Non-Equilibrium features of inelastic gases

Renaud Lambiotte
Supras, ULG (Belgium)

Overview

- Introduction
- HCS: anomalous velocity distributions
- Mixtures: non-equipartition of energy
- Granular Demon experiment: order-disorder transition, hysteresis, metastability, segregation, oscillations...
- Conclusion

Grains: smooth inelastic hard spheres (IHS)

$$\mathbf{v}_i^* = \mathbf{v}_i - \frac{(1+\alpha)}{2}\boldsymbol{\epsilon}(\boldsymbol{\epsilon}.\mathbf{v}_{ij})$$

$$\mathbf{v}_j^* = \mathbf{v}_j + \frac{(1+\alpha)}{2}\boldsymbol{\epsilon}(\boldsymbol{\epsilon}.\mathbf{v}_{ij})$$

Inelasticity coefficient:

$$\alpha \in]0:1]$$

The granular temperature $T(\mathbf{r};t)$

$$\frac{d}{2}T(\mathbf{r};t) = \frac{1}{n(\mathbf{r};t)}\int d\mathbf{v}\ \frac{m}{2}V^2 f(\mathbf{r},\mathbf{v};t) \qquad \mathbf{V} = \mathbf{v} - \mathbf{u}(\mathbf{r};t)$$

→ kinetic definition

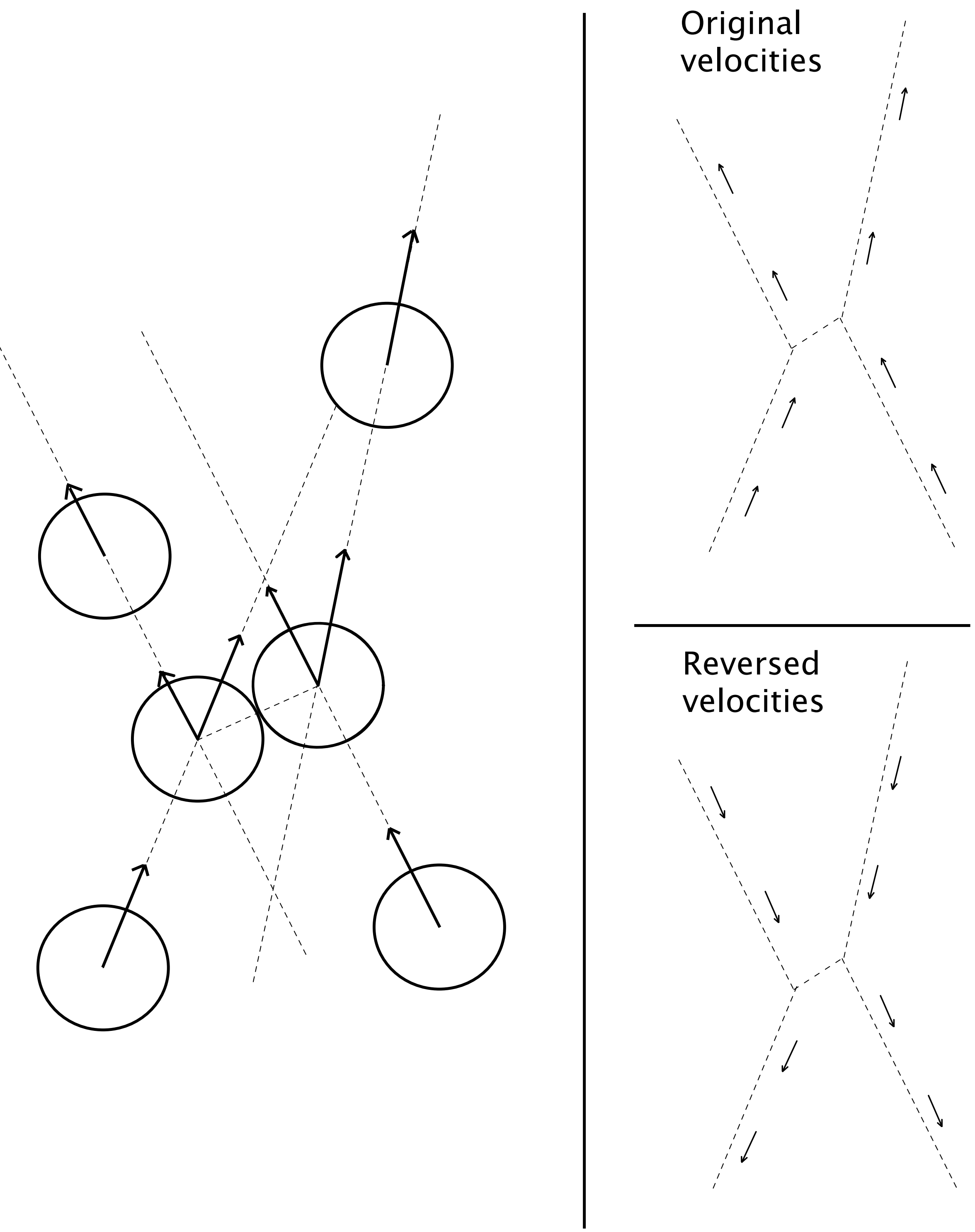
~ agitation of the grains

~ width of their velocity distribution

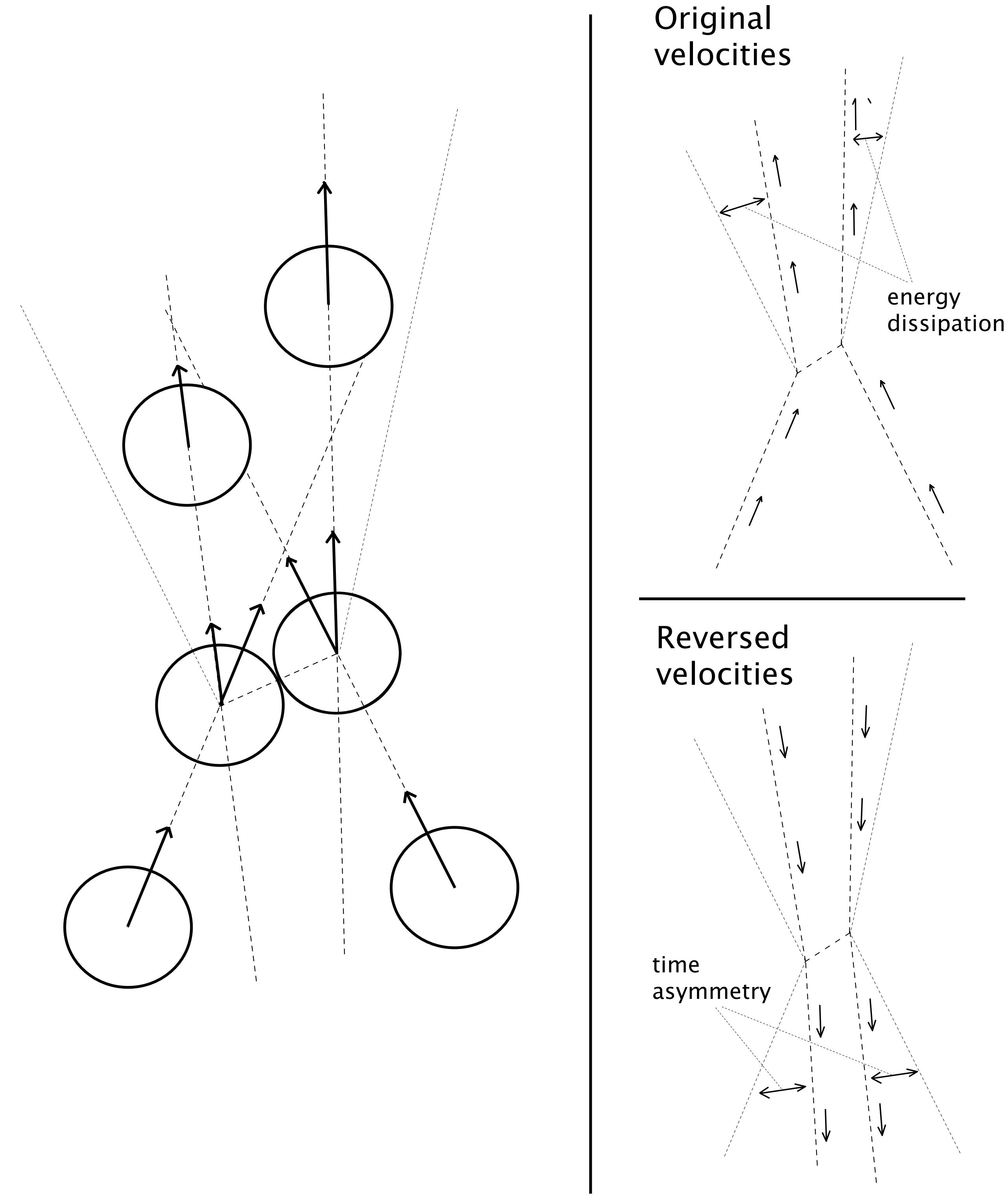
Low density + low inelasticity: inelastic Boltzmann equation

$$\frac{\partial f(\mathbf{r},\mathbf{v}_1;t)}{\partial t} + \mathbf{v}.\frac{\partial f(\mathbf{r},\mathbf{v}_1;t)}{\partial \mathbf{r}} = \sigma^{d-1}\int d\boldsymbol{\epsilon} d\mathbf{v}_2(\boldsymbol{\epsilon}.\mathbf{v}_{12})\Theta(\boldsymbol{\epsilon}.\mathbf{v}_{12})[\frac{1}{\alpha^2}f(\mathbf{r},\mathbf{v}_1^{'};t)f(\mathbf{r},\mathbf{v}_2^{'};t) - f(\mathbf{r},\mathbf{v}_1;t)f(\mathbf{r},\mathbf{v}_2;t)]$$

phase space contraction + time asymmetry



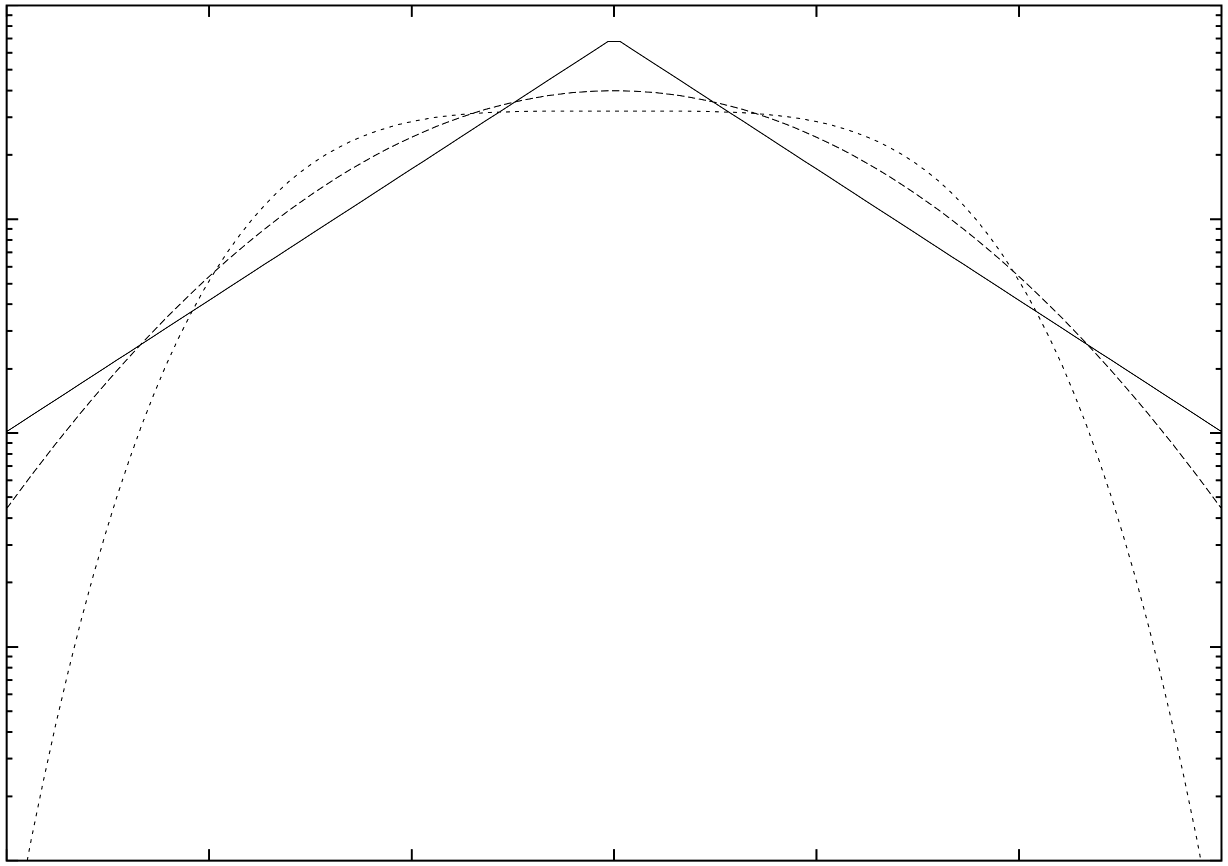
Elastic discs: energy conservation + time symmetry



