Dynamic facilitation approach to glasses

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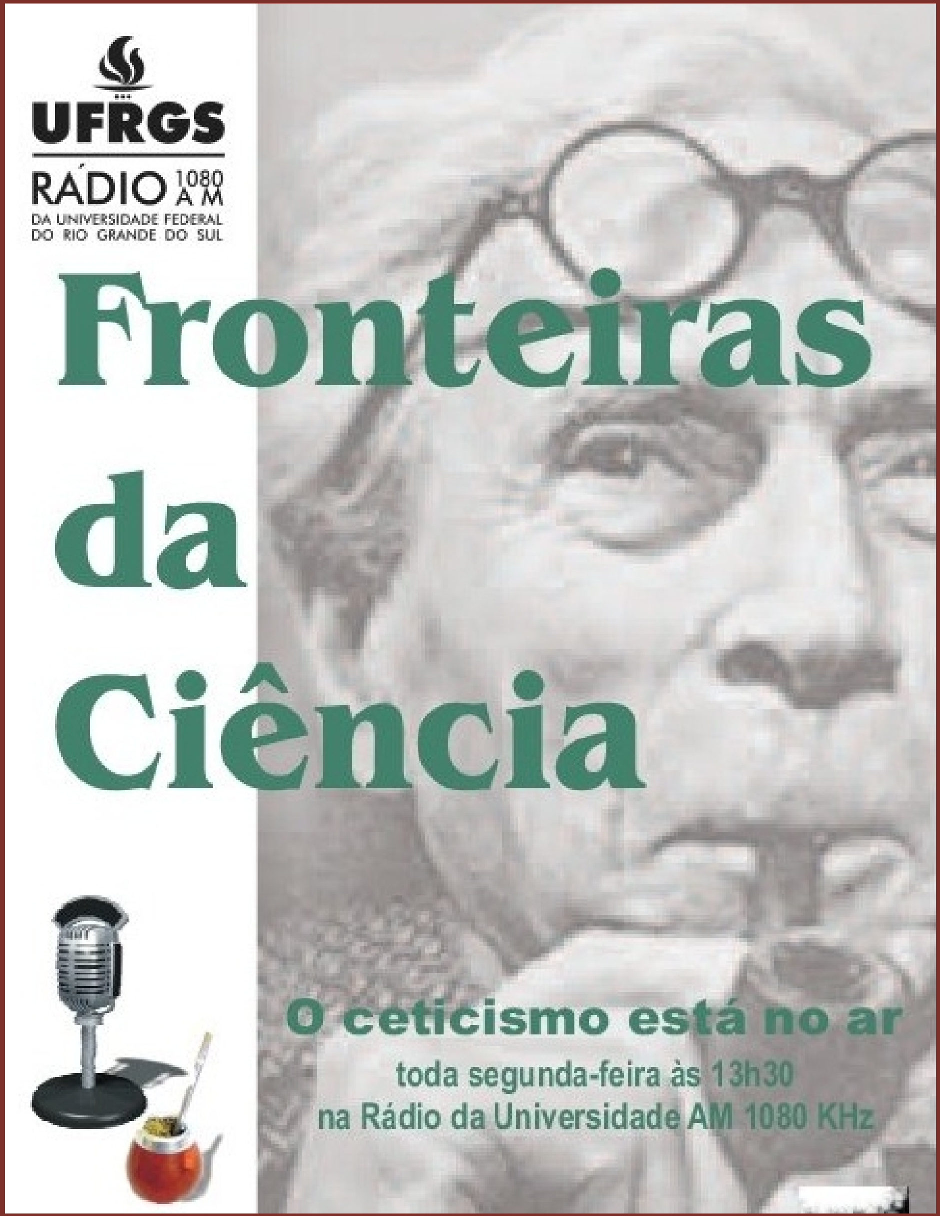
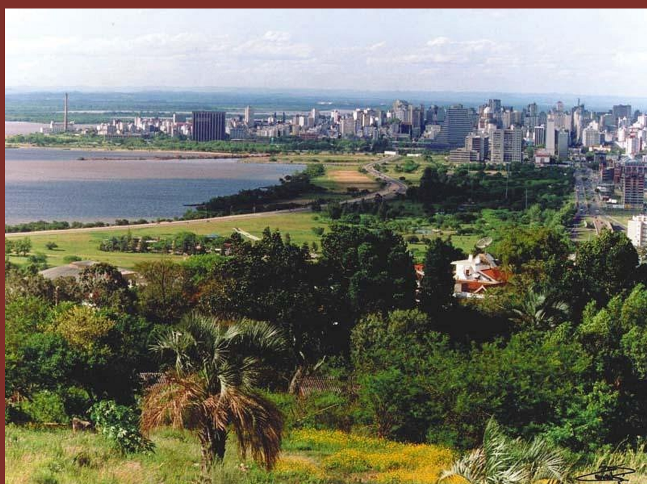


Collaborators

- Mauro Sellitto (Mostar, Bosnia and Herzegovina)
- Daniele de Martino (Trieste, Italy)
- Fabio Caccioli (Trieste, Italy)



The Pitch Drop Experiment 1927-. . .

Glasses are liquids that cannot flow (below T_g)

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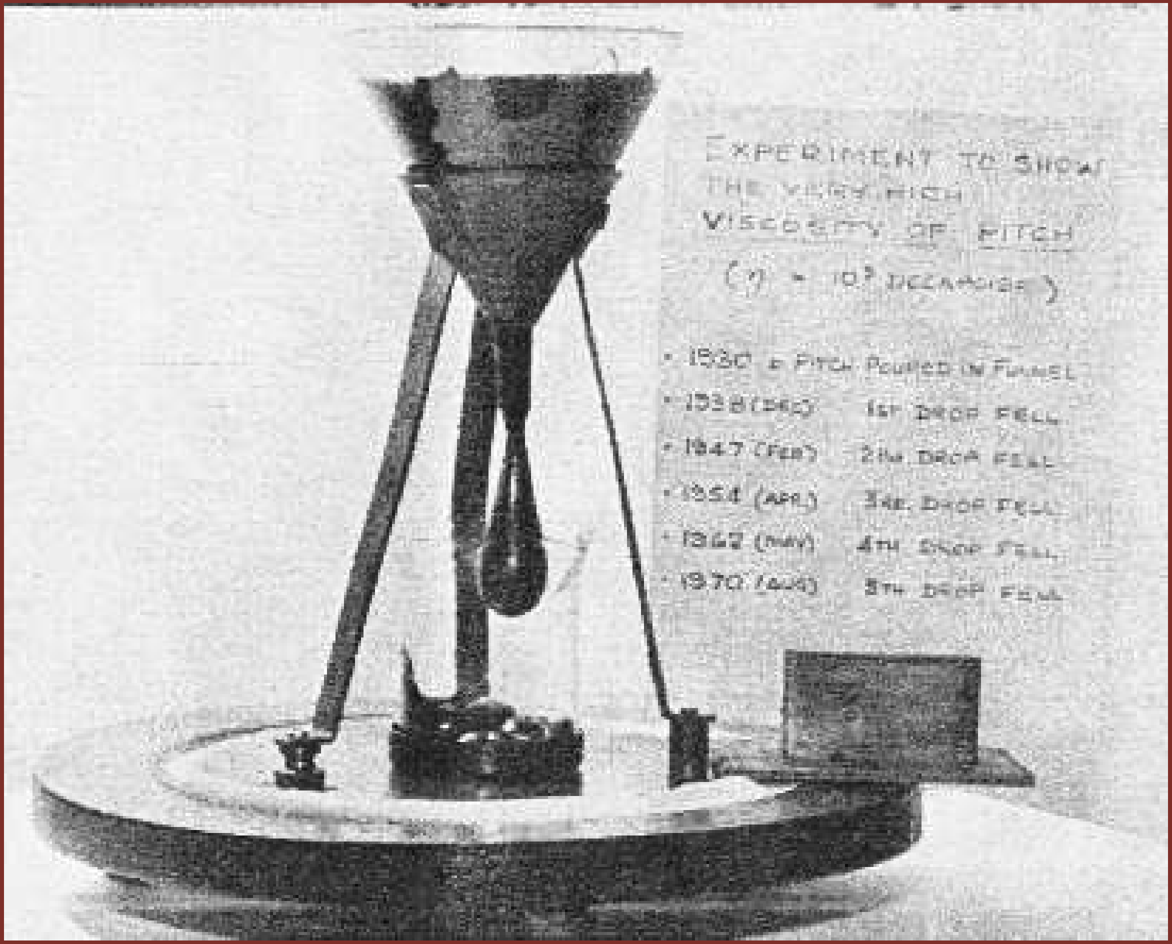

