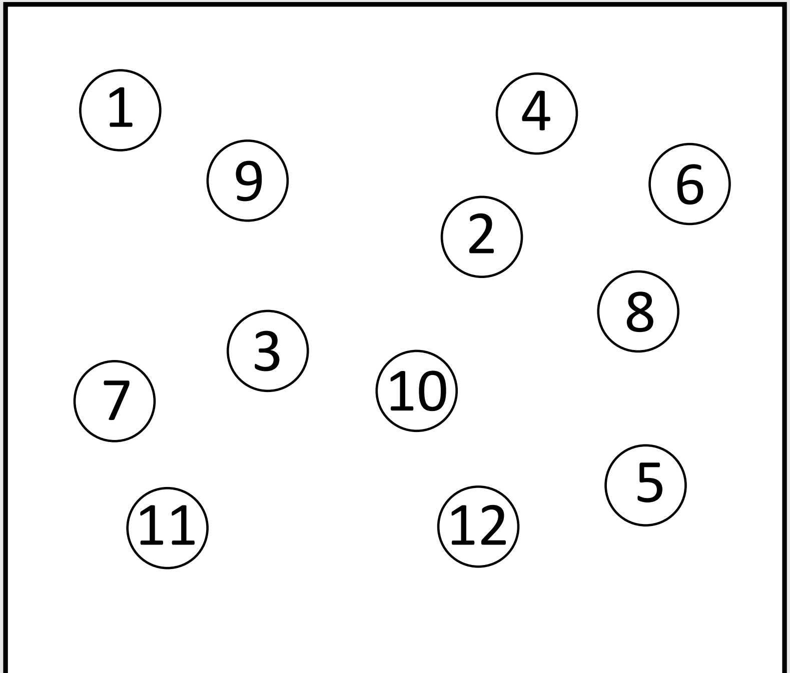
Toy Model: Distinguishable Monomers



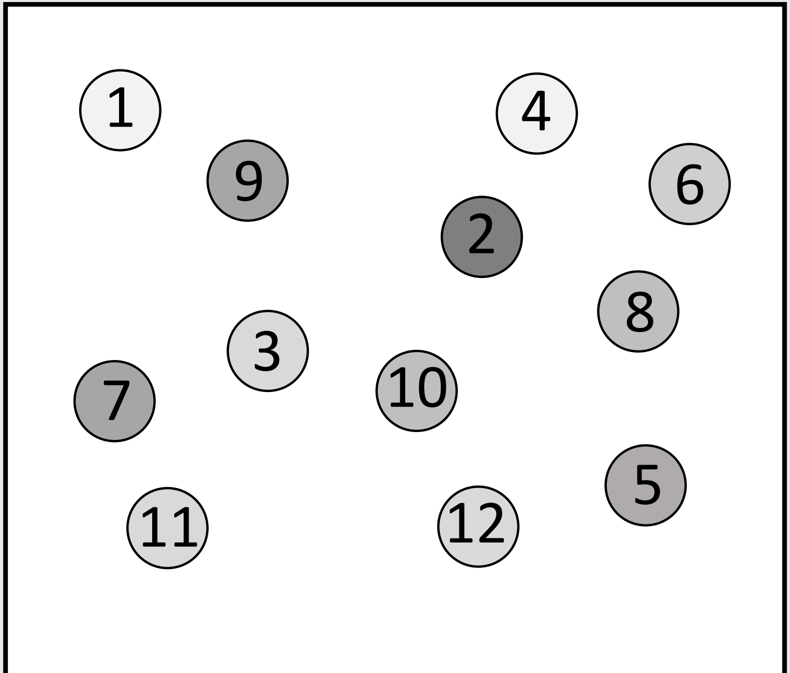
N Labeled Monomers

$$y_i \;\; \forall \;\; i \in [1, N]$$

$$r_{ij} = r_{ji} = R/2$$

$$p_{ij} = C(y_i, y_j)$$

Toy Model: Intrinsic Character



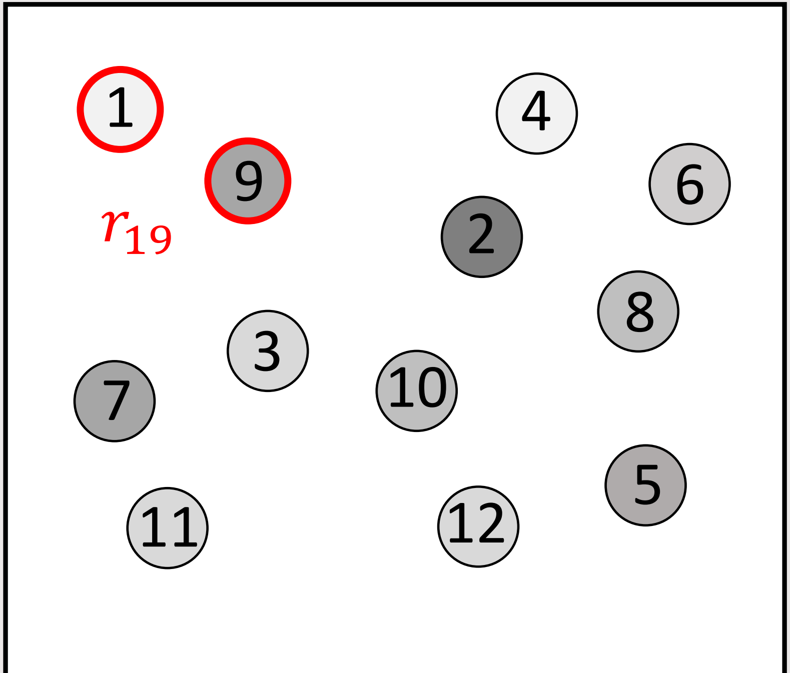
N Labeled Monomers

$$y_i \ \forall \ i \in [1, N]$$

$$r_{ij} = r_{ji} = R/2$$

$$p_{ij} = C(y_i, y_j)$$

Toy Model: Pairwise Interaction Rate



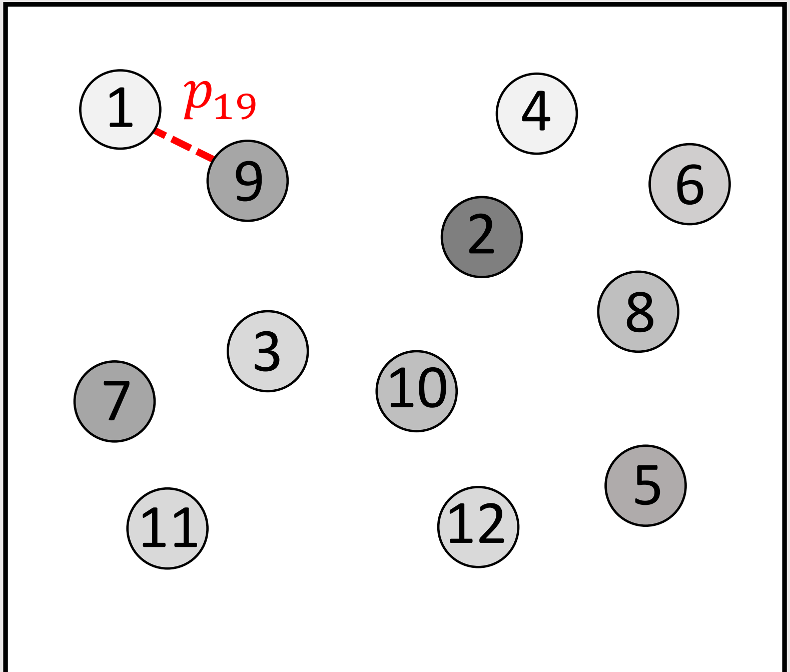
N Labeled Monomers

$$y_i \;\; \forall \;\; i \in [1, N]$$

$$r_{ij} = r_{ji} = R/2$$

$$p_{ij} = C(y_i, y_j)$$

Toy Model: Coalescence Probability Function



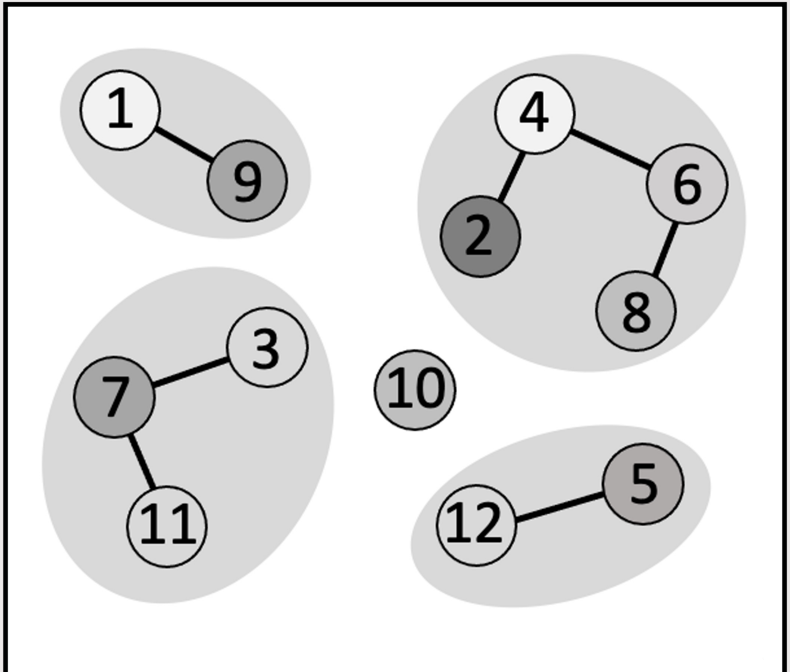
N Labeled Monomers

$$y_i \ \forall \ i \in [1, N]$$

$$r_{ij} = r_{ji} = R/2$$

$$p_{ij} = C(y_i, y_j)$$