Inelastic discs: no energy conservation + time asymmetry

Homogeneous Cooling State

self-similar solutions $f(\mathbf{v};t) = \frac{n}{v_0^d(t)}\tilde{f}(\frac{v}{v_0(t)})$ $\quad T(t) = \frac{1}{2}mv_0^2(t)$



In general, these asymptotic distributions exhibit overpopulated high energy tails

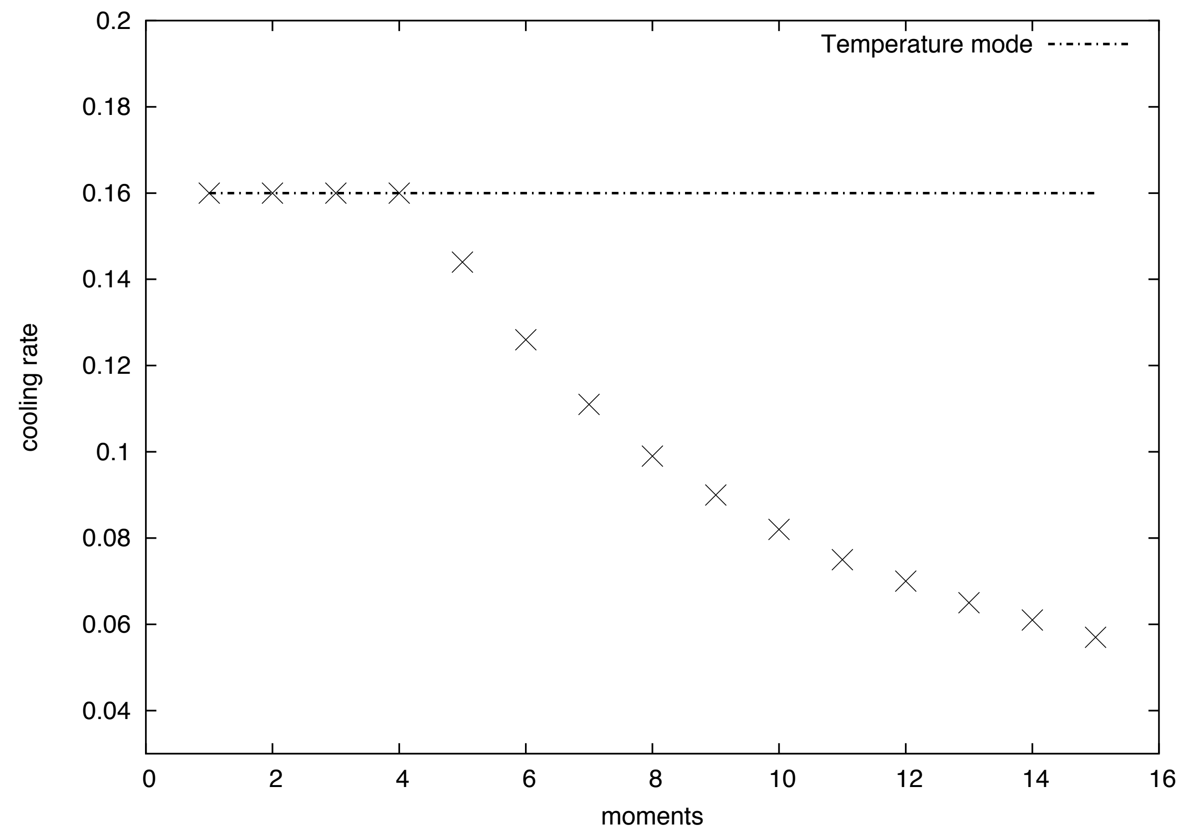
Simplified models => formation of non-Maxwellian tails: Inelastic Maxwell Models

Simplified cross section $v_{12} \approx \sqrt{T}$

Analytically tractable: Fourier analysis...

$$\frac{\partial f_1}{\partial t} + f_1 = \frac{1}{2\pi}\int d\theta d\mathbf{v}_2 \frac{1}{\alpha} f_1^{'} f_2^{'} \quad \text{<=>} \quad \frac{\partial \Phi(\mathbf{k};t)}{\partial t} + \Phi(\mathbf{k};t) = \frac{1}{2\pi}\int d\theta \Phi(\mathbf{k}_+;t)\Phi(\mathbf{k}_-;t)$$

IMM exhibit power laws, associated to multiscaling of the velocity moments



1D Lorentz model

Depending on their collisional history: different energy for the particles => favours overpopulated tails

$$\frac{\partial f(v;t)}{\partial t} = \frac{1}{\alpha} f(\frac{v}{\alpha};t) - f(v;t)$$

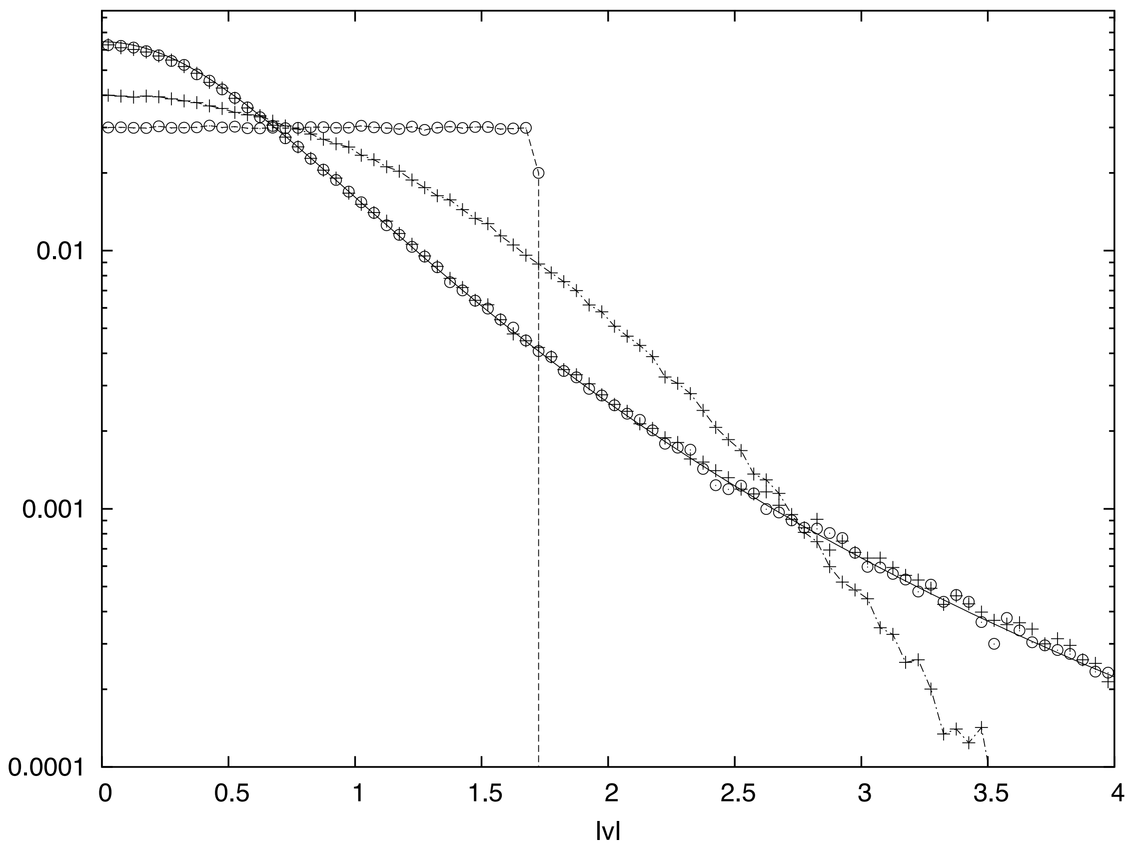
$$\frac{\partial \phi(k;t)}{\partial t} = \phi(\alpha k;t) - \phi(k;t)$$

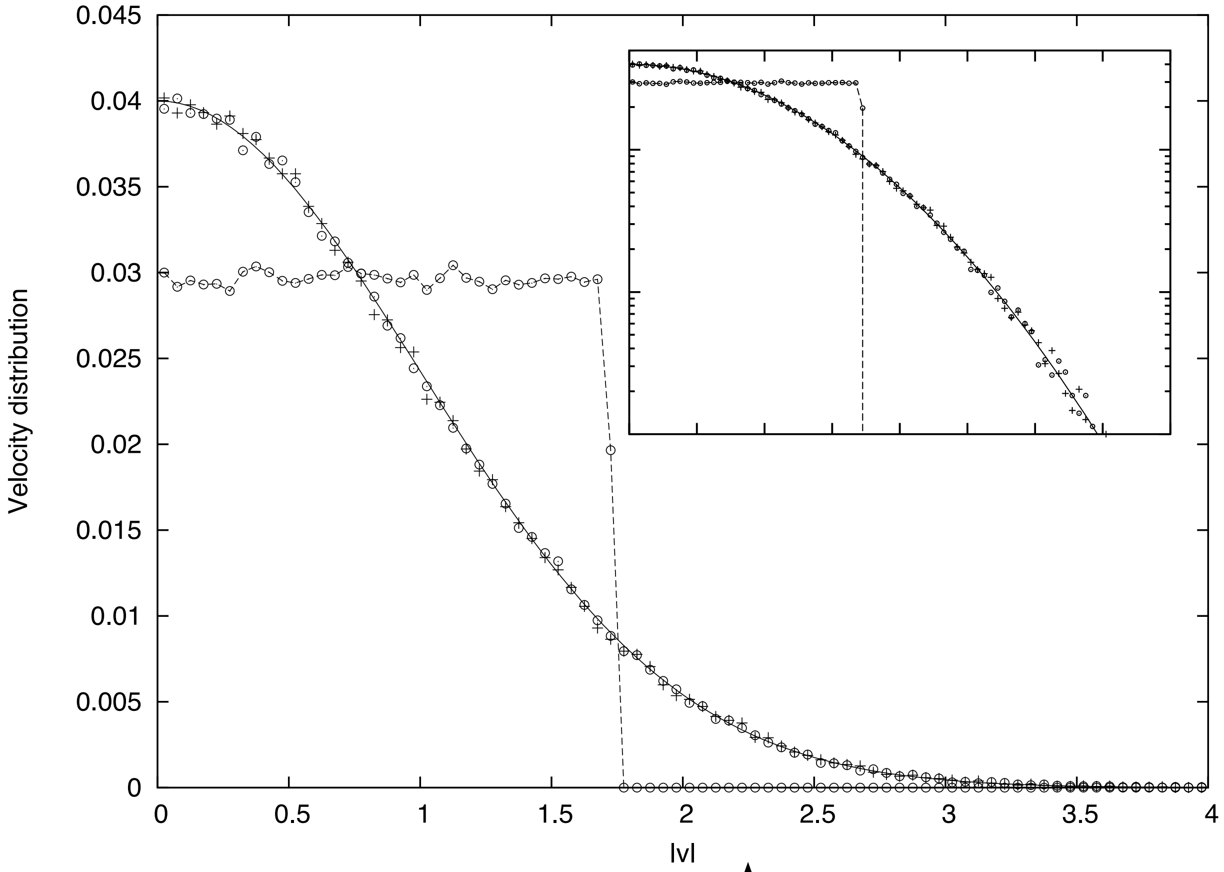
$$\phi(k;t) = \sum_{N=0}^{\infty} \frac{t^N e^{-t}}{N!} \phi_0(\alpha^N k;t)$$