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Complex media

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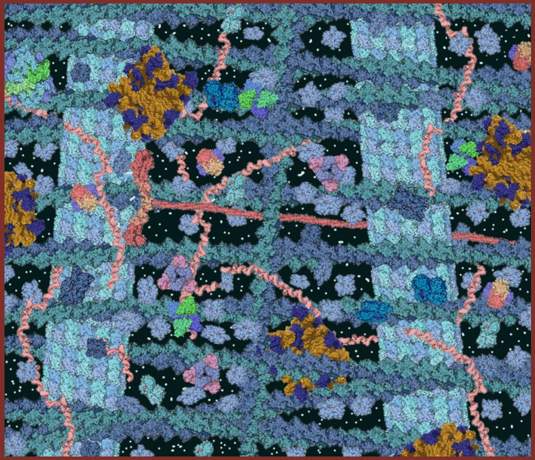
- transport properties in disordered media (e.g., molecular crowding, porous media, etc)



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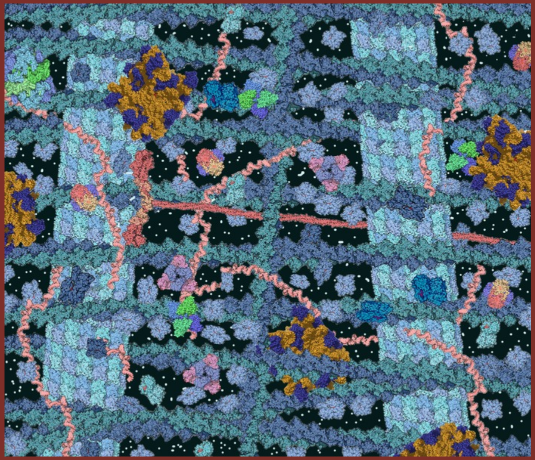

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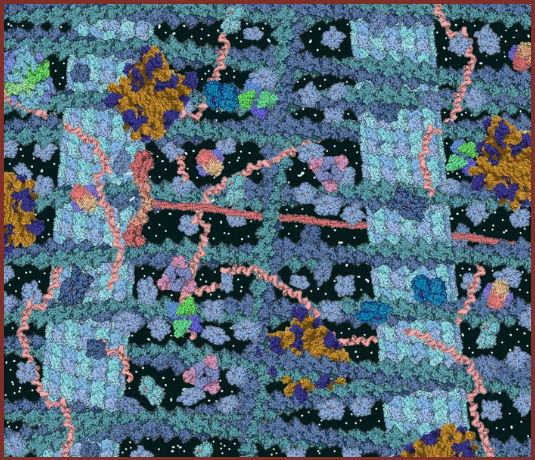
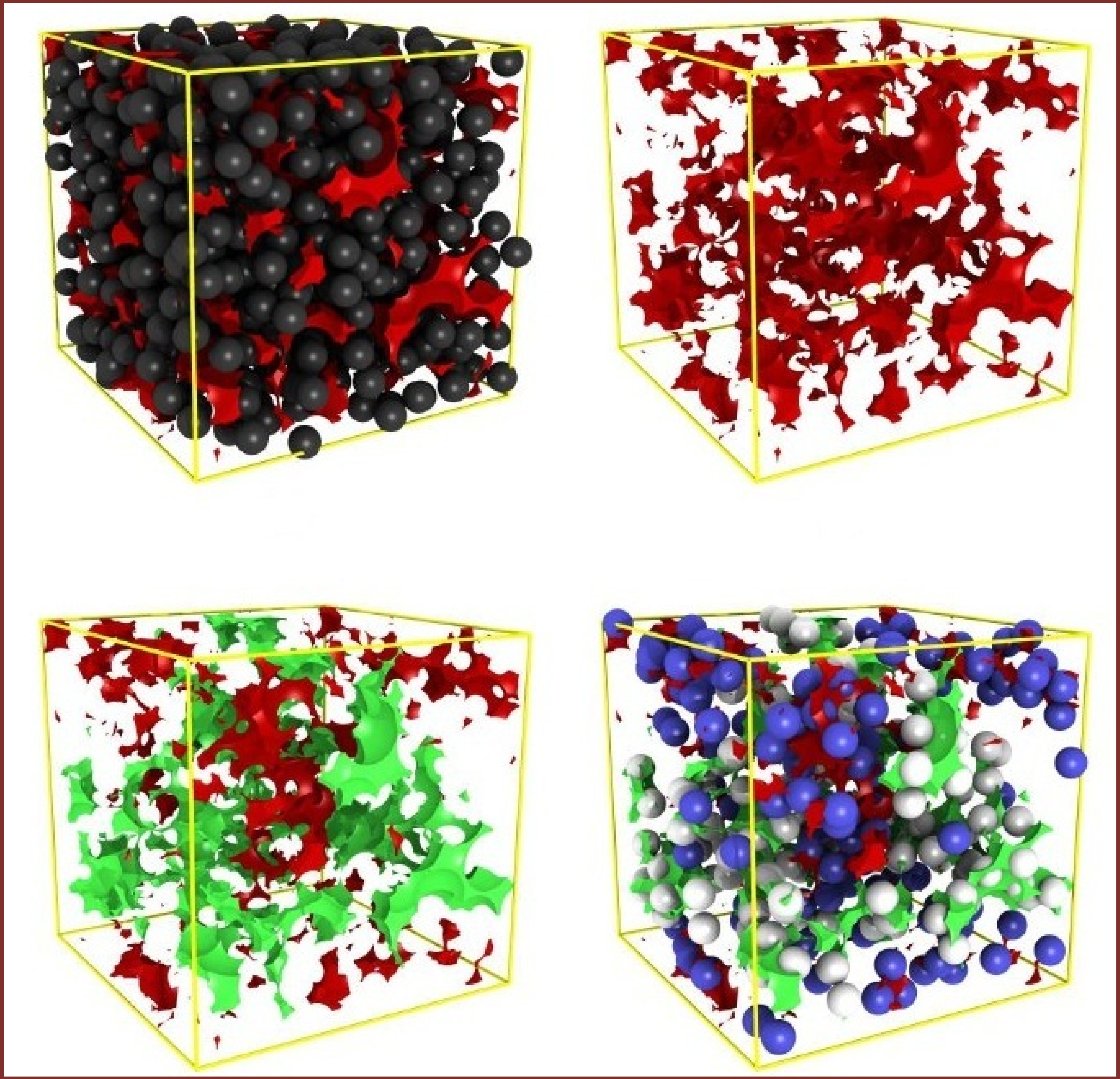


- asymmetric (binary) mixtures (colloids)
- quenched-annealed mixtures

Quenched-annealed mixtures

Kurzidim et al, arXiv:1012.1267



Quenched-annealed mixtures Krakoviack PRE 75 (2007) 031503, 79 (2009) 061501

- Quenched matrix: particles frozen in a (statistically homogeneous) disordered configuration
- Annealed particles: fluid, mobile particles

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- Quenched matrix: particles frozen in a (statistically homogeneous) disordered configuration
- Annealed particles: fluid, mobile particles
- Two possible scenarios:
  - discontinuous (type B) transition: dilute matrices (weak confinement)

$$\Phi - \Phi_c \propto (T - T_c)^{1/2}$$

  - continuous (type A) transition: dense matrices (strong confinement)

$$\Phi \propto T - T_c$$

where

$$\begin{aligned} \Phi &= \lim_{t \to \infty} \phi(t) \\ \Phi_c &= \Phi(T_c) \end{aligned}$$

