The role of diffusion in nonequilibrium phase transitions

Géza Ódor MTA MFA Hungary

- One of the primary goals is to explore universality classes like in equilibrium statistical physics
- Due to the lack of Gibbs distribution phase transitions (PT) may occur in low dimensions
- Which factors determine the PT universility class of a model of short range interactions ? Besides the spatial dimensions, boundaries, inhomogenities:
  1) Symmetries, conservation laws like in equilibrium (BAW2 ...)
  2) Initial conditions (temporal boundary condition) (PCP ...)
  3) Topological effects in low dimensions (multi-comp systems...)
  4) Dynamically generated long range memory (coupled systems...)
  5) Mean-field classes of RD : nA -> (n+k)A, mA-> (m-l)A --> /.
  6) For competing dynamics (diffusion) --> /.

See also: *G. Ódor, Rev. Mod. Phys. 76 (2004) no. 3.*

Mean-field classes of site restricted, one-component reaction-diffusion systems

- General, reaction-diffusion systems :

Order parameter ρ

$$n A \xrightarrow{\sigma} (n+k) A \qquad m A \xrightarrow{\lambda} (m-l) A \qquad 0\,A \overset{D}{\Leftrightarrow} A0$$

$$\partial \rho / \partial t = a k \sigma \rho^{n} (1-\rho)^{k} - a l \lambda \rho^{m}$$

$$\rho(t) \propto t^{-\alpha}$$
$$\rho(\infty) \propto \epsilon^{\beta}$$

- n = m : $\beta = 1, \alpha = 1/n$ $\qquad \sigma_c = l/(k+l)$
- n < m : $\beta = 1/(m-n), \alpha = 1/(m-1)$ $\qquad \sigma_c = 0$
- n > m : First order transition

n és m determine the mean-field class!
Diffusion does not play a role.

G. Ódor: PRE 67, 056114 (2003)

The dynamical cluster mean-field method

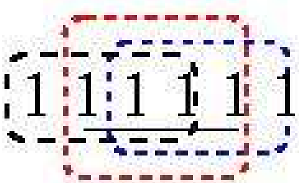
Master equations for N=1,2,... block probablities:

$\partial P_N(s_i)/\partial t = f(P_N(s_i)), \quad s_i = 0,1 \qquad P_{abcde} \simeq P_{abcd} P_{bcde} / P_{bcd}$

Example 4-Blocks:

Conf. 1 Conf. 2

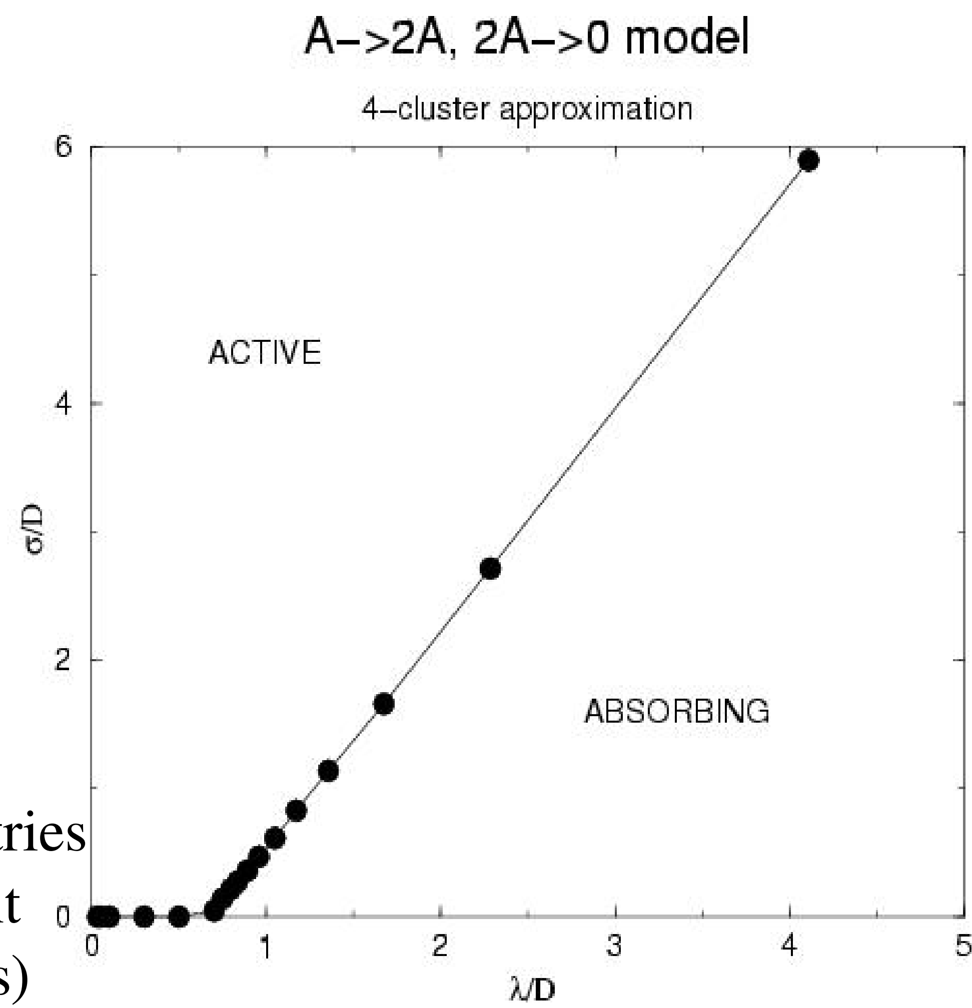
ANN



--> 1 1 1 1 0 0

$$\lambda \frac{P_{1111} P_{1111} P_{1111}}{\underbrace{(P_{1110} + P_{1111})}_{P_{111}}^{2}}$$

