3s^{-1}$. The step size for Δt in the simulation was $\frac{1}{2500000}$.