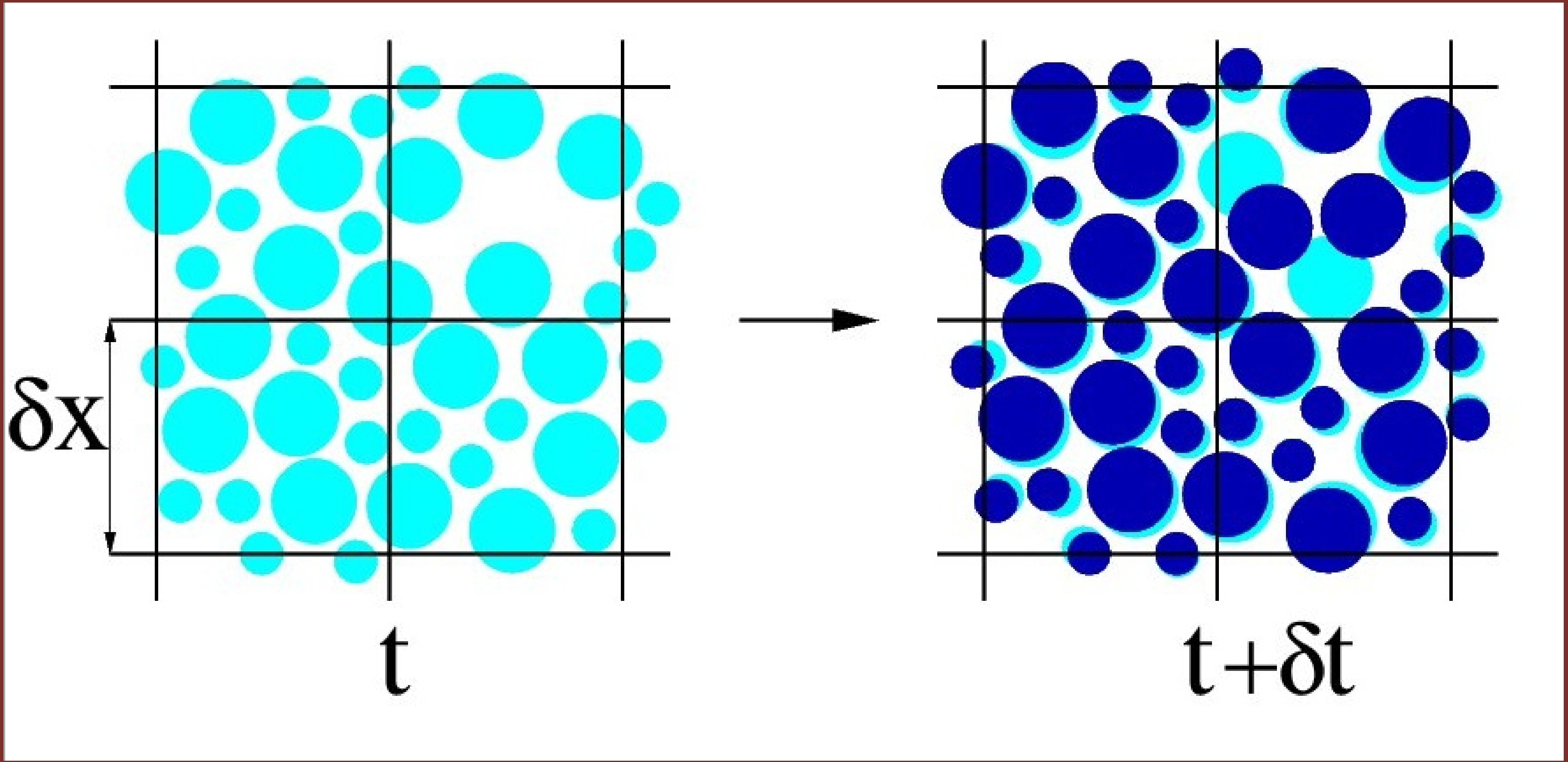
Kinetically

Constrained

Models

Heterogeneities

Ritort & Sollich, Adv. Phys. 52, 219 (2003)



Chandler & Garrahan, J. Chem. Phys. 123, 044511 (2005)

Coarse graining

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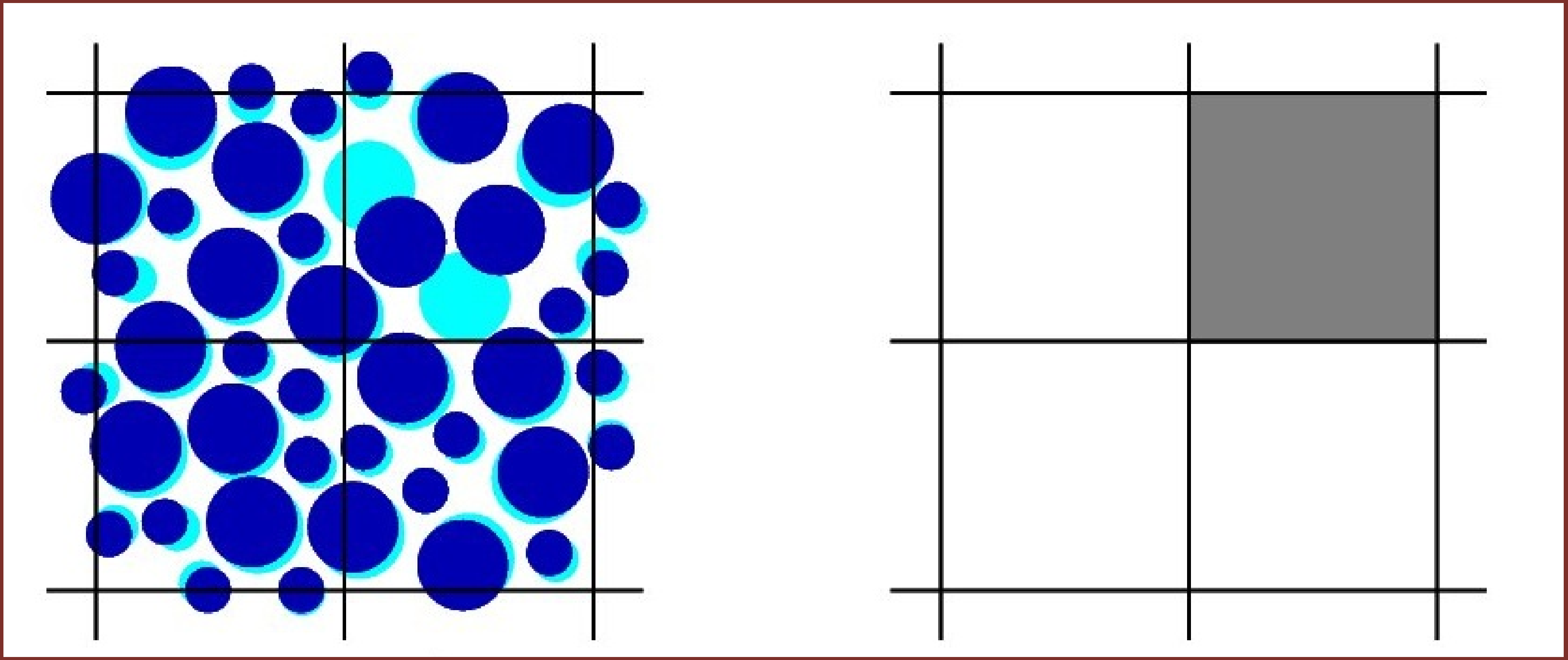