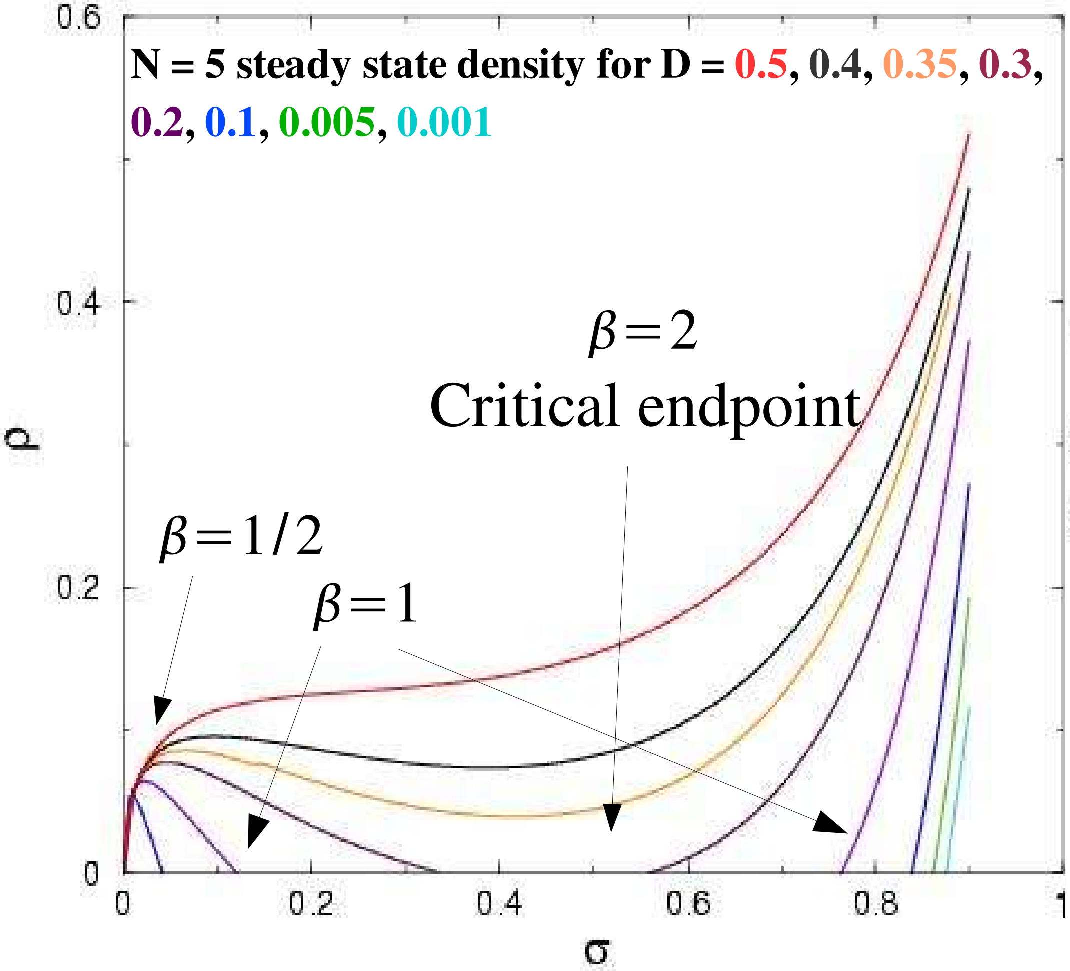
Taking into account symmetries for N=8 case 136 independent variables (block. probabilities)

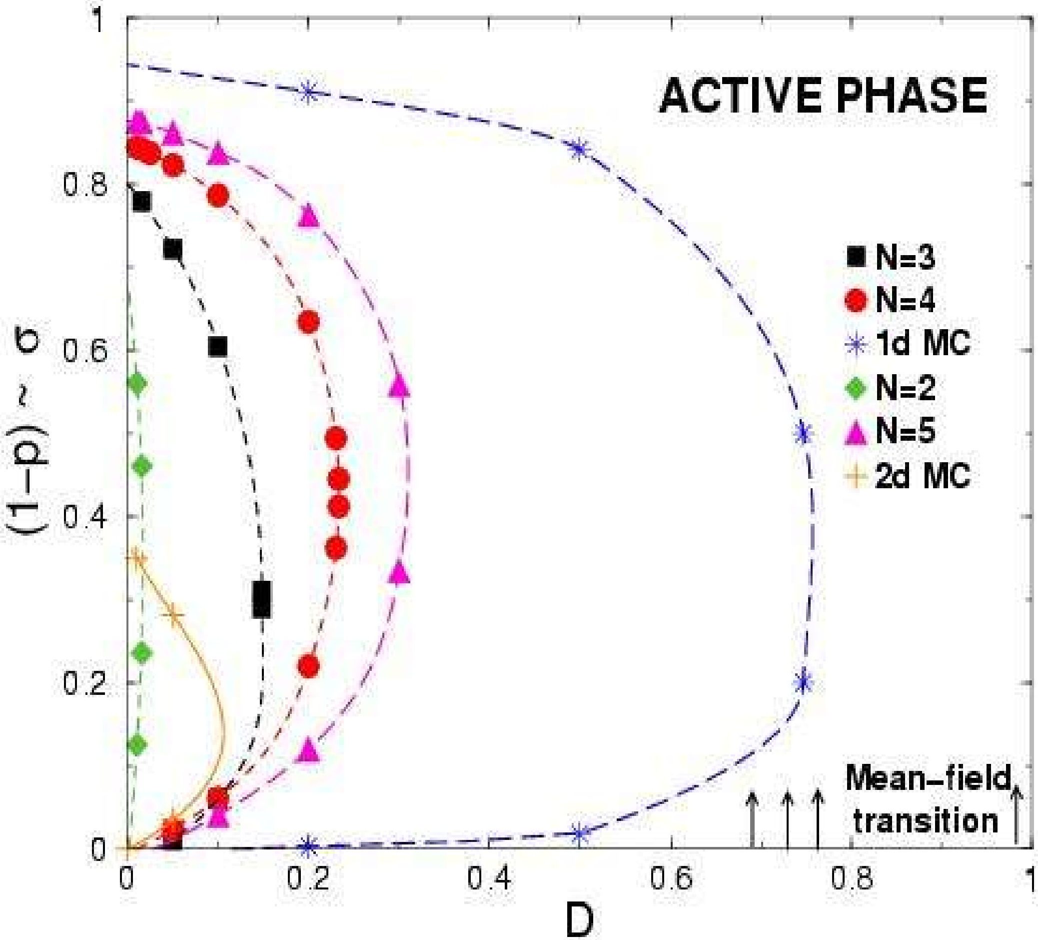


Cluster approximations for: 2A -> 3A, 4A -> 0 model

Steady state density for N >= 2 (diffusion dependence).