$$\phi_N(k;t) = \phi_0(\alpha^N k;t)$$

Continuous time process

$$\frac{\partial f(v_1;t)}{\partial t} + f(v_1;t) = \int_{-\infty}^{\infty} dv_2 \; (\frac{1}{\alpha}) f(v_1^{'};t) f(v_2^{'};t)$$





$$f_{N+1}(v_1;t) = \int_{-\infty}^{\infty} dv_2 \; (\frac{1}{\alpha}) f_N(v_1^{'};t) f_N(v_2^{'};t)$$

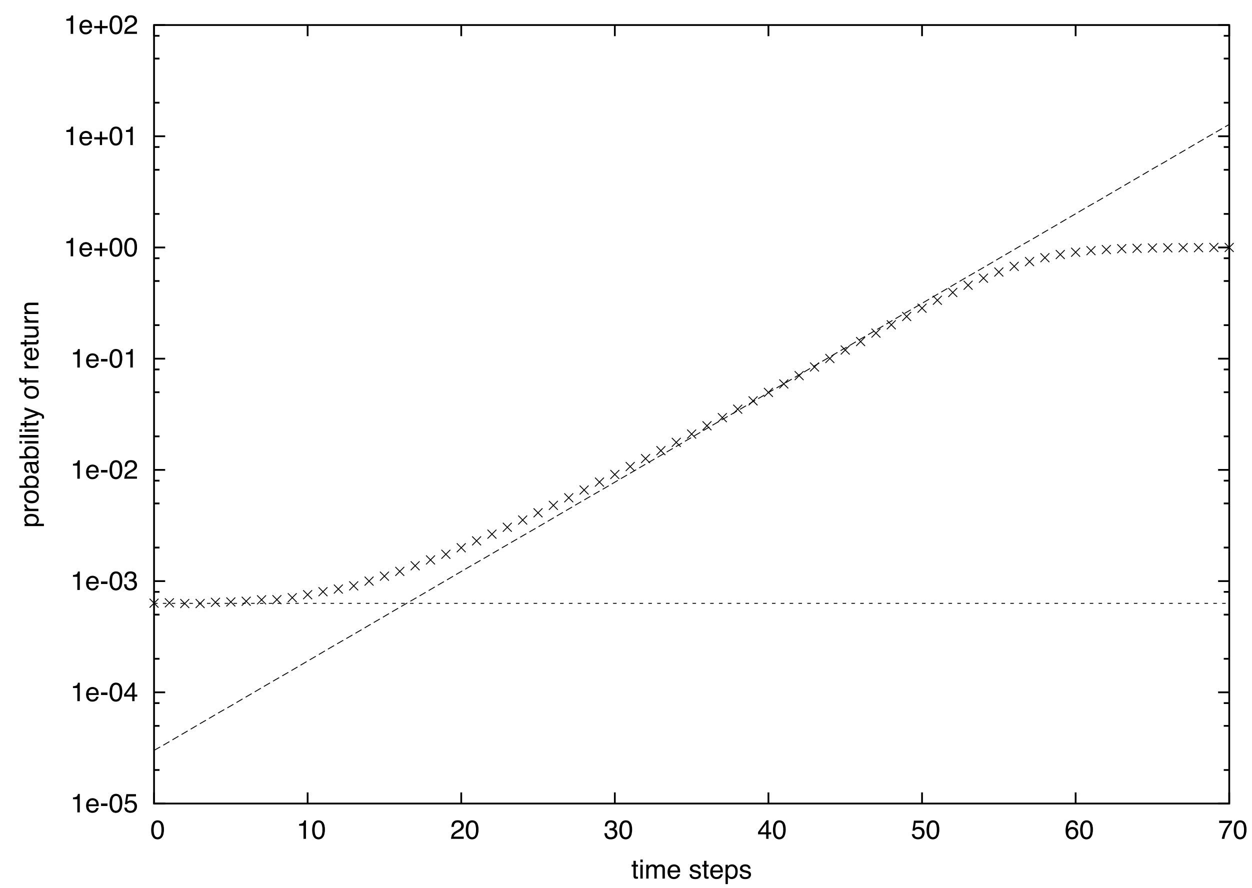
Discrete time process

In one dimension, a class of initial conditions converge toward a Lévy distribution

Equilibrium features: thermal bath

$$f(v) \rightarrow \frac{a}{\pi} \frac{1}{(a^2 + v^2)}$$

In simulations, truncated Lévy distribution: finite energy of the system.



BUT: 1) Asymptotic distribution depends on the modeling of the scattering cross section
2) comparison with a random walk is limited to Maxwell models

Equilibrium: microscopic time-reversibility + energy conservation

$$\frac{\partial f(\mathbf{v}_1)}{\partial t} = \int d\boldsymbol{\epsilon} d\mathbf{v}_2 (\boldsymbol{\epsilon}.\mathbf{v}_{12})\Theta(\boldsymbol{\epsilon}.\mathbf{v}_{12})[f_T(\mathbf{v}_1^{'})f_B(\mathbf{v}_2^{'}) - f_T(\mathbf{v}_1)f_B(\mathbf{v}_2)]$$

$$\Rightarrow \quad f_T(\mathbf{v}_1^{'})f_B(\mathbf{v}_2^{'}) = f_T(\mathbf{v}_1)f_B(\mathbf{v}_2)$$

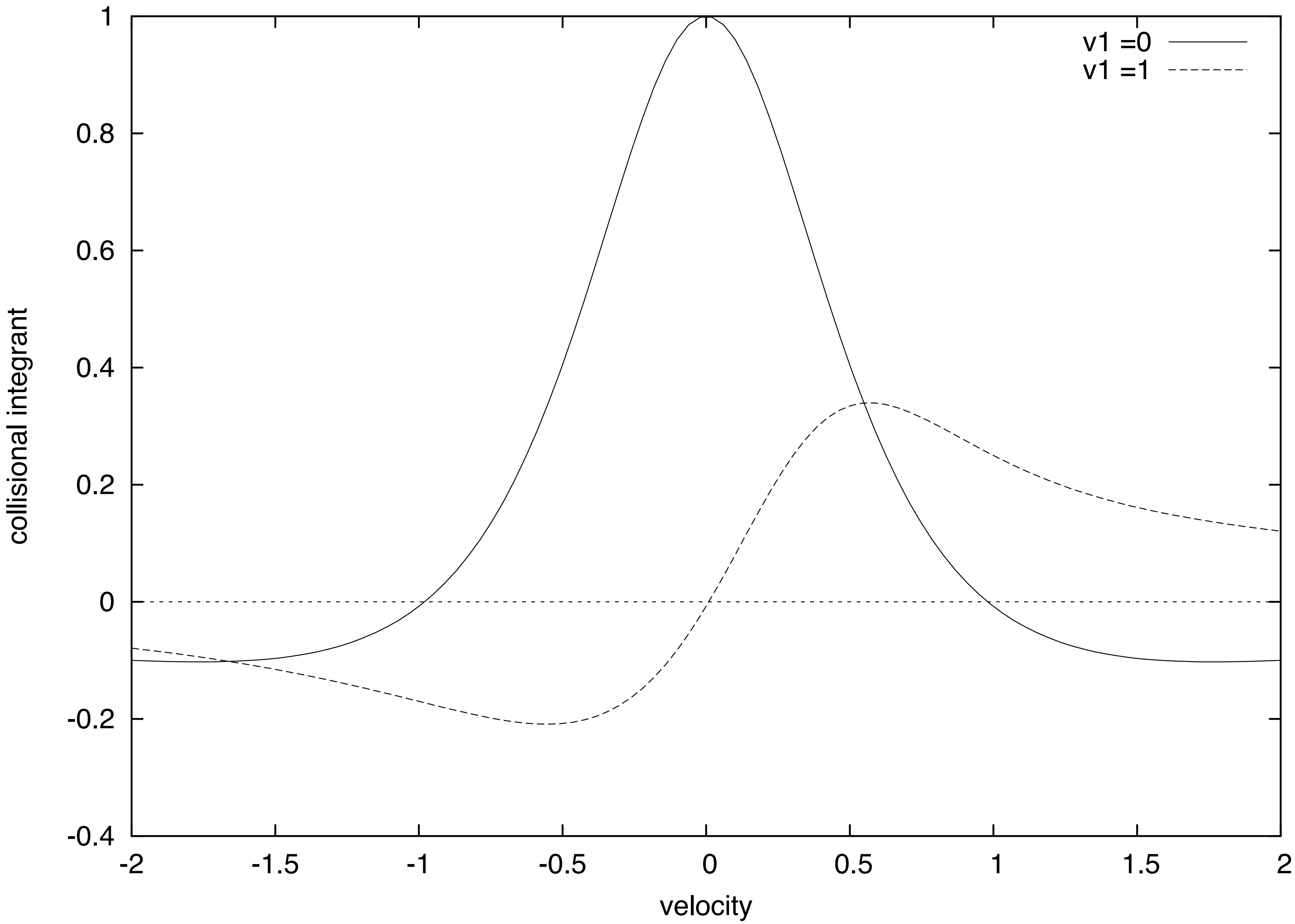
Non-equilibrium

$$\frac{\partial \phi(k;t)}{\partial t} = \int dk^{'}\gamma^{'}(k^{'})[\phi((\frac{1+\alpha}{2})k-k^{'};t)\phi((\frac{\alpha-1}{2})k+k^{'};t)-\phi(k-k^{'};t)\phi(k^{'};t)]$$

$$\partial_t\phi(k;t) + \phi(k;t) = \phi(\frac{1+\alpha}{2}k;t)\phi(\frac{\alpha-1}{2}k;t)$$

$$\Rightarrow \quad \int_{-\infty}^{\infty} dv_2 \; [\frac{1}{\alpha}f(v_1^{'};t)f(v_2^{'};t) - f(v_1;t)f(v_2;t)] = 0$$

$$I(v_2) = [\frac{1}{\alpha} f(v_1^{'}) f(v_2^{'}) - f(v_1) f(v_2)]|_{v_1}$$



Non-equipartition of energy

In the case of mixtures: different species have different "granular temperatures", but their ratio goes to a constant