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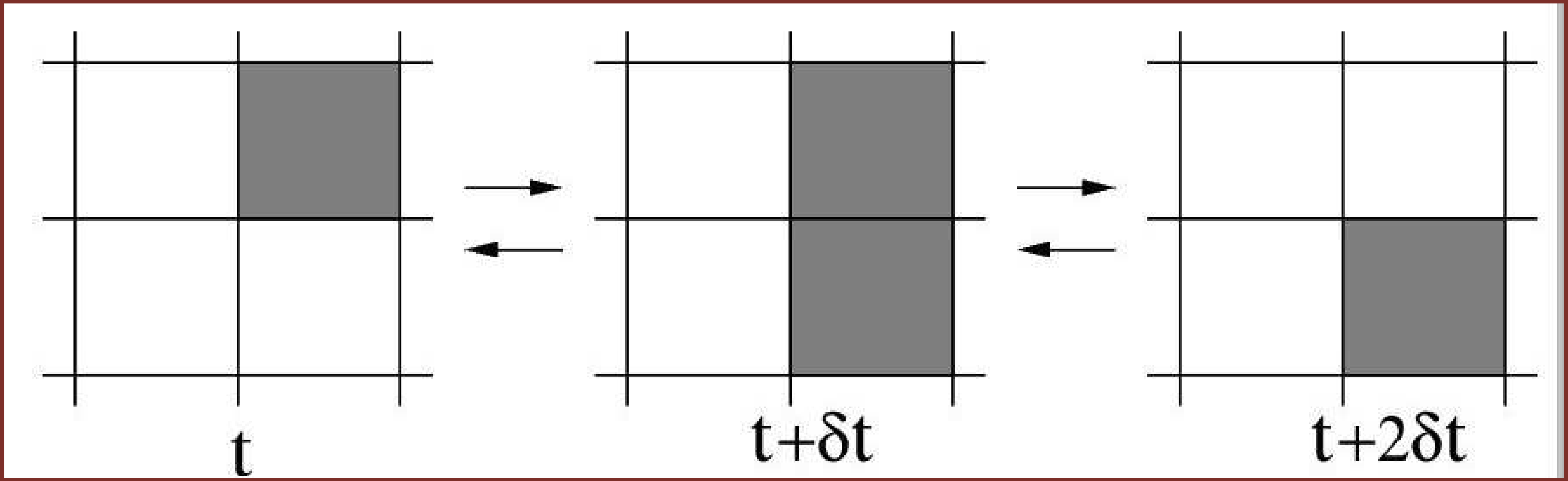
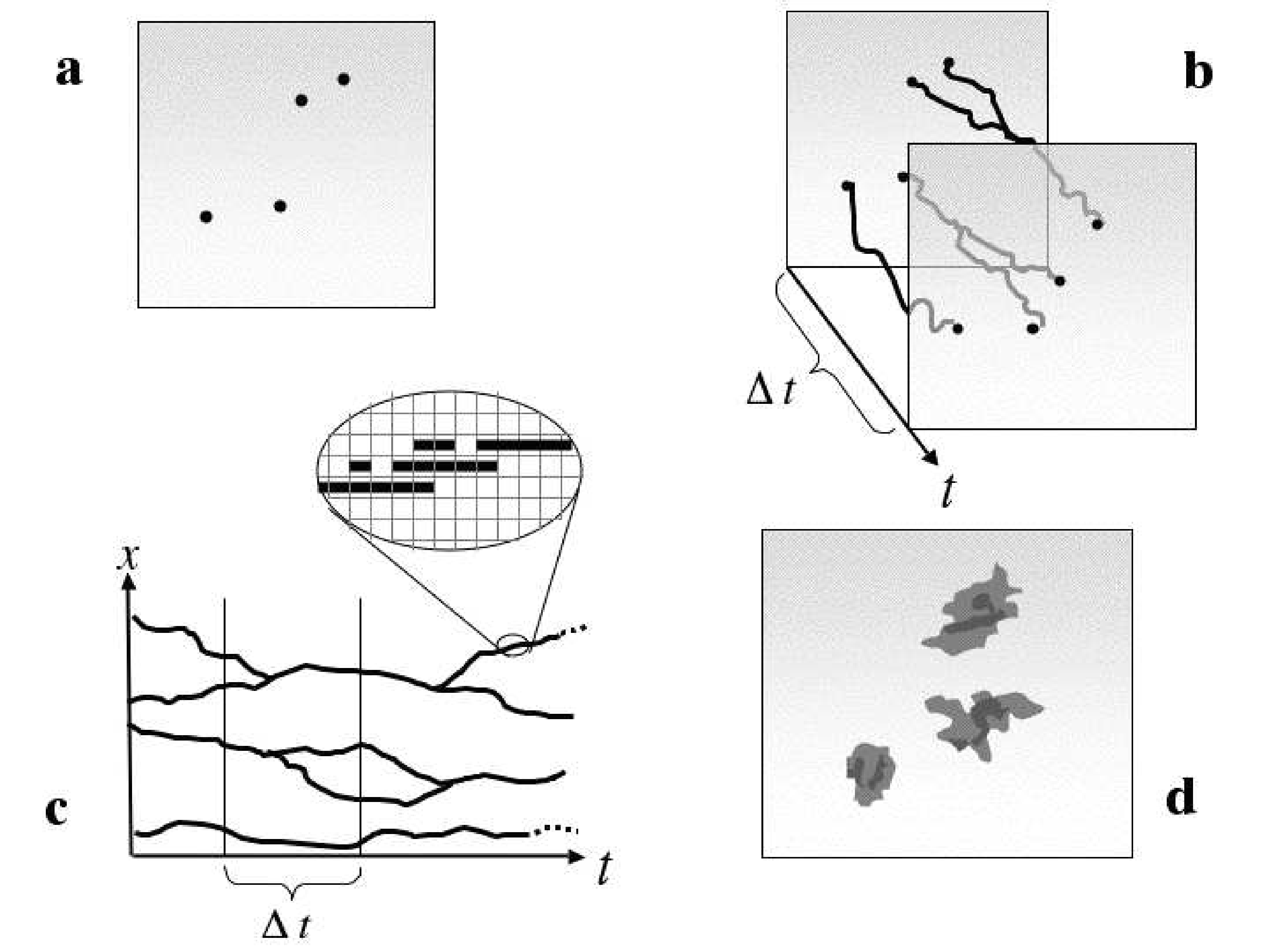


Chandler & Garrahan, J. Chem. Phys. 123, 044511 (2005)

- mobility field: $n_i(t) = 0, 1$
- facilitation: a cell can change $n_i \to 1 - n_i$ only if a neighbour cell has $n_j = 1$

Trajectories

Ritort & Sollich, Adv. Phys. 52, 219 (2003)



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Fredrickson-Andersen

Ritort & Sollich, Adv. Phys. 52 (2003) 219

On a lattice with coordination number z, we consider a system of N non interacting spins:

$$E = \sum_i n_i \qquad (n_i = 0, 1)$$

n_i can flip if and only if at least f of its z neighboring spins are up (facilitating spins).

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Put the focus on the dynamics:

- How much of the glassy phenomenology can be described without relying on non-trivial equilibrium behavior?
- Some properties are not grasped (e.g., crystallization)
- as T decreases, the number of facilitating spins decreases and the dynamics becomes slower

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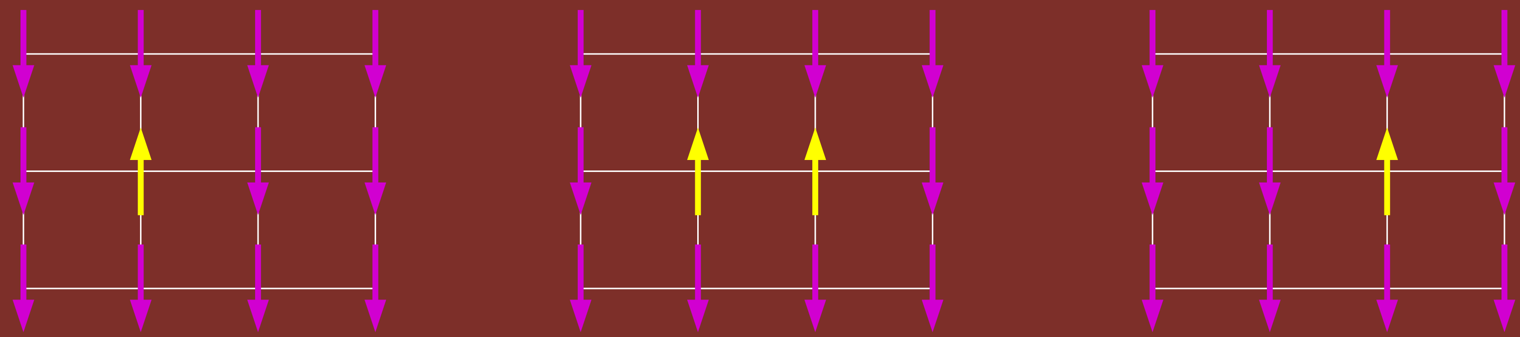
$f = 1$ (diffusive case):



