Problem Set 3. (due 5/1)

Problem 1 Consider the following situation. Receptor R binds a ligand present at fixed concentration $[L]$ and forms an active complex R^*. R^* gets deactivated with the rate $\alpha[Ca]$ (which depends on the concentration of Ca) to form inactive complex R'. Finally inactive complex R' dissociates releasing R which can bind the ligand again. This is described by reaction kinetics equations

$$\dot{R^*} = k[L]R - \alpha[Ca]R^* \tag{1}$$

$$\dot{R'} = \alpha[Ca]R^* - \beta R' \tag{2}$$

$$\dot{R} = -k[L]R + \beta R' \tag{3}$$

In the active state R^* generates an influx of [Ca] which is governed by

$$[\dot{Ca}] = R^* - \gamma[Ca] \tag{4}$$

The number of receptors is small, so fluctuations in R^* are important, however the influx of Ca ions is large enough that Ca dynamics can be treated deterministically.

a) (50) Formulate a suitable Gillespie procedure to simulate the event driven molecular dynamics of this process.

b) (50) Implement in Matlab (or your favorite alternative language) using $R + R^* + R' = 10$, $k[L] = 1$; $\alpha = \beta = 1$; $\gamma = 0.2$. What is the mean and the coefficient of variation of R*?