Inelastic impurity in an elastic bath

$$\Delta = < E_T^* - E_T >_{TB}$$

$$E_T = \frac{(1+\alpha)}{(2+(1-\alpha)\frac{m_B}{m_T})} E_B \leq E_B$$

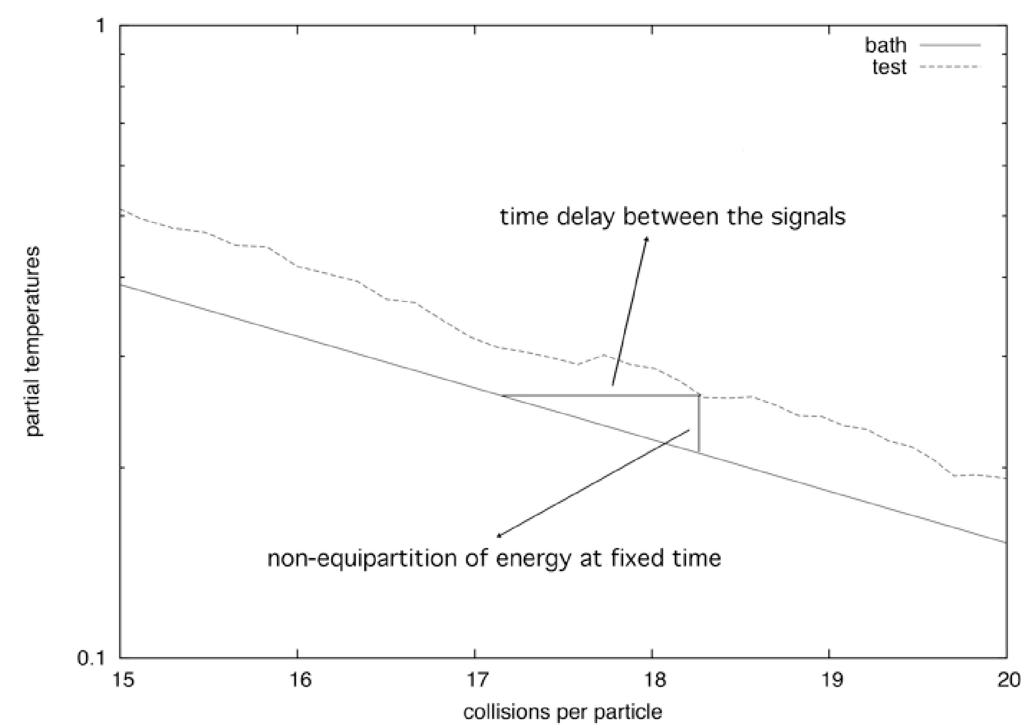
Elastic impurity in an inelastic bath

$$\frac{\partial T_T}{\partial t} = -\lambda_T (T_T - T_B)$$

$$\frac{\partial T_B}{\partial t} = -\lambda_B T_B$$

$$T_T(t) \to R_\infty \, T_B(t)$$

$$R_\infty = \frac{\lambda_T}{(\lambda_T - \lambda_B)}$$

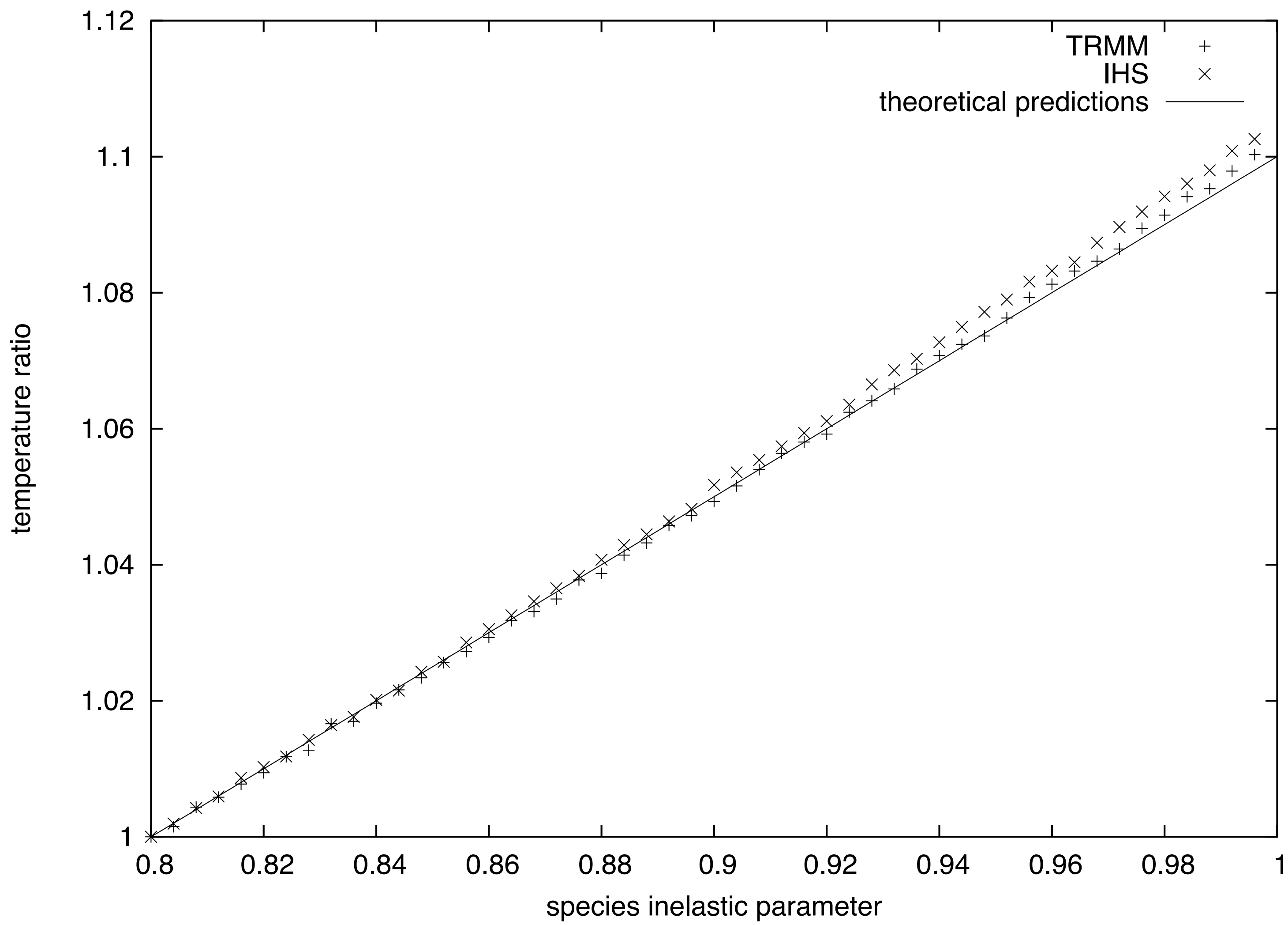


Mean field model (TRMM) for arbitrary mixtures: K components

Refined modeling of the collision rate: $\overline{\nu_{ij}} = \frac{1}{\sqrt{2}}\sqrt{\frac{T_i}{m_i} + \frac{T_j}{m_j}}$

$$\frac{\partial T_j}{\partial \tau} = \sum_n^K x_n \frac{1}{\sqrt{2}}\sqrt{R_j \frac{m_1}{m_j} + R_n \frac{m_1}{m_n}}$$
$$\times \mu_{nj}(2 - \epsilon_{jn})[(-2\mu_{jn} - \mu_{nj}\epsilon_{jn})T_j \; + \; (2\mu_{jn} - \mu_{jn}\epsilon_{jn})T_n]$$

with $R_j = \frac{T_i}{T_1}, \; \epsilon_{ij} = 1 - \alpha_{ij}, \; \mu_{ij} = \frac{m_i}{m_i + m_j}$

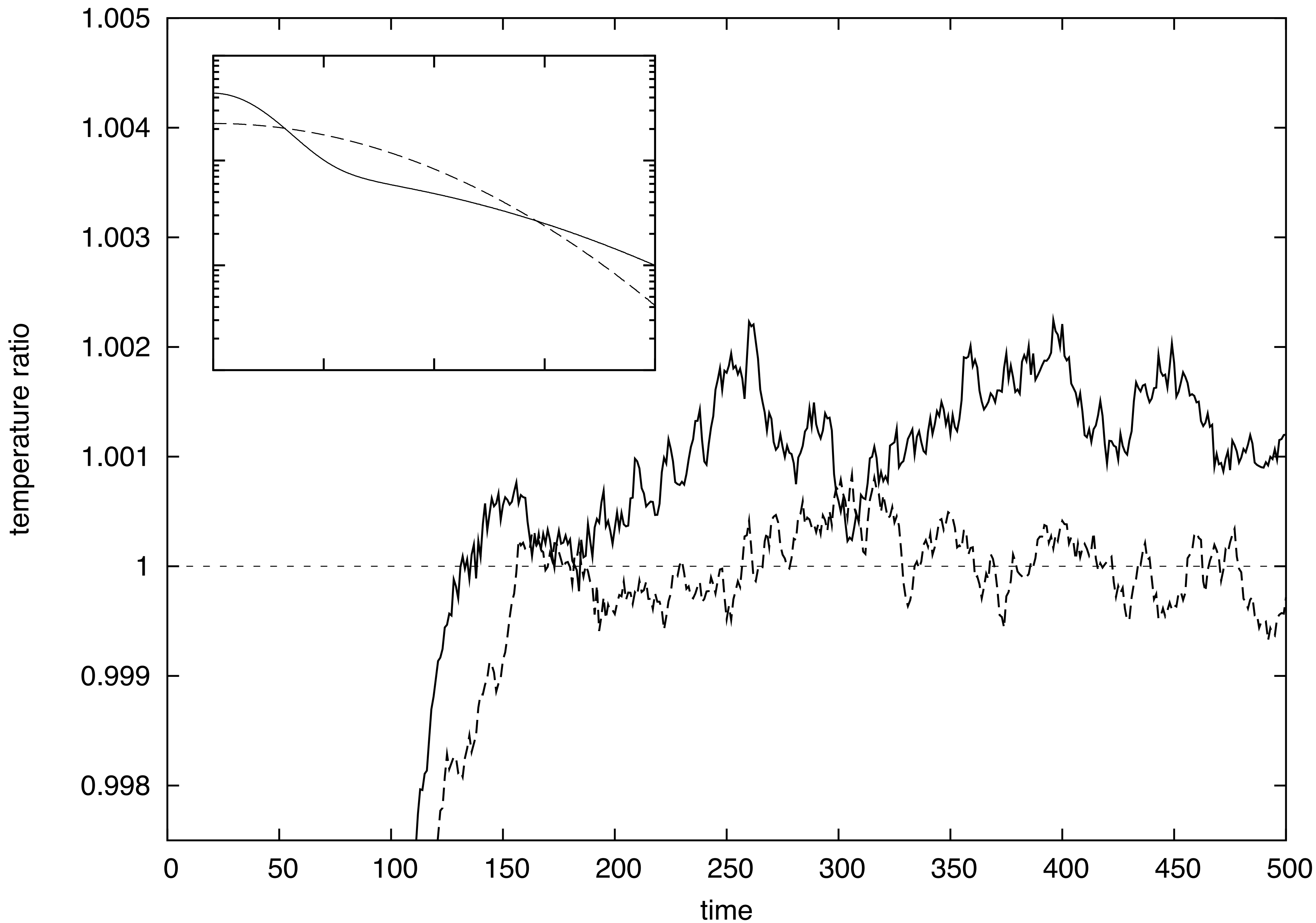


50 components:
$\alpha \in [0.8 : 1.0[$

Qualitative and quantitative agreement with DSMC and MD (2 components)