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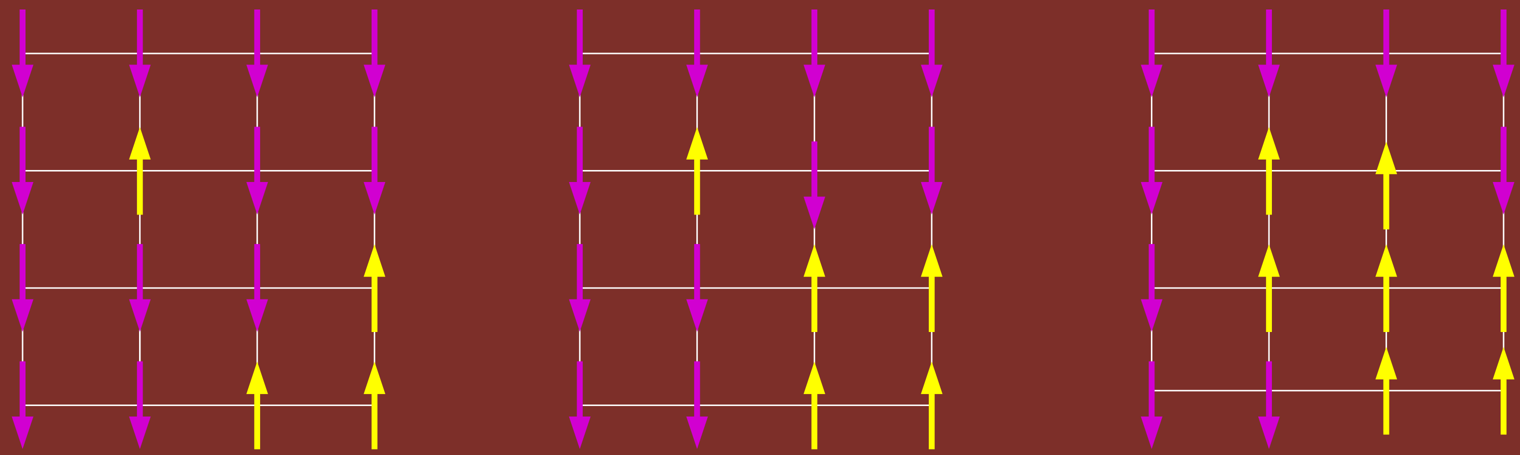
$f > 1$ (cooperative case):



Disordered facilitation

Sellitto, de Martino, Caccioli and Arenzon, PRL **105** (2010) 265704

Branco, J. Stat. Phys. **70** (1993) 1035

- $f \longrightarrow f_i$: site dependent quenched random variable $(1 \geq q \geq r \geq 0)$

$$P(f_i) = (1-q)\ \delta_{f_i,2} + (q-r)\ \delta_{f_i,3} + r\ \delta_{f_i,4}$$

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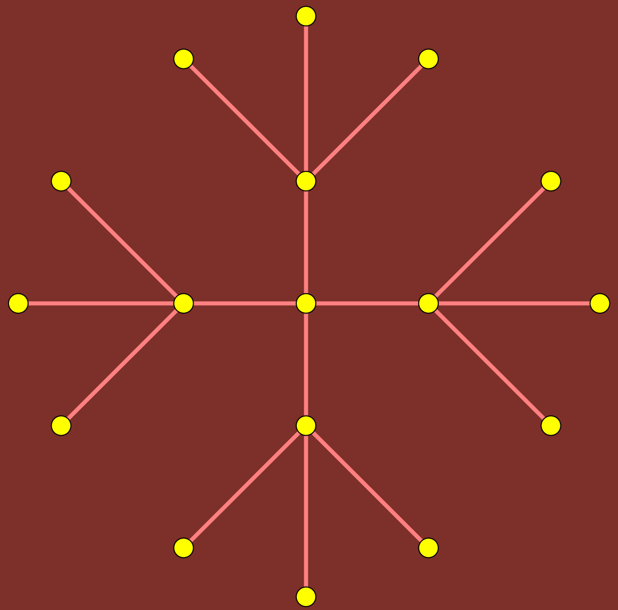
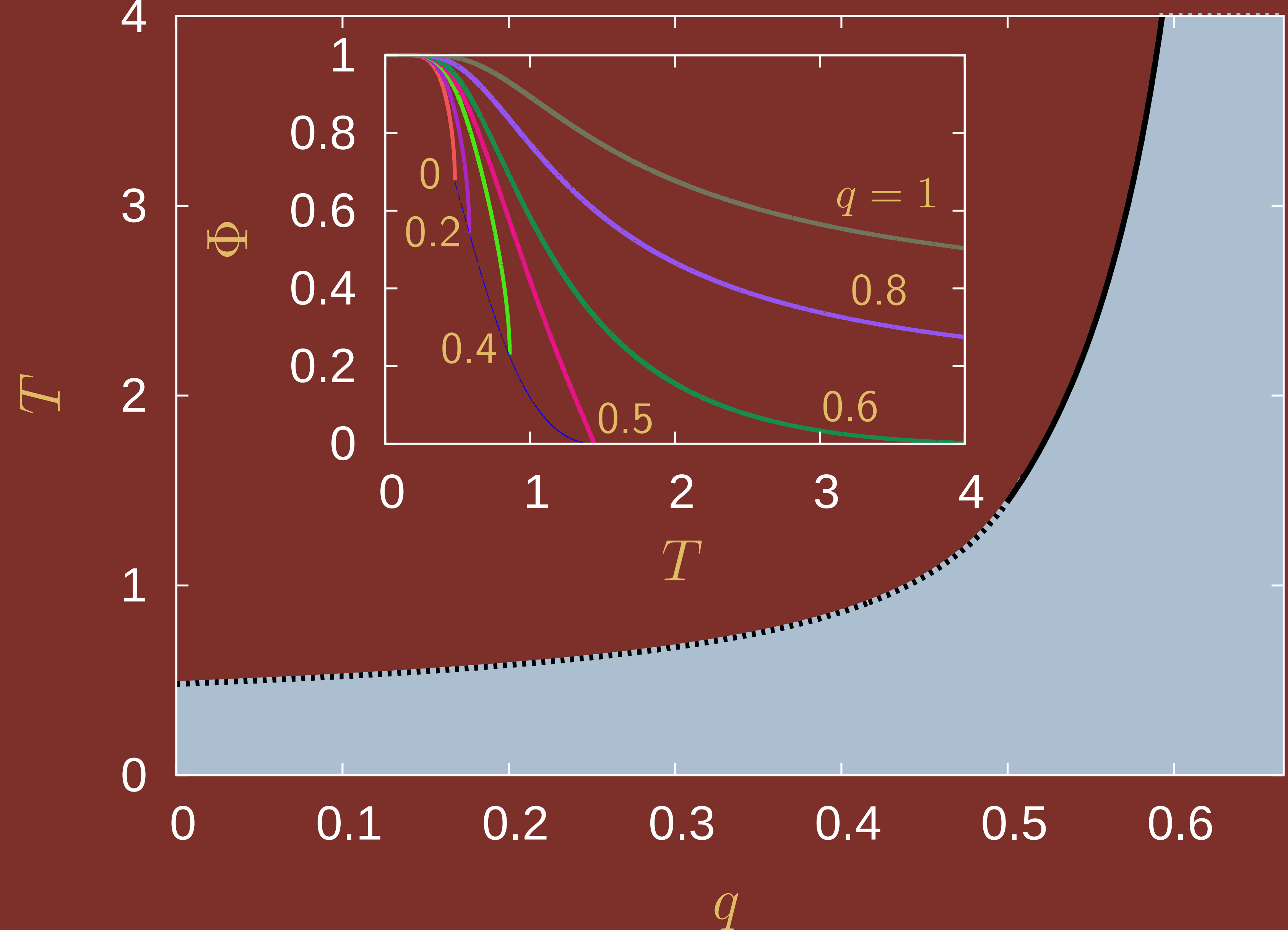
- Bethe lattice with $z = 4$: EXACT SOLUTION



