# Kinetics of Ring Formation

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E. Ben-Naim and P.L. Krapivsky, Phys. Rev. E **83**, 061102 (2011)

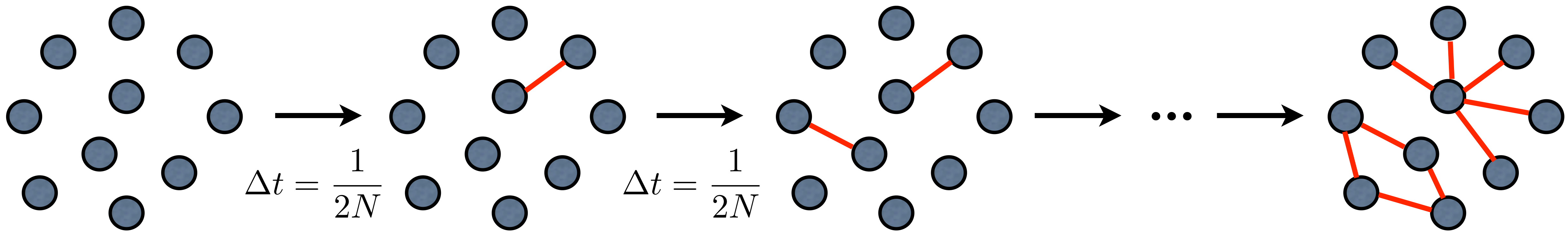
Talk, paper available from: http://cnls.lanl.gov/~ebn

ICIAM, Vancouver, BC, Canada, July 22, 2011

# Plan

1. Kinetics of random graphs
2. Kinetics of <u>regular</u> random graphs
   - Finite rings phase
   - Giant rings phase
3. Shuffling

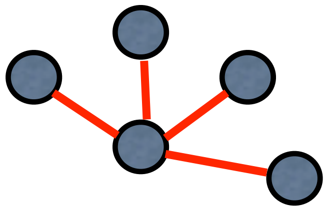
# Kinetics of Random Graphs



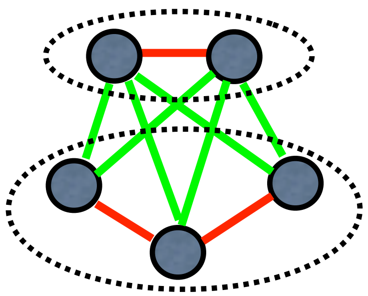

- Initial state: $N$ isolated nodes
- Dynamical linking
  1. Pick 2 nodes at random
  2. Connect the 2 nodes with a link
  3. Augment time $t \to t + \dfrac{1}{2N}$
- Each node experiences one linking event per unit time

Flory, Stockmeyer 43
Erdos, Renyi 60

# Aggregation Process



- Cluster = a connected graph component
- Aggregation rate = product of cluster sizes



$$K_{ij} = ij$$

- Master equation

$$\frac{dc_k}{dt} = \frac{1}{2}\sum_{i+j=k} ij c_i c_j - k c_k \qquad c_k(t=0) = \delta_{k,1}$$

- Cluster size density

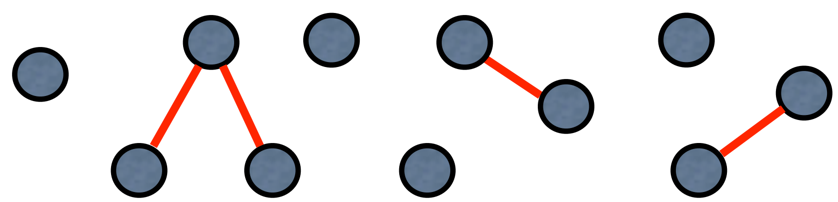
$$c_k(t) = \frac{1}{k \cdot k!}(kt)^{k-1} e^{-kt}$$

- Divergent second moment reveals percolation transition

$$M_2 = (1-t)^{-1} \qquad t_g = 1$$

Ziff 82
Leyvraz 03

# Cluster Phase ( t<1 )



- Microscopic clusters, tree structure
- Cluster size distribution contains <u>entire</u> mass

$$M(t) = \sum_{k=1}^{\infty} k\, c_k = 1$$

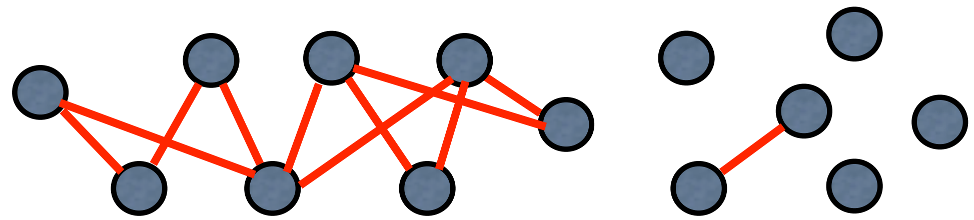
- Typical cluster size diverges near percolation point

$$k_* \sim (1-t)^{-2}$$

- Critical size distribution has power law tail

$$c_k(1) \simeq \frac{1}{\sqrt{2\pi}} k^{-5/2}$$

# Giant Component Phase ( t>1 )



- Macroscopic component exist, complex structure
- Cluster size distribution contains fraction of mass

