Clock Model: Vilar et al 2002, PNAS. Mechanisms of Noise-resistance in genetic oscillators.

Circadian Clock Oscillator Model:

	Reaction	k_{on} (or k_f)	k_{off}	k_a^{3D} (or k_f)	k_b	σ
1	PmrA⟶PrmA+mRNA_A	$50s^{-1}$	-	$50s^{-1}$	-	-
2ab	PrmA+A⇌PrmA_bound	$602\mu M^{-1}s^{-1}$	$50s^{-1}$	$4888.6nm^3\mu s^{-1}$	$244.5s^{-1}$	5nm
3	PrmA_bound ⟶PrmA_bound+mRNA_A	$500s^{-1}$	-	$500s^{-1}$	-	-
4	PrmR⟶PrmR+mRNA_R	$0.01s^{-1}$	-	$0.01s^{-1}$	-	-
5ab	PrmR+A⇌PrmR_bound	$602\mu M^{-1}s^{-1}$	$100s^{-1}$	$4888.6nm^3\mu s^{-1}$	$489s^{-1}$	5nm
6	PrmR_bound ⟶PrmR_bound+mRNA_R	$50s^{-1}$	-	$50s^{-1}$	-	-
7	mRNA_A⟶mRNA_A+A	$50s^{-1}$	-	$50s^{-1}$	-	-
8	mRNA_R⟶mRNA_R+R	$5s^{-1}$	-	$5s^{-1}$	-	-
9	A+R⟶C	$1204\mu M^{-1}s^{-1}$	-	$356263nm^3\mu s^{-1}$	-	8nm
10	C⟶R	$1s^{-1}$	-	$1s^{-1}$	-	-
11	A⟶Null	$1s^{-1}$	-	$1s^{-1}$	-	-
12	R⟶Null	$0.2s^{-1}$	-	$0.2s^{-1}$	-	-
13	mRNA_A⟶Null	$10s^{-1}$	-	$10s^{-1}$	-	-
14	mRNA_R⟶Null	$0.5s^{-1}$	-	$0.5s^{-1}$	-	-

For all species D_t=10μm^2/s, and D_R=0.
V=4.188 μm^3
Initial copies are 0 except for prmA=1 and prmR=1.
Use Δt=10μs, density can get high and 50μs is above suggested max time-step.

DATA FILES:
This directory contains A(t) R(t) for NERDSS trajectory. First column is Iteration, time=Itr*50us.
ar_iter_regDecay_NERDSS.dat
And for slower decay: ar_iter_slowDecay_NERDSS.dat

Files for ODE from Virtual Cell: ARode_vstime.dat
Files from PDE from Virtual Cell: ARpde_vstime.dat

ANALYSIS FILES: Read in trajectory [t, A(t), R(t)], calculate periods of oscillations and lag times.
`findOscillationPeriodFFTZeroPad.m`
`calc_peak_sepsAR.m`