Toy Model: Connected Components/Clusters

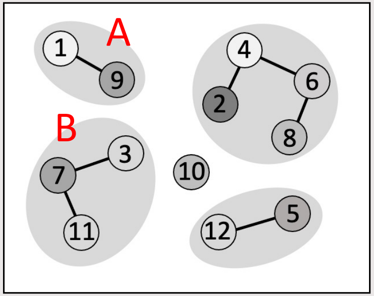


N Labeled Monomers

$$y_i \;\; \forall \;\; i \in [1, N]$$

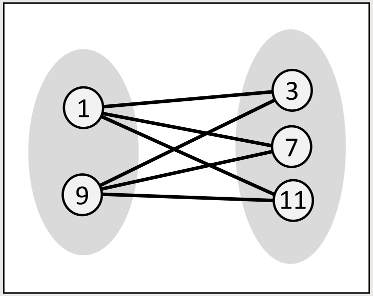
$$r_{ij} = r_{ji} = R/2$$

$$p_{ij} = C(y_i, y_j)$$



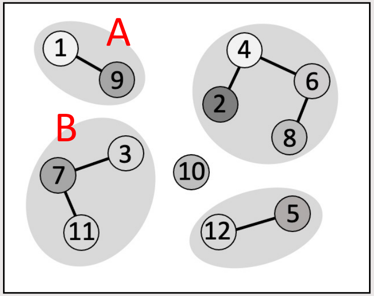
Transition Events

$$[A] + [B] \longrightarrow [A+B]$$



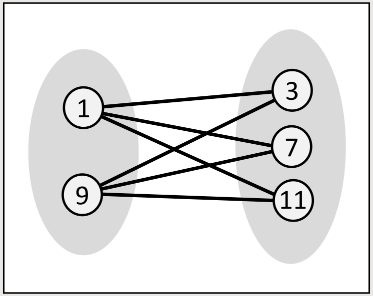
Microscopic Model

Coarse-Grained Model



Transition Events

$$\{y_1, y_9\} + \{y_3, y_7, y_{11}\} \longrightarrow \{y_1, y_3, y_7, y_9, y_{11}\}$$



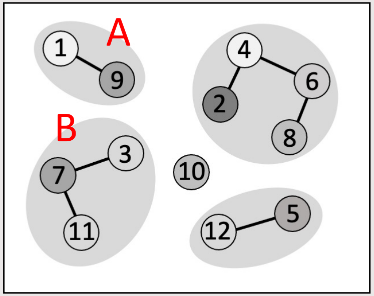
Microscopic Model

$$Y_A + Y_B \xrightarrow{R_a(Y_A, Y_B)} Y_A \cup Y_B$$

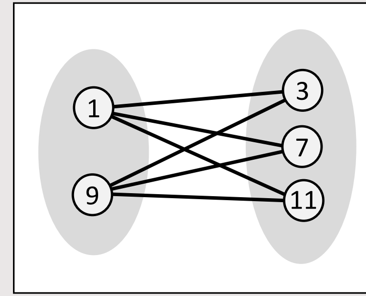
$$R_a(Y_A, Y_B) = \sum_{\forall y_m \in Y_a} \sum_{\forall y_n \in Y_b} R \times C(y_m, y_n)$$

Coarse-Grained Model

