Variables/Parameters - Descriptions and Values

	Description	Value
a_i	mRNA A Concentration in Cell i	0 - 0.1*
b_i	mRNA B Concentration in Cell i	0 - 0.1*
c_i	mRNA C Concentration in Cell i	0 - 0.1*
w_i	mRNA W Concentration in Cell i	0 - 0.1*
x_i	mRNA X Concentration in Cell i	0 - 0.1*
y_i	mRNA Y Concentration in Cell i	0 - 0.1*
z_i	mRNA Z Concentration in Cell i	0 - 0.1*
A_i	Protein A Concentration in Cell i	0 - 0.1*
B_i	Protein B Concentration in Cell i	0 - 0.1*
C_i	Protein C Concentration in Cell i	0 - 0.1*
W_i	Protein W Concentration in Cell i	0 - 0.1*
X_i	Protein X Concentration in Cell i	0 - 0.1*
Y_i	Protein Y Concentration in Cell i	0 - 0.1*
Z_i	Protein Z Concentration in Cell i	0 - 0.1*
S_i	Intracellular Autoinducer Concentration in Cell i	0 - 0.1*
S_e	Extracellular Autoinducer Concentration	0 - 0.1*
α	Rate of Transcription for A, B, and C	216
α_w	Rate of Transcription for W	Sweep from 216
α_x	Rate of Transcription for X	Sweep from 216
α_y	Rate of Transcription for Y	Sweep from 216
α_z	Rate of Transcription for Z	Sweep from 216
κ	Maximal C Transcription in the Presence of Saturating Concentration of Autoinducer	20
k_{deg}	mRNA Degradation Rate	1
β_i	Ratio of mRNA to Protein Lifetime	2
k_{s0}	Degradation Rate of Autoinducer	1
k_{s1}	Production Rate of Autoinducer	0.01
η	Autoinducer Diffusion Across the Cell Membrane	0.4433, 1.367, 2.67
k_{diff}	Diffusion of Extracellular Autoinducer	8
$k_{deg_{Se}}$	Degradation Rate of Extracellular Autoinducer	2
Q	Strength of Quorum Sensing	0.4, 0.63, 0.8
n	Hill Coefficient	2

Table 1: Model variables and parameters descriptions and inital values. *Initial value inside this range chosen randomly for each cell.

Phase1 - Paper Model - Equations

mRNA Equations

$$\frac{da_i}{dt} = \frac{\alpha}{1 + C_i^n} - k_{deg} \cdot a_i$$

$$\frac{db_i}{dt} = \frac{\alpha}{1 + A_i^n} - k_{deg} \cdot b_i$$

$$\frac{dc_i}{dt} = \frac{\alpha}{1 + B_i^n} + \frac{\kappa \cdot S_i}{1 + S_i} - k_{deg} \cdot c_i$$

Protein Equations

$$\frac{dA_i}{dt} = \beta_i \cdot (a_i - A_i)$$

$$\frac{dB_i}{dt} = \beta_i \cdot (b_i - B_i)$$

$$\frac{dC_i}{dt} = \beta_i \cdot (c_i - C_i)$$

Autoinducer Equations

$$\frac{dS_i}{dt} = -k_{s0} \cdot S_i + k_{s1} \cdot A_i + \eta \cdot (S_i - S_e)$$

$$\frac{dS_e}{dt} = k_{diff} \cdot (\overline{S_i} - S_e) - k_{deg_{Se}} \cdot S_e$$

In python scripts, extracellular autoinducer is calculated using steady state assumptions: $S_e = \overline{S_i} \cdot Q$

Phase2a - Adriana - Node W - Equations

mRNA Equations

$$\frac{da_i}{dt} = \frac{\alpha}{1 + C_i^n} + \frac{\alpha \cdot W_i^n}{1 + W_i^n} - k_{deg} \cdot a_i$$

$$\frac{db_i}{dt} = \frac{\alpha}{1 + A_i^n} - k_{deg} \cdot b_i$$

$$\frac{dc_i}{dt} = \frac{\alpha}{1 + B_i^n} + \frac{\kappa \cdot S_i}{1 + S_i} - k_{deg} \cdot c_i$$