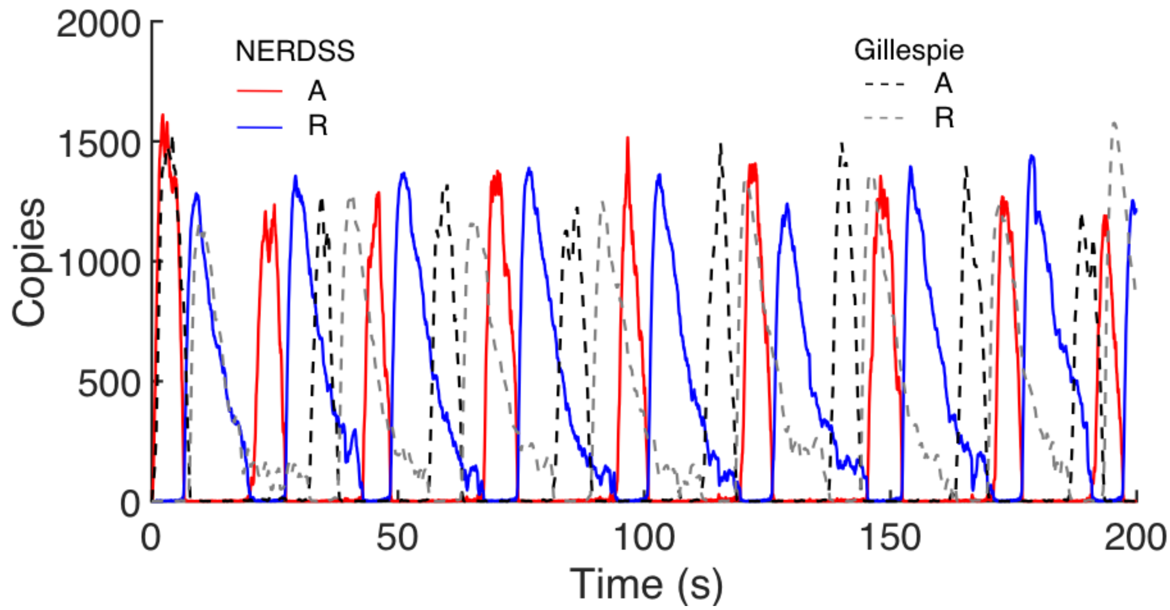

Fig 1. NERDSS simulations give periods of 24.5s, 24.75, 6.45s lag. ODE/PDE is 25.12, 25.12 and 6.55s. Based on FFt with zeropad to 5000s.

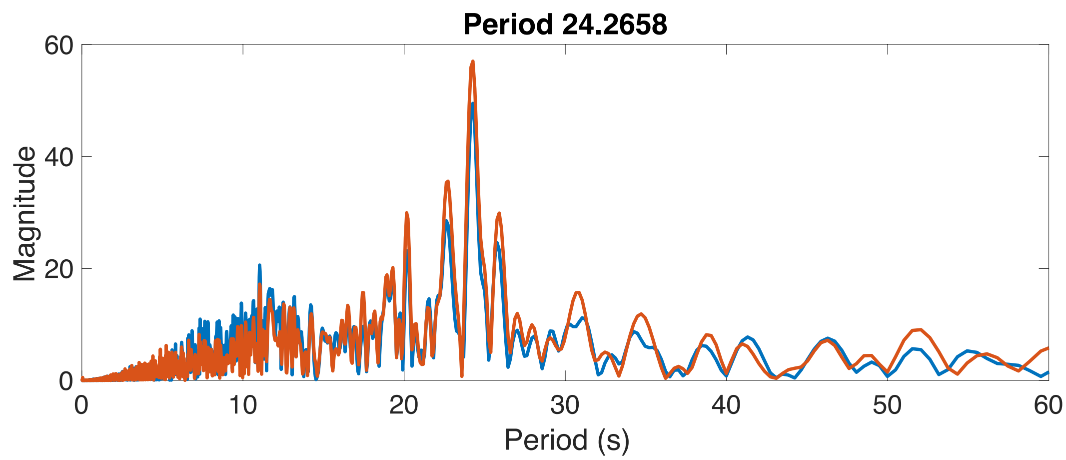

Fig 2. FFT of NERDSS A/R oscillations vs time, after zero padding to 500s. Largest amplitude is for oscillations at a period of 24.2658s, from this trajectory.

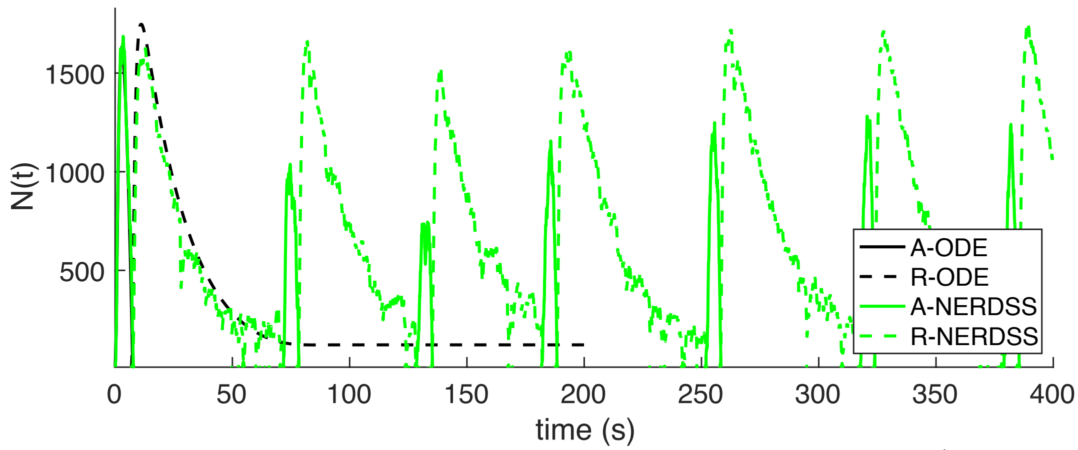

Fig 3. With slow R decay, (reaction #12, we drop the rate from 0.2 to 0.05 s^{-1}) oscillations disappear in deterministic solution but persist in stochastic simulations. Here, the single-particle NERDSS simulations were run for 1000s, producing oscillations with periods of 63.3 and 64.1s, or about twice as slow as the original model. The lag between A and R slowed to 7.95s.