Reaction-Diffusion Processes On regular and random graphs

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Thanks to

Federico Bianco Université Pierre et Marie Curie, Paris

Raffaella Burioni Università di Parma

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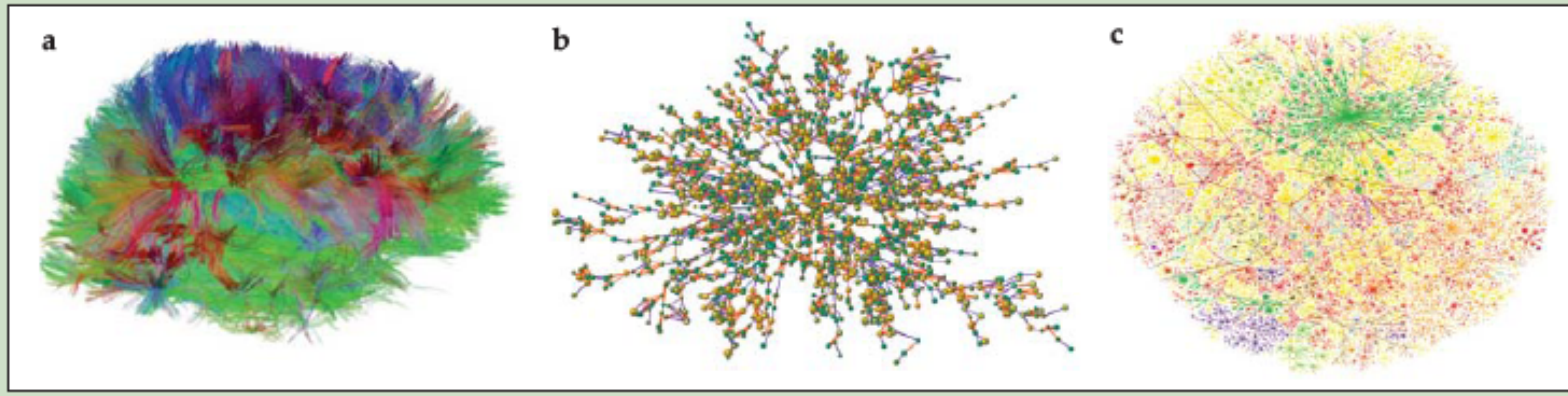
Davide Vergni IAC-CNR, Roma

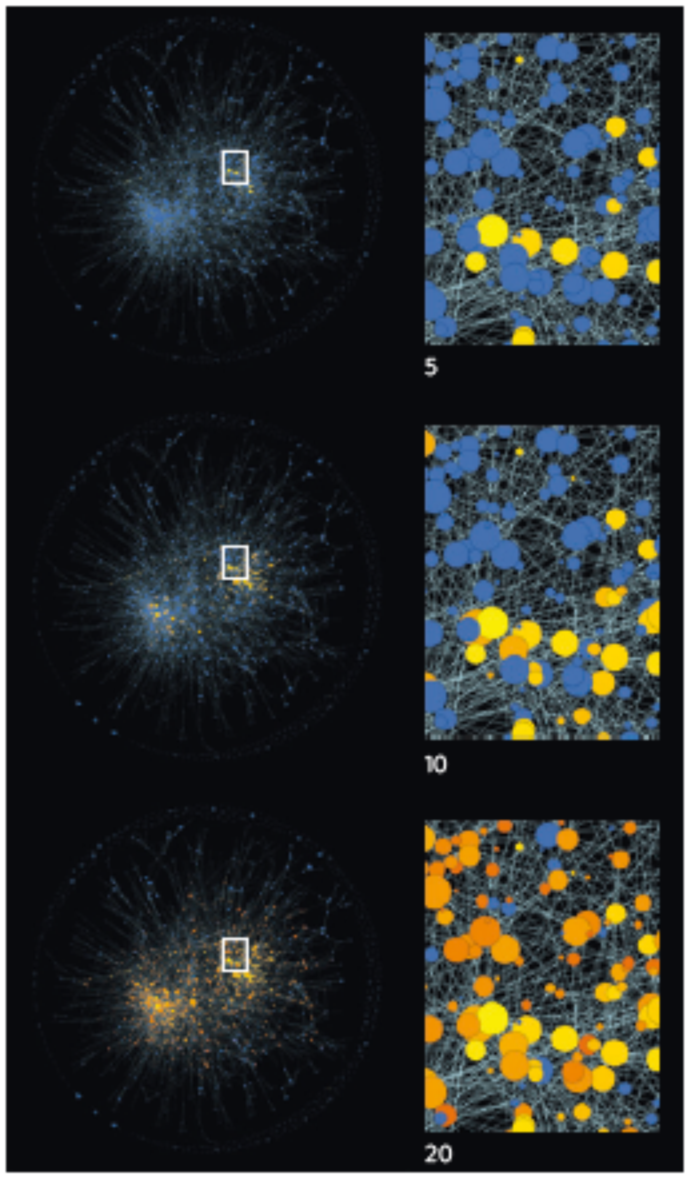
Burioni et al.
Reaction spreading on graphs
Physical Review E 86, 055101(R) (2012)

Bianco et al.
Reaction spreading on percolating clusters
Physical Review E 87, 062811 (2013)

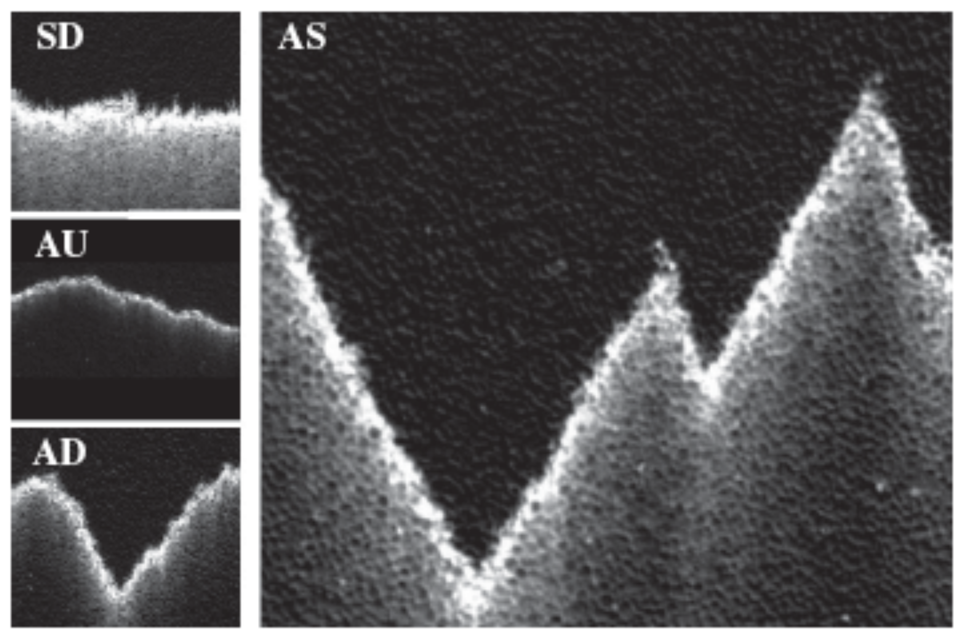
Motivations



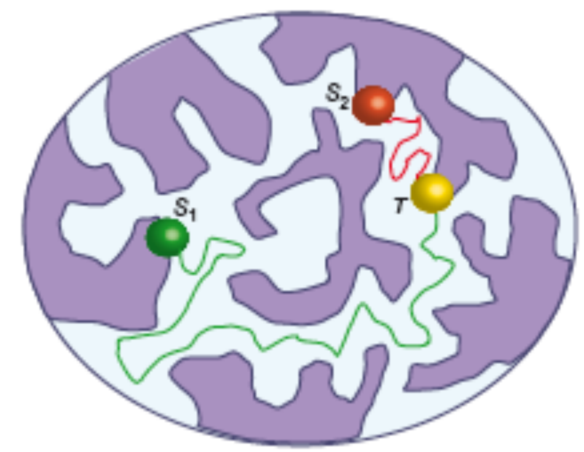
Brain, social network, internet



Progression of an epidemic process
Vespignani Nature Phys 2011



Chemical fronts in porous media
Atis, Saha, Auradou, Salin, Talon PRL 2013



Chemical kinetic
Benichou et al Nature Chem 2010

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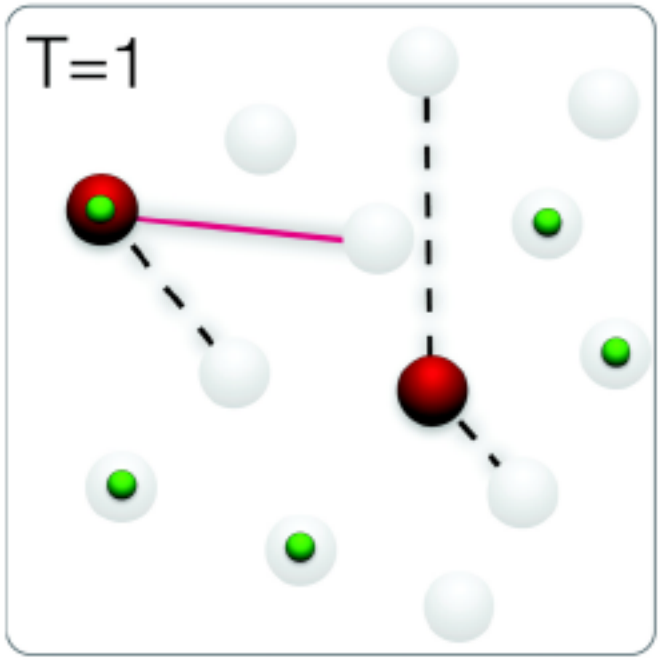
General framework



microscopic point of view, molecules:
diffusion (jumps)
advection (In presence of stirring)
reaction for ex. $(A + B \to 2A)$