Maxwell models => no dependence on the velocity distribution

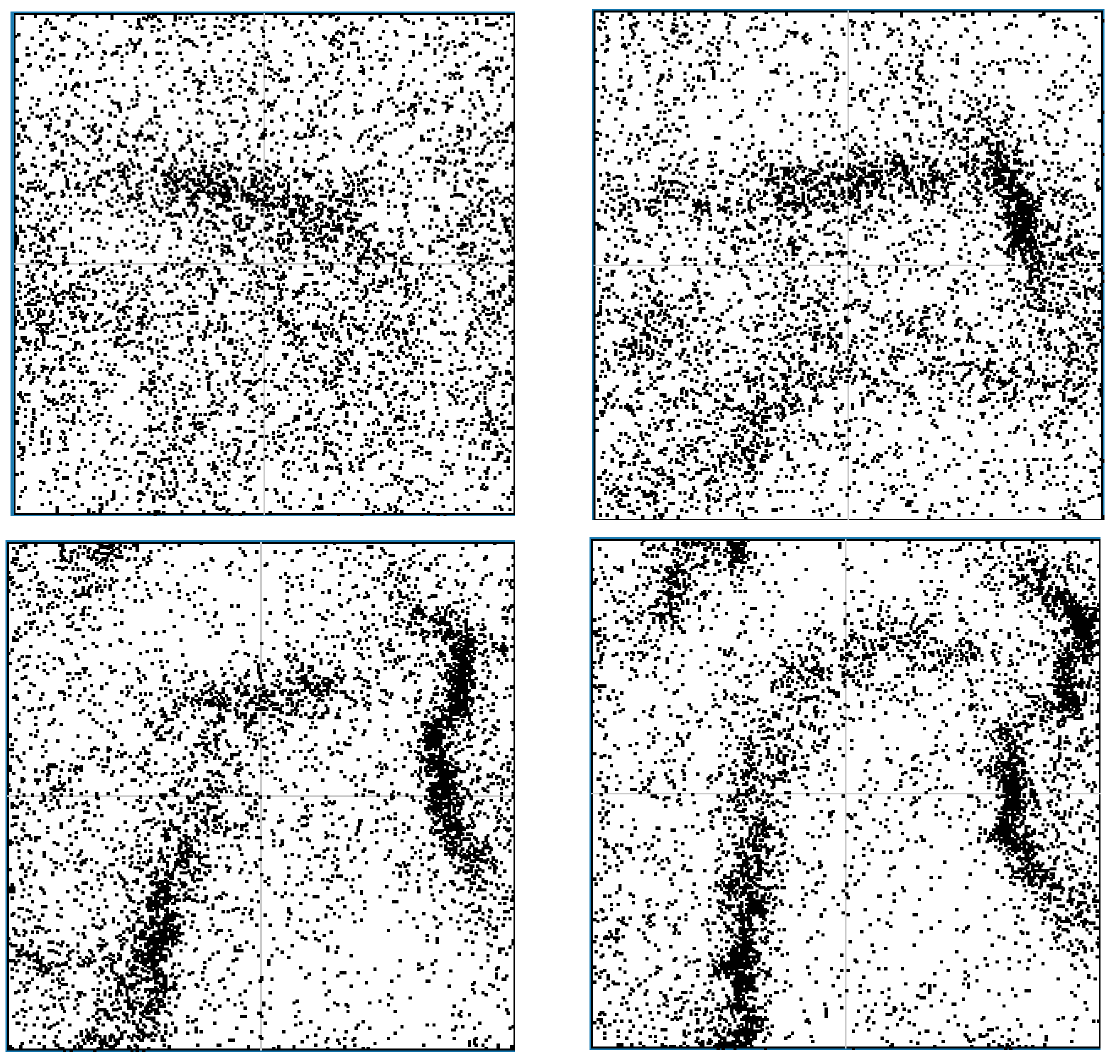
this dependence exists but is small for small $(1-\alpha)$
This behaviour also takes place for a non-equilibrium classical fluid!



Coupling between their energy and their density:

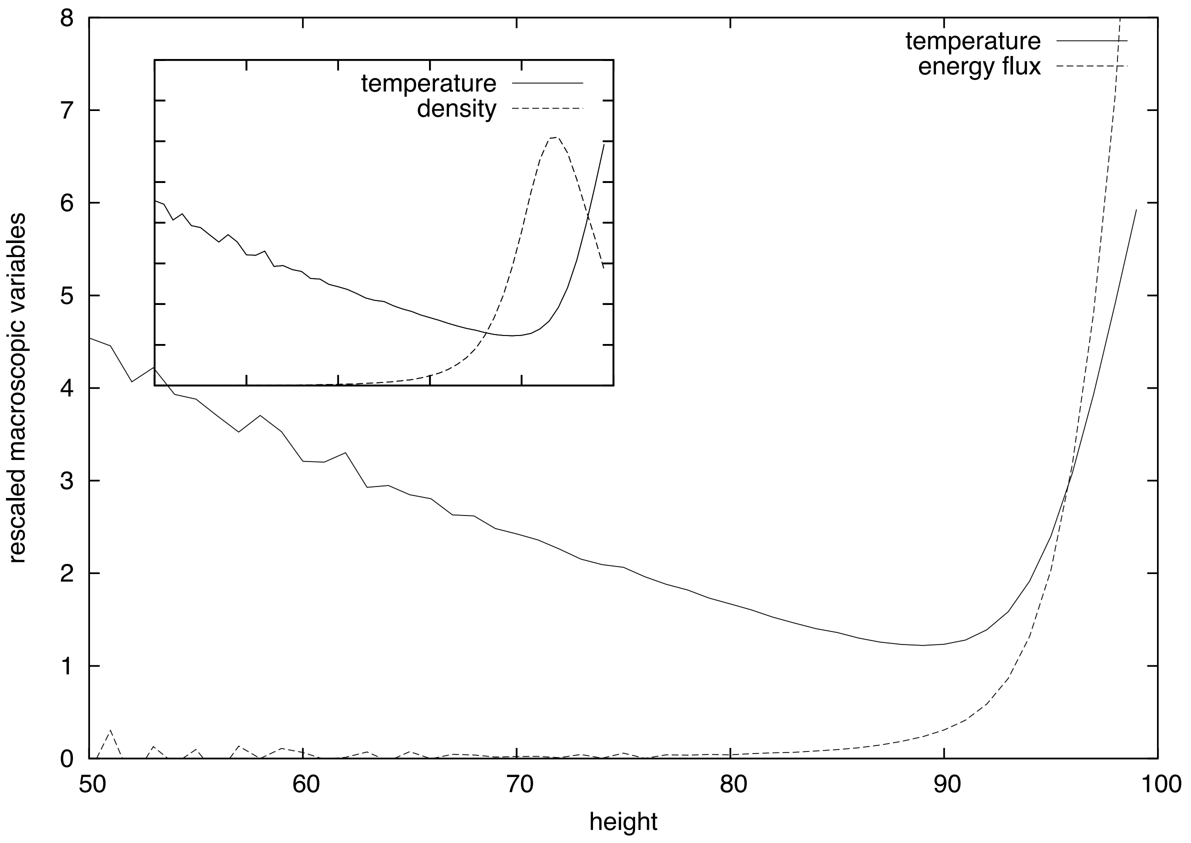
$$\partial_t T(\mathbf{r};t) \sim -n(\mathbf{r};t) T^{\frac{3}{2}}(\mathbf{r};t)$$

Natural tendency to aggregate, which may lead to clustering



Anomalous transport: emergence of anomalous transport relations

$$\mathbf{J}_T = -\kappa\, \partial_{\mathbf{r}} T(\mathbf{r};t) - \varsigma\, \partial_{\mathbf{r}} n(\mathbf{r};t)$$



Eggers theoretical approach:

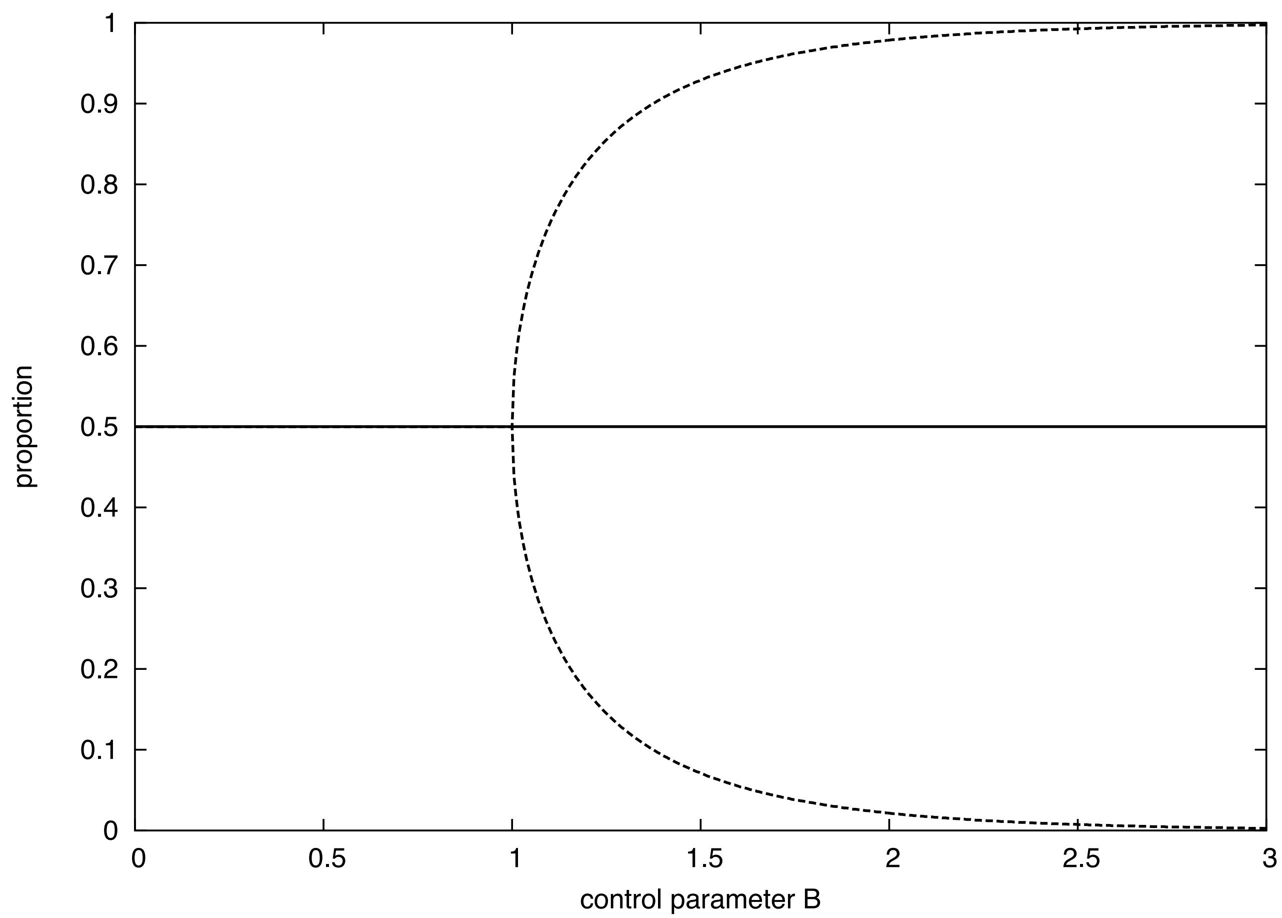
Escape rate: $$F_i = F(p_i) = p_i f(p_i)$$

Escape rate/grain: $$f(p_i) = \sqrt{B} p_i e^{-Bp_i^2}$$

Inelasticity parameter: $$B = 4\pi g r^2 (1-\alpha)^2 \frac{h}{(af)^2} (\frac{2R}{lN})^2$$

=> $$\partial_t p_1 = -p_1 f(p_1) + (1-p_1) f(1-p_1)$$

LOSS GAIN



The choice for *f(p)* is not critical. The main requirement is that *f(p)* is a decreasing function for large p

Eggers approach: no fluctuations

Lipowski et al. proposed a stochastic urn model, mixing the properties of the Eggers dynamics, and that of the Ehrenfest urn model

Original Ehrenfest urn model

=> Boltzmann approach to irreversibility: micro-reversibility vs macro-irreversibility

2R balls in two urns:

* pick a ball at random
* the ball changes urn

Granular urn model

=> thermodynamic-like formalism for the phase transition

2R balls in two urns:

* pick a ball at random
* with probability f(N), the ball changes urn, otherwise nothing happens.