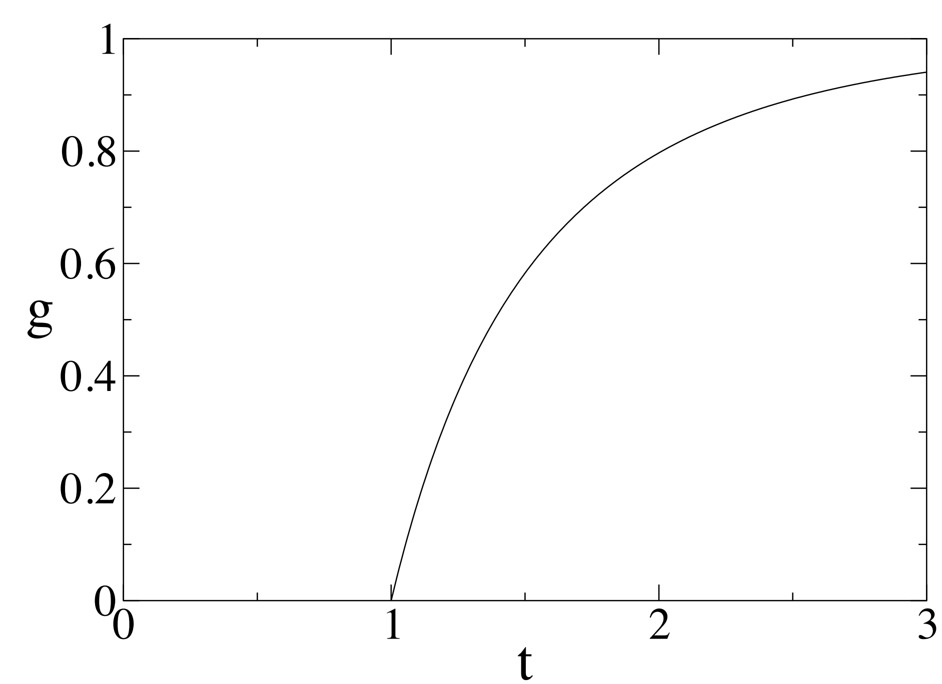
$$M(t) = \sum_{k=1}^{\infty} k c_k = 1 - g$$

- Giant component accounts for "missing" mass

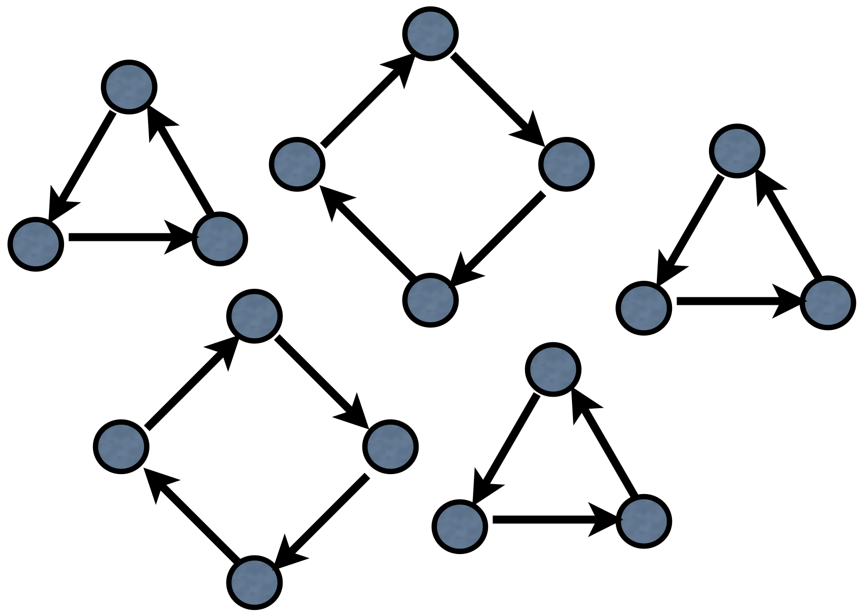
$$g = 1 - e^{-gt}$$

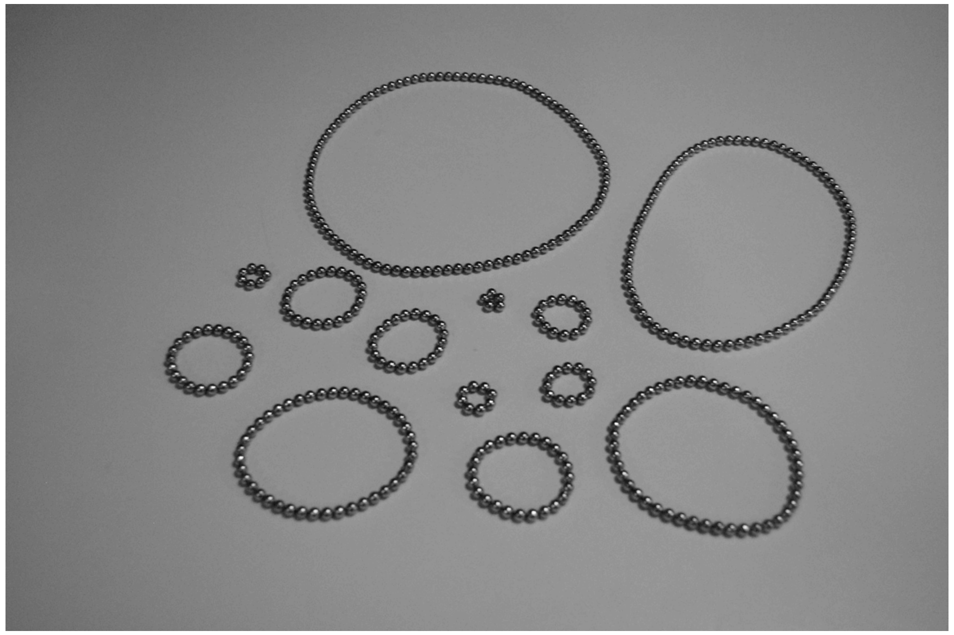
- Giant component takes over entire system

