Clathrin flat lattice in solution:

The theory line is always the analytical solution to the ODE from A+A⇌C

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Where A(t)+2C(t)=A0+2C0. We set A0=3Ntrimer, C0=0. Macroscopic rates are used.

All NERDSS input files use ka3D values. For clathrin leg labels that are distinct, (e.g. c1 and c2), 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. Dt=13um2/s, DR=0.03rad2/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).