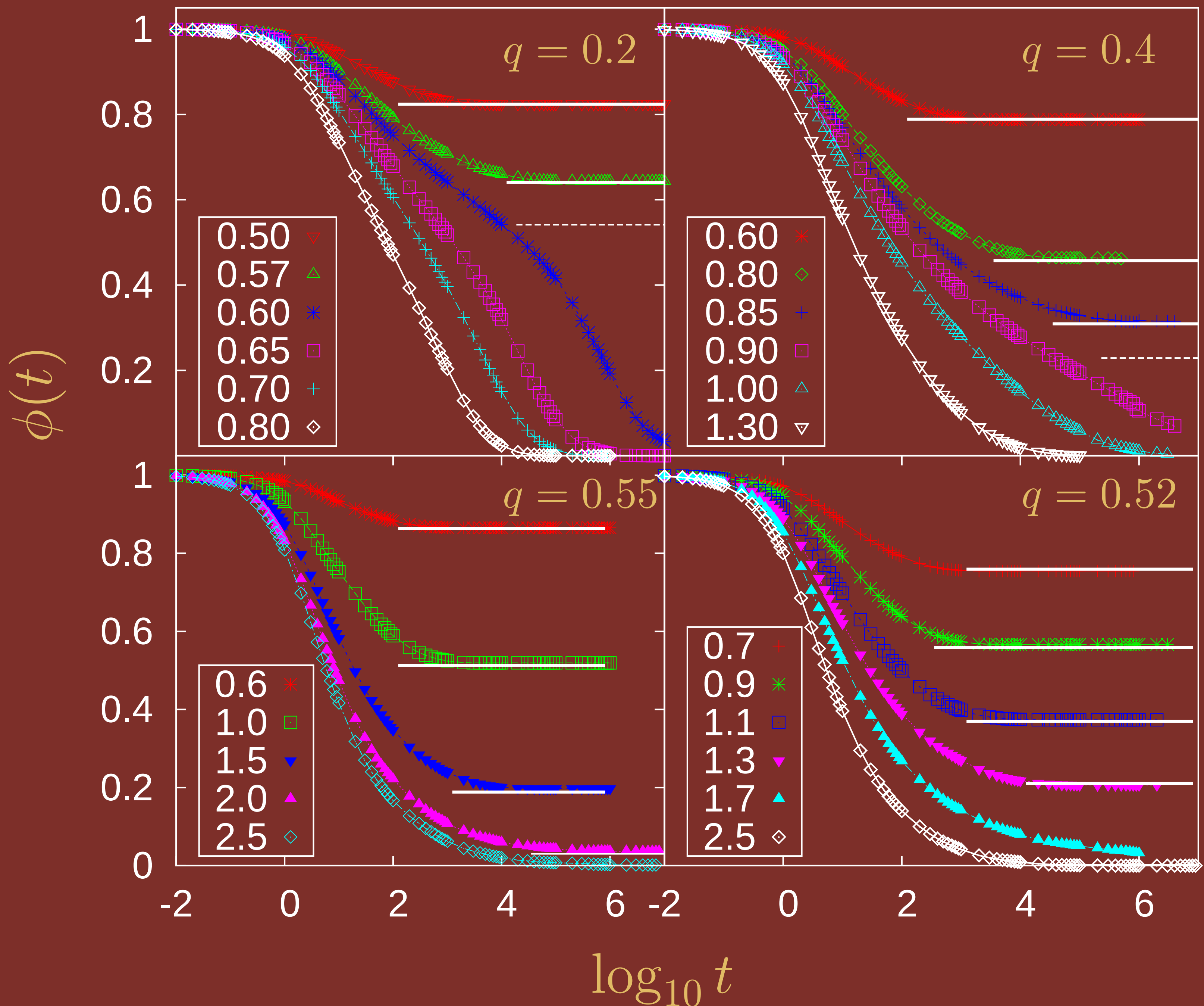
Phase diagram

Sellitto, de Martino, Caccioli and Arenzon, PRL 105 (2010) 265704



Persistence

Sellitto, de Martino, Caccioli and Arenzon, PRL 105 (2010) 265704



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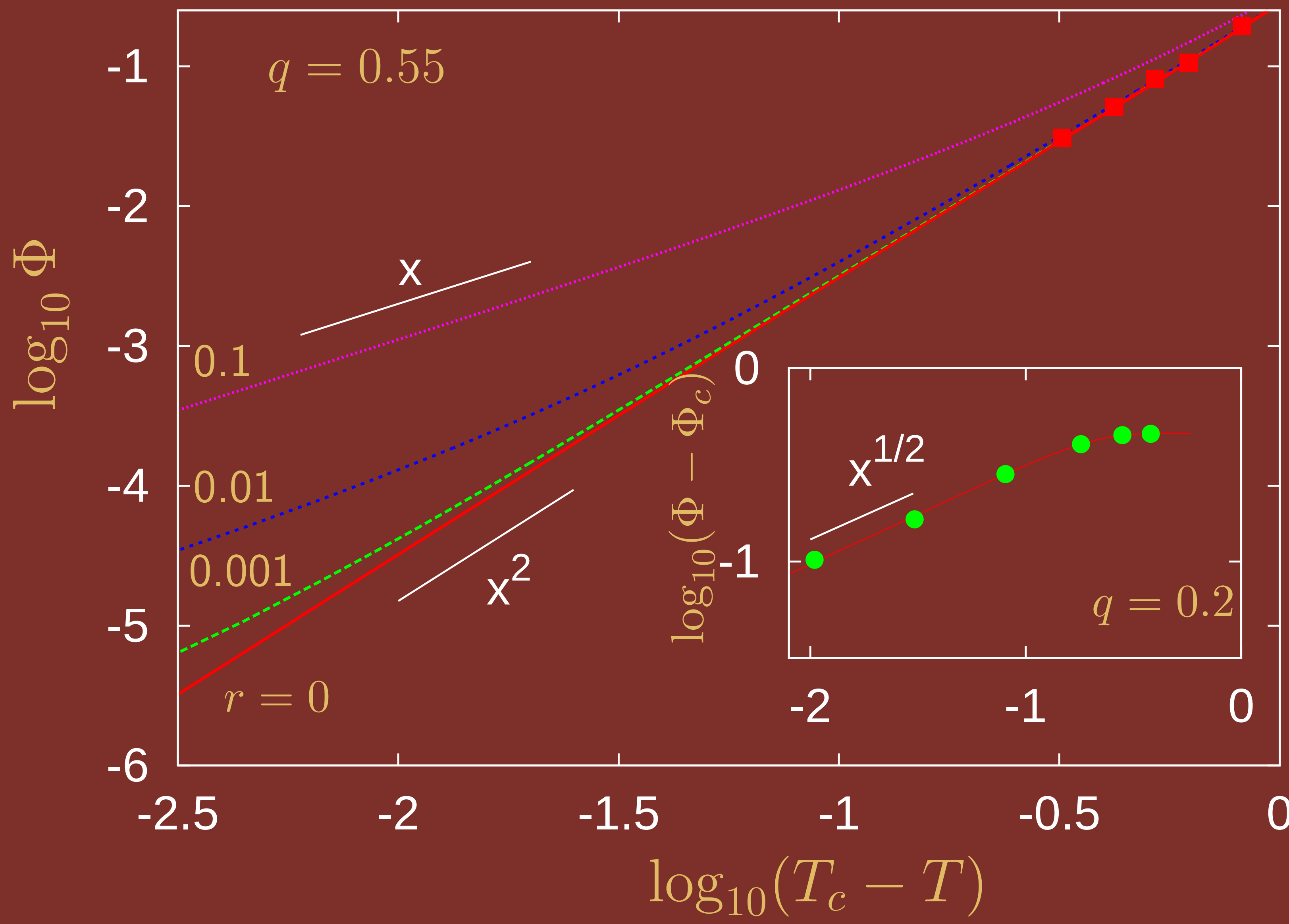