$$g \to 1$$



# Random Regular Graphs



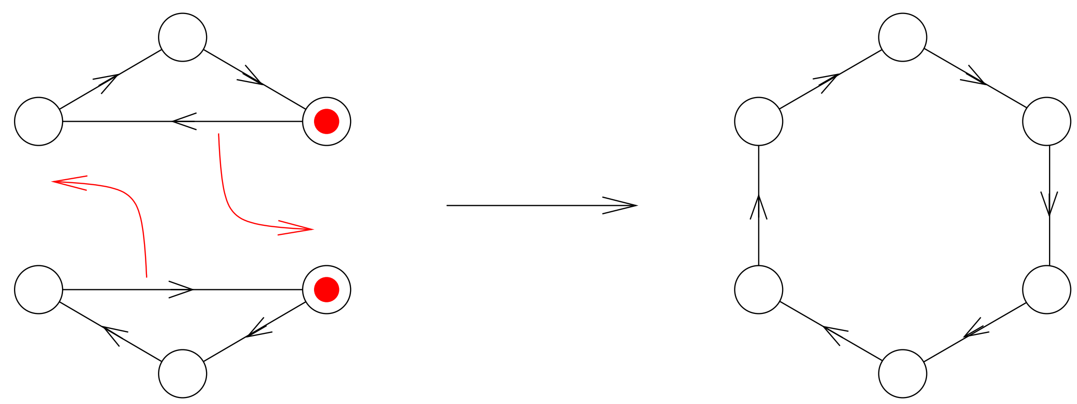


- All nodes have identical degree
- Motivation: rings of magnetic particles
- Consider simplest case: rings; all nodes have degree 2
- Consider directed links (without loss of generality)
- In a system of $N$ nodes, there are exactly $N$ links

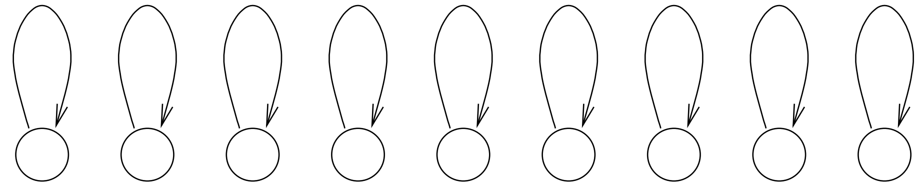
Number of links is conserved!

Kun 01

# Redirection Process

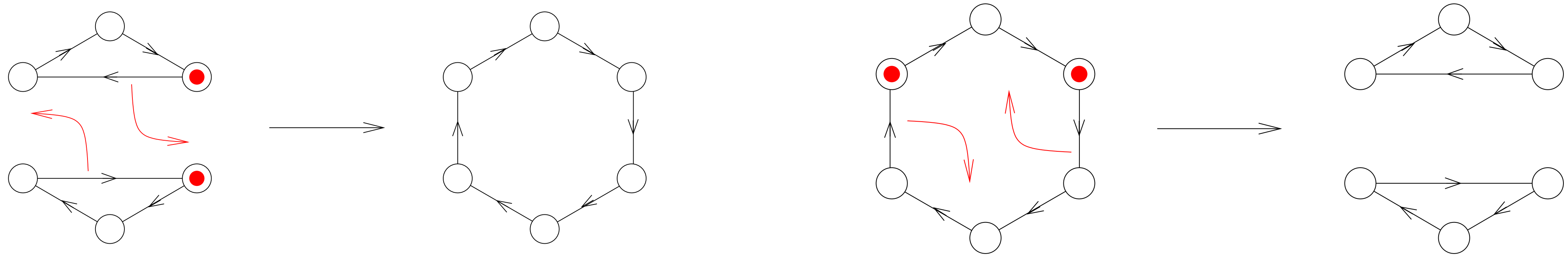


- Dynamical redirection
    1. Pick 2 nodes at random
    2. Connect 2 nodes by redirecting 2 associated links
    3. Augment time $t \to t + \dfrac{1}{2N}$
- A node experiences one redirection event per unit time
- Initial condition: isolated nodes, each has a self-link



Redirection process maintains ring topology

# Aggregation-Fragmentation Process



- **Aggregation**: inter-ring redirection

Identical to random graph process

$$i, j \xrightarrow{K_{ij}} i + j \qquad \text{with} \qquad K_{ij} = ij$$

- **Fragmentation**: intra-ring redirection

Fragmentation rate depends on system size!

$$i + j \xrightarrow{F_{ij}} i, j \qquad \text{with} \qquad F_{ij} = \frac{i+j}{N}$$

- Total fragmentation rate is quadratic

$$F_k = \sum_{i+j=k} F_{ij} = \frac{k(k-1)}{2N}$$

Reversible process

# Rate Equations

- Size distribution satisfies

$$\frac{dr_k}{dt} = \frac{1}{2}\sum_{i+j=k} ij\, r_i r_j - k\, r_k + \frac{1}{N}\left[\sum_{j>k} j\, r_j - \frac{k(k-1)}{2} r_k\right]$$

- Rate equation includes explicit dependence on $N$
- Perturbation theory

$$r_k = \underbrace{f_k}_{\text{finite rings}} + \frac{1}{N}\underbrace{g_k}_{\text{giant rings}}$$