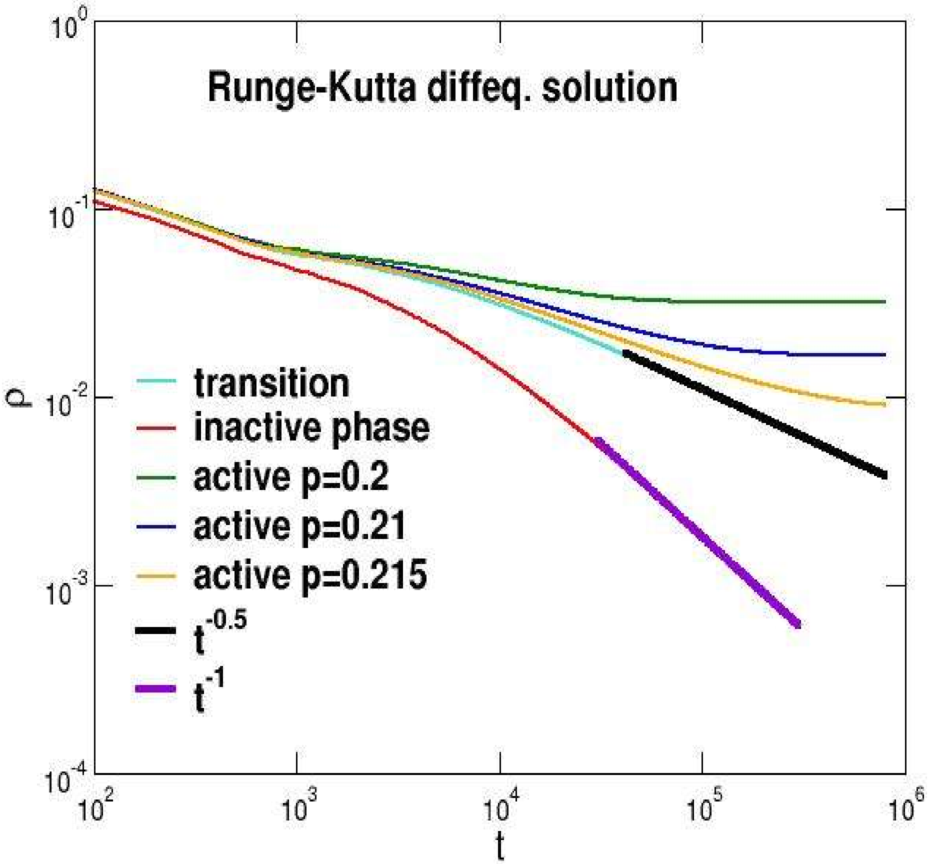
Unexpected phase transitions for $\sigma_c > 0$, with $\beta=1$ (*for n < m MF:* $\sigma_c = 0$)





Cluster approximations for: 2A -> 3A, 4A -> 0 model

Density decay solution for N = 3 at D=0.05 near σ_c> 0 critical point with exponent $\alpha = 0.5$ (2A -> 3A, 2A -> 0 (PCPD) behavior)



Simulations in 1 and 2 dimension support N-cluster results:

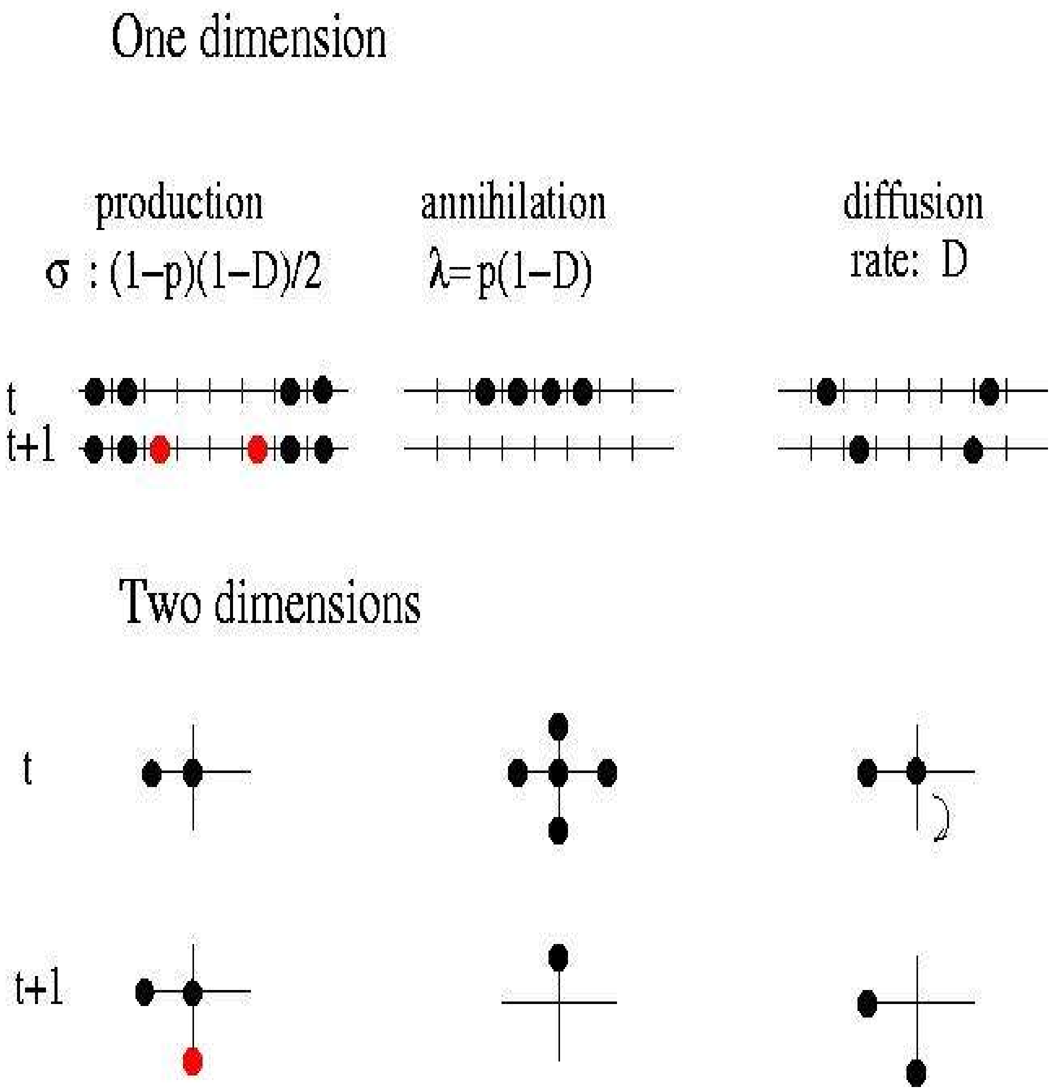
G. Ódor, PRE 69, 036112 (2004)

G. Ódor: cond-mat/0403562

Unexpected by perturbative RG

For low diffusions the : 2A->3A->4A->0 process becomes relevant !