$$\frac{dw_i}{dt} = \frac{\alpha_w \cdot A_i^n}{1 + A_i^n} - k_{deg} \cdot w_i$$

Protein Equations

$$\frac{dA_i}{dt} = \beta_i \cdot (a_i - A_i)$$

$$\frac{dB_i}{dt} = \beta_i \cdot (b_i - B_i)$$

$$\frac{dC_i}{dt} = \beta_i \cdot (c_i - C_i)$$

$$\frac{dW_i}{dt} = \beta_i \cdot (w_i - W_i)$$

Autoinducer Equations

$$\frac{dS_i}{dt} = -k_{s0} \cdot S_i + k_{s1} \cdot A_i + \eta \cdot (S_i - S_e)$$

$$\frac{dS_e}{dt} = k_{diff} \cdot (\overline{S_i} - S_e) - k_{deg_{Se}} \cdot S_e$$

In python scripts, extracellular autoinducer is calculated using steady state assumptions: $S_e = \overline{S_i} \cdot Q$

Phase2a - Sydney - Node x - Equations

mRNA Equations

$$\frac{da_i}{dt} = \frac{\alpha}{1 + C_i^n} - k_{deg} \cdot a_i$$

$$\frac{db_i}{dt} = \frac{\alpha}{1 + A_i^n} + \frac{\alpha \cdot X_i^n}{1 + X_i^n} - k_{deg} \cdot b_i$$

$$\frac{dc_i}{dt} = \frac{\alpha}{1 + B_i^n} + \frac{\kappa \cdot S_i}{1 + S_i} - k_{deg} \cdot c_i$$

$$\frac{dx_i}{dt} = \frac{\alpha_x \cdot A_i^n}{1 + A_i^n} - k_{deg} \cdot x_i$$

Protein Equations

$$\frac{dA_i}{dt} = \beta_i \cdot (a_i - A_i)$$

$$\frac{dB_i}{dt} = \beta_i \cdot (b_i - B_i)$$

$$\frac{dC_i}{dt} = \beta_i \cdot (c_i - C_i)$$

$$\frac{dX_i}{dt} = \beta_i \cdot (x_i - X_i)$$

Autoinducer Equations

$$\frac{dS_i}{dt} = -k_{s0} \cdot S_i + k_{s1} \cdot A_i + \eta \cdot (S_i - S_e)$$

$$\frac{dS_e}{dt} = k_{diff} \cdot (\overline{S_i} - S_e) - k_{deg_{Se}} \cdot S_e$$

In python scripts, extracellular autoinducer is calculated using steady state assumptions: $S_e = \overline{S_i} \cdot Q$

Phase2a - Sean - Node Y - Equations

mRNA Equations

$$\frac{da_i}{dt} = \frac{\alpha}{1 + C_i^n} - k_{deg} \cdot a_i$$

$$\frac{db_i}{dt} = \frac{\alpha}{1 + A_i^n} - k_{deg} \cdot b_i$$

$$\frac{dc_i}{dt} = \frac{\alpha}{(1 + B_i^n)(1 + Y_i^n)} + \frac{\kappa \cdot S_i}{1 + S_i} - k_{deg} \cdot c_i$$

$$\frac{dy_i}{dt} = \frac{\alpha_y \cdot B_i^n}{1 + B_i^n} - k_{deg} \cdot y_i$$

Protein Equations

$$\frac{dA_i}{dt} = \beta_i \cdot (a_i - A_i)$$

$$\frac{dB_i}{dt} = \beta_i \cdot (b_i - B_i)$$

$$\frac{dC_i}{dt} = \beta_i \cdot (c_i - C_i)$$

$$\frac{dY_i}{dt} = \beta_i \cdot (y_i - Y_i)$$

Autoinducer Equations

$$\frac{dS_i}{dt} = -k_{s0} \cdot S_i + k_{s1} \cdot A_i + \eta \cdot (S_i - S_e)$$

$$\frac{dS_e}{dt} = k_{diff} \cdot (\overline{S_i} - S_e) - k_{deg_{Se}} \cdot S_e$$

In python scripts, extracellular autoinducer is calculated using steady state assumptions: $S_e = \overline{S_i} \cdot Q$