- Fragmentation irrelevant for finite rings $F_k \sim \dfrac{k^2}{N}$

$$\frac{df_k}{dt} = \frac{1}{2}\sum_{i+j=k} ij\, f_i f_j - k\, f_k$$

Recover random graph equation

# Finite Rings Phase ( t<1 )

- All rings are finite in size

$$M(t) = \sum_{k=1}^{\infty} f_k = 1$$

- Size distribution

$$f_k(t) = \frac{1}{k \cdot k!}(kt)^{k-1} e^{-kt}$$

- Second moment diverges in finite time $M_2 = \sum_k k^2 f_k$

$$\frac{dM_2}{dt} = M_2^2 \quad \Longrightarrow \quad M_2 = (1-t)^{-1}$$

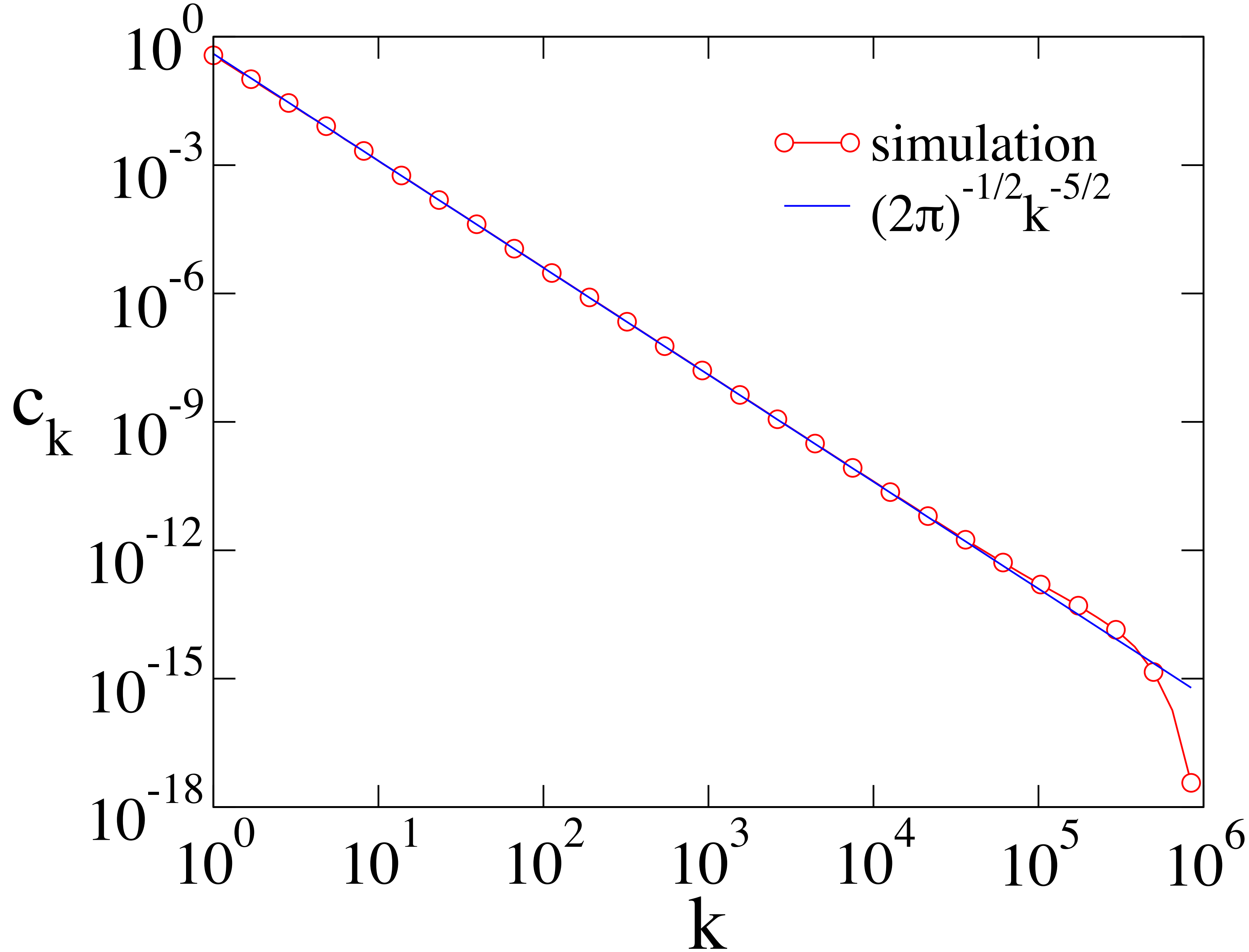
- Critical size distribution

$$f_k(1) \simeq \frac{1}{\sqrt{2\pi}} k^{-5/2}$$

Identical behavior to good-old random graph

# Critical Size Distribution

Simulation results




Excellent agreement between theory and simulation

# Giant Rings Phase ( t>1 )

- Finite rings contain only a fraction of g all mass

$$M(t) = \sum_{k=1}^{\infty} k f_k = 1 - g$$

- "Missing Mass" 1-g must be found in giant rings

$$g = 1 - e^{-gt}$$

- Expect giant, macroscopic rings

- Very fast aggregation and fragmentation processes

$$F_k \sim \frac{k^2}{N} \sim N \quad \text{when} \quad k \sim N$$

Fragmentation comparable to aggregation
No longer negligible

# Distribution of giant rings

- Quantify giant rings by normalized size $\ell = \dfrac{k}{N}$
- Average number of giant rings of normalized size $\ell$

$$g(t) = \int_0^{g(t)} d\ell\, \ell\, G(\ell, t)$$

- Rate equation

$$\cancel{\frac{1}{N}\frac{\partial G(\ell,t)}{\partial t}} = \overbrace{\frac{1}{2}\int_0^{\ell} ds\, s(\ell - s)G(s,t)G(\ell - s, t)}^{\text{agg gain= } \ell/2} - \overbrace{\ell(g-\ell)G(\ell,t)}^{\text{agg loss= } g-\ell}$$
$$+ \overbrace{\int_\ell^{g} ds\, s\, G(s,t)}^{\text{frag gain= } g-\ell} - \overbrace{\frac{1}{2}\ell^2 G(\ell,t)}^{\text{frag loss= } \ell/2}$$