At macro-hydrodynamic level ADR equation

$$\partial_t \theta = \hat{L}\theta + \frac{1}{\tau} f(\theta)$$

$\hat{L}$ General advection-diffusion operator

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ADR eq.

$$\hat{L} = -\mathbf{u} \cdot \nabla + D\Delta$$

Advection by a fluid flow and Diffusion

$f(\theta)/\tau$ Non-linear local reaction

τ reaction time-rate

$$\hat{L} = \frac{1}{r^{d-1}} \frac{\partial}{\partial r} \left(k(r) r^{d-1} \frac{\partial}{\partial r} \right)$$

Effective diffusion

(Richardson, Procaccia O'Shaughnessy)

Probabilistic interpretation

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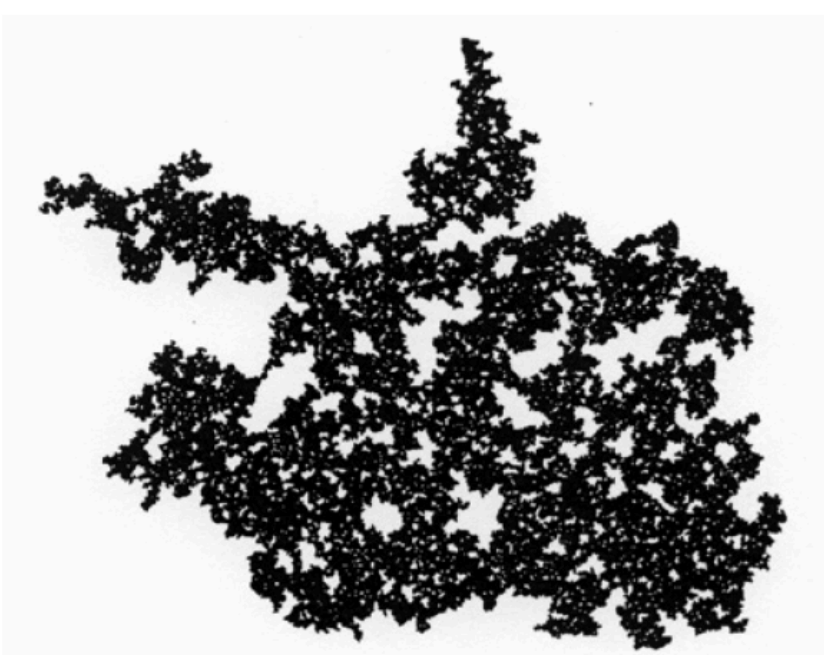
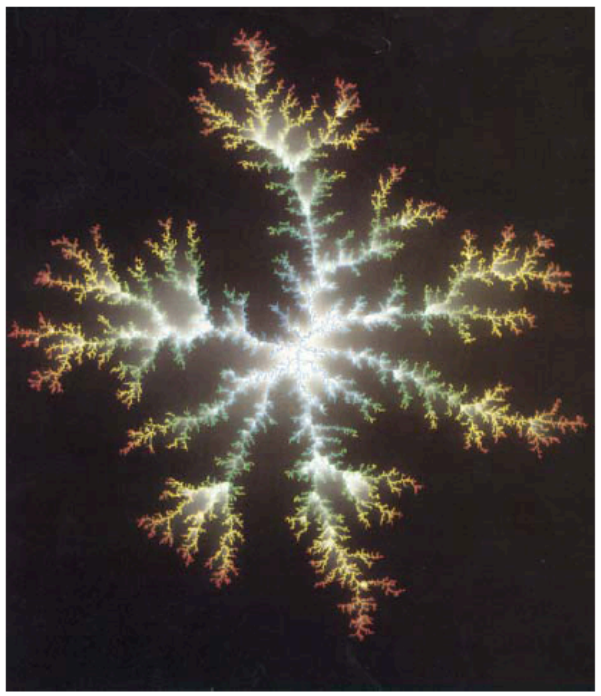
$$\hat{L} = -\mathbf{u} \cdot \nabla + D\Delta \quad \longleftrightarrow \quad \mathrm{d}\mathbf{x}/\mathrm{d}t = \mathbf{u} + \sqrt{2D}\boldsymbol{\eta}$$

advection-reaction=Fokker-Planck

$$\theta(\mathbf{x},t) = \left\langle \theta(\mathbf{x},0) \exp\left(\frac{1}{\tau} \int_0^t \frac{f(\theta(\mathbf{x}(s;t),s))}{\theta(\mathbf{x}(s;t),s)} ds \right) \right\rangle$$

transport + reaction
Freidlin formula





Complex geometry

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Time Discretisation

Limit case $\delta - \text{impulse}$ $f(\theta) = \sum_{n=-\infty}^{\infty} g(\theta)\delta(t - n\Delta t)$

Lagrangian and reaction maps

$$\mathbf{x}(t+\Delta t) = \mathbf{F}_{\Delta t}(\mathbf{x}(t)), \qquad \theta(t+\Delta t) = G_{\Delta t}(\theta(t))$$

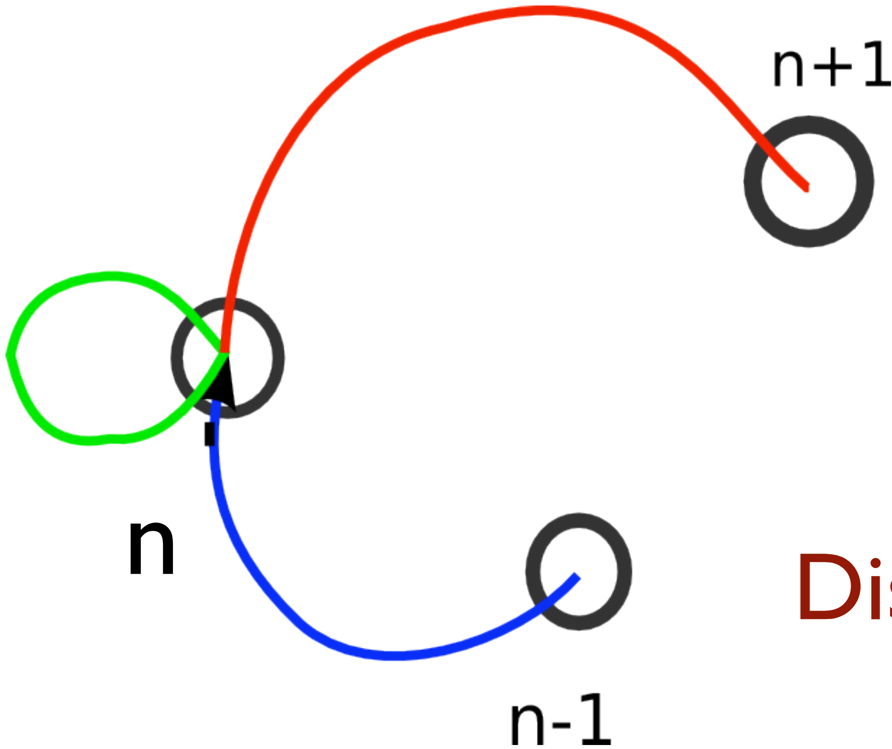
discrete-time ARD

$$\theta(\mathbf{x}, t+\Delta t) = \langle G_{\Delta t}(\theta(\mathbf{F}^{-1}_{\Delta t}(\mathbf{x} - \sqrt{2D\Delta t}\mathbf{w}), t))\rangle_{\mathbf{w}}$$

Even for non-gaussian diffusion

$$\theta(\mathbf{x}, t+\Delta t) = \int d\mathbf{w}\, G_{\Delta t}(\theta(\mathbf{x} - \mathbf{w}, t))\, p_{\Delta t}(\mathbf{w})$$

Space Discretisation



$$\theta(x, t+\Delta t) = \int_{-\infty}^{+\infty} \mathrm{d}w P_{\alpha,\Delta t}(w)\theta(x-w, t+0^+)$$

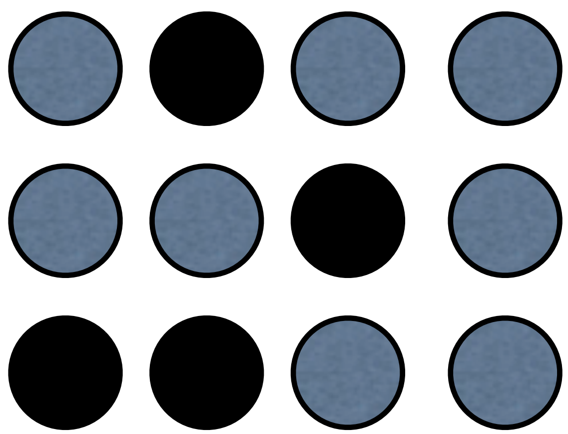
$$= \int_{-\infty}^{+\infty} \mathrm{d}w P_{\alpha,\Delta t}(w) G(\theta(x-w,t))$$

Discrete process

$$\theta_n(t+\Delta t) = \sum_j P^{(\Delta t)}_{j\to n}\theta_j(t)$$

$$P^{(\Delta t)}_{n\to n} = 1 - 2W\Delta t \qquad P^{(\Delta t)}_{n\to n-1} = P^{(\Delta t)}_{n\to n+1} = W\Delta t$$

Discretisation: master eq.



