Counting connected components in random temporal networks

Verena Schamboeck

Spring meeting WSC 2017, Antwerpen, 15.5.2017

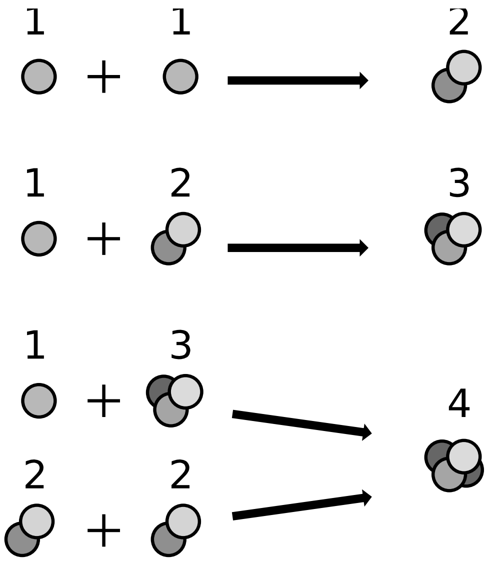
Universiteit van Amsterdam

Smoluchowski coagulation problem

- Coagulation problem: **$C_r + C_s \rightarrow C_{r+s}$**
- Master equation:

$$\boxed{\frac{dc_r}{dt} = \frac{1}{2}\sum_{s=1}^{r-1} a_{s,r-s} c_s c_{r-s} - \sum_{s=1}^{\infty} a_{r,s} c_r c_s}$$

- Applications in
  - Colloidal physics
  - Crowd dynamics
  - Social sciences
  - Astrophysics
  - Polymer chemistry



M. von Smoluchowski
Drei Vorträge über Diffusion, Brown'sche Molekularbewegung und Koagulation von Kolloidteichen
Physik. Z., 17 (1916), pp. 557–571

Smoluchowski coagulation problem

- Master equation:

$$\boxed{\frac{dc_r}{dt} = \frac{1}{2}\sum_{s=1}^{r-1} a_{s,r-s}c_s c_{r-s} - \sum_{s=1}^{\infty} a_{r,s}c_r c_s}$$

Reaction constant: $a_{r,s}=rs$

$$\Downarrow$$

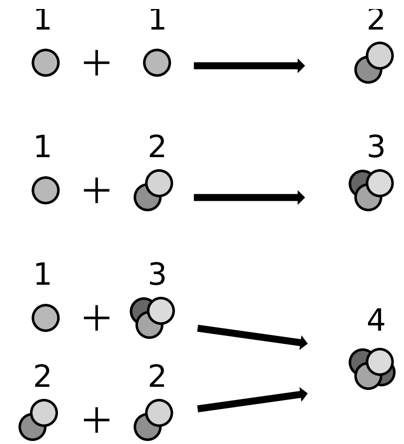
Transformation using generating function: $C(z,t) = \sum_{r=1}^{\infty} c_r(t)e^{-rz}$

Substitution: $u(z,t) = -\frac{\partial C(z,t)}{\partial z}$

$$\Downarrow$$

→ inviscid Burgers equation: $\boxed{\frac{\partial u}{\partial t} = (M_1(t) - u)\frac{\partial u}{\partial z}}$

($M_1(t)$ – 1. moment of c_r)

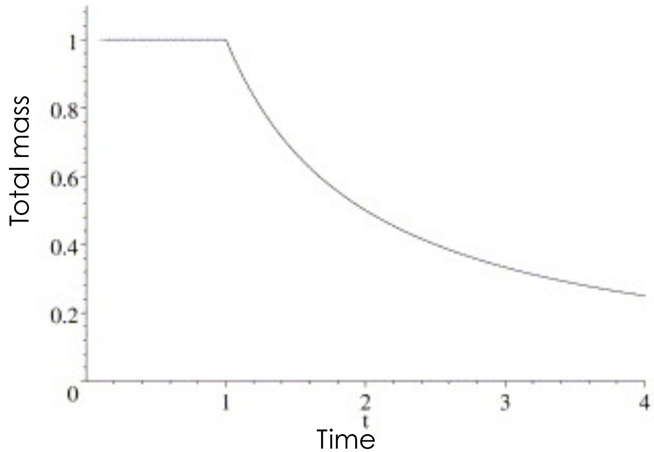


J. Wattis
An introduction to mathematical models of coagulation-fragmentation processes: A discrete deterministic mean-field approach
Physica D, 222 (2006), pp. 1–20