Phase2a - Olivia - Node Z - Equations

mRNA Equations

$$\frac{da_i}{dt} = \frac{\alpha}{1 + C_i^n} - k_{deg} \cdot a_i$$

$$\frac{db_i}{dt} = \frac{\alpha}{(1 + A_i^n)(1 + Z_i^n)} - k_{deg} \cdot b_i$$

$$\frac{dc_i}{dt} = \frac{\alpha}{1 + B_i^n} + \frac{\kappa \cdot S_i}{1 + S_i} - k_{deg} \cdot c_i$$

$$\frac{dz_i}{dt} = \frac{\alpha_z \cdot B_i^n}{1 + B_i^n} - k_{deg} \cdot z_i$$

Protein Equations

$$\frac{dA_i}{dt} = \beta_i \cdot (a_i - A_i)$$

$$\frac{dB_i}{dt} = \beta_i \cdot (b_i - B_i)$$

$$\frac{dC_i}{dt} = \beta_i \cdot (c_i - C_i)$$

$$\frac{dZ_i}{dt} = \beta_i \cdot (z_i - Z_i)$$

Autoinducer Equations

$$\frac{dS_i}{dt} = -k_{s0} \cdot S_i + k_{s1} \cdot A_i + \eta \cdot (S_i - S_e)$$

$$\frac{dS_e}{dt} = k_{diff} \cdot (\overline{S_i} - S_e) - k_{deg_{Se}} \cdot S_e$$

In python scripts, extracellular autoinducer is calculated using steady state assumptions: $S_e = \overline{S_i} \cdot Q$

Phase2b - Group Model - Equations

mRNA Equations

$$\frac{da_i}{dt} = \frac{\alpha}{1 + C_i^n} + \frac{\alpha \cdot W_i^n}{1 + W_i^n} - k_{deg} \cdot a_i$$

$$\frac{db_i}{dt} = \frac{\alpha}{(1 + A_i^n)(1 + Z_i^n)} + \frac{\alpha \cdot X_i^n}{1 + X_i^n} - k_{deg} \cdot b_i$$

$$\frac{dc_i}{dt} = \frac{\alpha}{(1 + B_i^n)(1 + Y_i^n)} + \frac{\kappa \cdot S_i}{1 + S_i} - k_{deg} \cdot c_i$$

$$\frac{dw_i}{dt} = \frac{\alpha_w \cdot A_i^n}{1 + A_i^n} - k_{deg} \cdot w_i$$

$$\frac{dx_i}{dt} = \frac{\alpha_x \cdot A_i^n}{1 + A_i^n} - k_{deg} \cdot x_i$$

$$\frac{dy_i}{dt} = \frac{\alpha_y \cdot B_i^n}{1 + B_i^n} - k_{deg} \cdot y_i$$

$$\frac{dz_i}{dt} = \frac{\alpha_z \cdot B_i^n}{1 + B_i^n} - k_{deg} \cdot z_i$$

Protein Equations

$$\frac{dA_i}{dt} = \beta_i \cdot (a_i - A_i)$$

$$\frac{dB_i}{dt} = \beta_i \cdot (b_i - B_i)$$

$$\frac{dC_i}{dt} = \beta_i \cdot (c_i - C_i)$$

$$\frac{dW_i}{dt} = \beta_i \cdot (w_i - W_i)$$

$$\frac{dX_i}{dt} = \beta_i \cdot (x_i - X_i)$$

$$\frac{dY_i}{dt} = \beta_i \cdot (y_i - Y_i)$$

$$\frac{dZ_i}{dt} = \beta_i \cdot (z_i - Z_i)$$

Autoinducer Equations

$$\frac{dS_i}{dt} = -k_{s0} \cdot S_i + k_{s1} \cdot A_i + \eta \cdot (S_i - S_e)$$

$$\frac{dS_e}{dt} = k_{diff} \cdot (\overline{S_i} - S_e) - k_{deg_{Se}} \cdot S_e$$

In python scripts, extracellular autoinducer is calculated using steady state assumptions: $S_e = \overline{S_i} \cdot Q$

Quantification Metrics

Average Amplitude

Find all points where $\frac{db_i}{dt} = 0$ and get the value of b_i in each cell.
Calculate the average amplitude at that time point and add to a list.
Take the average of the list to find the average amplitude of all cells across all time points.

Synchronization Metric

At each time point where a derivative is taken, find the variance in b_i across all ten cells.
Average of variances at each time point is synchronization score. Lower score means more synchronization (lower variance between cells at any given time point).