$$A_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0 & \text{if } (i,j) \notin E \end{cases}$$

$$\frac{d\theta_i}{dt} = \mathsf{W} \sum_j \Delta_{ij} \theta_j + \frac{1}{\tau} f(\theta_i)$$

$$\theta_n(t + \Delta t) = \sum_j P_{j \to n}^{(\Delta t)} \theta_j(t)$$

$$\begin{aligned} P_{i \to j}^{(\Delta t)} &= W A^{ij} \Delta t \text{ if } i \neq j \\ P_{i \to i}^{(\Delta t)} &= 1 - k_i W \Delta t \text{ if } i \neq j \end{aligned}$$

$$\theta_n(t + \Delta t) = G_{\Delta t} \left(\sum_j P_{j \to n}^{(\Delta t)} \theta_j(t) \right)$$

$$\boxed{G(\theta) = \theta + \frac{\Delta t}{\tau} \theta (1 - \theta)}$$

FKPP

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Topology and geometry of the graphs

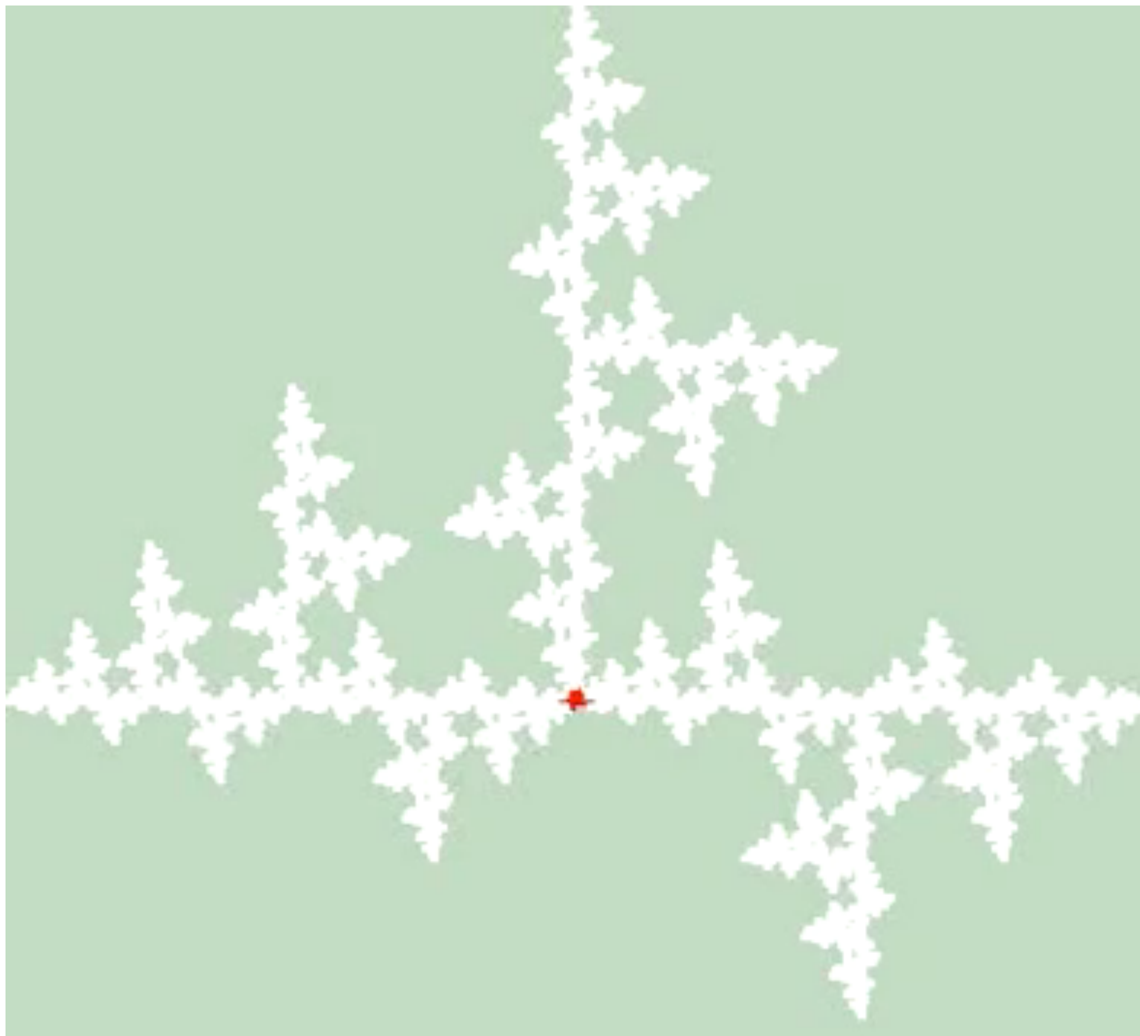
Connectivity dimension d_l $\#(l) \sim l^{d_l}$

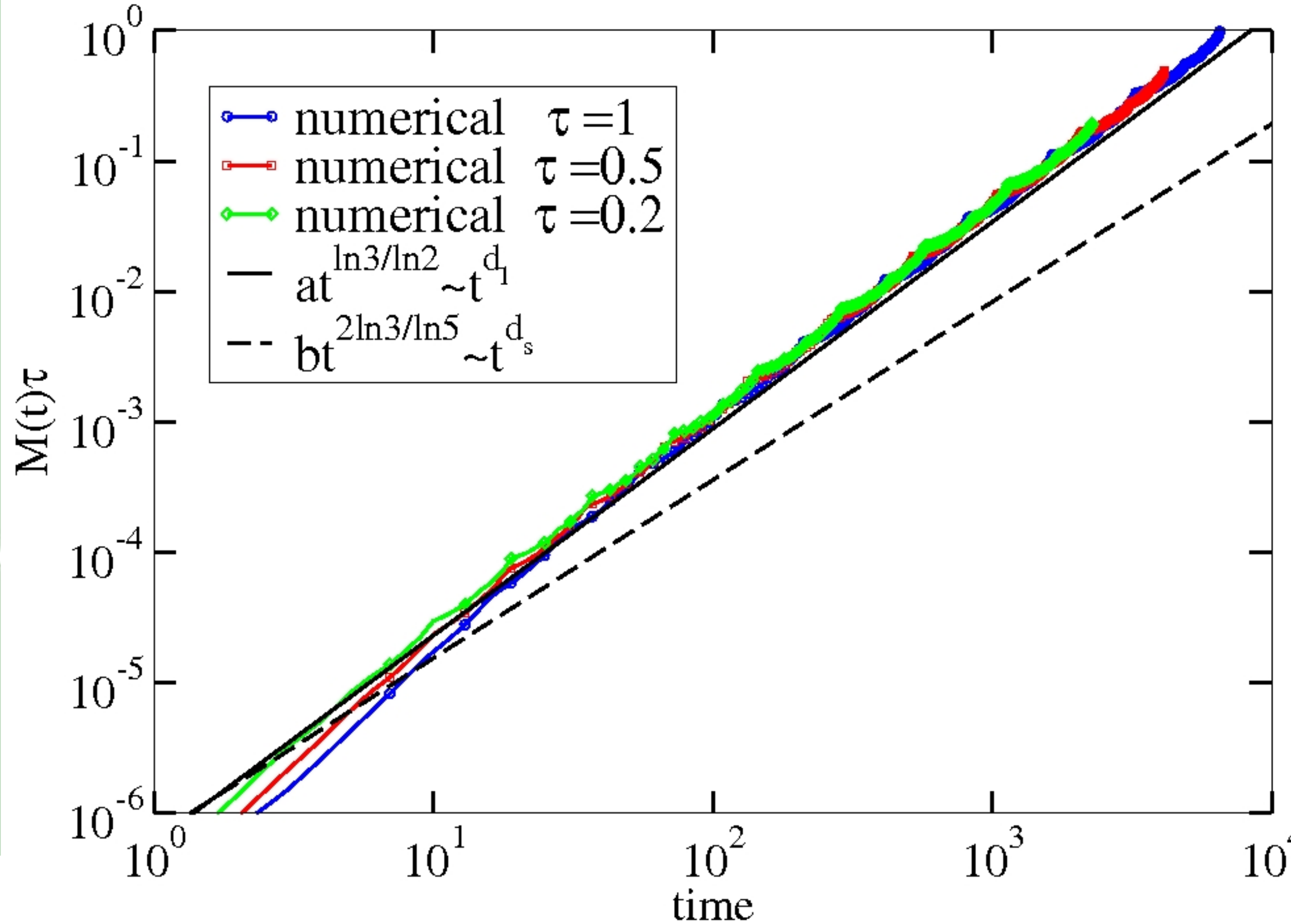
Spectral dimension $$d_s = \lim_{t \to \infty} -2 \frac{\ln P_{ii}(t)}{\ln t}$$

fractal dimension d_f $\#(r) \sim r^{d_f}$

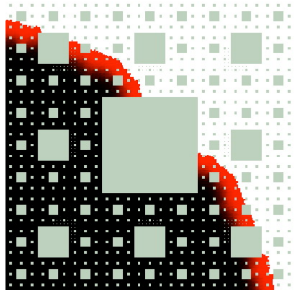
total quantity of the reaction product $$M(t) = \frac{1}{N} \sum_{i \in V} \theta_i(t)$$