Original Ehrenfest urn model

urn phase space

$$\mathbf{x} = (x_1, .., x_j, .., x_{2R})$$

1: urn 1
0: urn 2

Microscopic time reversibility

$$(0, 0, .., 0)$$

$$\downarrow \frac{1}{2R} \qquad \uparrow \frac{1}{2R}$$

$$(1, 0, .., 0)$$

$$\gamma(\mathbf{x}) = \frac{1}{2R}$$

Granular urn model

urn phase space

$$\mathbf{x} = (x_1, .., x_j, .., x_{2R})$$

1: urn 1
0: urn 2

Microscopic time irreversibility

$$(0, 0, .., 0)$$

$$\downarrow \frac{f(2R)}{2R} \qquad \uparrow \frac{f(1)}{2R}$$

$$(1, 0, .., 0)$$

$$\rho(\mathbf{x}) = \frac{1}{Z} \prod_{\delta=-R}^{\Delta(\mathbf{x})-1} \frac{f(R-\delta)}{f(R+\delta+1))}$$

where: $\Delta(\mathbf{x}) = N_1(\mathbf{x}) - R$

In the following, we use a simpler expression for the escape probability:

$$f(N_1) = e^{-A\frac{N_1}{2R}}$$

The probability in phase space $\rho(\mathbf{x})$, and the probability $P(p)$ of observing a proportion $p = \frac{N_1}{2R}$ are therefore:

$$\rho(\mathbf{x}) = \frac{1}{Z}e^{-2R[A\ \ p(\mathbf{x})(1-p(\mathbf{x}))]}$$

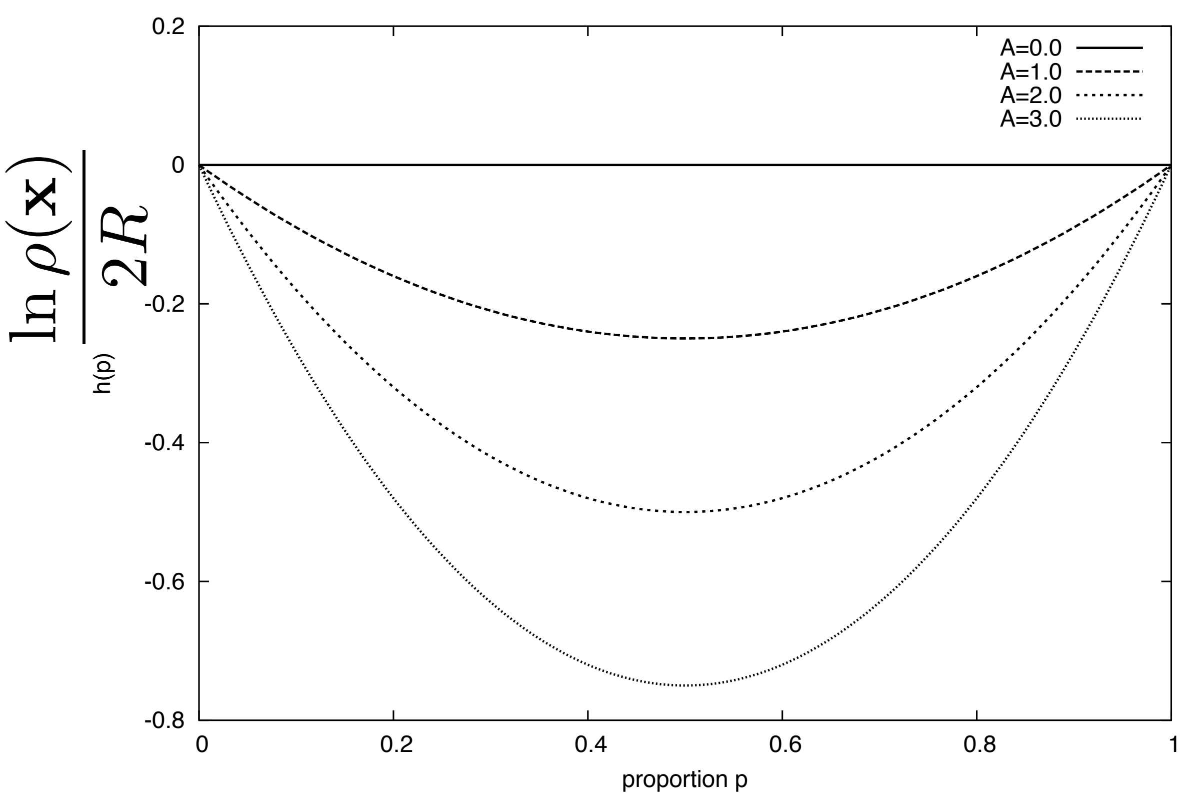
$$P(p) = \frac{1}{Z}e^{-2R\ \ [p\ln(p)+(1-p)\ln(1-p)+A\ \ p(1-p)]}$$

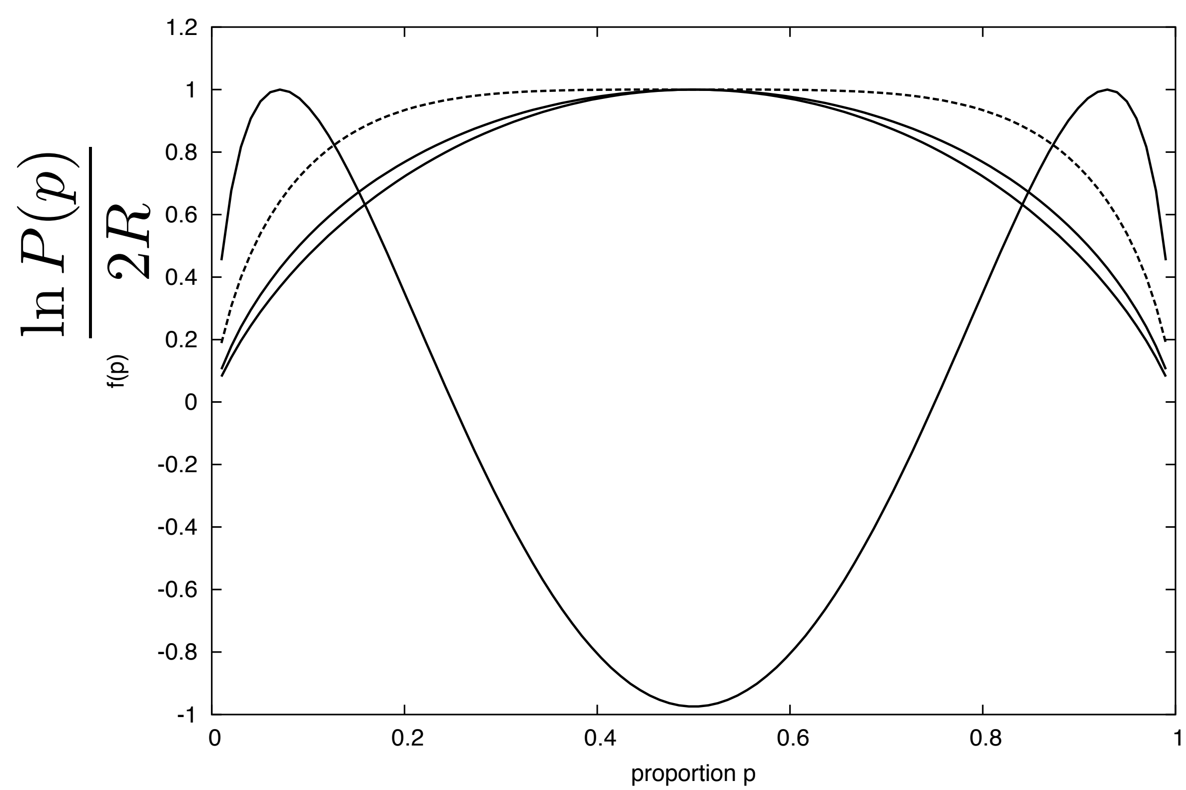
$$\rho(\mathbf{x}) = \frac{1}{Z}e^{-\beta H(\mathbf{x})} \quad \beta \leftrightarrow A$$

$$H(\mathbf{x}) \leftrightarrow 2R\ p_1(\mathbf{x})(1-p_1(\mathbf{x}))$$

Inelasticity discriminates phase space: order-disorder transition entropy (disorder phase) <=> energy (order phase)

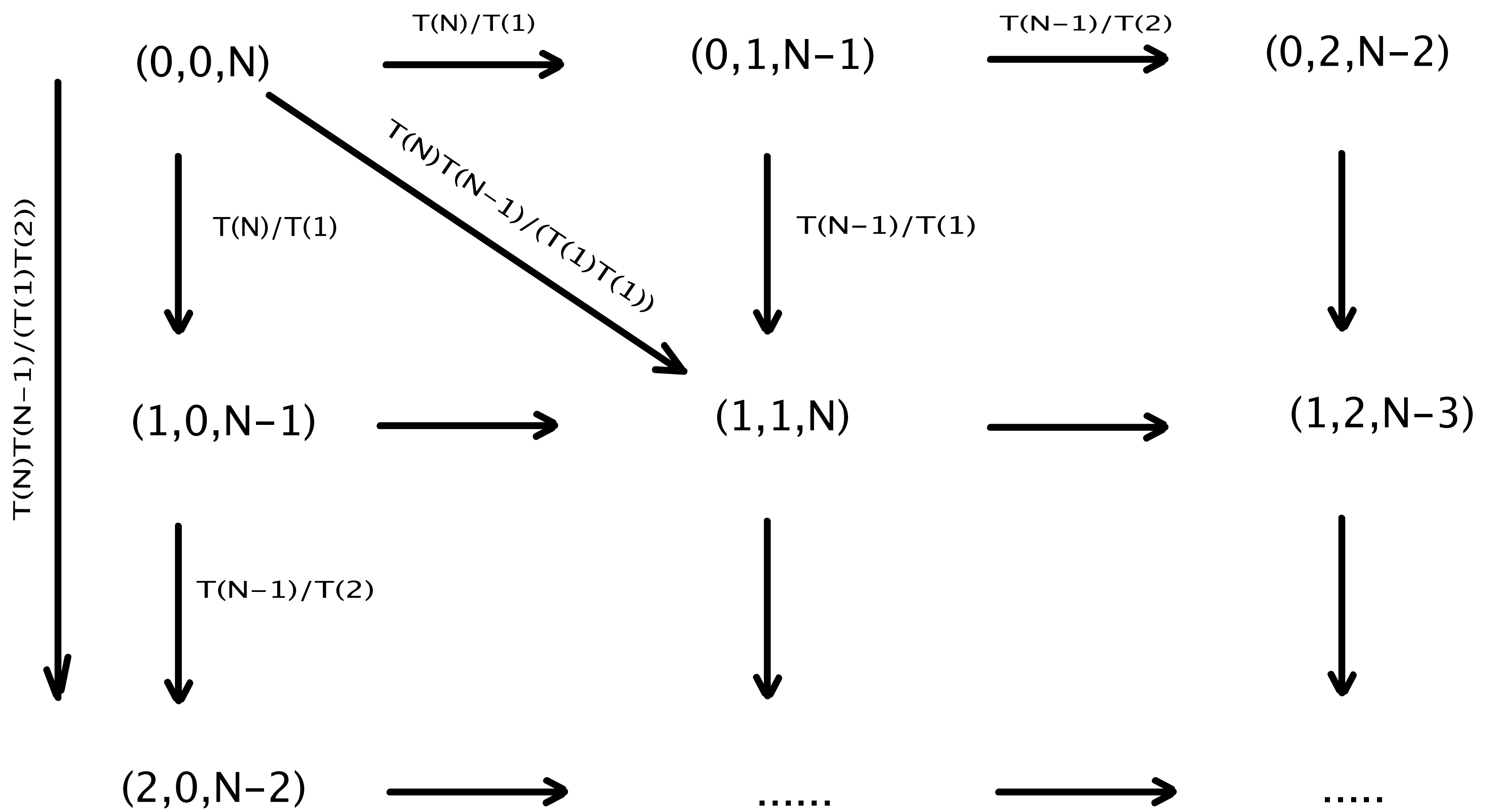
Thermodynamic formalism: partition function, free energy, average energy <H>...
Second order transition at the critical point A=2: <H> continuous at the transition