Transition Events



$$[2] + [3] \longrightarrow [5]$$



Microscopic Model

$$Y_A + Y_B \xrightarrow{R_a(Y_A, Y_B)} Y_A \cup Y_B$$

$$R_a(Y_A, Y_B) = \sum_{\forall y_m \in Y_a} \sum_{\forall y_n \in Y_b} R \times C(y_m, y_n)$$

Coarse-Grained Model

$$[i] + [j] \xrightarrow{K(i,j)} [k]$$

$$K(i,j) = R \times F \times (i \times j)$$

$$F = \int_0^1 \int_0^1 C(y_m, y_n) q(y_m) q(y_n) dy_m dy_n$$

Coarse-Grained Model: Deterministic Formulation

Aggregation Rate Kernel

- Product Kernel $\boxed{K(i,j) = R\times F\times(i\times j)}$
- Mean-Field Coalescence Probability $\boxed{F = \int_0^1 \int_0^1 C(y_m, y_n) q(y_m) q(y_n) dy_m dy_n}$

Smolukhowski Coagulation Equation

$$\boxed{\frac{d}{dt} n_k(t) = (R\times F)\ \frac{1}{2} \sum_{i+j=k} ij\, n_i(t) n_j(t) - (R\times F)\ k n_k(t) \sum_{i\geq 1} i\, n_i(t)}$$