Results: fractals

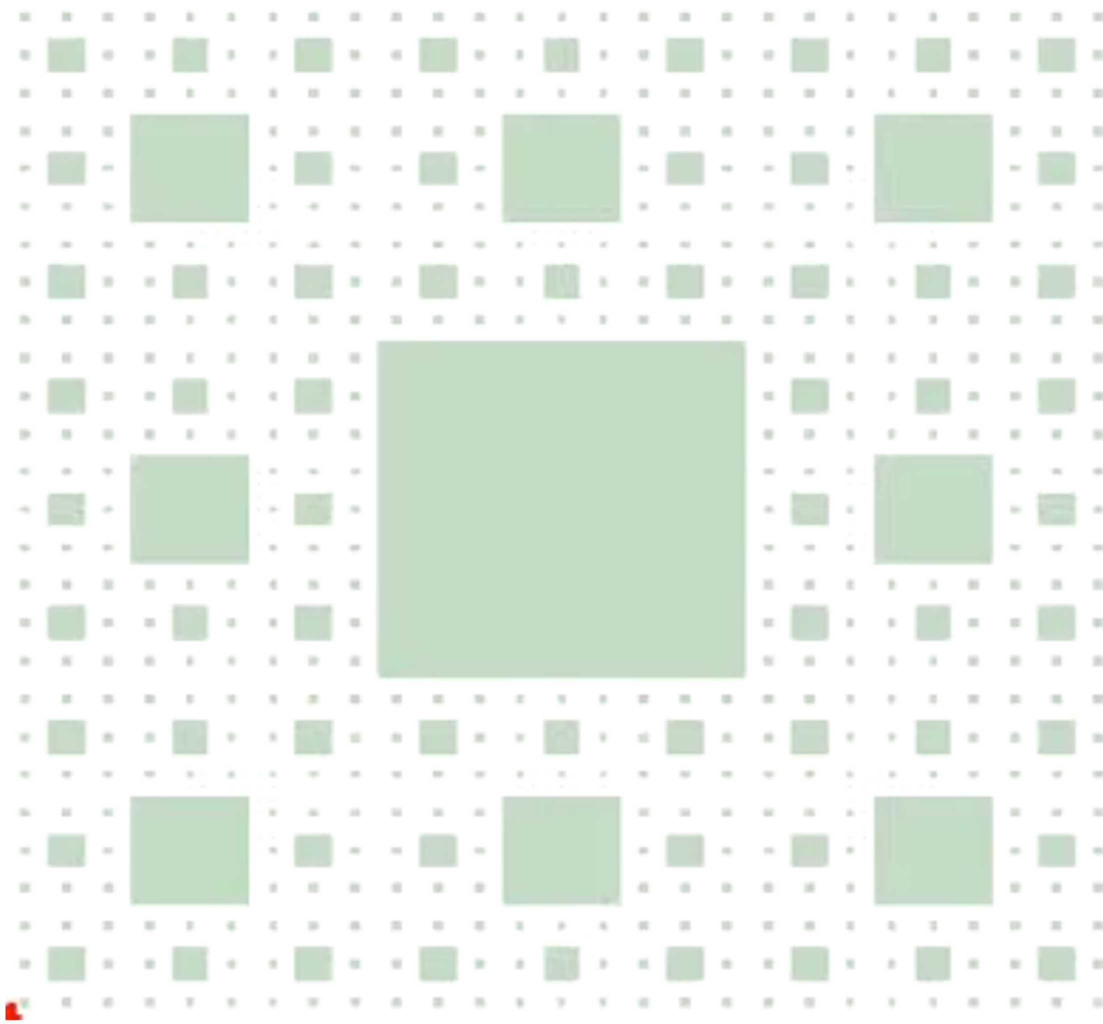


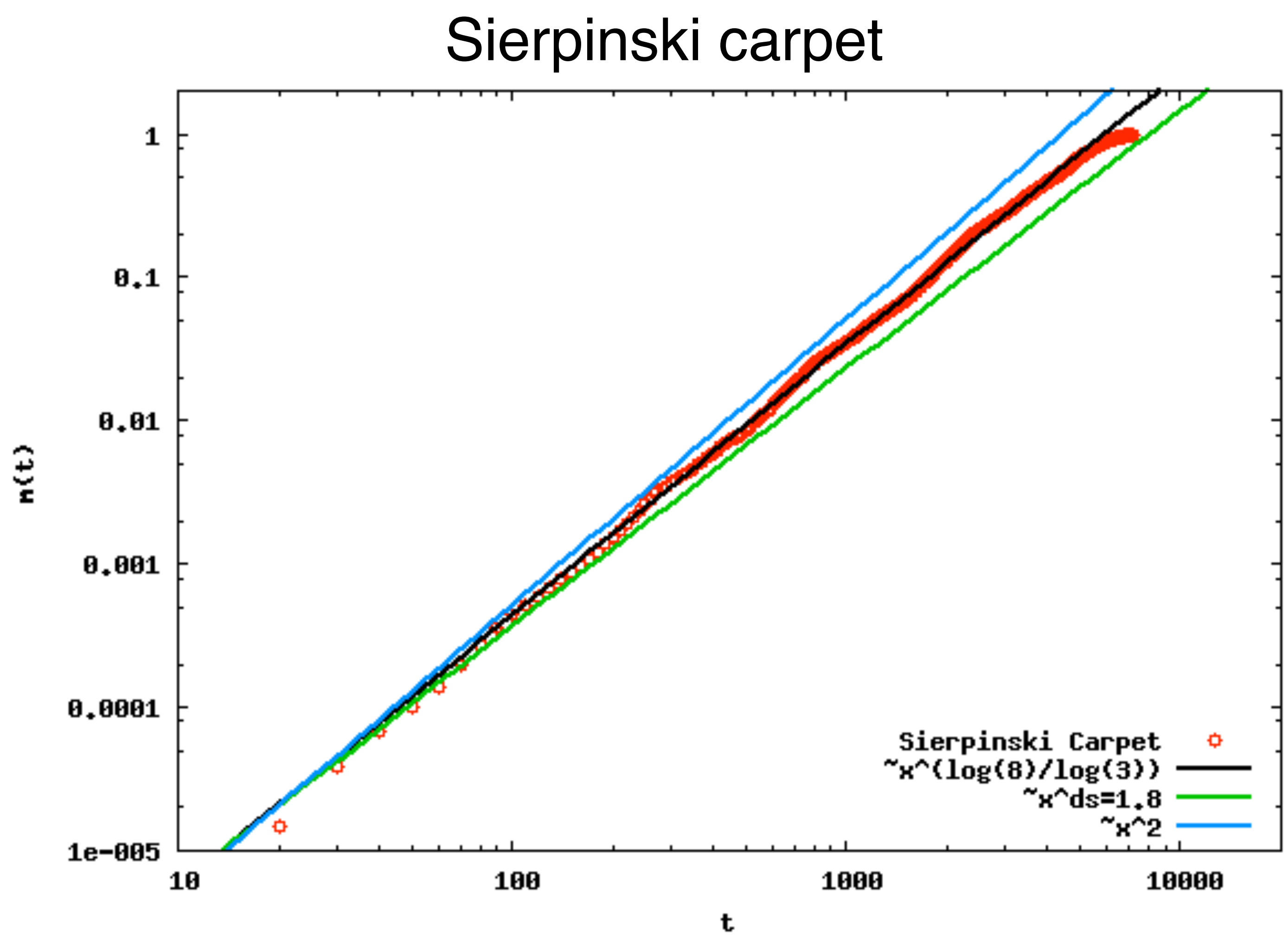


Spreading on a T-fractal where the front is in red. The percentage of quantity of product $M(t)\tau$ vs t. Numerical results for Equation with $w = 0.5$ are compared to prediction t^{d_l}. For this graph $d_l = \ln 3/\ln 2 \simeq 1.585$, $d_s = 2\ln 3/\ln 5 \simeq 1.365$.



Results: fractals





Main result

$$M(t) \sim t^{d_l}$$

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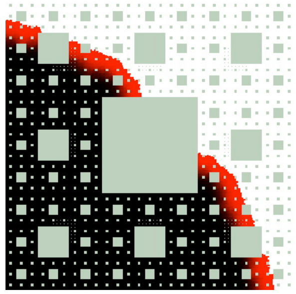

Results: fractals

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reaction spreading <=> short-time n random walkers

