Clathrin flat lattice in solution:
The theory line is always the analytical solution to the ODE from A+A⇌C
$\frac{dA(t)}{dt} = -2k_{on}A(t)^2 + 2k_{off}C(t)$,
Where A(t)+2C(t)=A_0+2C_0. We set A_0=3N_{trimer}, C_0=0. Macroscopic rates are used.
All NERDSS input files use k_a^{3D} values. For clathrin leg labels that are distinct, (e.g. c_1 and c_2), the input rates must be multiplied by 2 to enforce the same binding free energies for all binding reactions.

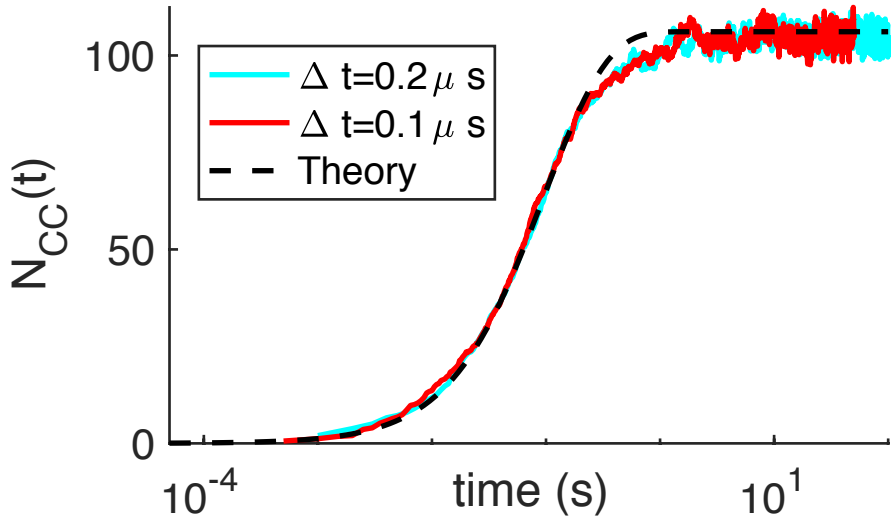

Fig 1. Bound clathrin legs, initially 100 trimers in V=(0.494um)^3. Same volume for other simulations. Kd=1uM, kon=1uM-1s-1, koff=1s-1. Theory is for 300 independent legs, so no spatial or structural effects. LoopCoopFactor f=5.9E-6. D_t=13um^2/s, D_R=0.03rad^2/s. Nbound_eq=106.1 for independent sites.

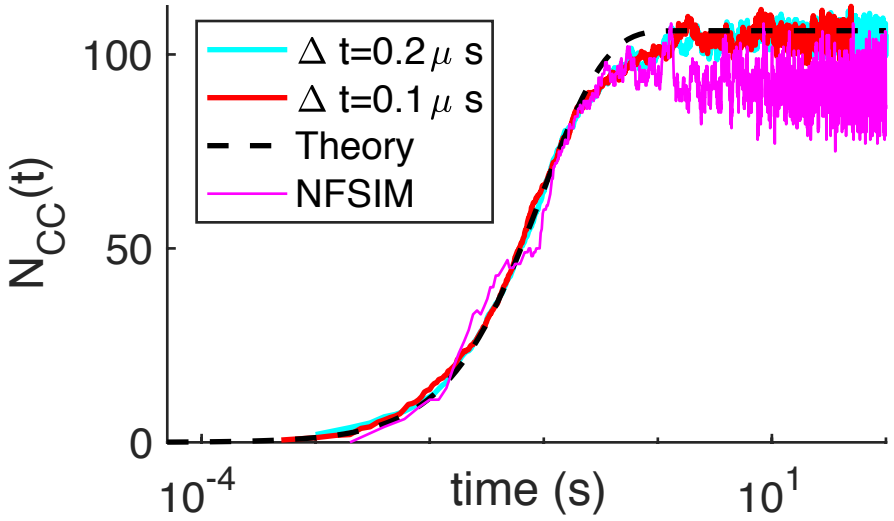

Fig 2. Here NFSim has intramolecular binding included. Note that for NFsim, must multiply initial self-rates by 2, as done in the .bngl file. For output, note homodimers (A(a!).A(a!)) are double counted because the pattern appears twice.