Monodispersed I.C.
$n_k(t=0) = N\delta_{1k}$

Detection of Critical Time

- Moments

$$\boxed{M_n(t) = \sum_{k\geq 1} k^n n_k(t)}$$

- Moment Divergence $n \geq 2$

$$\boxed{M_n(t) \to \infty \text{ as } t \to t_c}$$

- Critical Time

$$\boxed{t_c = \frac{1}{RFN}}$$

Coarse–Grained Model: $n_k(t)$

Generating Function

$$\mathcal{E}(x,t) = \sum_{k\geq 1} k\, n_k e^{kx}$$

- Inviscid Burgers equation $n_k(t) \leftrightarrow \mathcal{E}(x,t)$

$$\dot{\mathcal{E}}(x,t) - \frac{1}{t_c}\left(\frac{\mathcal{E}(x,t)}{N} - 1\right)\frac{\partial}{\partial x}\mathcal{E}(x,t) = 0$$

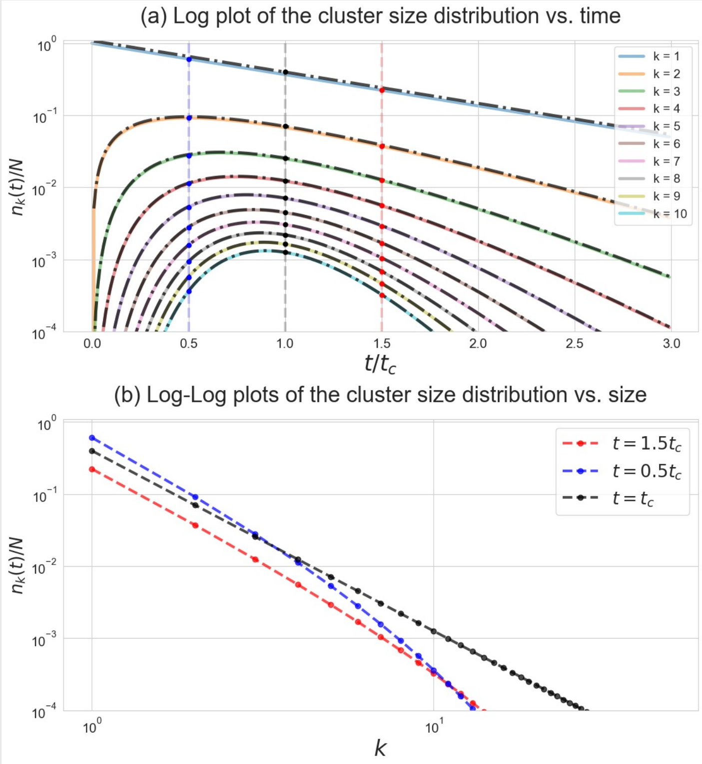
Cluster Size Distribution

$$n_k(t) = N\,\frac{k^{k-2}}{k!}\,\alpha(t)^{k-1}\,exp\big(-k\,\alpha(t)\big)$$

$$\alpha(t) = t/t_c$$

- $t = t_c$

$$\boxed{n_k(t_c) = \frac{N}{\sqrt{2\pi}}k^{-5/2}}$$



Coarse-Grained Model: Monomer Concentration and Gel Fraction

Monomer Concentration

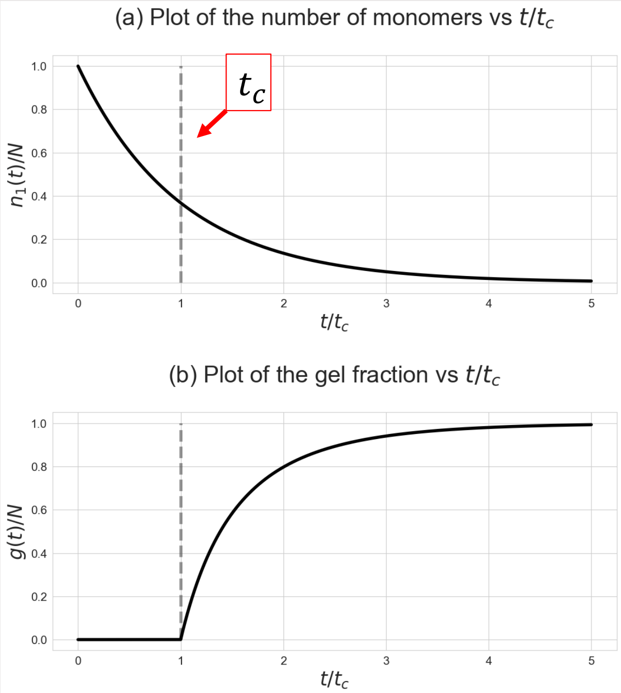
$$\alpha(t) = t/t_c$$

$$n_1(t) = N\,exp\big(-\alpha(t)\big)$$

Gel Fraction

$$M_1(t) = N\big(1 - g(t)\big)$$

$$g(t) = 1 + \frac{W_0\Big(-\alpha(t)\,exp\big(-\alpha(t)\big)\Big)}{\alpha(t)}$$