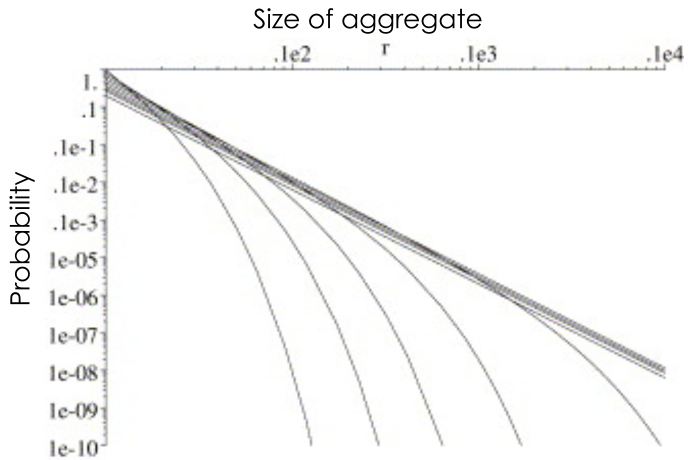
Smoluchowski coagulation problem

- Already highly non-trivial behavior:

$\boxed{C_r + C_s \rightarrow C_{r+s}}$



Mass conservation violated after critical time t_C



Change in the asymptotic decay of the size distribution at t_C: exponential → algebraic

J. Wattis
An introduction to mathematical models of coagulation-fragmentation processes: A discrete deterministic mean-field approach
Physica D, 222 (2006), pp. 1–20

What about the topology?

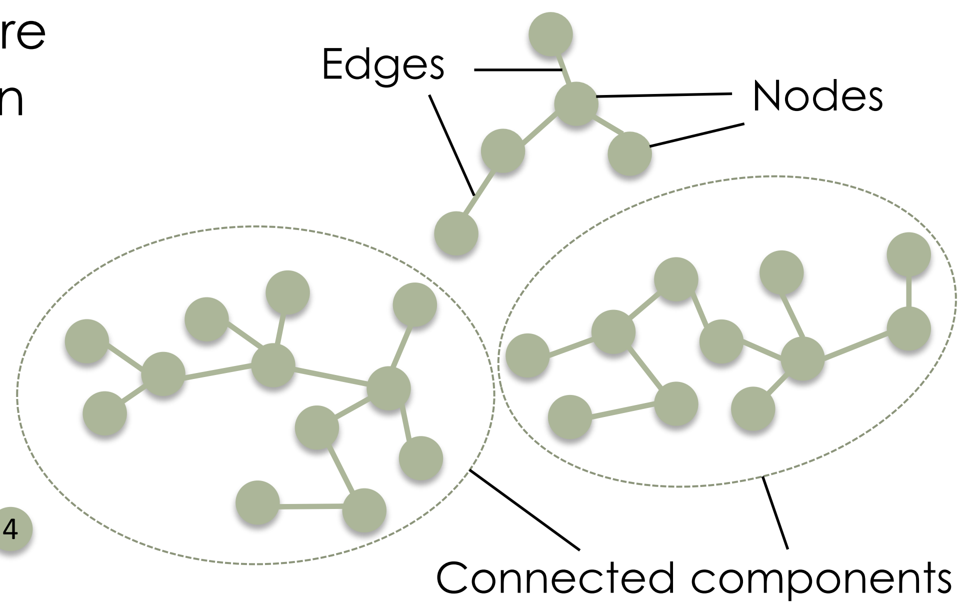
- Smoluchowski coagulation problem:
  - Aggregates treated as a ‘blob’ without inner structure

- **Challenge:**
  Find a model for growing discrete structures, e.g. highly crosslinked networks evolving in time

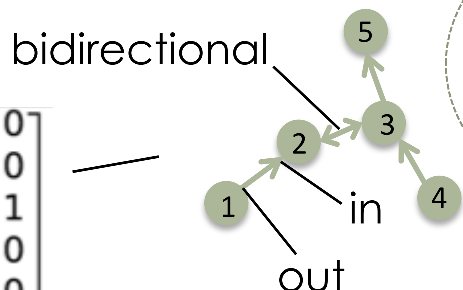
- From local to global:
  - Local topology determined by arbitrary process that grows the network
  - Modeling the network as a random graph to extract global properties