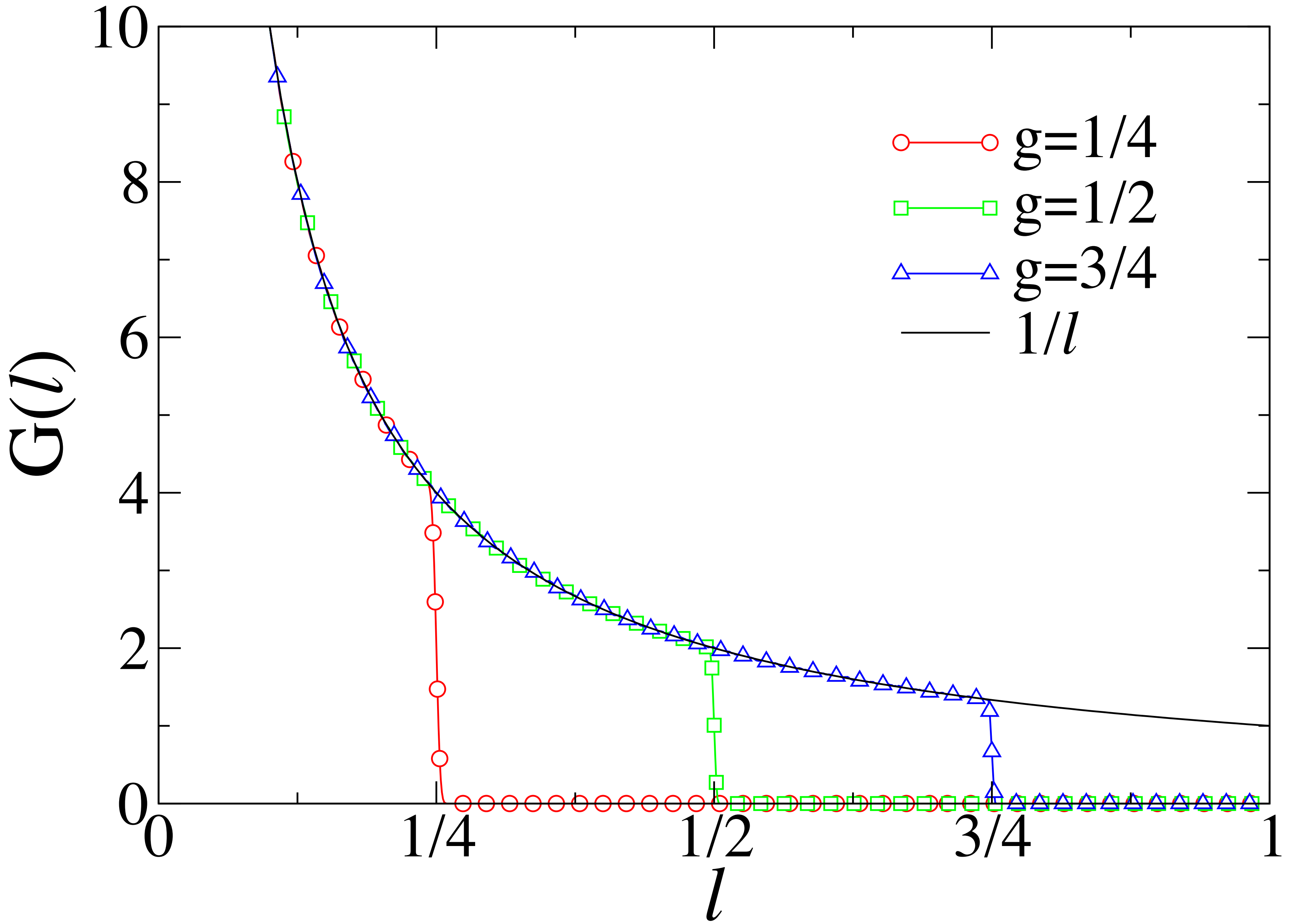
- Quasi steady-state

$$G(\ell, t) = \begin{cases} \ell^{-1} & \ell < g(t), \\ 0 & \ell > g(t). \end{cases}$$

Universal distribution, span grows with time

# Average Number of Giant Rings

Simulation results




$$G(\ell, t) = \begin{cases} \ell^{-1} & \ell < g(t), \\ 0 & \ell > g(t). \end{cases}$$

# Comments

- Rate equation for average number of giant rings

$$\cancel{\frac{1}{N}\frac{\partial G(\ell,t)}{\partial t}} = \frac{1}{2}\int_0^\ell ds\, s(\ell-s)G(s,t)G(\ell-s,t) - \ell(g-\ell)G(\ell,t)$$
$$+ \int_\ell^g ds\, s\, G(s,t) - \frac{1}{2}\ell^2 G(\ell,t)$$

- Practically closed equation; coupling to finite rings only through total mass $g(t)$

- Steady flux $N\, dg/dt$ from finite rings to giant rings

- Number of giant rings is not proportional to $N$!