Probability first passage at time t

$$F_{0j}(t)$$

Probability no passage in j at time t

$$C_{0j}(t) = 1 - \sum_{\tau=0}^{t} F_{0j}(\tau).$$

Independent n walkers ⟶

$$P(no\, j)_n = C_{0j}(t)^n$$

$$P(j)_n = 1 - C_{0j}(t)^n$$

Number of sites visited by n walkers

$$S_n(t) = \sum_{j=0}^{N} 1 - C_{0j}(t)^n$$

$$n \to \infty \to S_n(t) \sim t^{d_l}$$

Validity regime

$$P_m = <k>^{-t} \qquad nP_m \gg 1 \qquad t < \bar{t} \sim \log n$$

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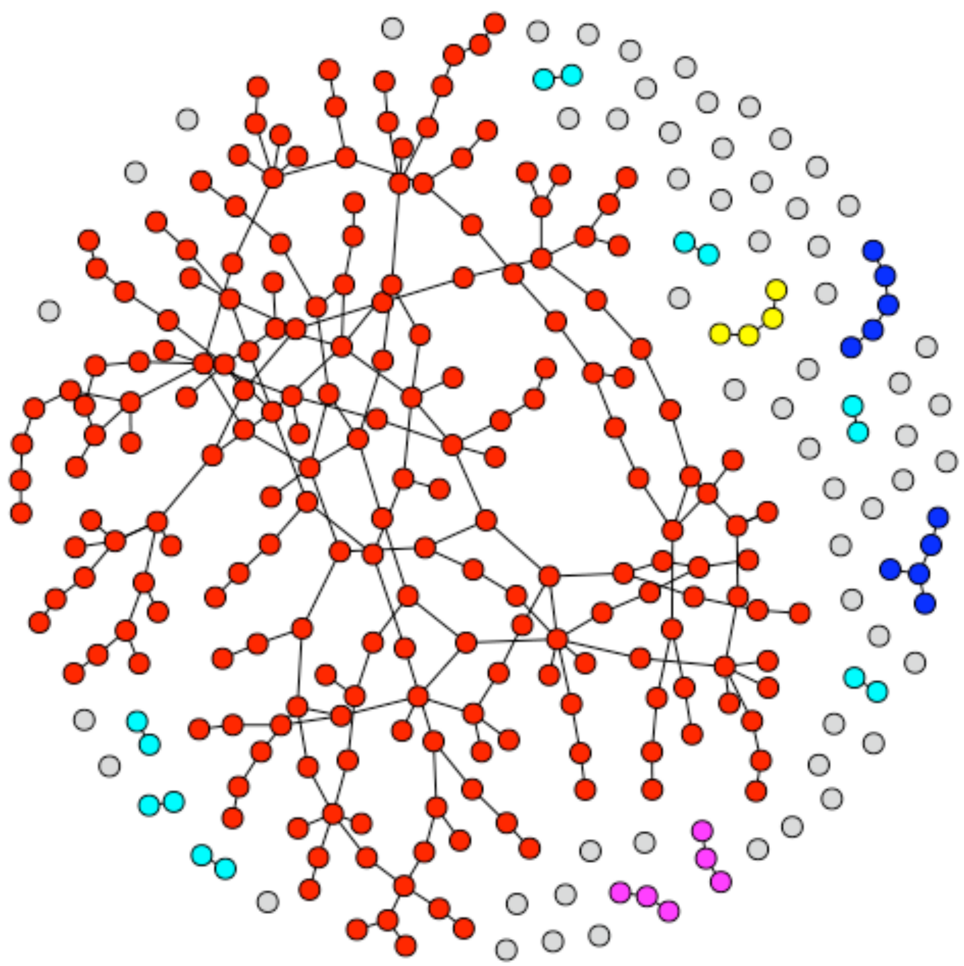
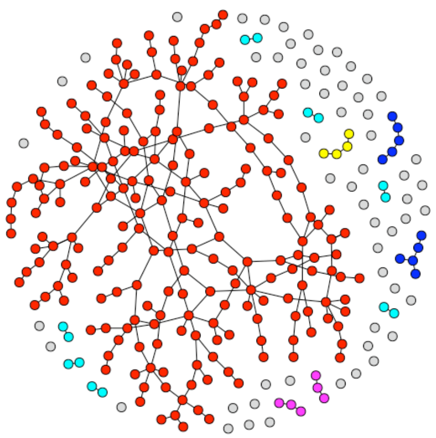
Erdos-Renyi random graph

$$< k >= p(N-1) \qquad d_l = \infty \qquad \#(t) \sim e^t$$

if $p > \frac{\log(N)}{N}$ the graph is globally connected

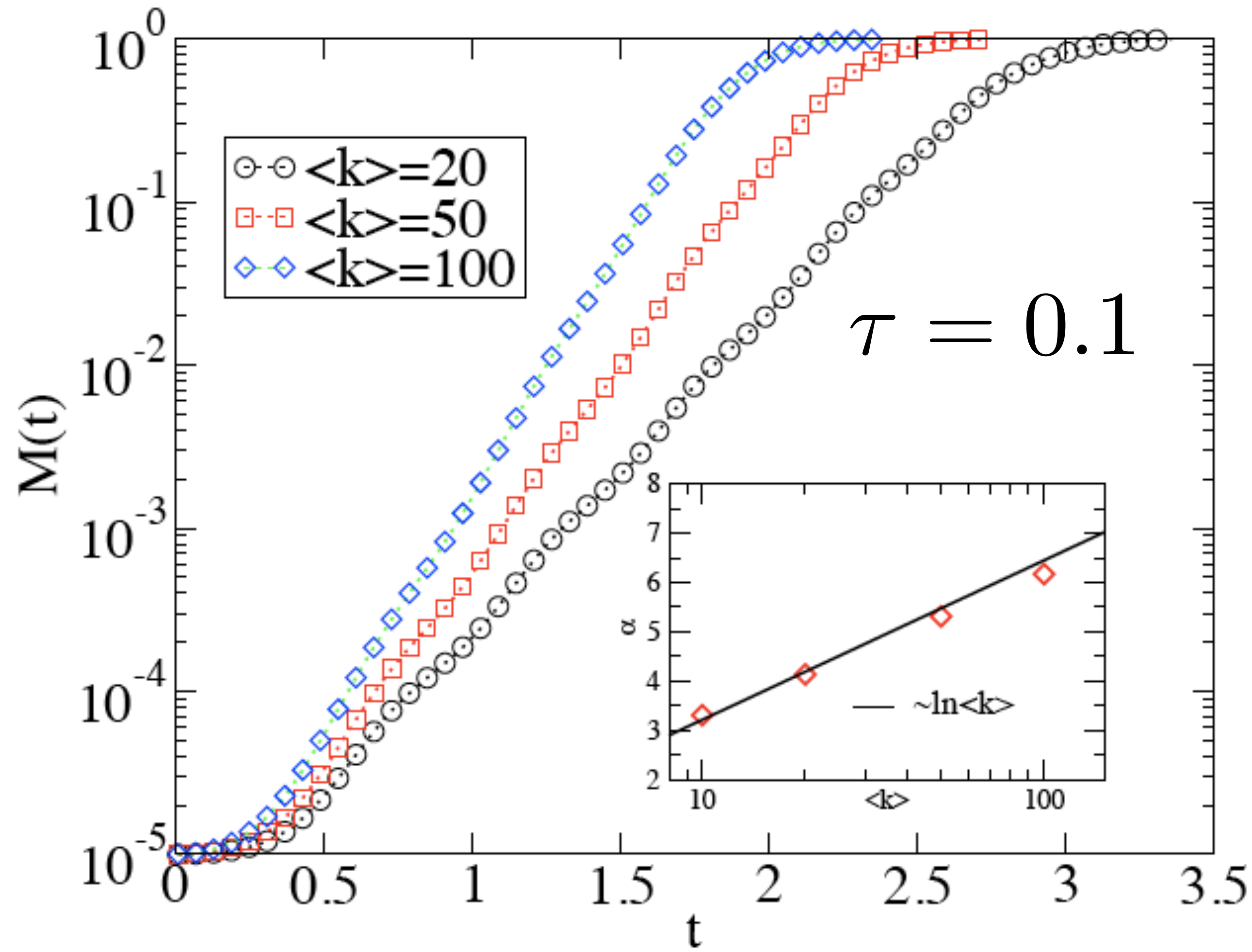


Erdos-Renyi random graph



Scaling

$$M(t) \sim e^{\alpha t}$$



Slow reaction $\alpha = 1/\tau$

Fast reaction $\alpha(k,\tau) \simeq C\tau^{\beta} \log < k >$

Mean-field eq. $\partial_t \rho(t) = \tau^{\beta} \log(< k >)\rho(t)(1-\rho(t))$

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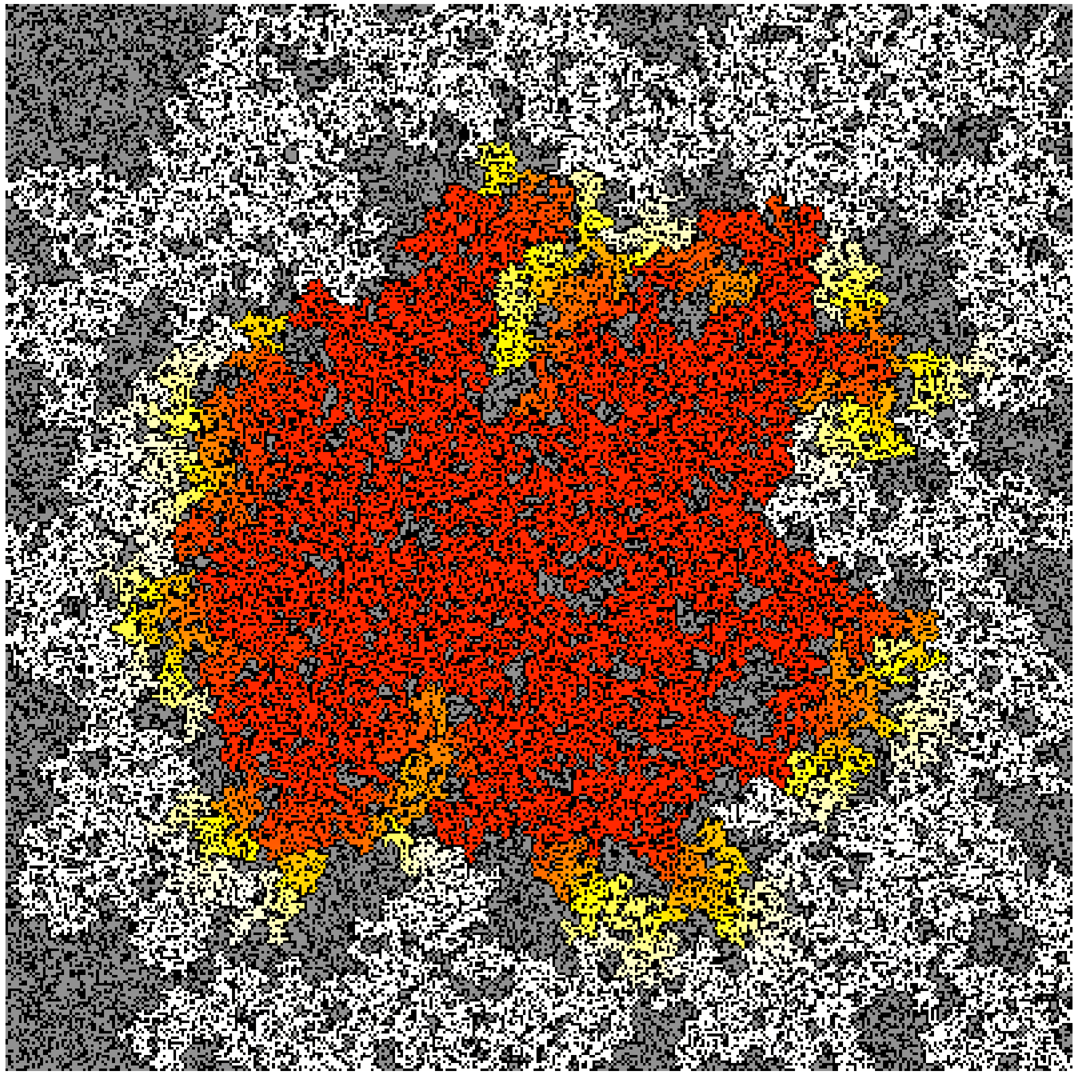
Percolation