Network theory

- Graph:
  - Set of nodes connected by edges
    - Nodes: Degree (number of edges), various attributes
    - Edges: Directional (in & out), bidirectional
  - Topology of a structure
  - No spatial information

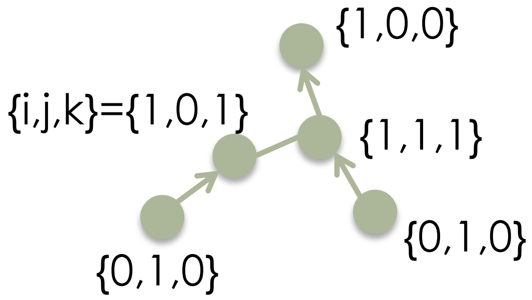


$$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$



Network theory

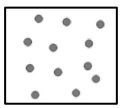
- Random graph with arbitrary degree distribution:
  - Degree distribution u(i,j,k):
    - Probability of a node for having
      - i in-edges
      - j out-edges
      - k bidirectional edges



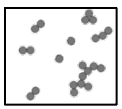
  - Random graph:
    - Probability distribution over all possible graphs
    - Maximizes the entropy for a given degree distribution

Network theory

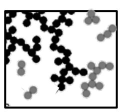
- Degree distribution:
  - Imagine global process governing the degree distribution



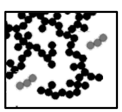
- t_0: No component with s>1



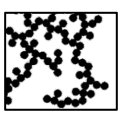
- $t_0<t<t_c$: Growth of component



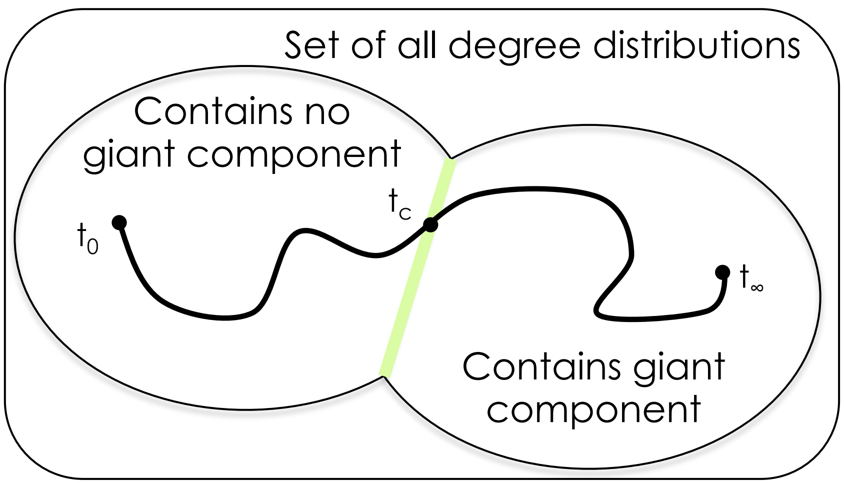
- t_c: Phase transition – Emergence of the ‘giant component’
  Giant component: scales linear with size of system



- $t>t_c$: Weight fraction of giant component increases



- t_∞: No aggregate with s>1, only giant component



The degree distribution

- **State of a node** defined by
  - Properties that alter the probability of a node to connect: v, p
  - # in-edges, i
  - # out-edges, j
  - # bidirectional edges, k

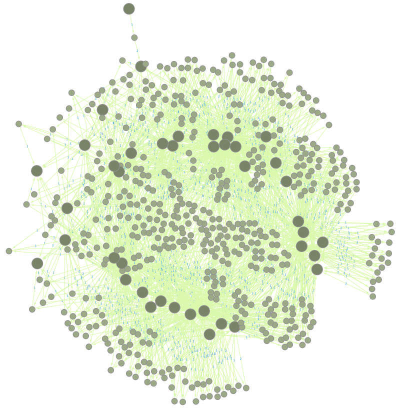
  Information on history of edge formation

- Concentration of states of nodes determined by polymerization reactions:

Master equation:

$$\begin{aligned}G_{v,p,i,j,k} = k_i[I]\big((v+1)g_{v+1,p-1,i,j,k} - vg_{v,p,i,j,k}\big) \\ + k_p c_{rd}\big((v+1)g_{v+1,p-1,i-1,j,k} - vg_{v,p,i,j,k}\big) \\ + k_p c'_{db}\big((p+1)g_{v,p+1,i,j-1,k} - pg_{v,p,i,j,k}\big) \\ + 2k_{td}c_{rd}\big((p+1)g_{v,p+1,i,j,k} - pg_{v,p,i,j,k}\big) \\ + 2k_{tc}c_{rd}\big((p+1)g_{v,p+1,i,j,k-1} - pg_{v,p,i,j,k}\big).\end{aligned}$$

Reaction network:



From local to global

- **Goal: Extract size distribution of connected components from local information**

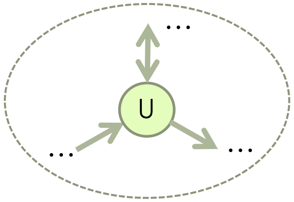
- Random graph with arbitrary degree distribution u(i,j,k) determined by the reaction mechanism

- **Transformation** to the domain of **generating function**:
  - Original degree distribution: $u(i,j,k) \;\rightarrow\; U(x,y,z) = \sum_{i,j,k}^{\infty} u(i,j,k)x^i y^j z^k$
  - Probability distribution for a node reached by an edge to be connected to further nodes:
    - Reached by in-edge $$u_{\text{in}}(i,j,k) = \frac{1}{\mu_{100}} \underbrace{(i+1)}_{\text{more in-edges} \rightarrow \text{higher probability to be reached}} u(\underbrace{i+1}_{\text{Minimum connectivity: 1}},j,k) \;\rightarrow\; U_{in} = \frac{1}{\mu_{100}}\frac{\partial}{\partial x}U(x,y,z)$$

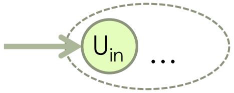
      Normalization
    - Reached by out-edge $u_{\text{out}}(i,j,k) \;\rightarrow\; U_{out}(x,y,z)$
    - Reached by bidirectional edge $u_{\text{bi}}(i,j,k) \;\rightarrow\; U_{bi}(x,y,z)$

From local to global

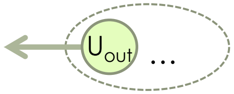
- Connected components:
  - Size distribution $w(s) \rightarrow W(x)$



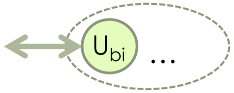
  - Biased size distribution:
    Size distribution of connected component reached by
    - In-edge $w_{in}(s) \rightarrow W_{in}(x)$



    - Out-edge $w_{out}(s) \rightarrow W_{out}(x)$



    - Bidirectional edge $w_{bi}(s) \rightarrow W_{bi}(x)$



From local to global

- Size distribution of connected component reached by in-edge w_{in}
  - Size distribution of i out-components:

    Convolution: $\underbrace{w_{out}(s)*w_{out}(s)*\ldots*w_{out}(s)}_{\text{i-times}} \rightarrow W_{out}(x)^i$

  - Size distribution of i out-, j in- and k bidirectional components:

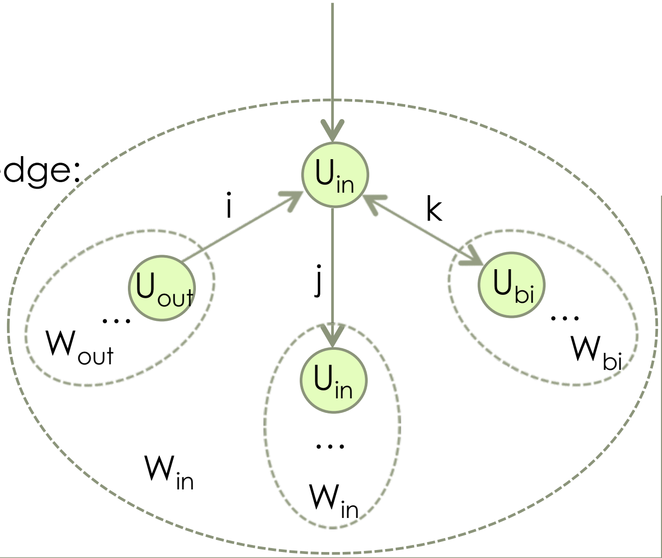
    $\underbrace{w_{out}*\ldots*w_{out}}_{\text{i-times}}*\underbrace{w_{in}*\ldots*w_{in}}_{\text{j-times}}*\underbrace{w_{bi}*\ldots*w_{bi}}_{\text{k-times}} \rightarrow W_{out}^i\, W_{in}^j\, W_{bi}^k$