Homophily in Heterogenous Networks

Coalescence Probability Function

$$\boxed{C(y_m, y_n) = (1 - |y_m - y_n|)^s}$$

Mean-Field Coalescence Probability

$$\boxed{F = \frac{2}{s+2}}$$

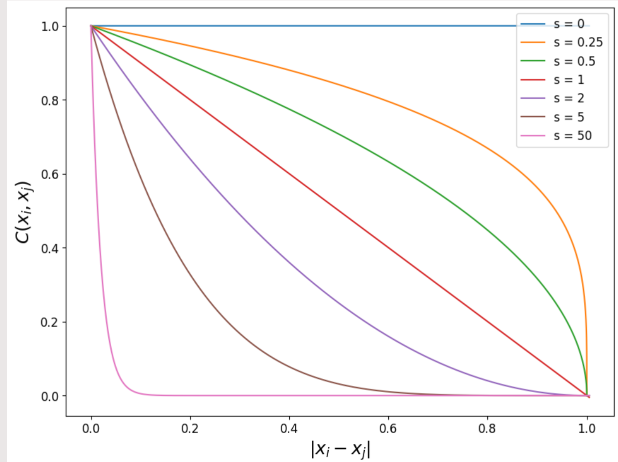
- Random Aggregation $s \to 0 \Rightarrow F \to 1$
- No Aggregation $s \to \infty \Rightarrow F \to 0$

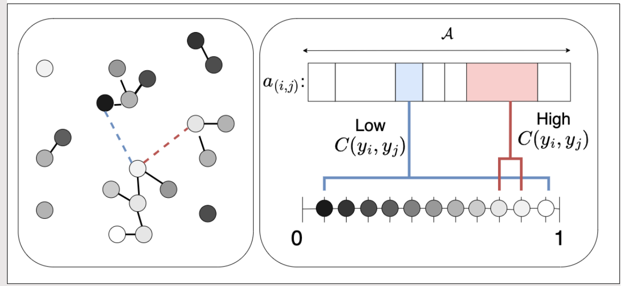
System Parameters $\boxed{(N, s)}$

- N : System Size
- s : Monomer Selectivity
- $R = \frac{2}{N(N-1)} \approx \frac{2}{N^2}$: pair-wise interaction rate
- $R_{tot} = \sum_{all\ pairs} R = 1$