Lattice simulations

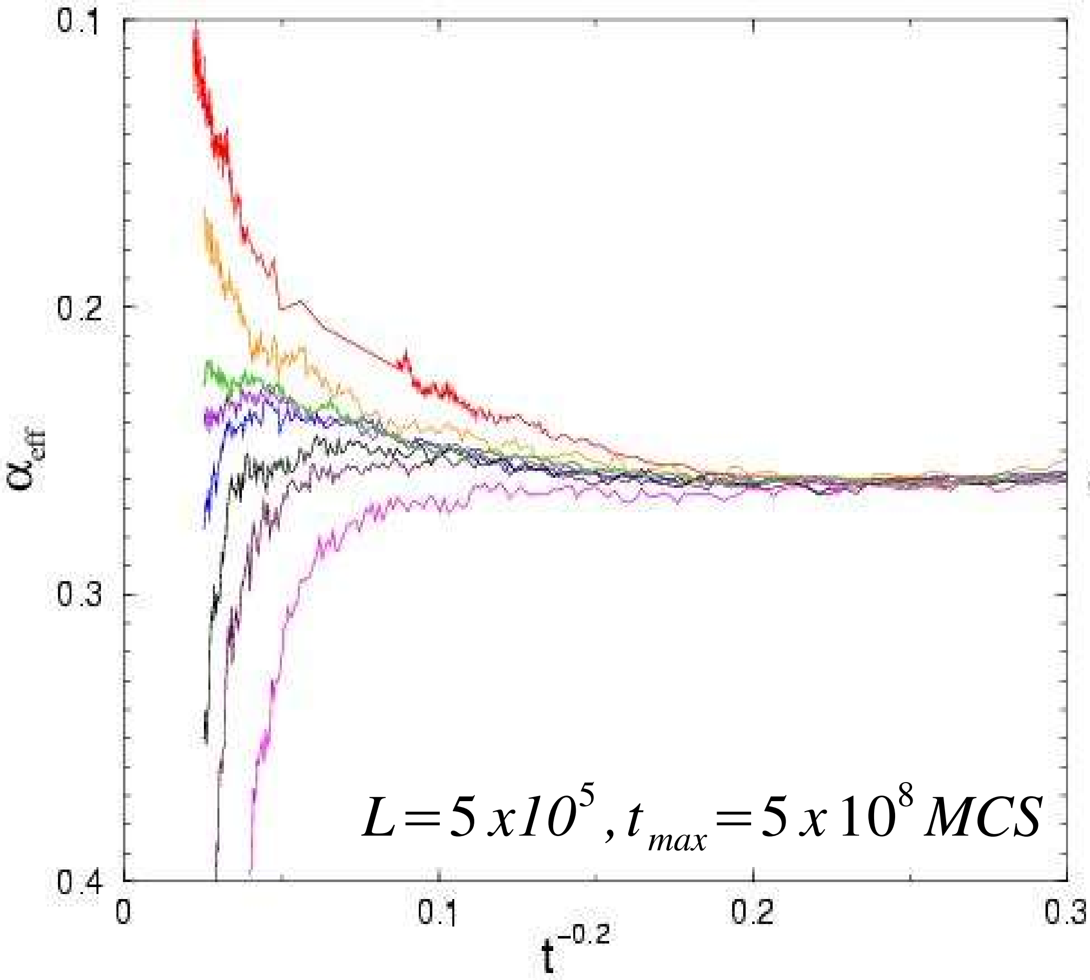


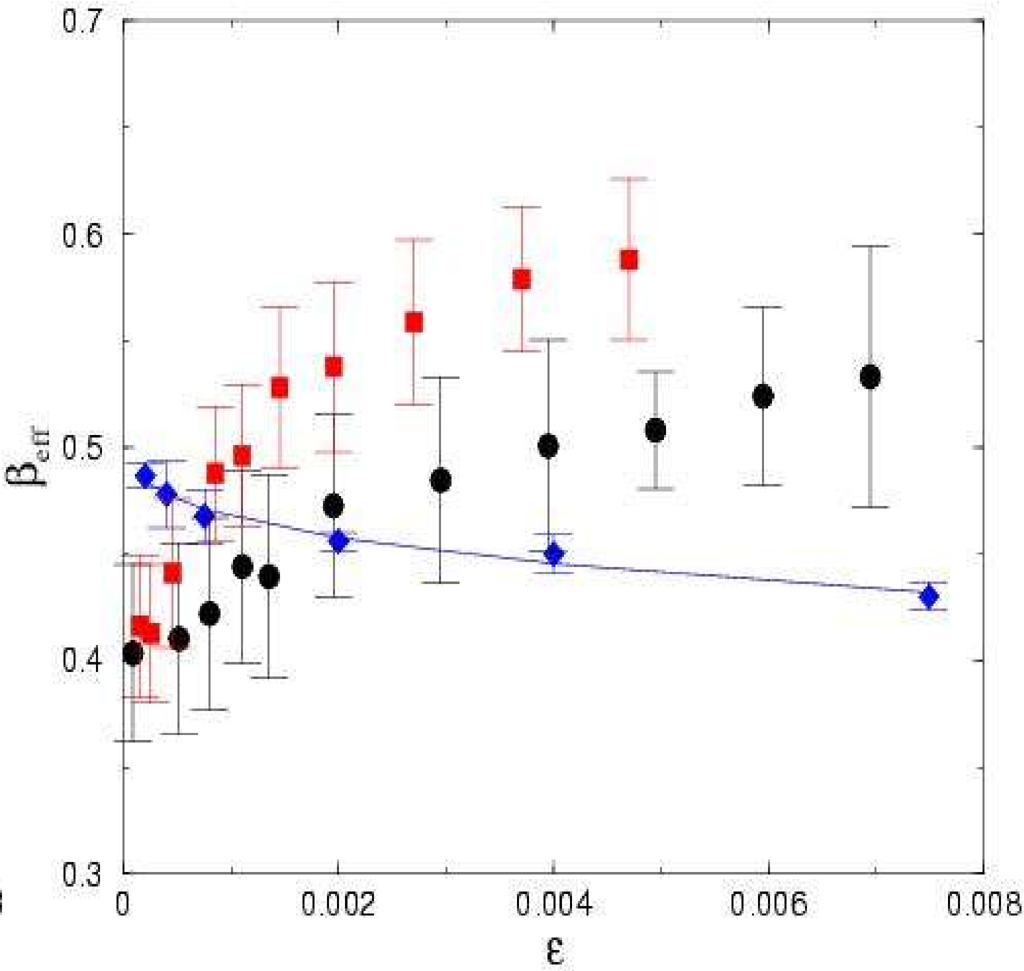
- Random sequential update of occupied sites
- Full or random half filled initial conditions
- L <= 500 000 in 1d,
  L <= 7000 x 7000 in 2d
  periodic boundary conditions
- t_max <= 5x10^8 MCS
- Master-slave parallel algotihms on international computing GRIDS (~ 100 - 500 CPU-s)

Simulation results for the 2A -> 3A, 4A -> 0 model in 1 dimension

Density decay local exponents with : $\alpha = 0.21(2)$ (~PCPD), at $D = 0.5$, $\sigma_c = 0.42075$.