Percolation in a square lattice

critical point $p \approx 0.595$



$$d_f \simeq 1.896$$
$$d_l \simeq 1.67$$
$$d_s \simeq 1.36$$

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Percolation: reaction spreading

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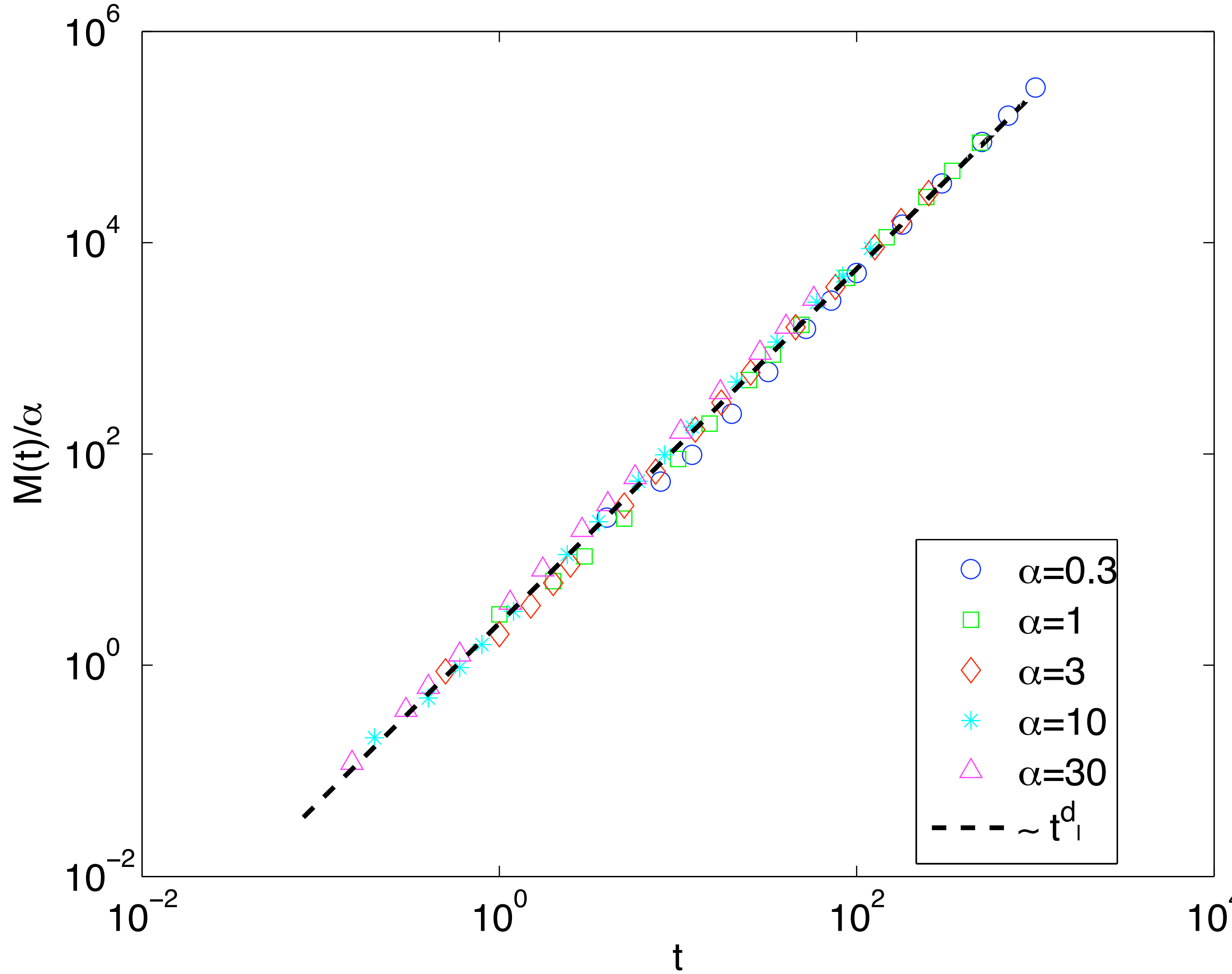
$$p = p_c$$

$$M(t) \simeq \alpha t^{d_l}$$



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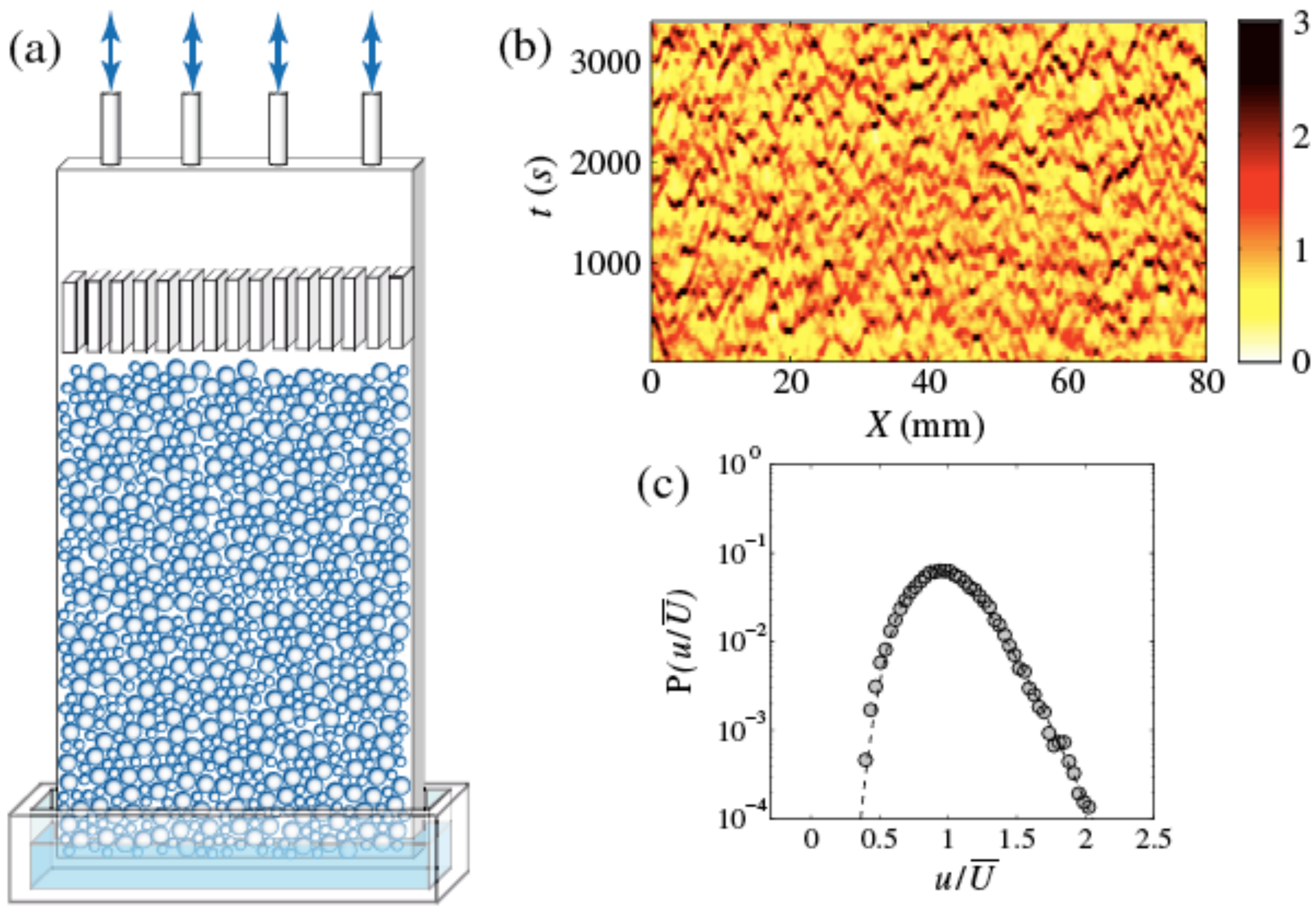
Percolation: travelling front