Critical Time of Gelation

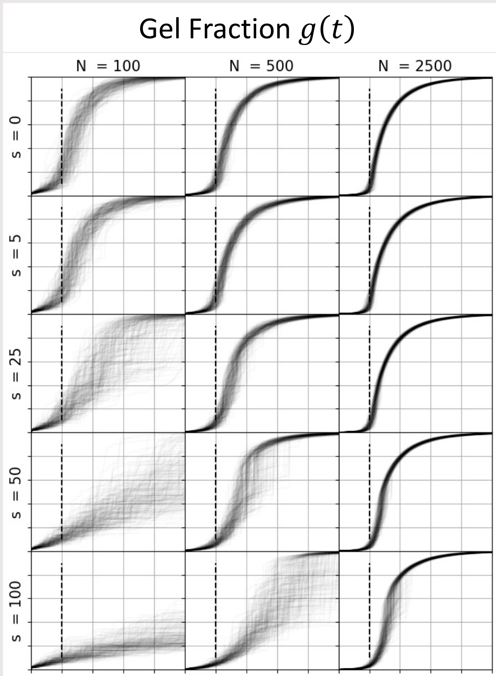
$$\boxed{t_c = \frac{N(s+2)}{4}}$$

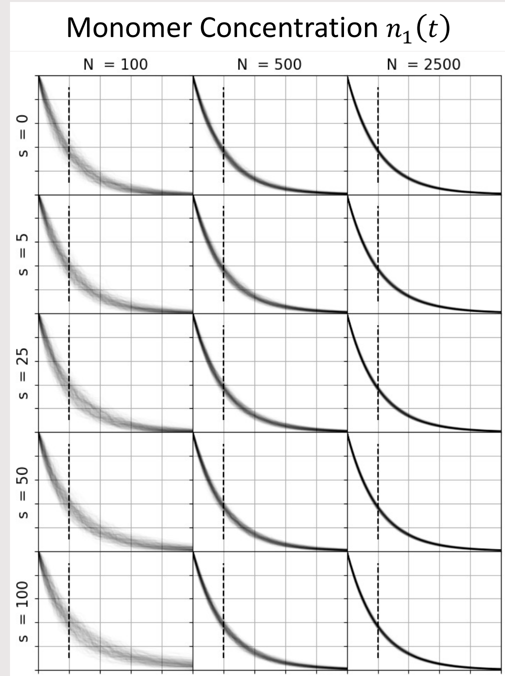




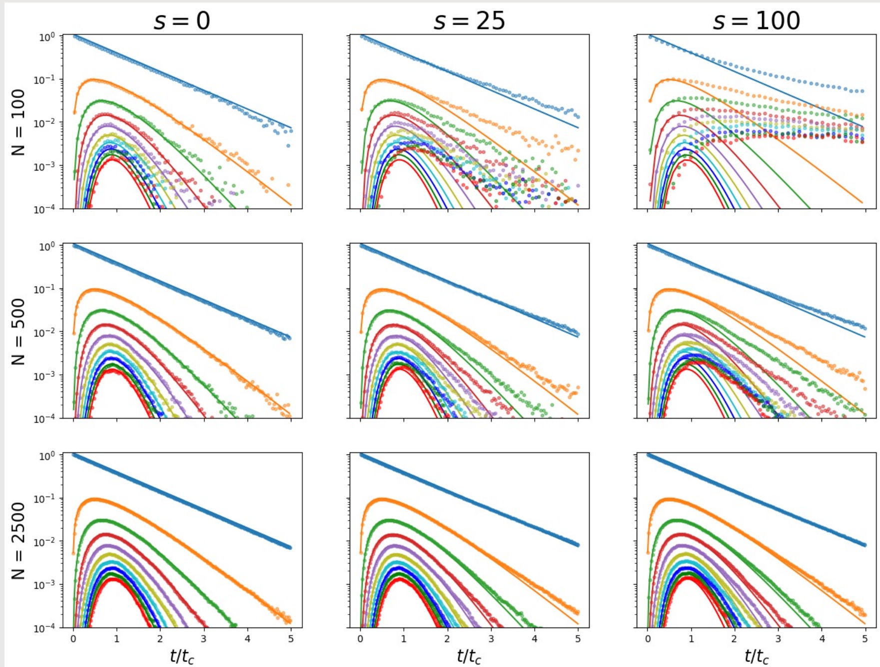
Homophily: Trajectories of Numerical Simulation