Three-compartment case

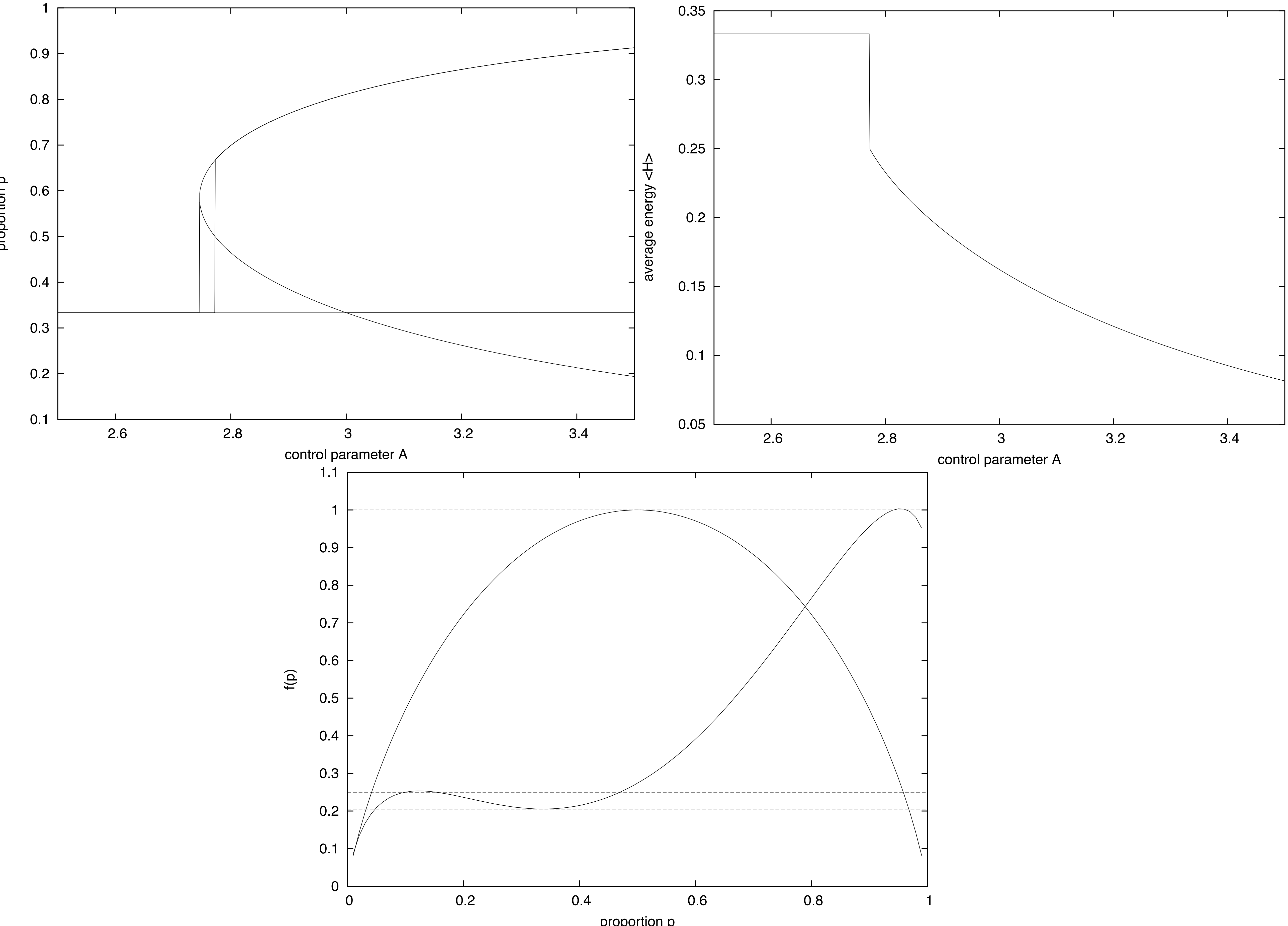
The previous methods also apply to the three-compartment Demon experiment, where one shows that by similar methods:

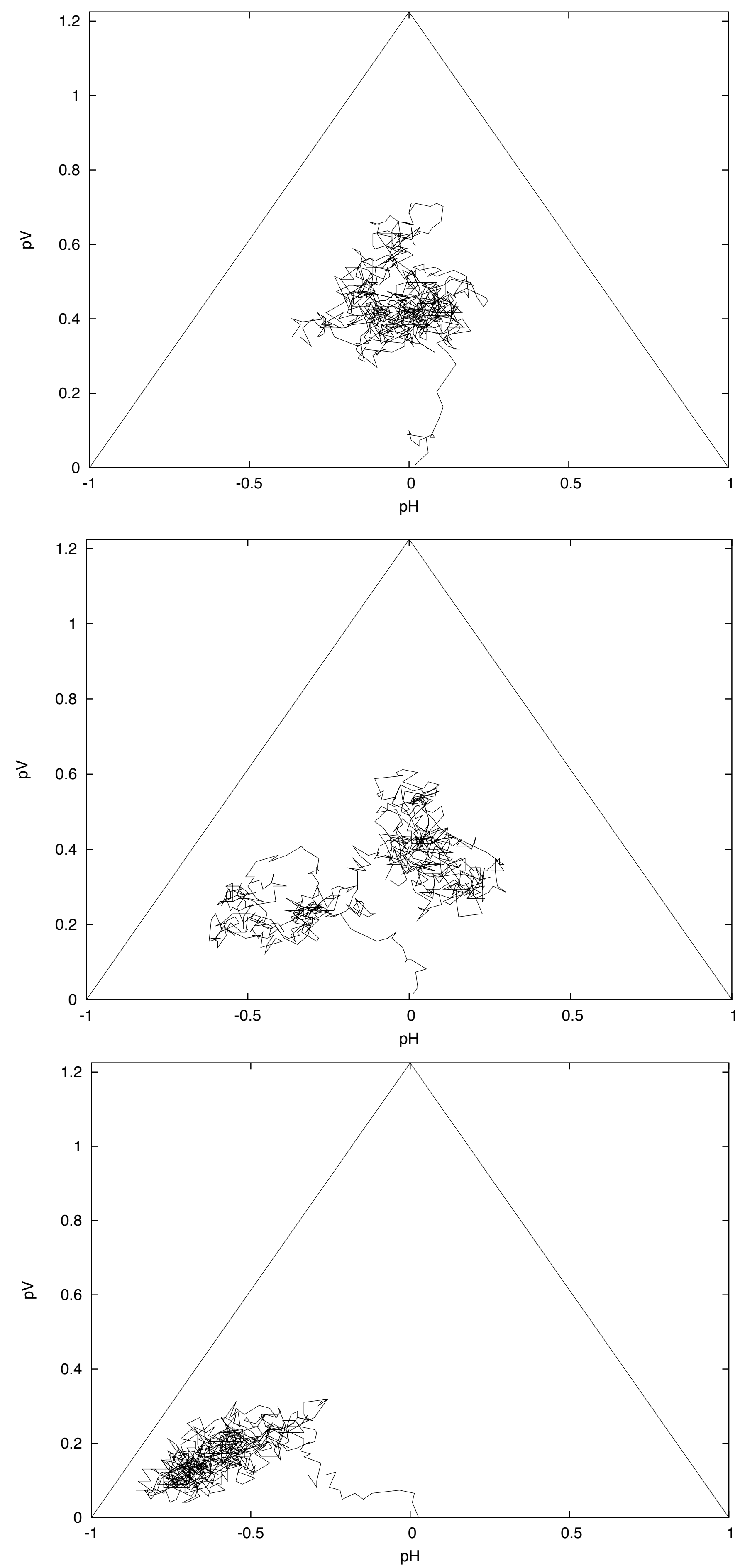


$$\rho(\mathbf{x}) = \frac{1}{Z} e^{-\beta H(\mathbf{x})} \qquad \beta \leftrightarrow A$$

$$H(\mathbf{x}) \leftrightarrow 3R \left(p_1 + p_2 - (p_1^2 + p_2^2 + p_1 p_2)\right)$$

Hysteretic behaviour, associated with a first order phase transition




pV
pH
0
0.2
0.4
0.6
0.8
1
1.2
-1
-0.5
0
0.5
1

Generalization to K urns

$$\varrho_\infty(\mathbf{N}) = \frac{\prod_j^{\sum_{i=1}^{K-1} N_i} T(KR - k + 1)}{\prod_{k=1}^{K-1} \prod_{j=1}^{N_k} T(j)}$$

$$\mathbf{N} = (N_1, ..., N_j, ..., N_K)$$

$$P(\mathbf{N}) = e^{-KR\ [\sum_{i=1}^{K} p_i \ln p_i + \frac{A}{2}(\sum_{i=1}^{K} p_i (1 - p_i))]}$$

Asymmetric Demon experiment

The analogy with an equilibrium phase transition can be enhanced by studying the coupling of the system with an anisotropic field.
=> ferromagnetic-like behaviour, characterized by hysteresis and a strong metastability.
In the previous models, the energy is injected in the same way in each compartment => the system is symmetric under the change $p \leftrightarrow (1-p)$

By heating differently each box, this symmetry is broken: a different escape probability for each compartment:

$$T_{12}(N_1) = e^{-\frac{AN_1}{2R}} \qquad T_{21}(N_1) = e^{-\frac{B(2R-N_1)}{2R}}$$