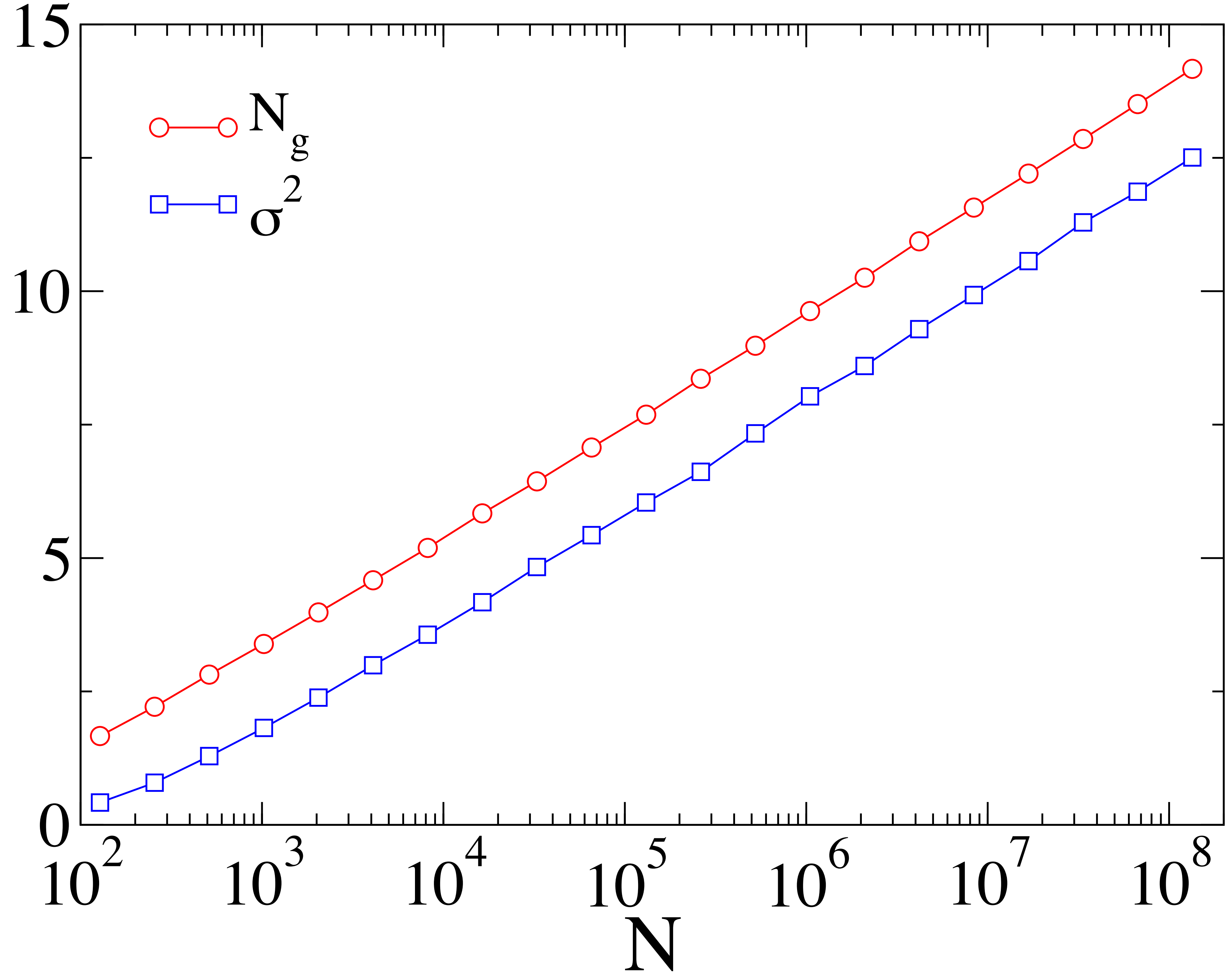
$$N_g \simeq \ln N$$

Number of microscopic rings proportional to $N$

Number of macroscopic rings logarithmic in $N$

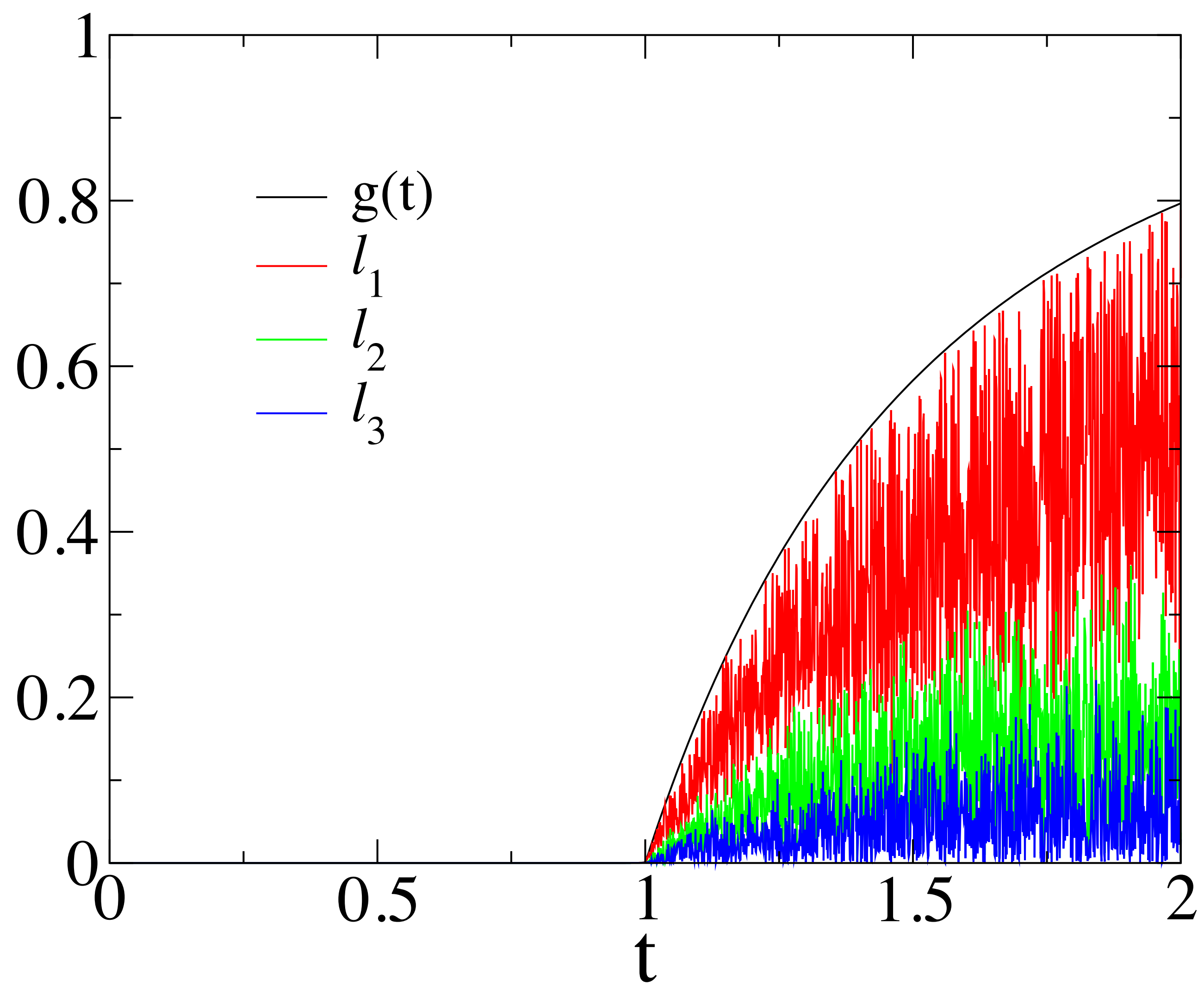
# Total Number of Giant Rings

Simulation results




Law of large numbers

# Multiple Coexisting Giant Rings




Total mass of giant rings is a deterministic quantity
Mass of an individual giant ring is a stochastic quantity!
Giant rings break and recombine very rapidly

# Limiting Distribution

- Steady-state size distribution satisfies