Steady state local exponents near σ_c=0.42 for D = 0.5, 0.2, with $\beta = 0.40(2)$ (~PCPD). For D = 0.9: only mean-field with β =1/2. 2A -> 0 process becomes irrelavant !



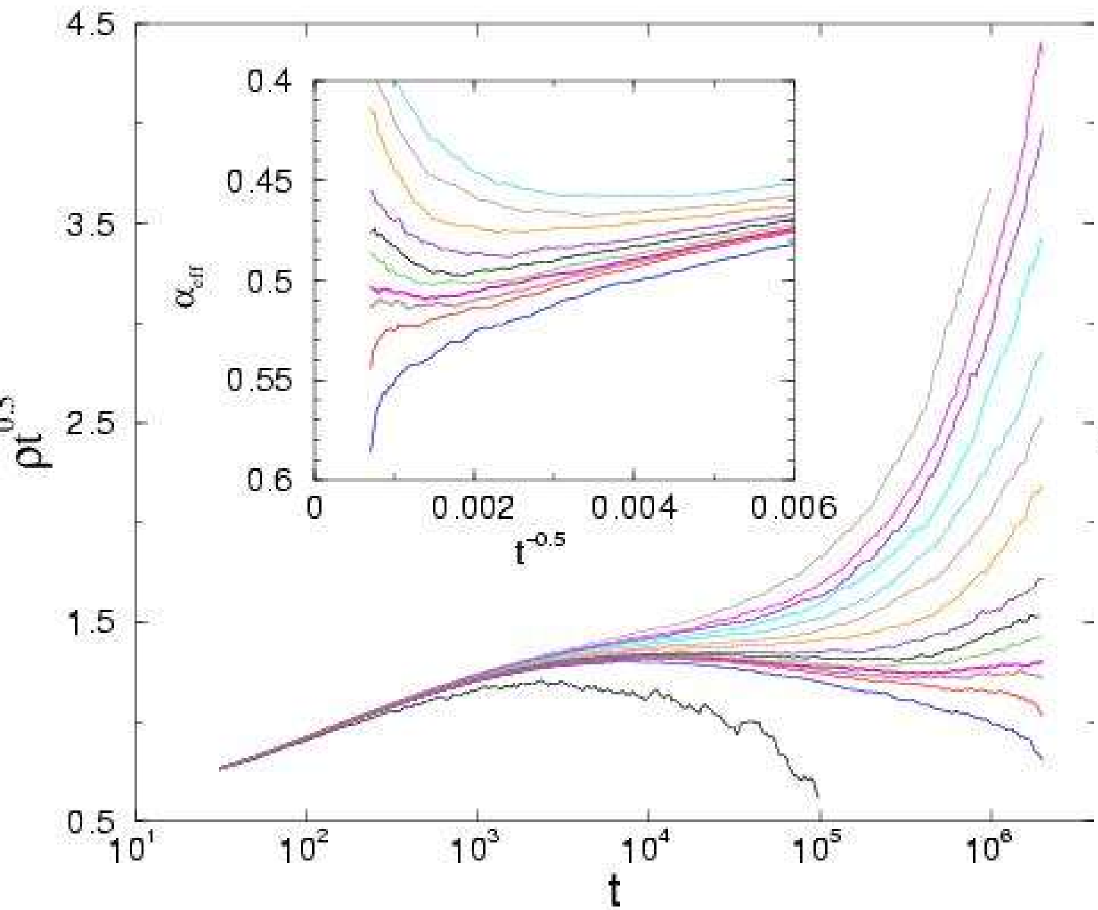


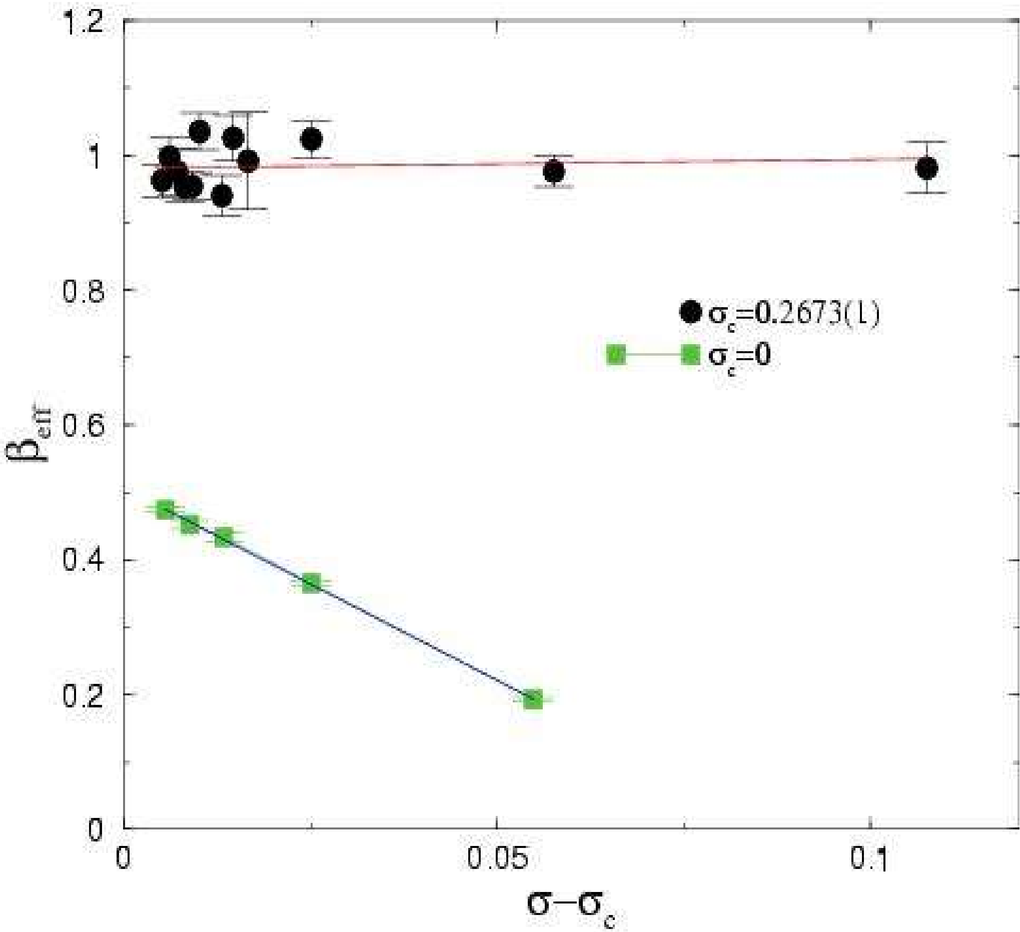
Simulation results for the 2A -> 3A, 4A -> 0 model in 2 dimensions