Increasing Selectivity s

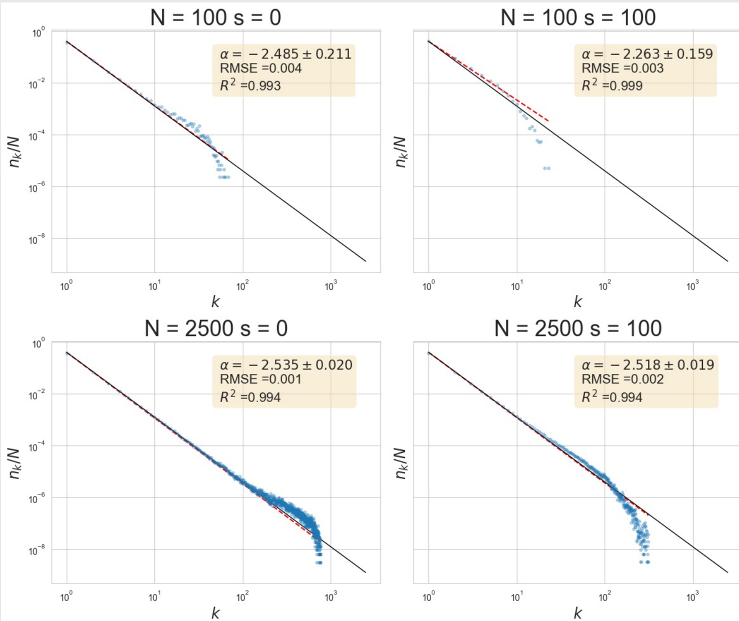


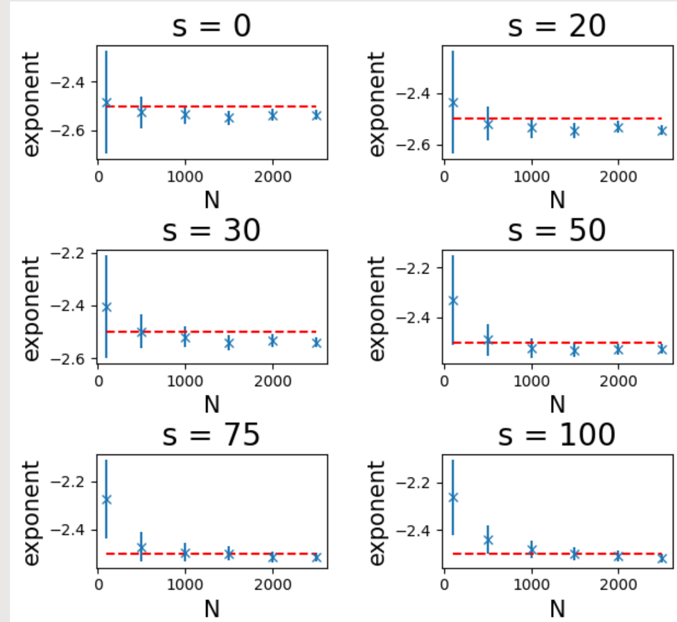


Homophily: Cluster Size Distribution $n_k(t_c)$

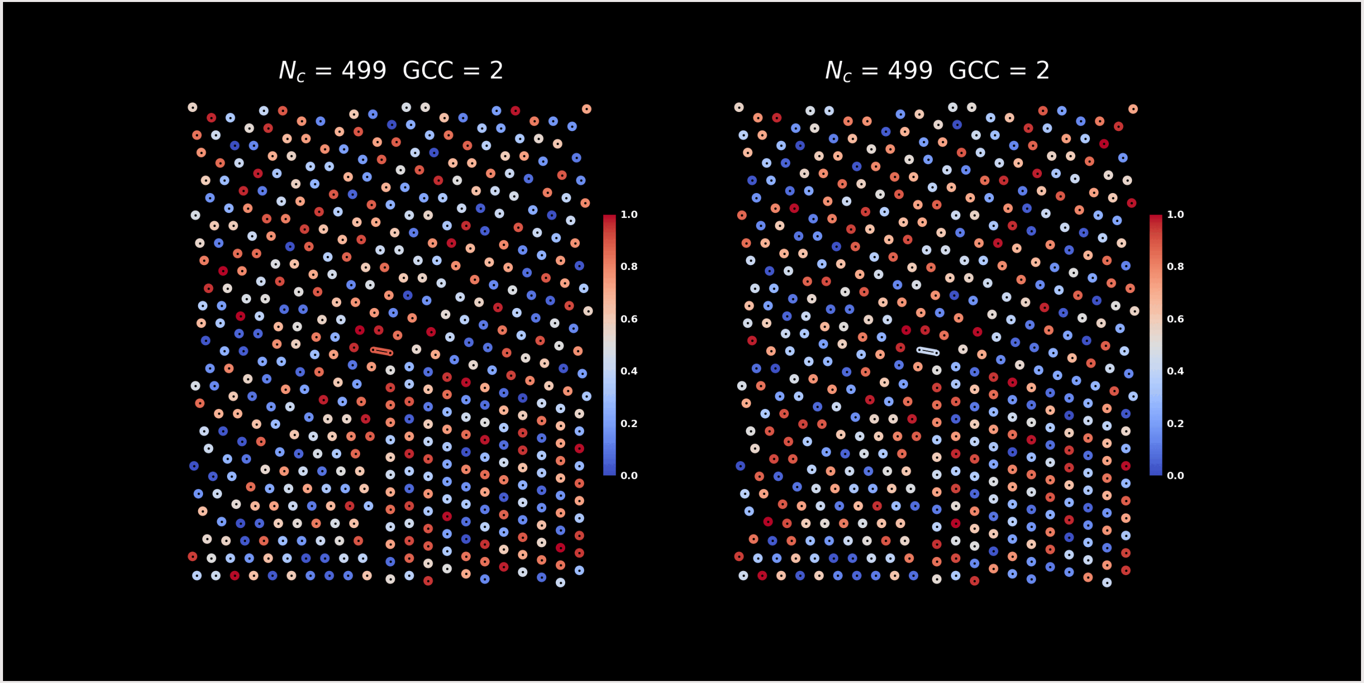


Homophily: $n_k(t = t_c) \propto k^{-5/2}$

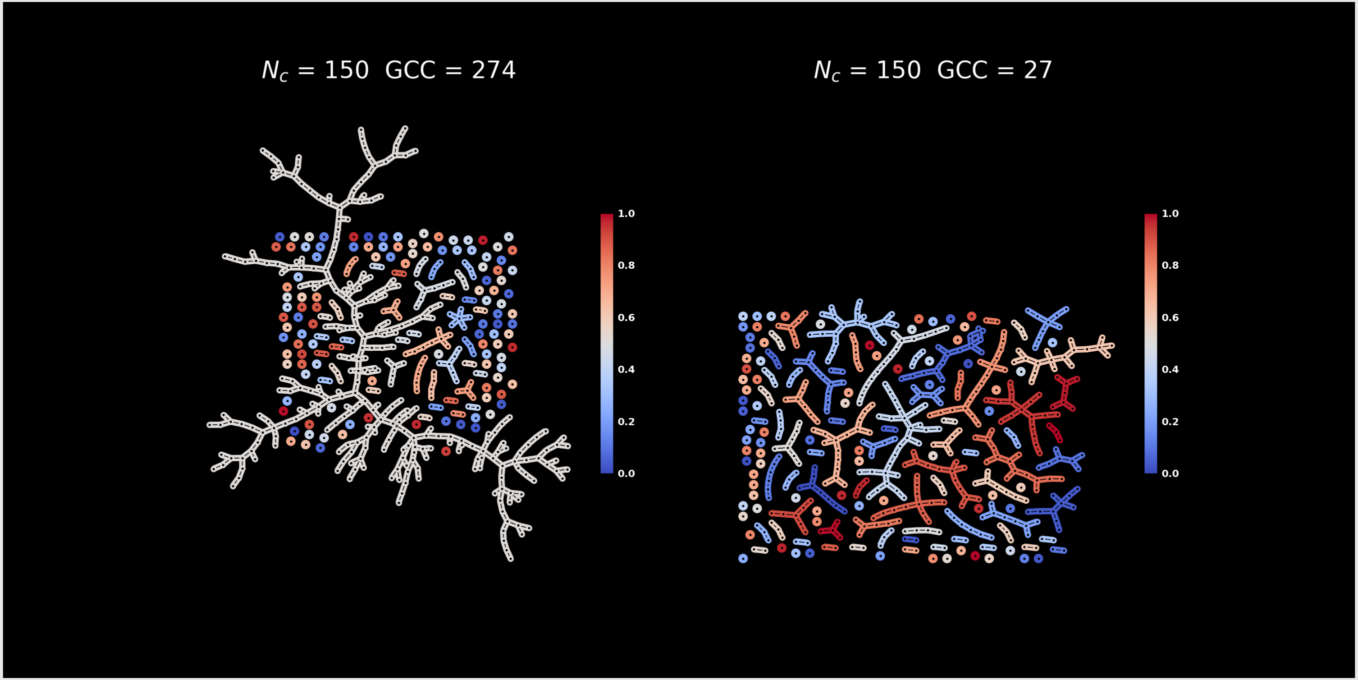