$$0 = \frac{1}{2}\sum_{i+j=k} K_{ij}\, c_i\, c_j - c_k \sum_{j\geq 1} K_{kj}\, c_j + \sum_{j\geq 1} F_{kj}\, c_{j+k} - \frac{1}{2}\, c_k \sum_{i+j=k} F_{ij}$$

- Detailed balance condition

$$K_{ij}\, c_i\, c_j = F_{ij}\, c_{i+j}$$

Lowe 95

- Substitute aggregation and fragmentation rates

$$K_{ij} = ij \qquad F_{ij} = \frac{i+j}{N}$$

- Steady-state solution

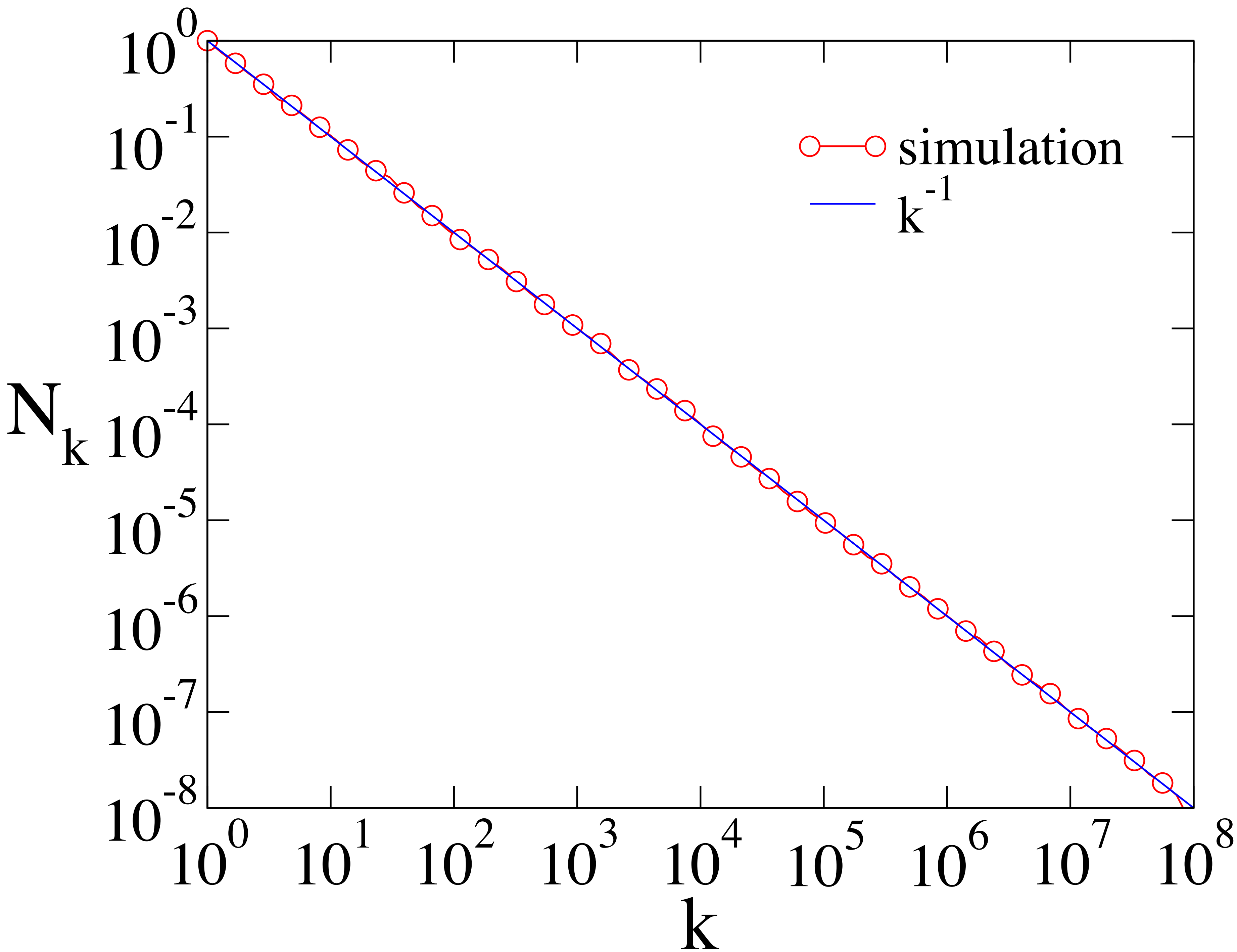
$$(ic_i)(jc_j) = \frac{1}{N}(i+j)c_{i+j} \quad \Longrightarrow \quad Nc_k = \frac{1}{k}$$