  - GF of size distribution for component reached by in-edge:

    $W_{in}=x \sum_{i,j,k}^{\infty} u_{in}(i,j,k)\ W_{out}^i\, W_{in}^j\, W_{bi}^k$

    $\boxed{W_{in}=x\ U_{in}(W_{out},W_{in},W_{bi})}$

    $\boxed{\begin{array}{l} W_{out}=x\ U_{out}(W_{out},W_{in},W_{bi}) \\ W_{bi}=x\ U_{bi}(W_{out},W_{in},W_{bi}) \end{array}}$



From local to global

- 3 coupled functional equations:

$$W_{in} = x\, U_{in}(W_{out}, W_{in}, W_{bi})$$

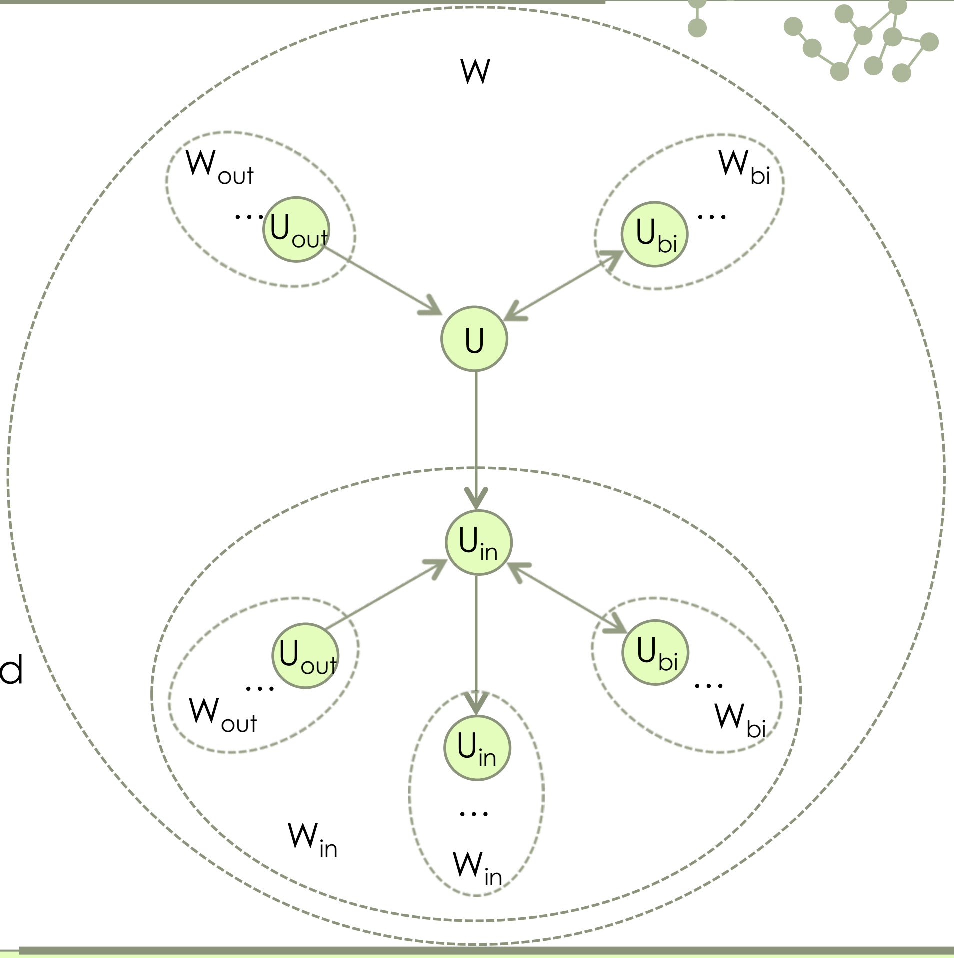
$$W_{out} = x\, U_{out}(W_{out}, W_{in}, W_{bi})$$