Porous media: experiments with glass spheres



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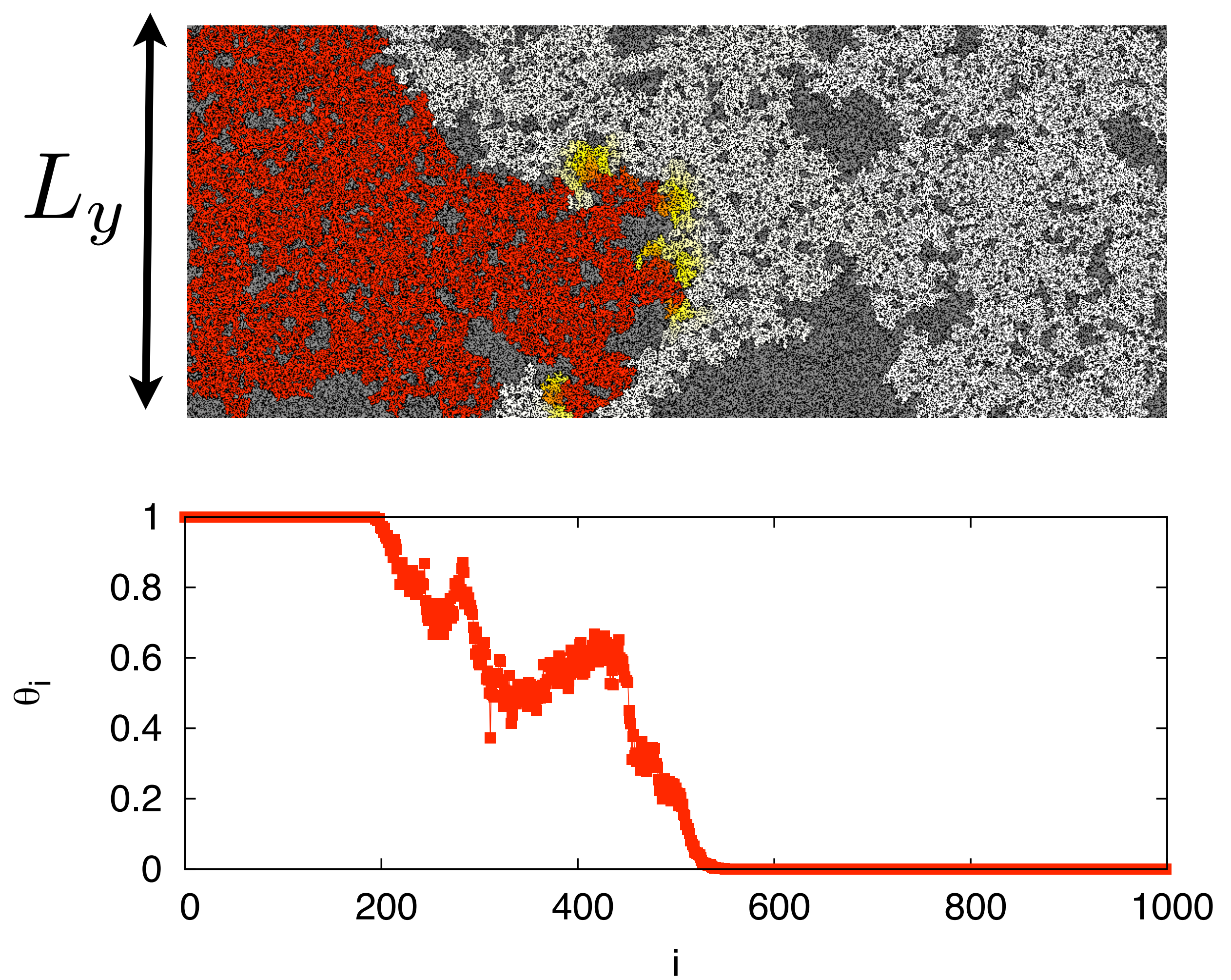
Numerical simulations



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Percolation: travelling front

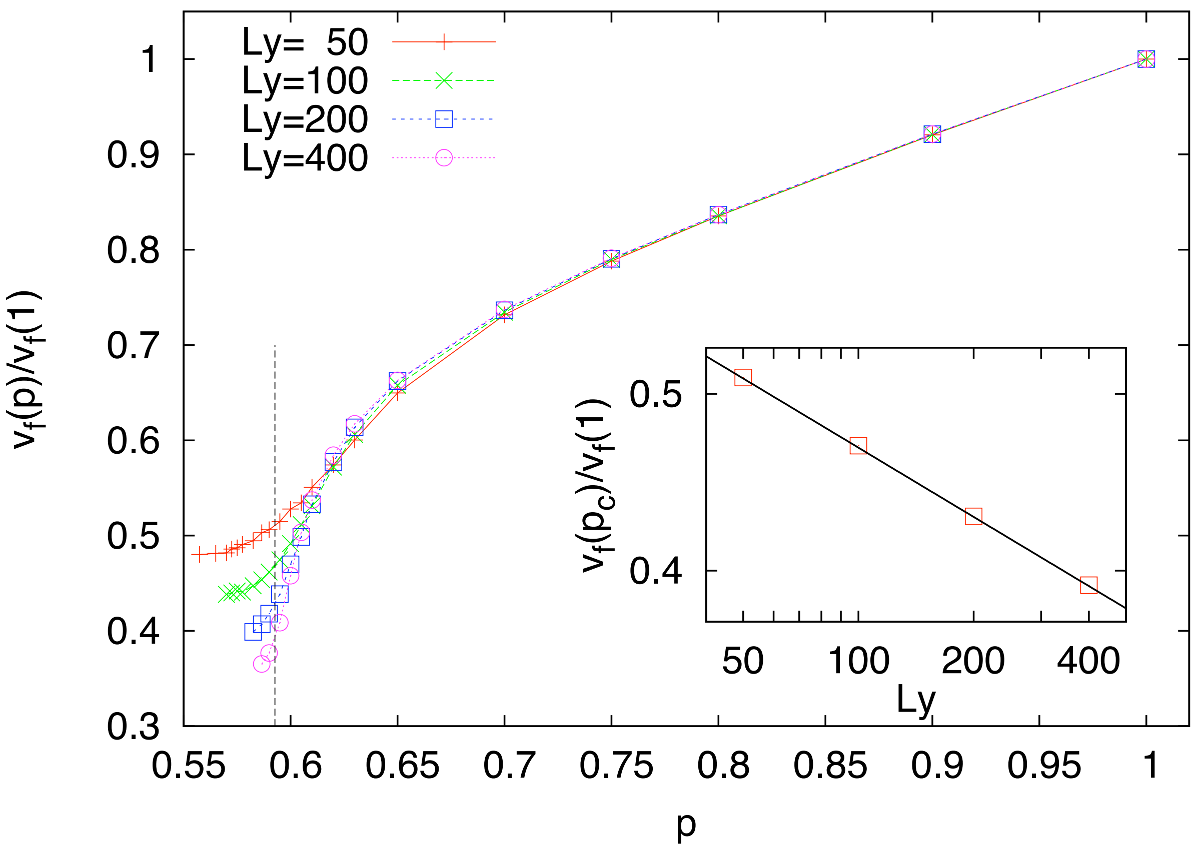
Velocity

$$M(t) \simeq N_p v t$$

$$p \approx p_c, N_p \sim \frac{L_y^{d_f}}{L_y} = L_y^{d_f - 1}$$

$$p \gg p_c, N_p \simeq p L_y$$

$$v = \lim_{t \to \infty} \frac{M(t)}{N_p t} \qquad u(p) = P(p) \frac{v_f(p)}{v_f(1)}$$



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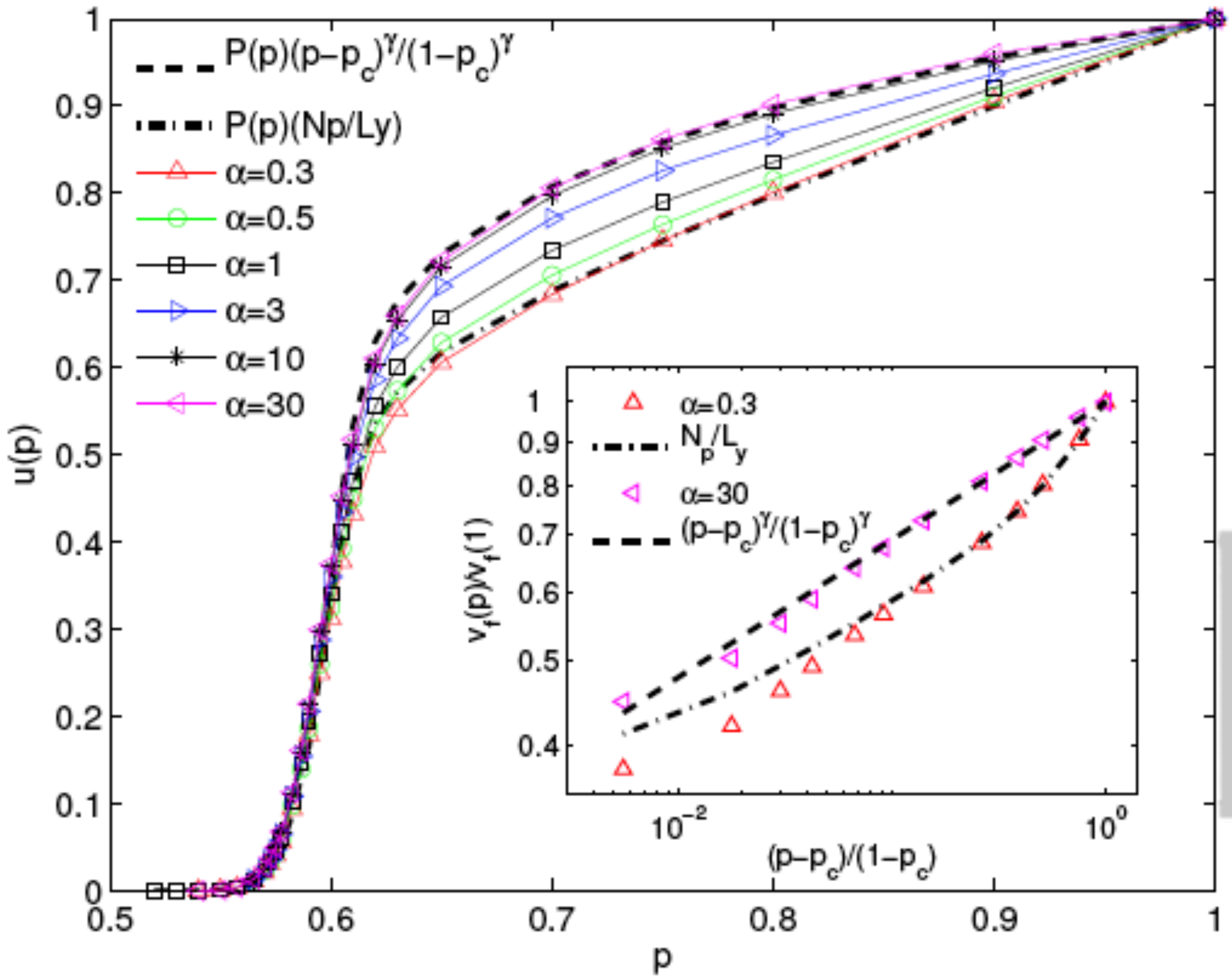
Percolation: travelling front