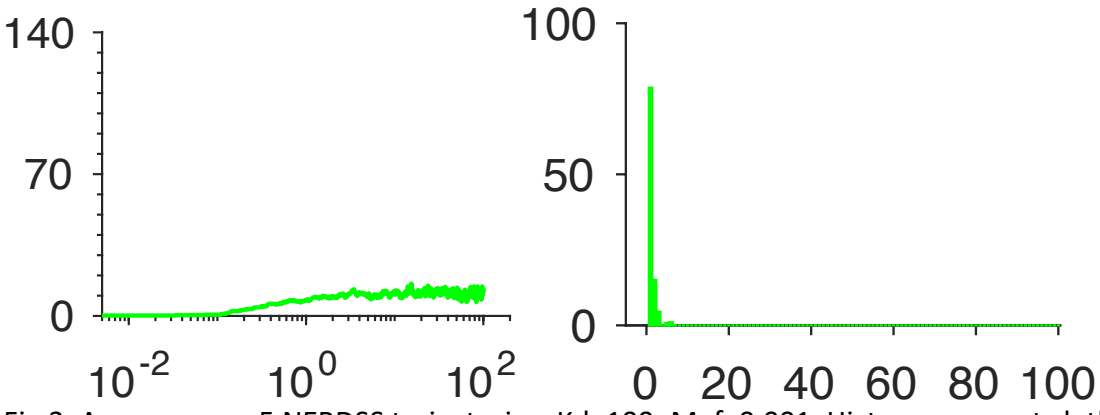

Fig 3. Average over 5 NERDSS trajectories, Kd=100uM, f=0.001. Histogram: most clathrin are in dimers or monomers, a few larger multi-mers exist.