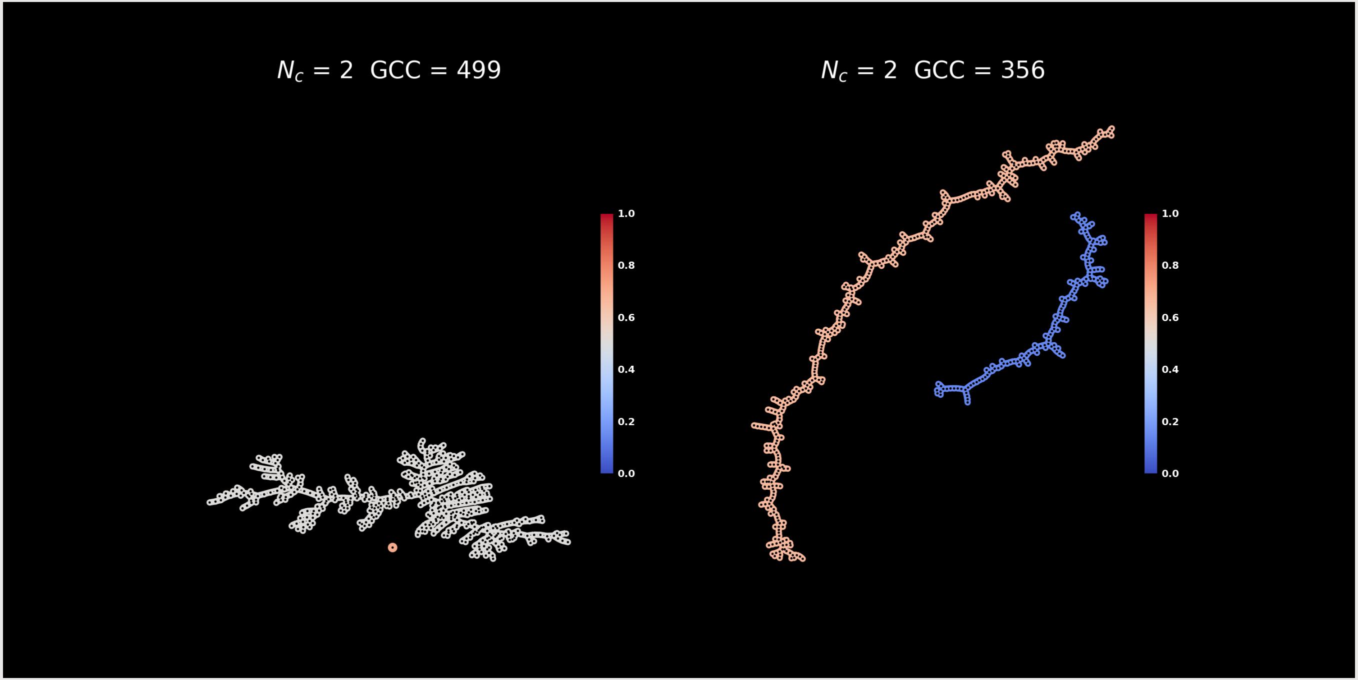
Homophily: Example Simulations



Homophily: Example Simulation

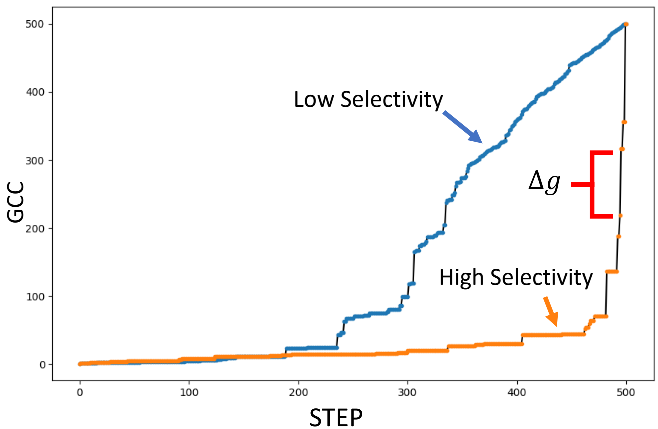


Homophily: Example Simulation



Homophily: Gap Size

Evolution of
Giant-Connected-Component/Gel



Average Maximum Gap Size