Algorithm

1. Master process:

   (a) Launch initial cell population (parallel slave processes) on the biochemical network model with a set of default model parameter values (specified in the biochemical network model).

   (b) Send MPI messages (instructions) to each slave processes (living cells). The messages should contain one or more of the following: cell-specific new parameter values, initial concentrations (protein copy numbers), and extracellular environment. These values will replace the default model parameters and concentrations of the initial population. Wait until the slave processes communicate by sending MPI messages. The slave processes will communicate after all of them have propagated simulation (Gillespie algorithm) for Δt period.

   (c) Read MPI messages from the slave processes (cells). The messages contain the current simulation data (state variables, such as species concentrations).

   (d) For each cell i, check and execute death. Calculate probability $p_{death}^{(i)} = 1 - e^{-k_{death}^{(i)} \Delta t}$. Draw a uniform random number between 0 and 1, $U^{(i)}(0,1)$. If $U^{(i)}(0,1) < p_{death}^{(i)}$, kill the cell (terminate the slave process).

   (e) For each cell i, check and execute division. Calculate the probability $P_{division}^{(i)} = 1 - e^{-k_{division} \Delta t}$. Draw $U^{(i)}(0,1)$, a uniform random number between 0 and 1. If $U^{(i)}(0,1) < pdivision$, execute division. Launch a new parallel slave process (simulation) to create a new cell.

   (f) Evaluate the new rate constant for cell death $k_{death}^{(i)} = k_{death,0} + \alpha P^{(i)}(t)$, where $P^{(i)}(t)$ is the current concentration of P in cell i.

   (g) Evaluate the change in extracellular signal, ΔI. The new concentration of the environment should be $I(t) + \Delta I$.

   (h) Go back to step (b) and iterate until the end of the simulation time.

2. Slave process i:

   (a) Receive and read the message sent by the master process. If applicable, replace the old parameters and state variables related to the cell attributes, species concentrations, and extracellular environment. Set a variable $t_{new} = t$, where t represents the current simulation time.

   (b) Calculate subcellular reaction rates: $a_1^{(i)} = k_{syn}$, $a_2^{(i)} = (k_f I)S^{(i)}$, $a_3^{(i)} = k_r P^{(i)}(t)$, $a_4^{(i)} = k_{deg}^{(i)} S^{(i)}$. Calculate sum of the reactions: $a_{tot} = \sum_{j=1}^{4} a_j^{(i)}$.

(c) Draw $U^{(i)}(0,1)$, a uniform random number between 0 and 1. Identify the smallest value of $a_k = \sum_{j=1}^{k} a_j^{(i)}$ for which $a_k \geq U(0,1)a_{tot}$. Execute reaction k, and update the network.

(d) Advance time: $t = t - \ln(U(0,1))/a_{tot}$.

(e) Go back to step (b) and iterate until $t - t_{new} \geq \Delta t$.

(f) Send a message to the master process. The message should contain information regarding the current state of the cell object (species concentrations, extracellular environment, and other state variables).