

Pseudocode for whole-cell simulation of translation

Data:

Genes:

Total number of genes = n

Ribosomes:

Total number of ribosomes = R^t

mRNAs:

Number of mRNAs of gene $i = A_i$

tRNAs:

Number of tRNAs of type $\phi(j) = T_{\phi(j)}^t$

Total number of tRNAs $\sum T_{\phi(j)}^t = T^t$

List of other parameters

Characteristic time of ribosomes = τ_r

Characteristic time of tRNAs = τ_t

Discrete positions a ribosome can occupy in a yeast cell = N_r

Discrete positions a tRNA can occupy in a yeast cell = N_t

Wobble parameter = w

Scaling coefficient due to tRNA competition = s

Also see Table S1

while $time < t$ (*total simulation time*) **do**

 Calculate

 Fraction of mRNAs of gene i that are *initiable*, f_i - i.e., those mRNAs with first 10 codons unbound.

 Number of *elongatable* ribosomes waiting at codon j , $R^b(j)$ - ribosomes with next 10 codons unbound.

 Rates of all possible events (see Table S2)

 Total initiation rate: $\rho^t = \sum_{i=1}^n \frac{R^f f_i A_i p_i}{\tau_r N_r}$

 Total elongation rate: $\epsilon^t = \sum_{j=1}^{61} \frac{R^b(j) T_{\phi(j)}^f w_j s}{\tau_t N_t}$

 Probability of each possible event (see Table S2)

 Randomly select an event based on its probability of occurrence (see Table S2)

 Update the changes in the state of the cell (see $\Delta State$ in Table S2)

 Increment $time$ by $\frac{1}{\rho^t + \epsilon^t}$

 Update the number of free ribosomes, R^f

 Update the number of free tRNAs of type $\phi(j)$, $T_{\phi(j)}^f$

end