Density decay local exponents with :
$\alpha = 0.50(1)$ (MF-PCPD) at $\sigma_c = 0.26715$

$$L = 7000, t_{max} = 2\,x\,10^6\,MCS\,,\,D = 0.05$$

Steady state local exponents at D = 0.05
with $\beta = 0.98(2)$ (MF-PCPD).
For D=0.9: only mean-field with β=1/2.
2A -> 0 process becomes irrelavant !





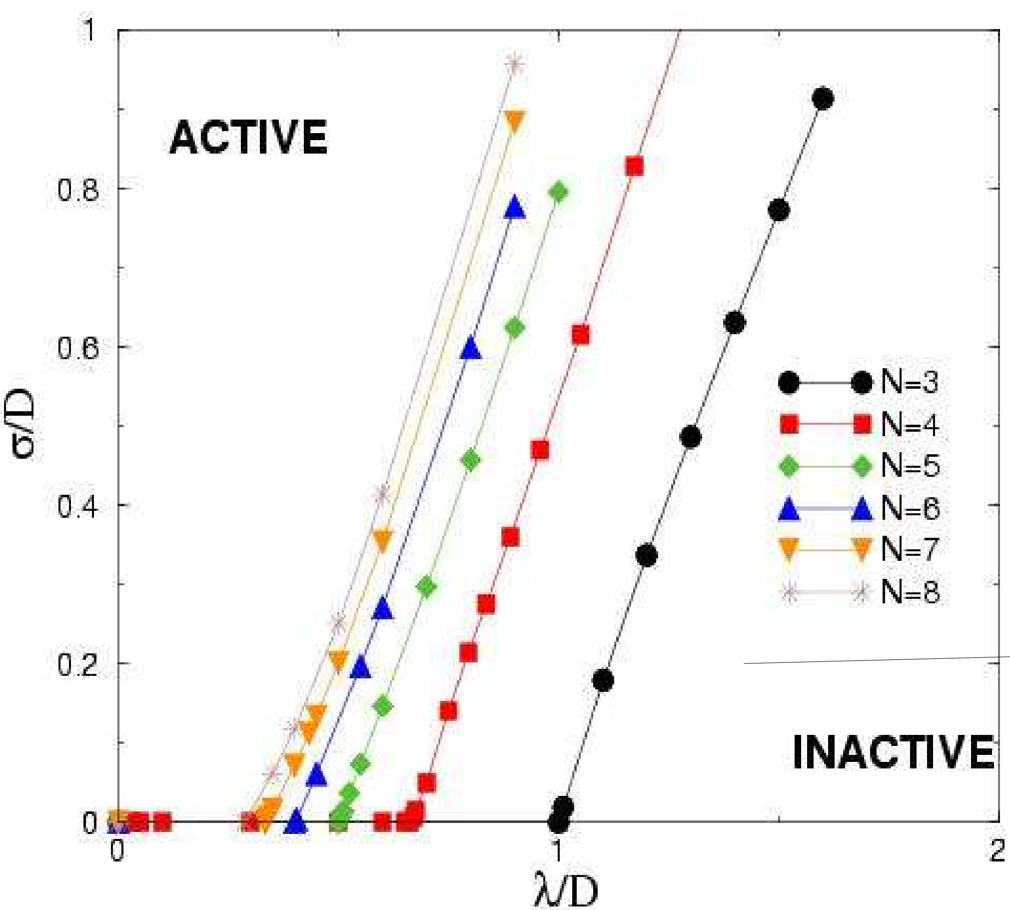
Cluster mean-field for BARW(unary)

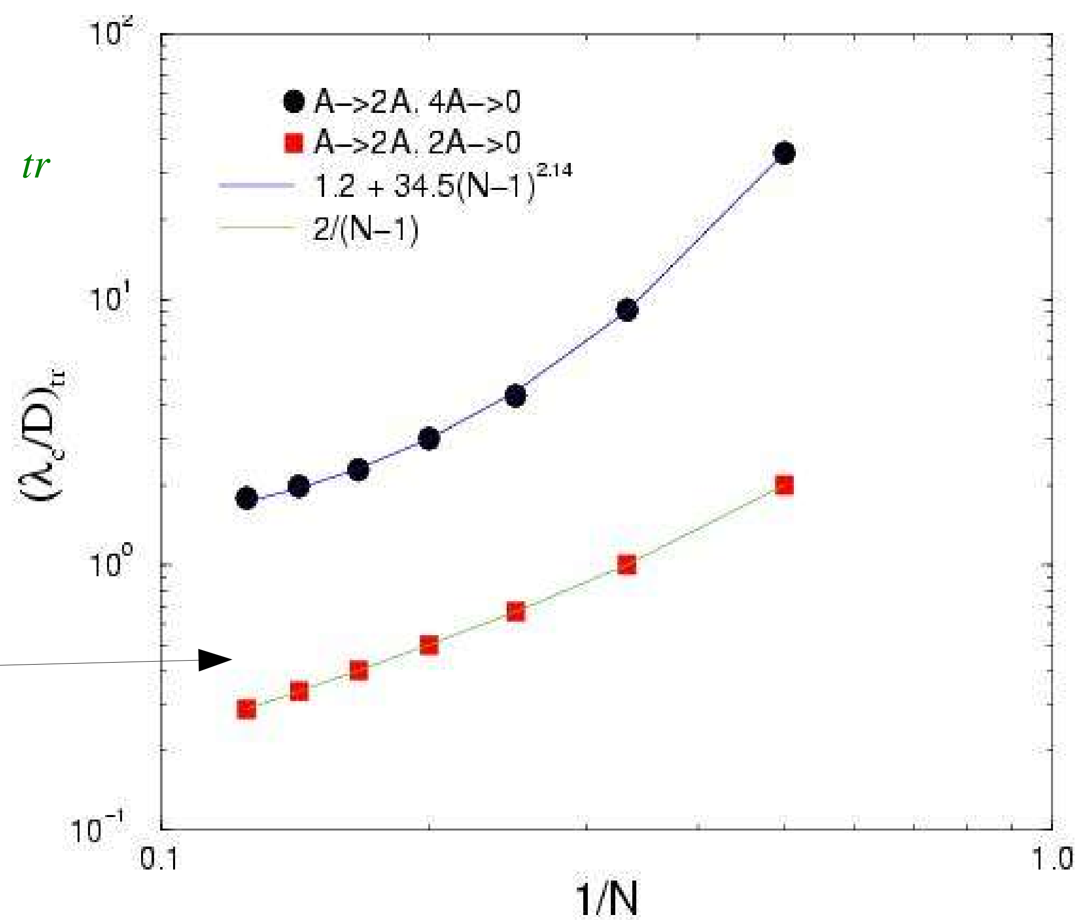
1) A -> 2A, 2A -> 0: (Canet, Chaté, Delamotte, cond-mat/0403432, NPRG)

