Appendix C: Stochastic Simulation of Plasmid Dynamics

C1. Overview

To capture demographic stochasticity in finite populations, a Gillespie-style stochastic simulation algorithm is employed. The system is modelled as a continuous-time Markov jump process, in which birth, death, plasmid loss, and conjugation events occur as Poisson processes with state-dependent rates.

C2. Reaction Channels and Propensities

Let $F(t)$ and $P(t)$ denote the number of plasmid-free and plasmid-bearing cells at time t, respectively, with total population size $N = F + P$.

The possible reactions and their propensities are:

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

C3. Gillespie Algorithm

At each simulation step, the total event rate is:

$$a_0 = \sum_{i=1}^{6} a_i$$

The time to the next event is exponentially distributed:

$$\tau \sim Exponential(a_0)$$

reflecting the memoryless nature of Poisson reaction processes.

An event is selected with probability a_i/a_0, and the system state is updated accordingly. Simulations proceed until a specified final time or population extinction.

C4. Pseudocode

```
while t < TMAX and F + P > 0:

    N = F + P
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    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

    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
```