$$W_{bi} = x\, U_{bi}(W_{out}, W_{in}, W_{bi})$$

→ solve numerically

- GF of size distribution of connected component

$$W = x\, U(W_{out}, W_{in}, W_{bi})$$



From local to global

- Back transform:
  - Derivatives

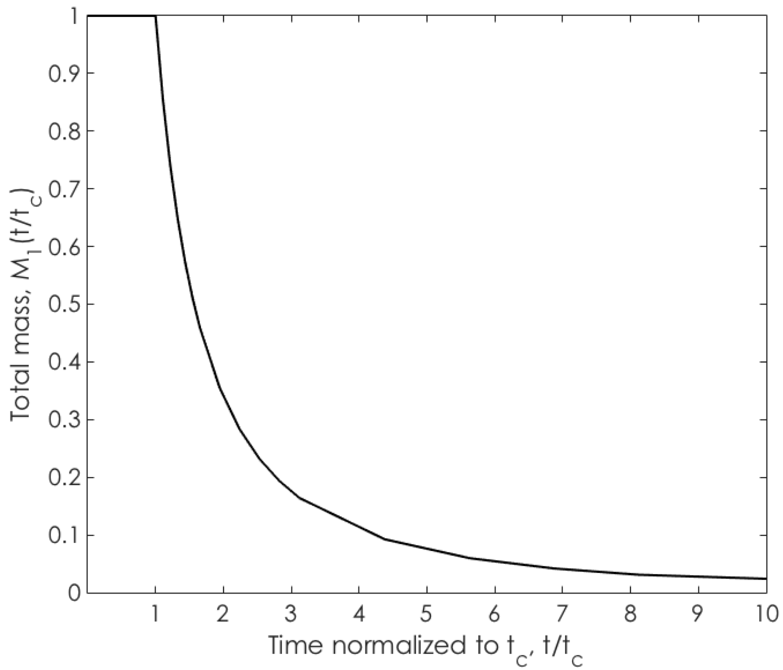
$$w(s) = \left[\left(\frac{\partial}{\partial x} \right)^n W(x) \right] \Bigg|_{x=0}$$

    - Problem: Numerically unstable (only feasible until s~30)
  - Inverse Fourier transform:

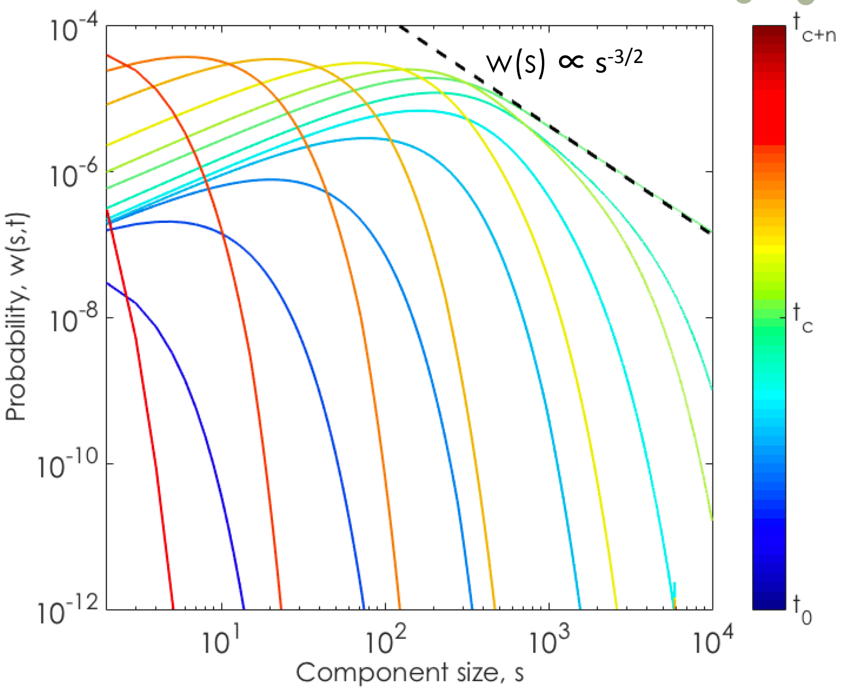
$$w(s) = \mathcal{F}^{-1}\big(W(x)\big), \;\; \text{with} \;\; x = e^{-\frac{2\pi i}{N}}$$