Exact relation: $(\lambda_c/D)_{tr} = 2/(N-1)$ found. For 1d: $(\lambda_c/D)_{tr}$ -> 0 as N -> inf.

2) A -> 2A, 4A -> 0: $(\lambda_c/D)_{tr}$ -> ~ 1.2 as N -> inf.

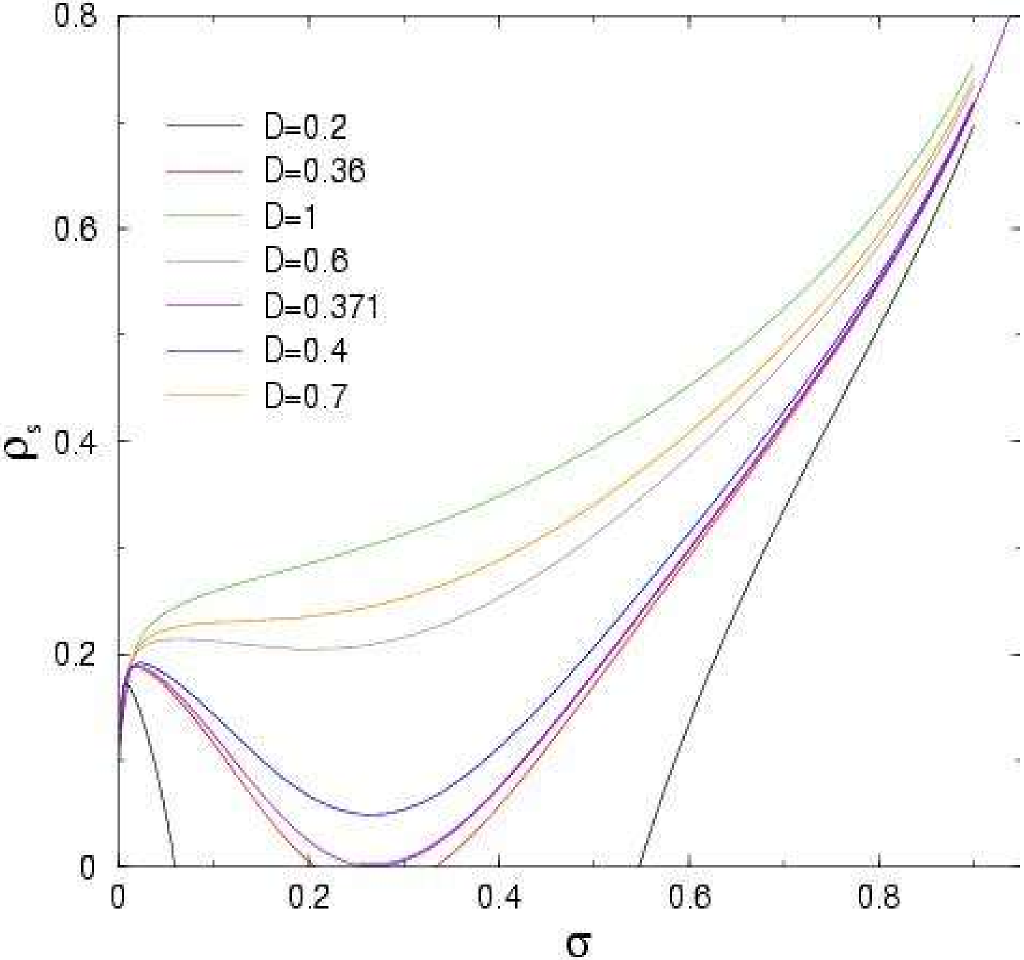
$$MF: m > n: \beta = 1/(m-n), \alpha = 1/(m-1), \sigma_c = 0$$



