

Appendix C: Stochastic Simulation Algorithm for Plasmid Dynamics

C.1 Overview

To capture stochasticity in plasmid-free (F) and plasmid-bearing (P) populations, a Gillespie-style stochastic simulation algorithm (SSA) was implemented. This simulates individual birth, death, plasmid loss, and conjugation events, allowing population trajectories to vary between runs and capturing fluctuations that deterministic ODEs cannot.

C.2 Reactions and Propensities

Reaction	Description	Propensity function, a_i
$F \rightarrow F + 1$	Birth of plasmid-free cell	$a_1 = r(1 - s) \left(1 - \frac{N}{K}\right) F$
$P \rightarrow P + 1$	Birth of plasmid-bearing cell	$a_2 = r(1 - c) \left(1 - \frac{N}{K}\right) P$
$F \rightarrow F - 1$	Death of plasmid-free cell	$a_3 = \mu F$
$P \rightarrow P - 1$	Death of plasmid-bearing cell	$a_4 = \mu P$
$P \rightarrow P - 1$ $F \rightarrow F + 1$	Plasmid loss (segregation)	$a_5 = \delta P$
$F \rightarrow F - 1$ $P \rightarrow P + 1$	Plasmid transfer (conjugation)	$a_6 = \frac{\beta FP}{K}$

where $N = F + P$ is the total population.

C.3 Gillespie Algorithm

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while t < TMAX and F + P > 0:

    N = F + P

    Compute logistic growth rates:
        wF = max(0, r*(1-s)*(1 - N/K))
        wP = max(0, r*(1-c)*(1 - N/K))

    Compute propensities:
        a1 = wF * F           # F birth
        a2 = wP * P           # P birth
        a3 = mu * F           # F death
        a4 = mu * P           # P death
        a5 = delta * P        # Plasmid loss
        a6 = beta * F * P / K # Conjugation

    a0 = sum(a1..a6)
    if a0 == 0: break

    Sample next reaction time: tau ~ Exponential(1/a0)
    t = t + tau

    Choose reaction i with probability a_i / a0
    Update F and P according to reaction i
    Ensure F >= 0 and P >= 0
```

Record F, P, t

Return time series of t, F, P