- Consistent with

$$G(\ell, t=\infty) = \frac{1}{\ell} \quad \text{for all} \quad \ell < 1$$

# Final Distribution

Simulation results



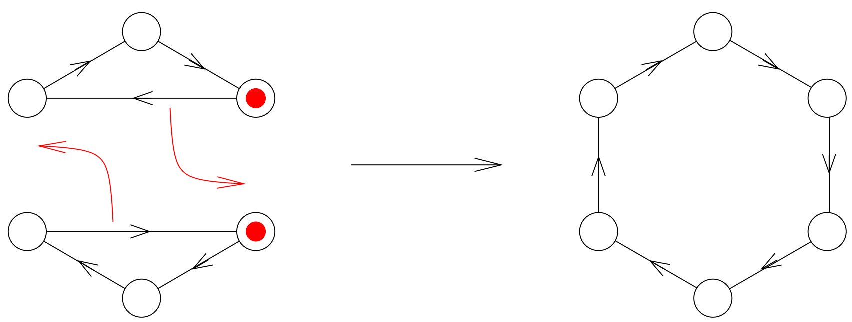
# Shuffling Algorithm

$$1\,\underline{2}\,3\,4\,\underline{5}\,6 \to 1\,5\,\underline{3}\,\underline{4}\,2\,6 \to 1\,5\,4\,3\,2\,6 \to \cdots$$

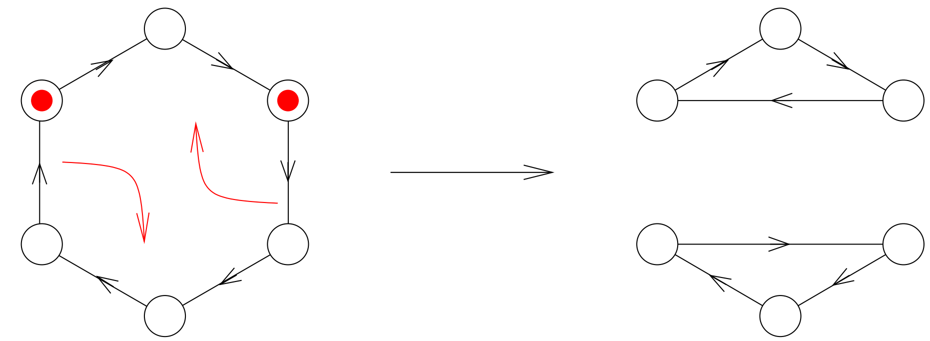
- Initial configuration: $N$ ordered integers
- Pairwise shuffling:
    1. Pick 2 numbers at random
    2. Exchange positions
    3. Augment time $t \to t + \dfrac{1}{2N}$
- Each integer is shuffled once per unit time
- Efficient algorithm, computational cost is $\mathcal{O}(N)$

Isomorphic to dynamical regular random graph!

# Cycles and Permutations



$$(1\underline{2}3)(4\underline{5}6) \to (156423)$$



$$(1\underline{5}64\underline{2}3) \to (123)(456)$$

- Cycle structure of a permutation

$$134265 \quad \Longrightarrow \quad (1)(234)(56)$$

- **Aggregation**: <u>inter</u>-cycle shuffling

$$i, j \xrightarrow{K_{ij}} i + j \qquad \text{with} \qquad K_{ij} = ij$$

- **Fragmentation**: <u>intra</u>-cycle shuffling

$$i + j \xrightarrow{F_{ij}} i, j \qquad \text{with} \qquad F_{ij} = \frac{i + j}{N}$$

Identical aggregation and fragmentation rates

# Implications to Shuffling

- $N$ pairwise shuffles generate a giant cycle
- Size of emergent giant cycle is $N^{2/3}$
- $N \ln N$ pairwise shuffles generate random order

Golomb 61
Flatto 85
Diaconis 86

# Summary

- Kinetic formulation of a regular randm graph
- Equivalent to: (i) aggregation-fragmentation (ii) shuffling
- Finite rings phase: fragmentation is irrelevant
- Giant rings phase
  - Multiple giant rings coexist
  - Number of giant rings fluctuates
  - Total mass is a deterministic quantity
  - Very rapid evolution