Front speed

$$v = \lim_{t\to\infty} \frac{M(t)}{N_p t}$$

$$u(p) = P(p)\frac{v_f(p)}{v_f(1)}$$



small α

$$u(p) = P(p)\frac{v_f(p)}{v_f(1)} \sim P(p)\frac{N_p}{L_y}$$

large α

$$u(p) = P(p)\frac{v_f(p)}{v_f(1)} \sim P(p)\left(\frac{p-p_c}{1-p_c}\right)^{\gamma}$$

$$\gamma = -\nu(1-d_{\min})$$

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Percolation: travelling front

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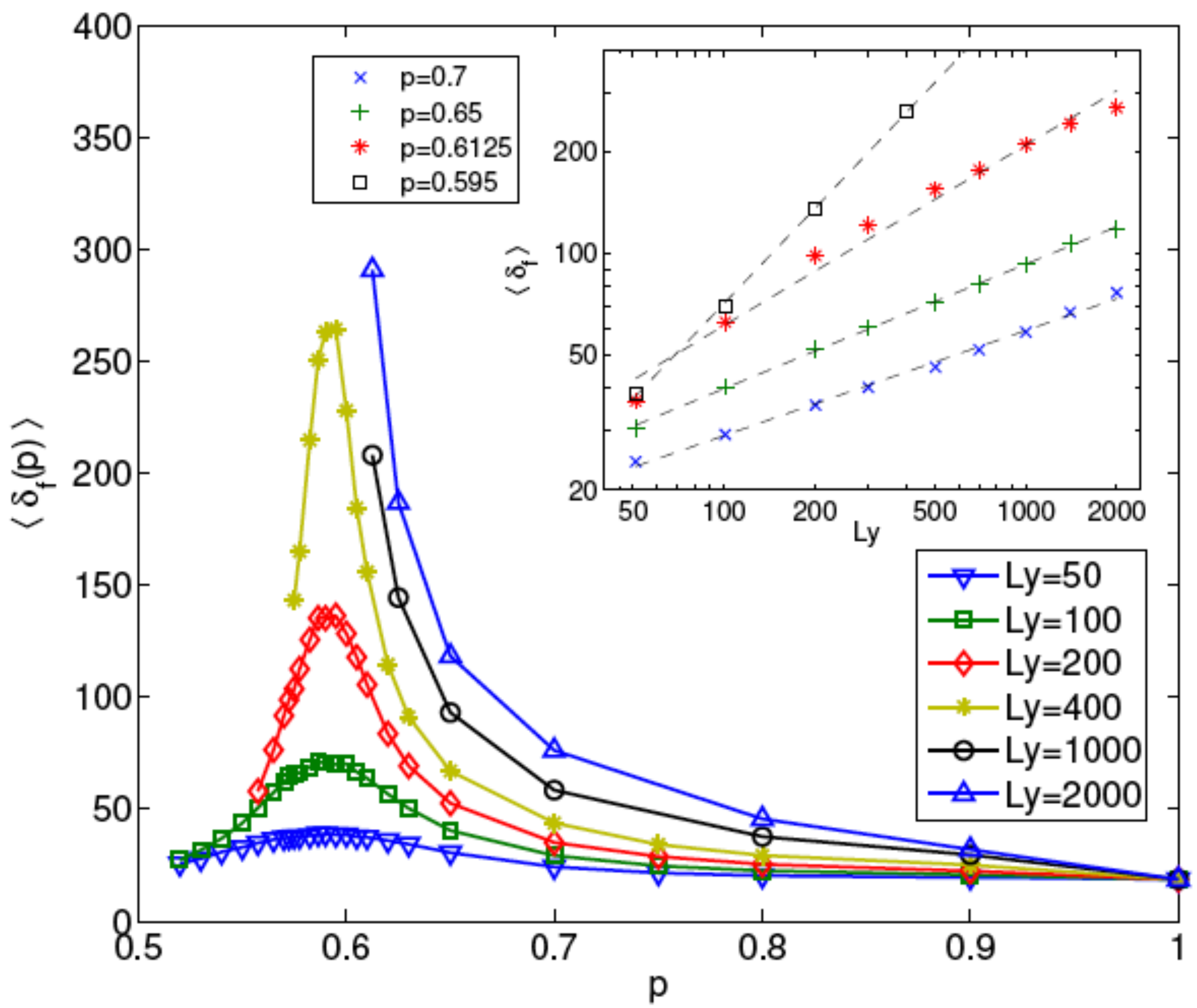
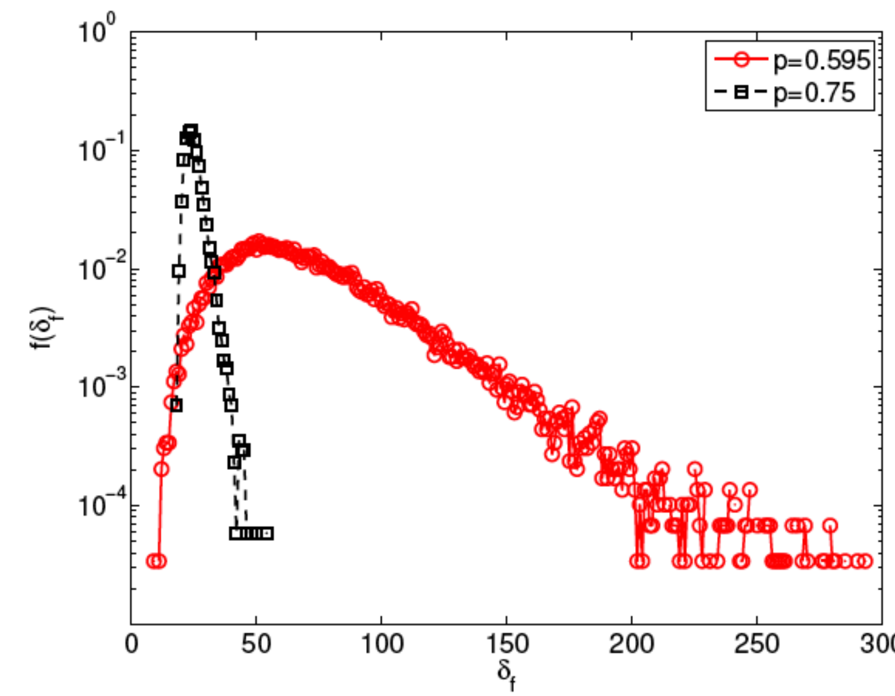
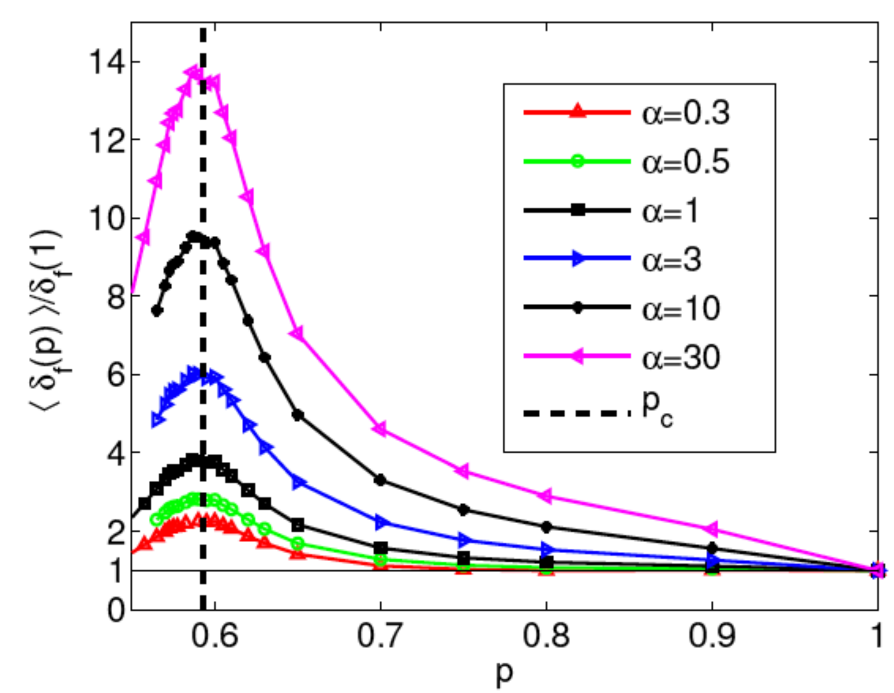
Front width







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Conclusions and perspectives

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- Advection-Reaction-Diffusion fundamental framework
  - Complex heterogeneous geometry
  - Finite-size effects
  - prevalence of fluctuations

- Flow-chemistry interaction
- Analysis of experiments in porous media
- Realistic simulations for epidemics networks
- Chemistry Role

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$m(t) \sim t^{d_l}$. $m(t) \sim r(t)^{d_f}$. Therefore $r(t) \sim t^{d_l/d_f}$, and $v = \frac{dr}{dt} \sim t^{d_l/d_f - 1} \sim r^{1-d_m in}$, where $d_m in = \frac{d_f}{d_l}$. Furthermore, if the linear size of the region is $r < \xi$, where ξ is the correlation length the cluster is self-similar and then $v \sim \xi^{1-d_m in}$. Moreover, analysis of the percolation phase transition gives $\xi \sim |p - p_c|^{-\nu}$, with $\nu = 4/3$ for $d = 2$ [?], which gives the final scaling $v \sim (p - p_c)^{\gamma}$, where $\gamma = -\nu(1 - d_m in)$. For the average velocity, the scaling is:

$$u(p) = P(p)\frac{v_f(p)}{v_f(1)} \sim P(p)\left(\frac{p - p_c}{1 - p_c}\right)^{\gamma} .d_f \quad (1)$$

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