    - Advantage: stable, faster (s log(s))
    - Disadvantage: evaluation for all s necessary

Component size distribution



Violation of the conservation of mass after t_c



$t<t_c$: $w(s) \propto e^{-s}$
$t=t_c$: $w(s) \propto s^{-3/2}$
$t>t_c$: $w(s) \propto e^{-s}$

Analytic criterion for existence of the giant component

- Weight average component size defined as

$$\langle s \rangle = W'(x)|_{x=0}$$

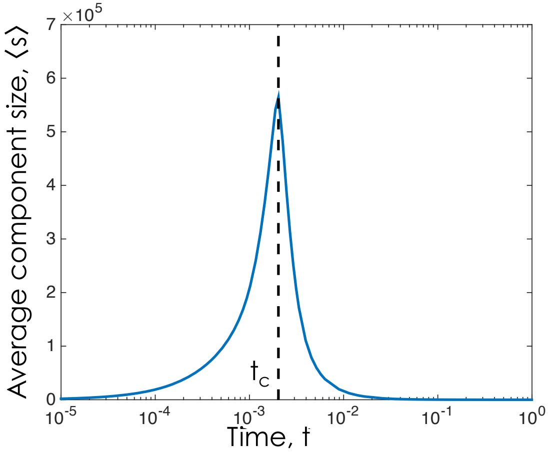
with

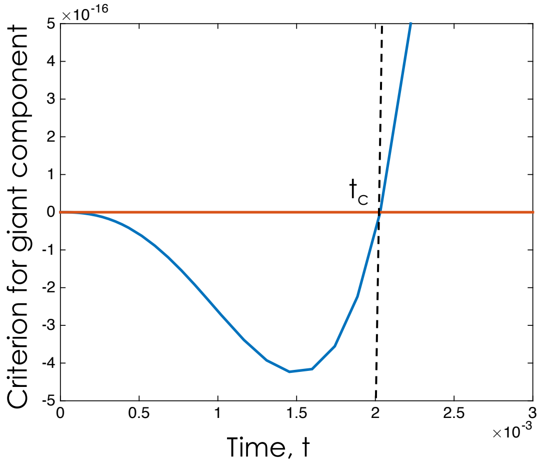
$$W(x) = xU(W_{\mathrm{out}}(x), W_{\mathrm{in}}(x), W_{\mathrm{bi}}(x))$$

⟨s⟩ → infinity

$$\boxed{\begin{aligned}&\mu_{110}^2(2\mu_{001}-\mu_{002})+\mu_{011}^2(\mu-\mu_{200})+\mu_{101}^2(\mu-\mu_{020})\\&+\mu(\mu_{200}+\mu_{020}-2\mu_{110})(2\mu_{001}-\mu_{002})\\&+2\mu_{101}\mu_{011}(\mu_{110}-\mu)+\mu_{200}\mu_{020}(\mu_{001}-\mu_{002})=0\end{aligned}}$$

with the partial moments μ_{lmn} of u(i,j,k)





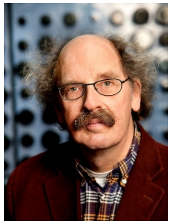
Summary

- Growing particles have discrete structure
- Modeling the structure as a network
  - Random graph with arbitrary trivariate degree distribution
  - Degree distribution determined by Master equation, reaction network, …
  - Extract size distribution of connected components
  - Ananlytic criterion for emergence of giant component

Acknowledgements

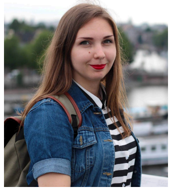
- Computational polymer chemistry group at the University of Amsterdam

Piet Iedema



Ivan Kryven

Yuliia Orlova



UNIVERSITEIT VAN AMSTERDAM

- Océ Technologies B.V.

océ

A CANON COMPANY

Technology Foundation STW

STW

connecting innovators