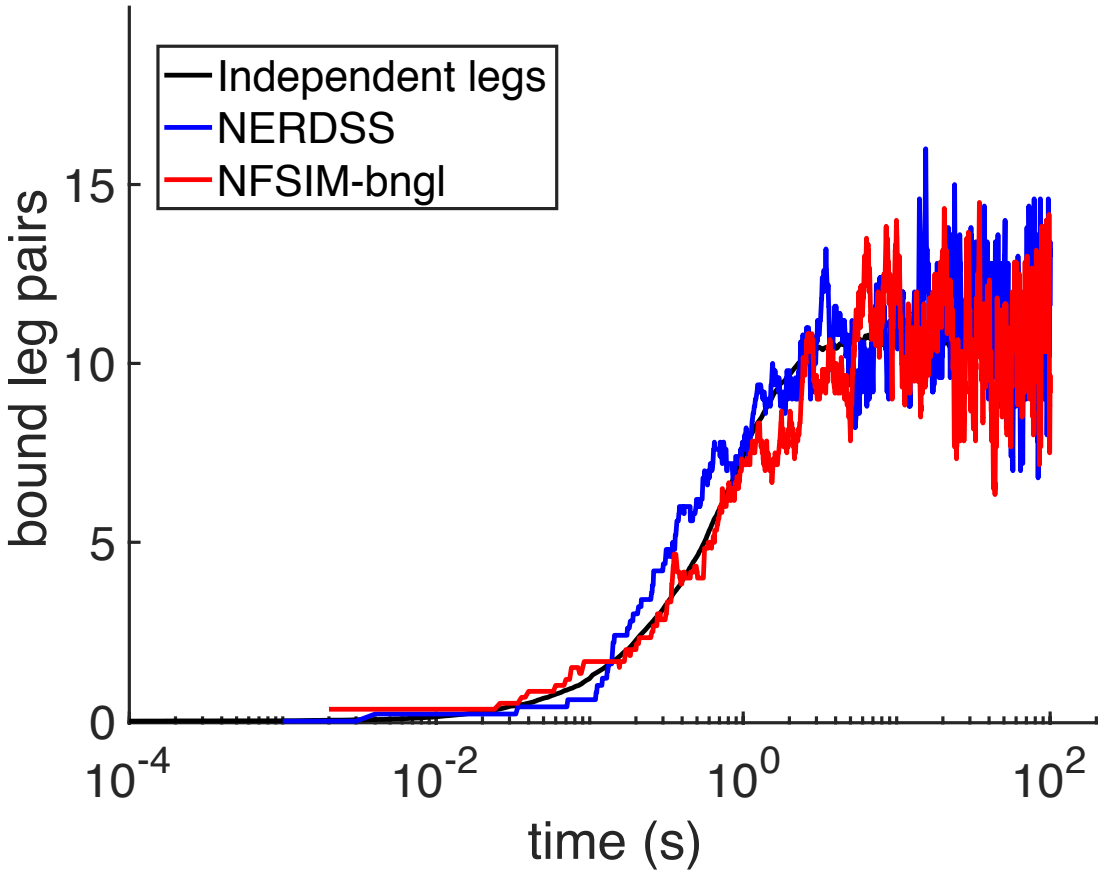

Fig 4. NERDSS is 3 trajectories. Kd=100uM, f=0.001. NFsim has no intra binding. Black is Gillespie here, but same result for independent legs, Nbound_eq=10.7.

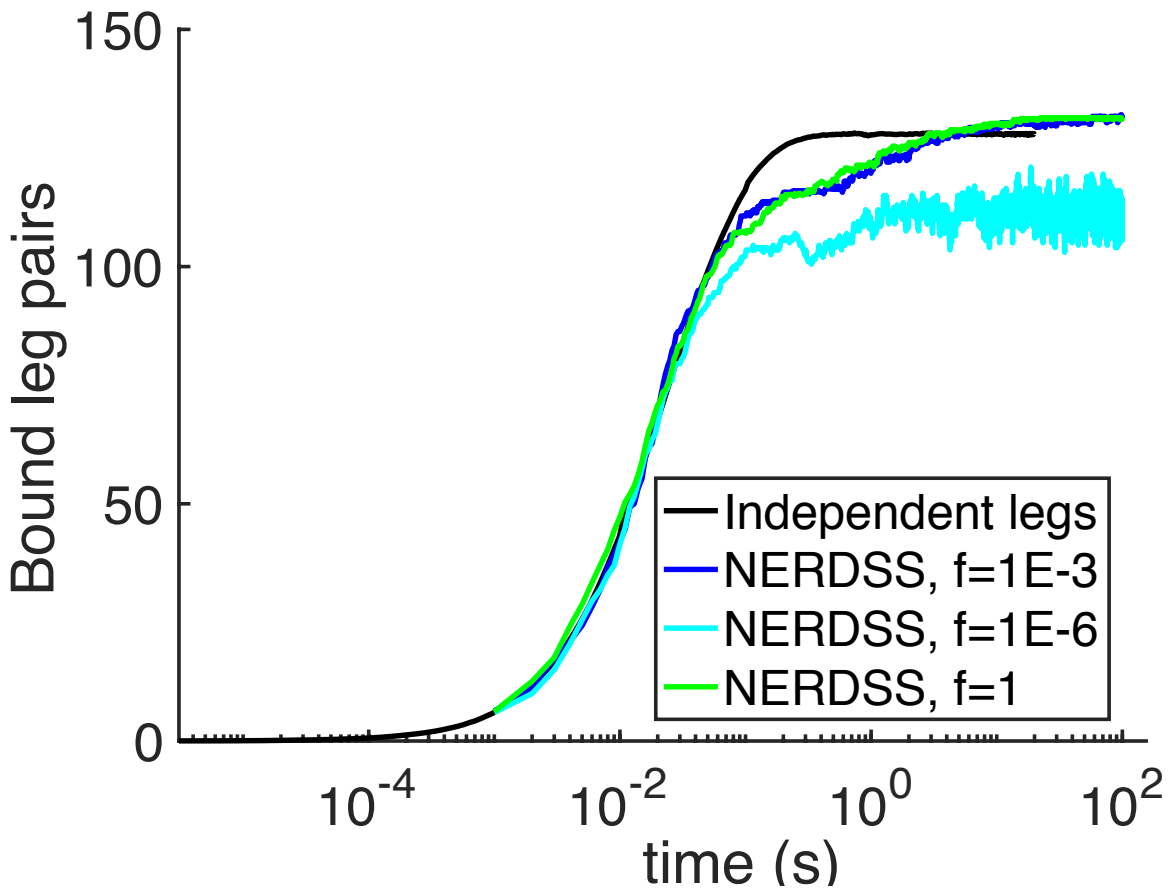

Fig 5. Clathrin 100 trimers, Kd=0.2uM. Decreasing f will de-stabilize loops, if it is low enough, causing fewer bound leg pairs. Nbound_eq=128.4 (for independent sites).