Predictions (MCT)

- at $T = T_c$, the approach to the plateau (even if it is 0) is power-law:

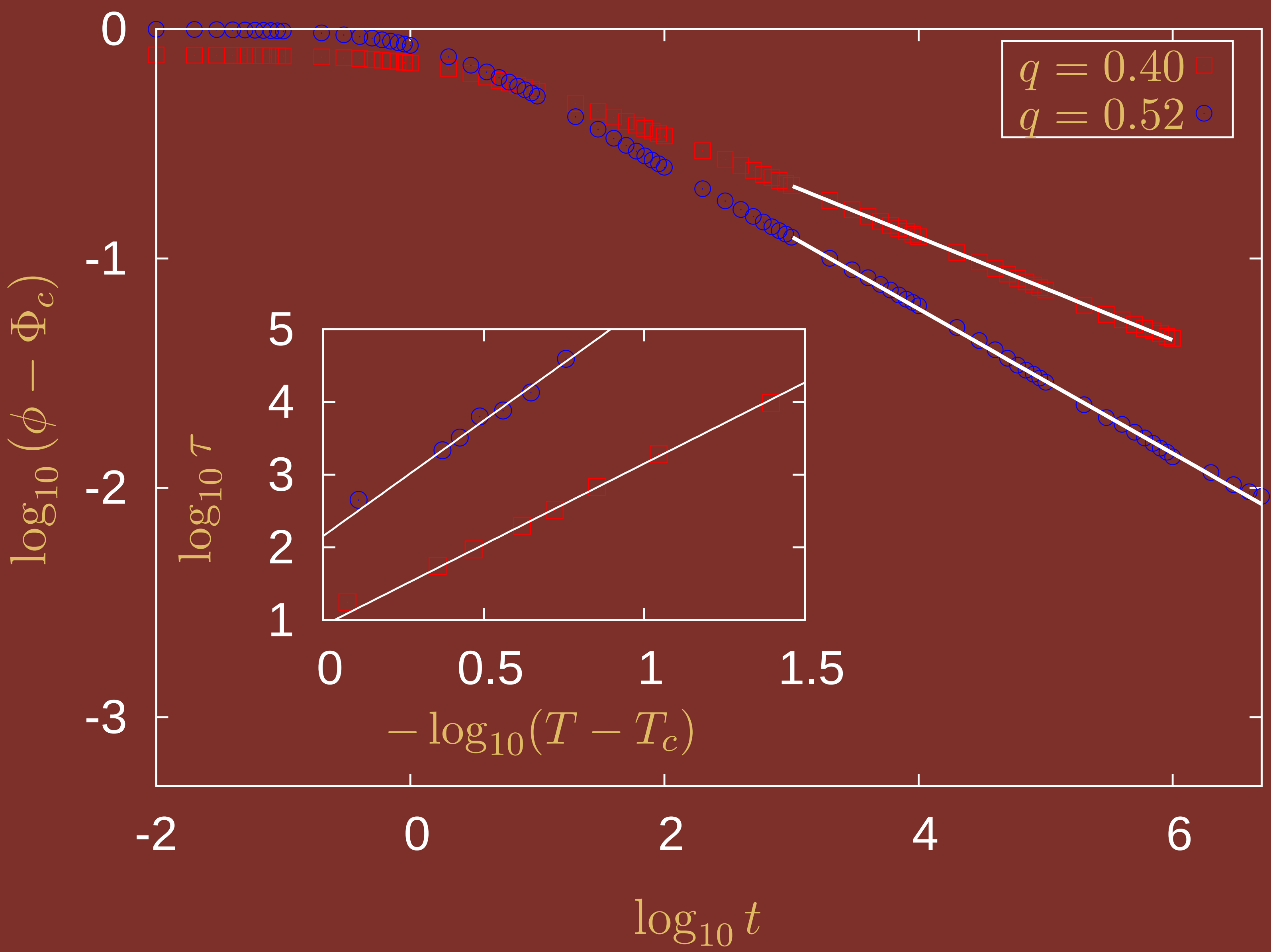
$$\phi(t) - \Phi_c \sim t^{-a(q)}$$

- For the β relaxation:

$$\tau \sim \begin{cases} (T - T_c)^{-\dfrac{1}{2a(q)}} & \text{(discontinuous)} \\ (T - T_c)^{-\dfrac{1}{a(q)}} & \text{(continuous)} \end{cases}$$