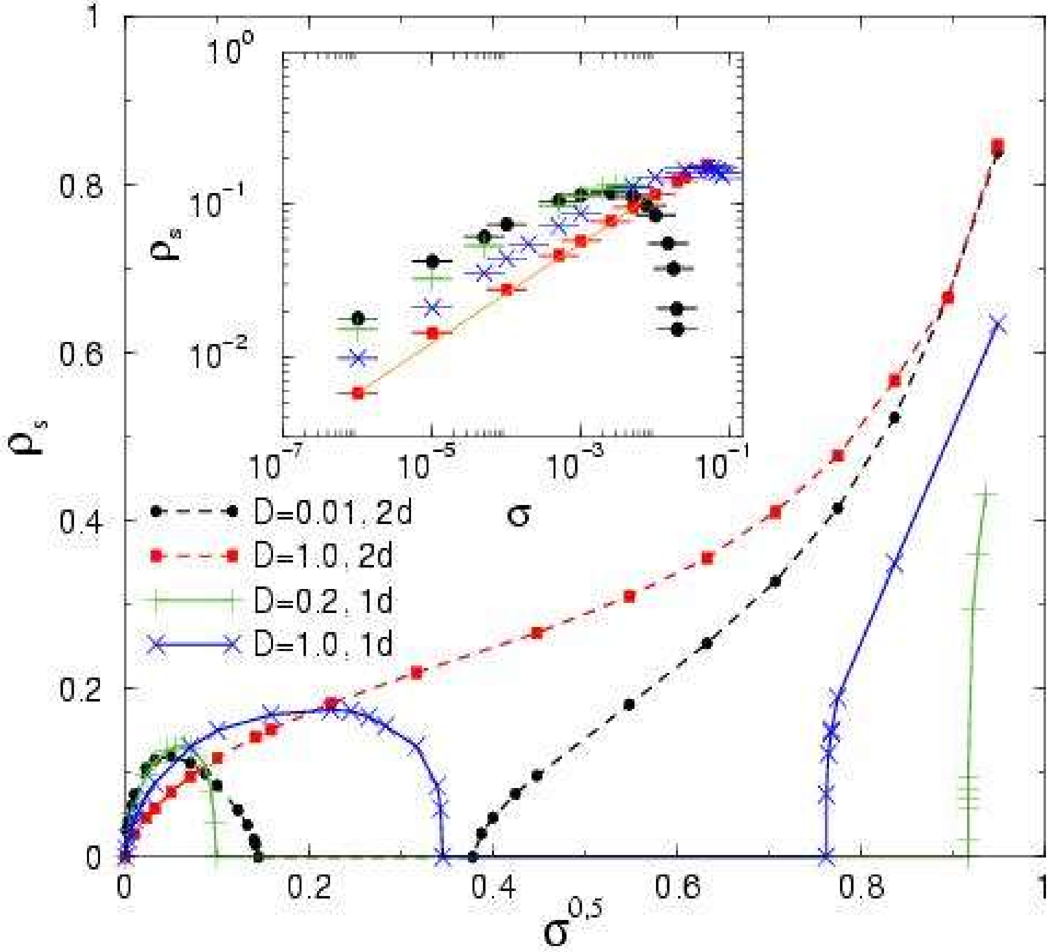


A->2A, 4A->0: Reentrant phase diagram

N-cluster approximation



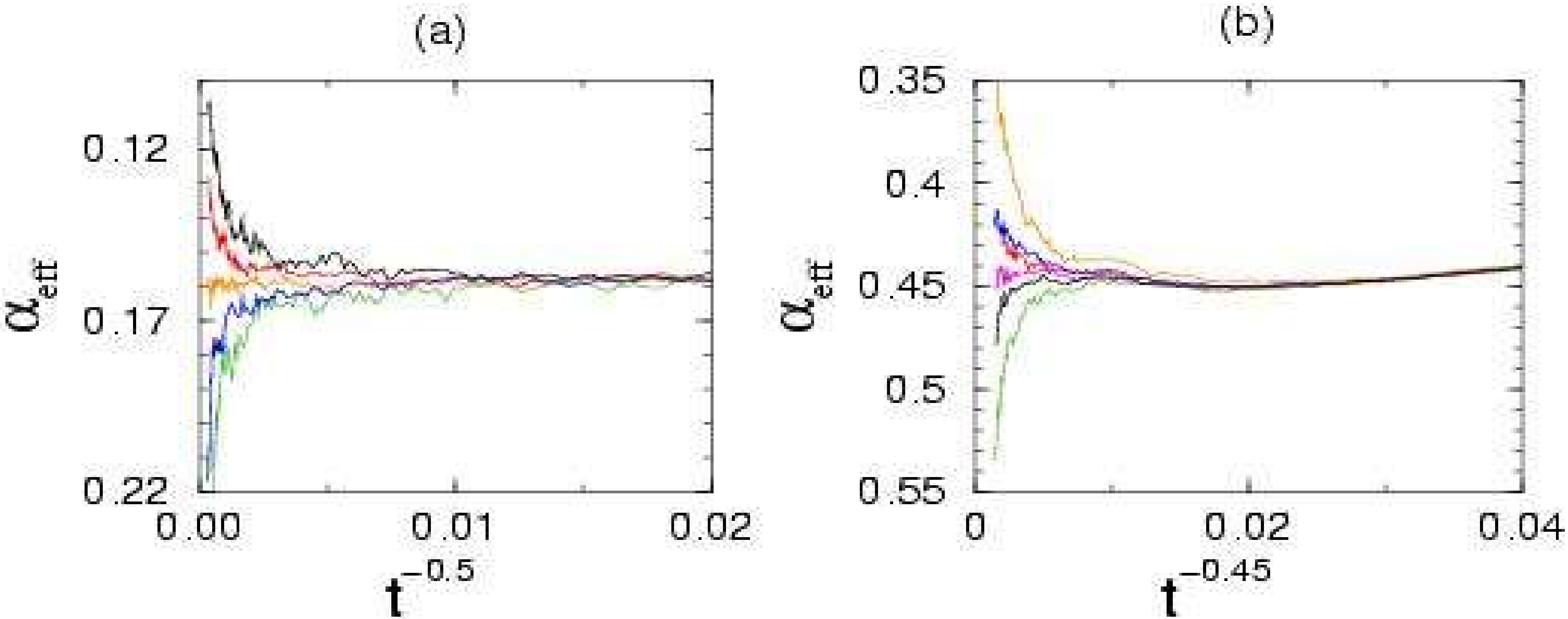
Simulations:
2d: L= 4000x4000, 1d: L= 100000



Critical point decay at $\sigma_c > 0$ in (a): one and (b): two dimensions

DP class value in 1d: $\alpha = 0.159464(6)$ (I. Jensen)

2d: $\alpha = 0.4505(10)$ (Voigt and Ziff)



For low diffusions the : A->2A->3A->4A->0 process becomes relevant !

Summary

- In general (site restricted) reaction-diffusion systems the mean-field universality class is determined by the number of reacting particles (n,m)
- Diffusion may become relevant in case of competing reactions by changing the phase diagram and introducing nontrivial fixed points
- Diffusion dependence has been found in similar systems:
  - *R. Dickman*: A -> 2A, 3A -> 0, *PRA42, 6985 (1990)*
  - *M. Paessens, G. Schütz :* bosonic PCPD, *JPA37, 4709 (2004)*
  - *N. Menyhárd, G. Ódor :* NEKIM-A, *PRE68, 056106 (2003)*
- Perturbative RG results should be revised !
- References : *G. Ódor: PRE 67, 056114 (2003)*
  G. Ódor: PRE 67, 016111 (2003)
  G. Ódor: PRE 69, 036112 (2004)
  G. Ódor: Rev. Mod. Phys. 76 (2004) , cond-mat/0205644
  G. Ódor: cond-mat/0403562, to appear in PRE
  G. Ódor: cond-mat/0406247