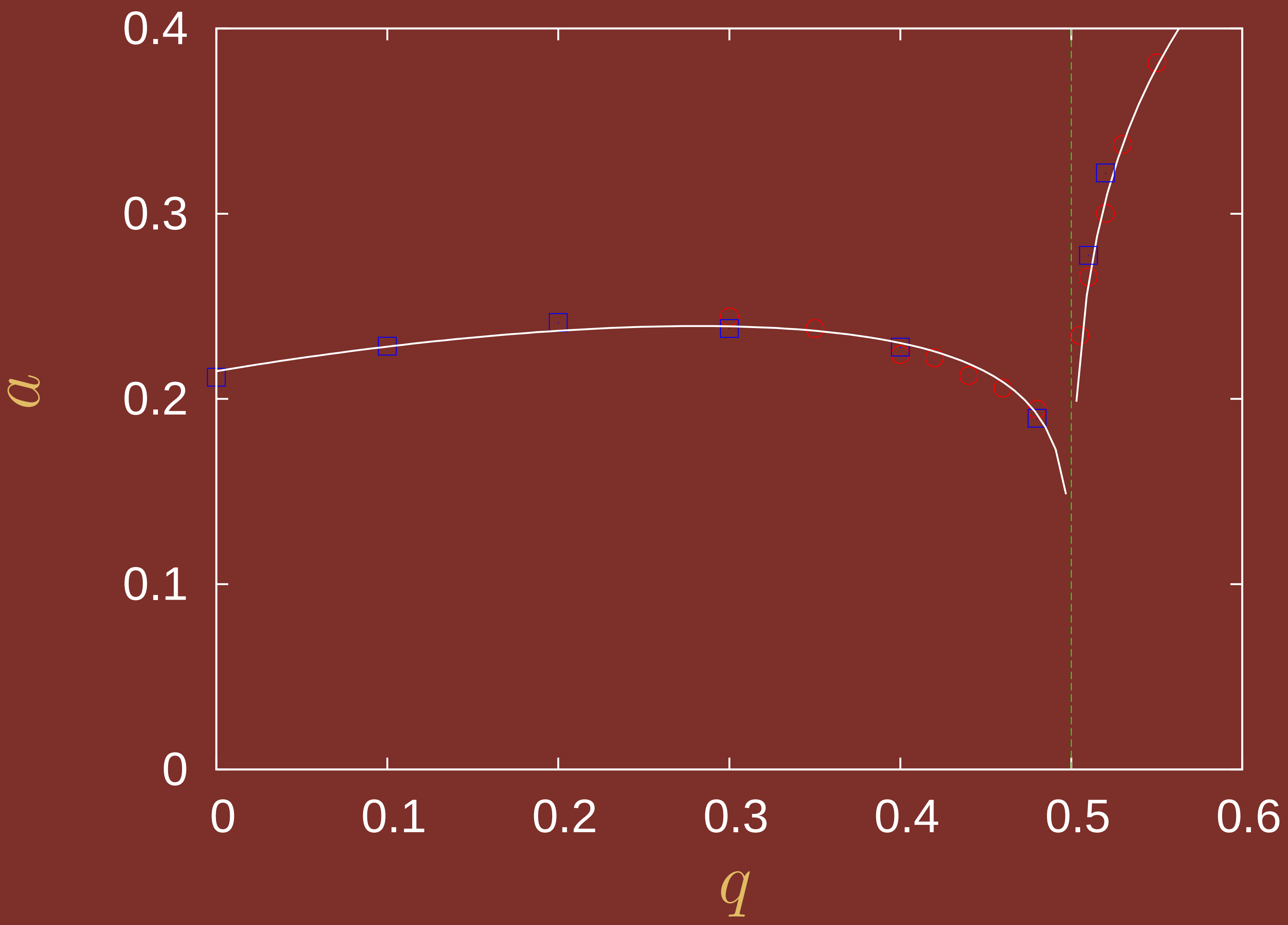
Persistence at $T_c(q)$

Sellitto, de Martino, Caccioli and Arenzon, PRL 105 (2010) 265704



Persistence at $T_c(q)$

Arenzon and Sellitto, 2011



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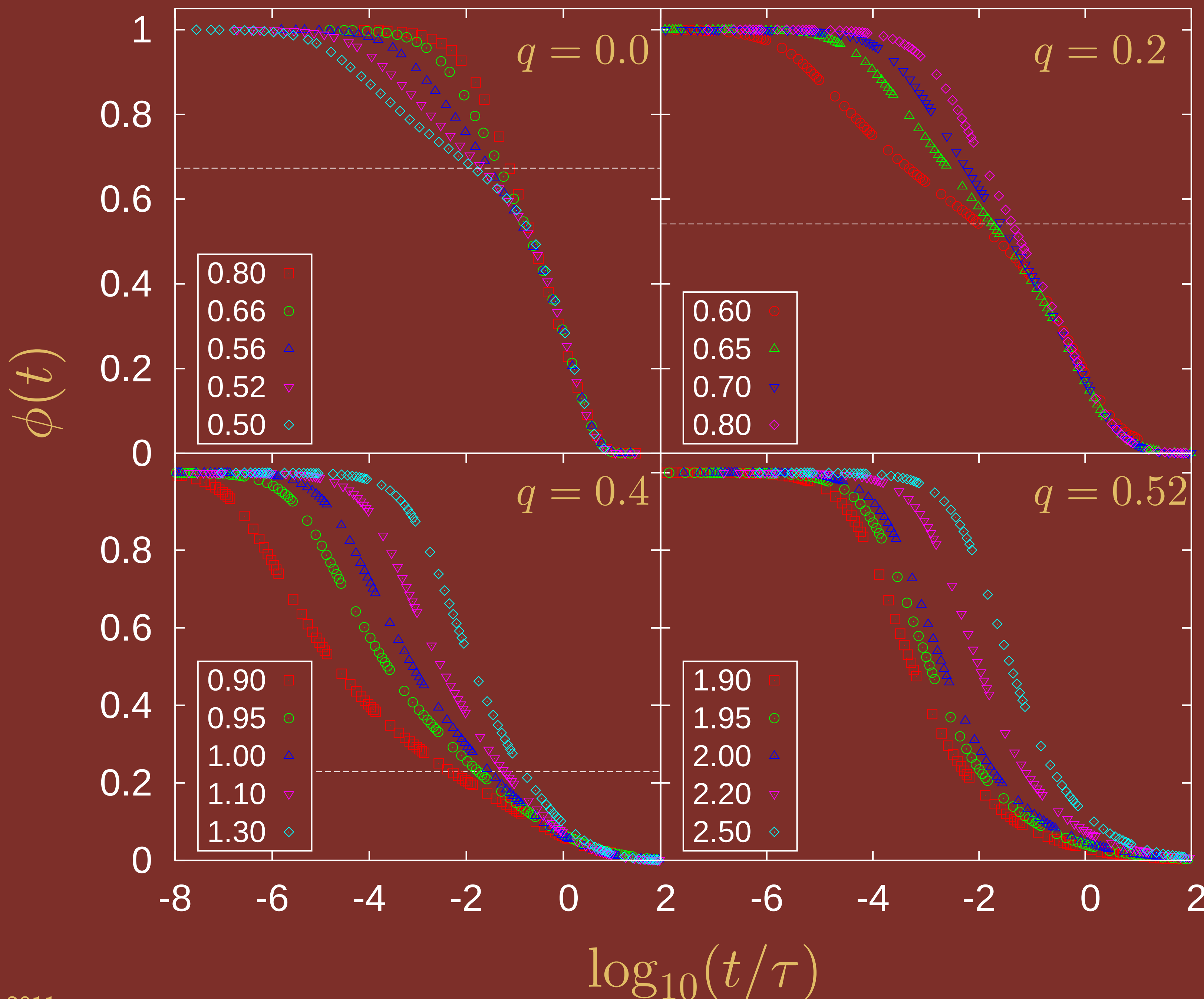
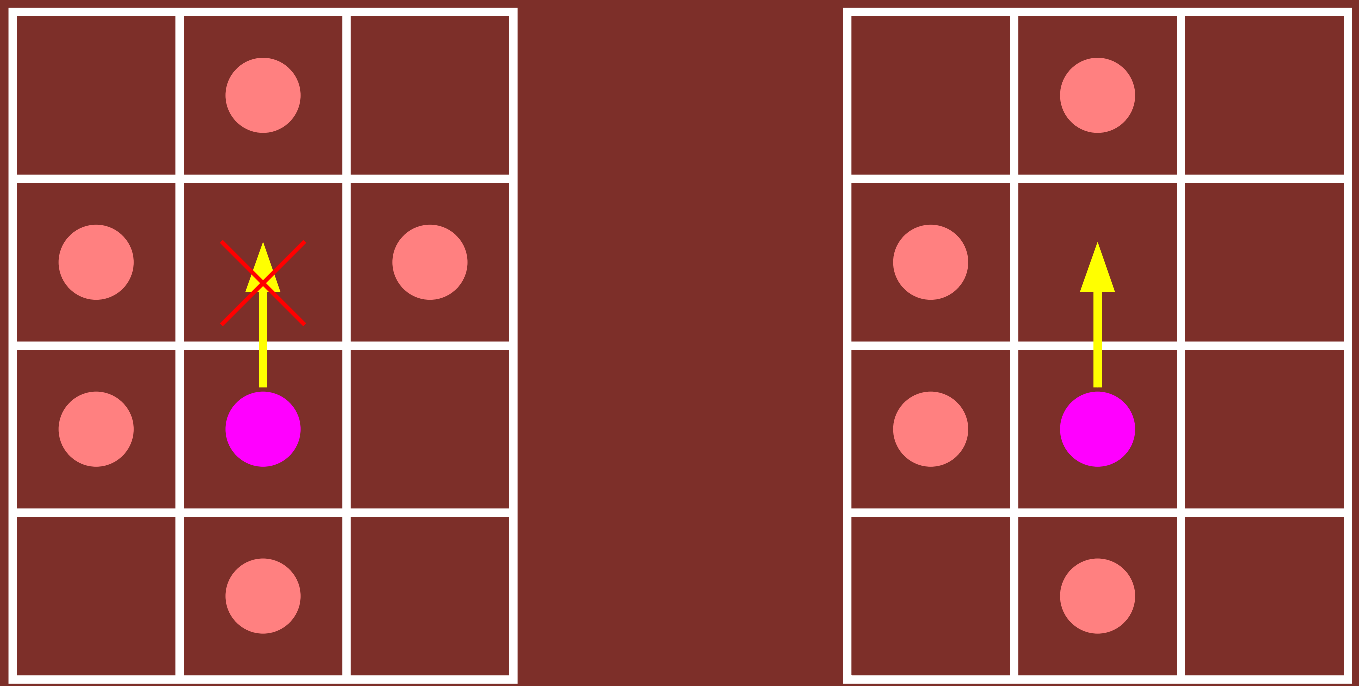


Kob-Andersen

Kob and Andersen, PRE 58 (1993) 4364

- cage effect
- no static interaction but hardcore exclusion: $\mathcal{H} = 0$
- N particles on a d-dimensional lattice diffusing if
  - the neighbor is empty and
  - the particle, before and after the jump, has less than m occupied neighbors
- EX.: $d = 2$, $m = 3$



- Other extensions: static atraction (reentrant behavior), finite dimensions.

Conclusions

- Facilitated spin mixtures with a crossover from a discontinuous to a continuous glass transition.
- Equivalent results are obtained for fixed facilitation and distributed connectivity.
- Microscopic realization of MCT for quenched-annealed binary mixtures:
  - although very schematic model,
  - quantitative agreement!

  We thus probe the universality of MCT beyond the context in which it was derived.