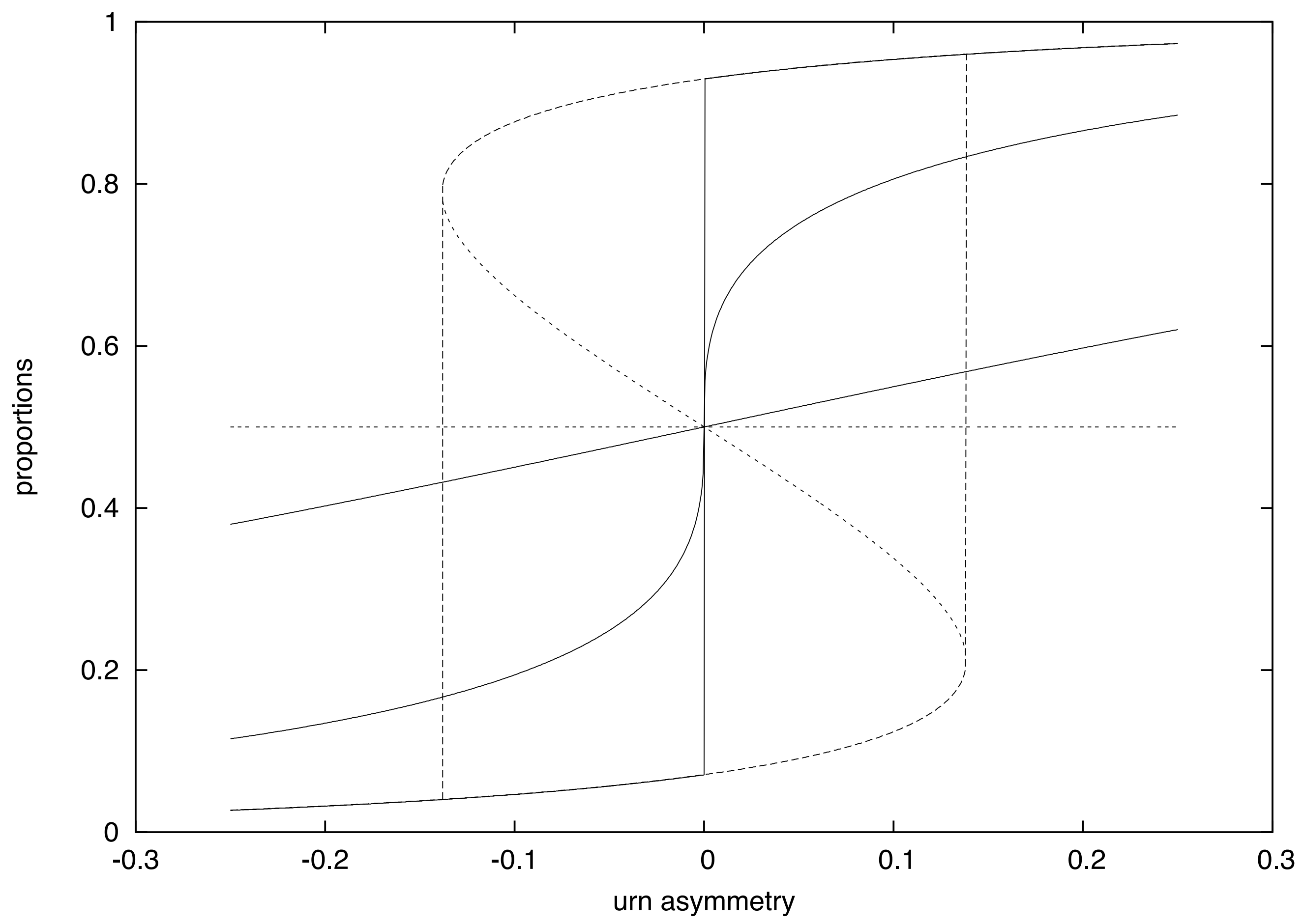
We derive the following canonical distribution:

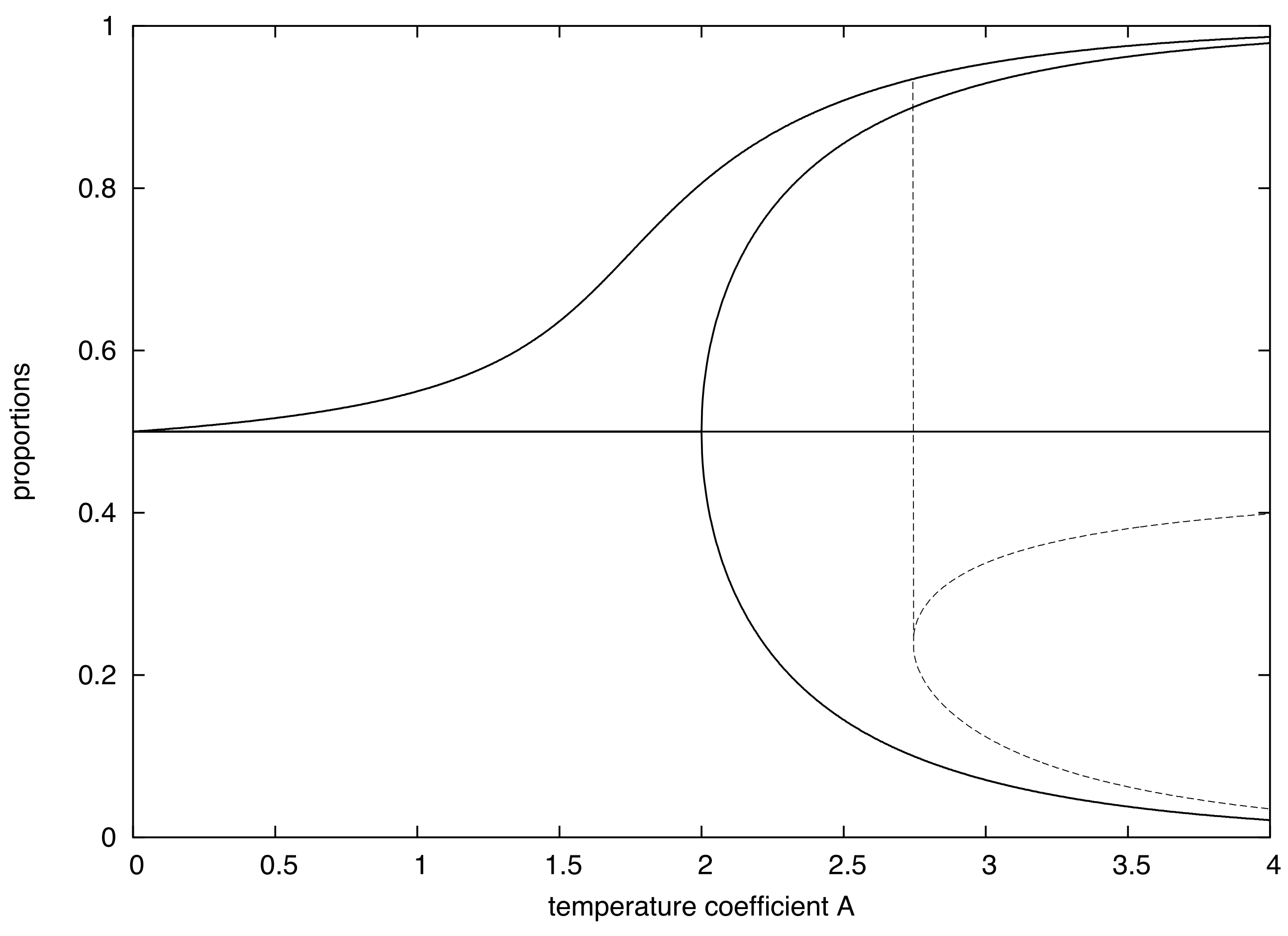
$$\rho(\mathbf{x}) = \frac{1}{Z} e^{-\beta(H(\mathbf{x})+E(\mathbf{x}))}$$

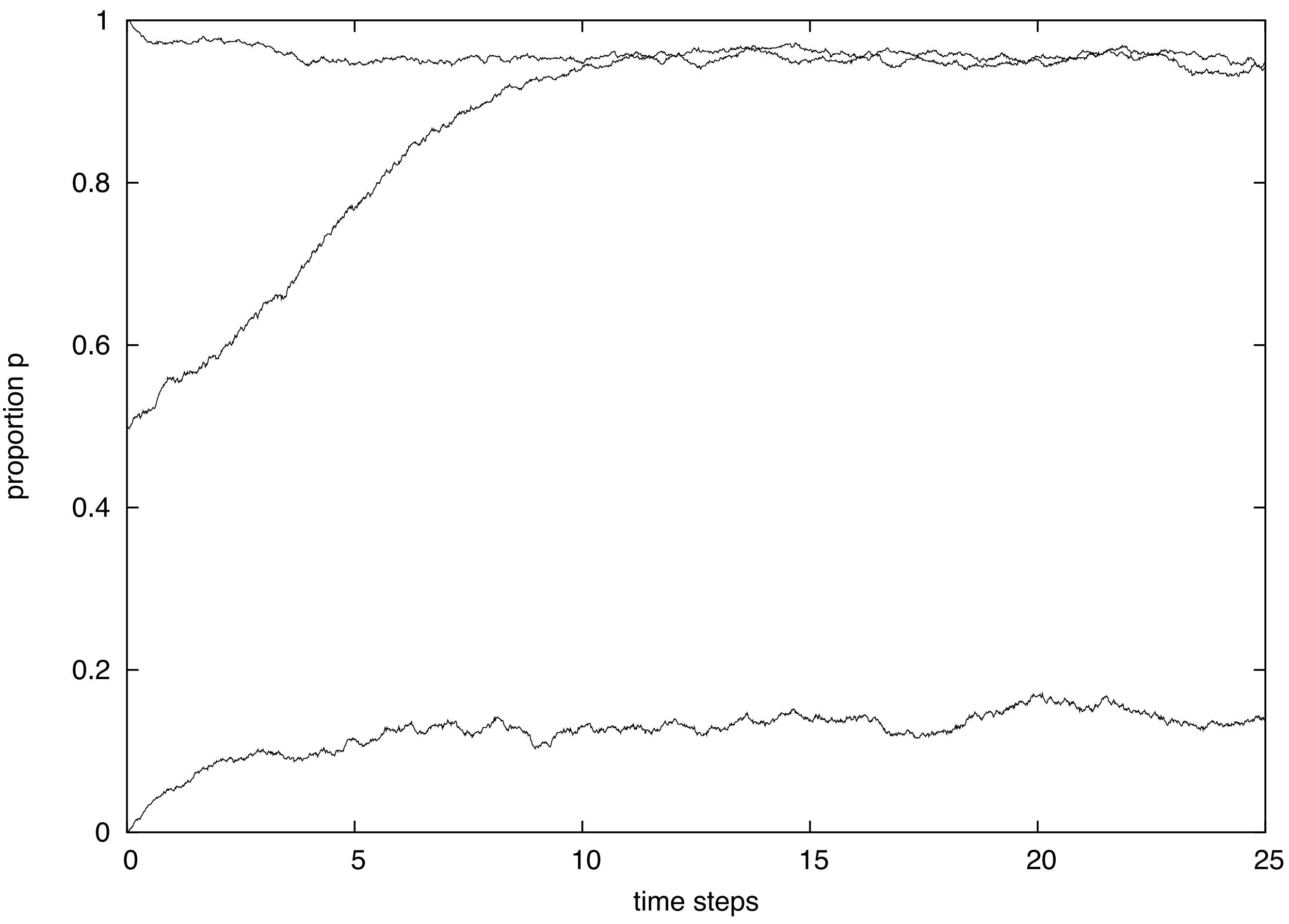
The original hamiltonian: $H(\mathbf{x}) \leftrightarrow 2R\, p_1(\mathbf{x})(1-p_1(\mathbf{x}))$

Coupling with the asymmetric field $E(\mathbf{x}) = -2R\, \epsilon p(\mathbf{x})$

$$\beta \leftrightarrow \frac{A+B}{2} \qquad 1-\epsilon = \frac{2B}{A+B}$$







Behaviour similar to that of ferromagnetic crystal

Curie temperature T=1/2

Asymmetric field <=> external magnetic field

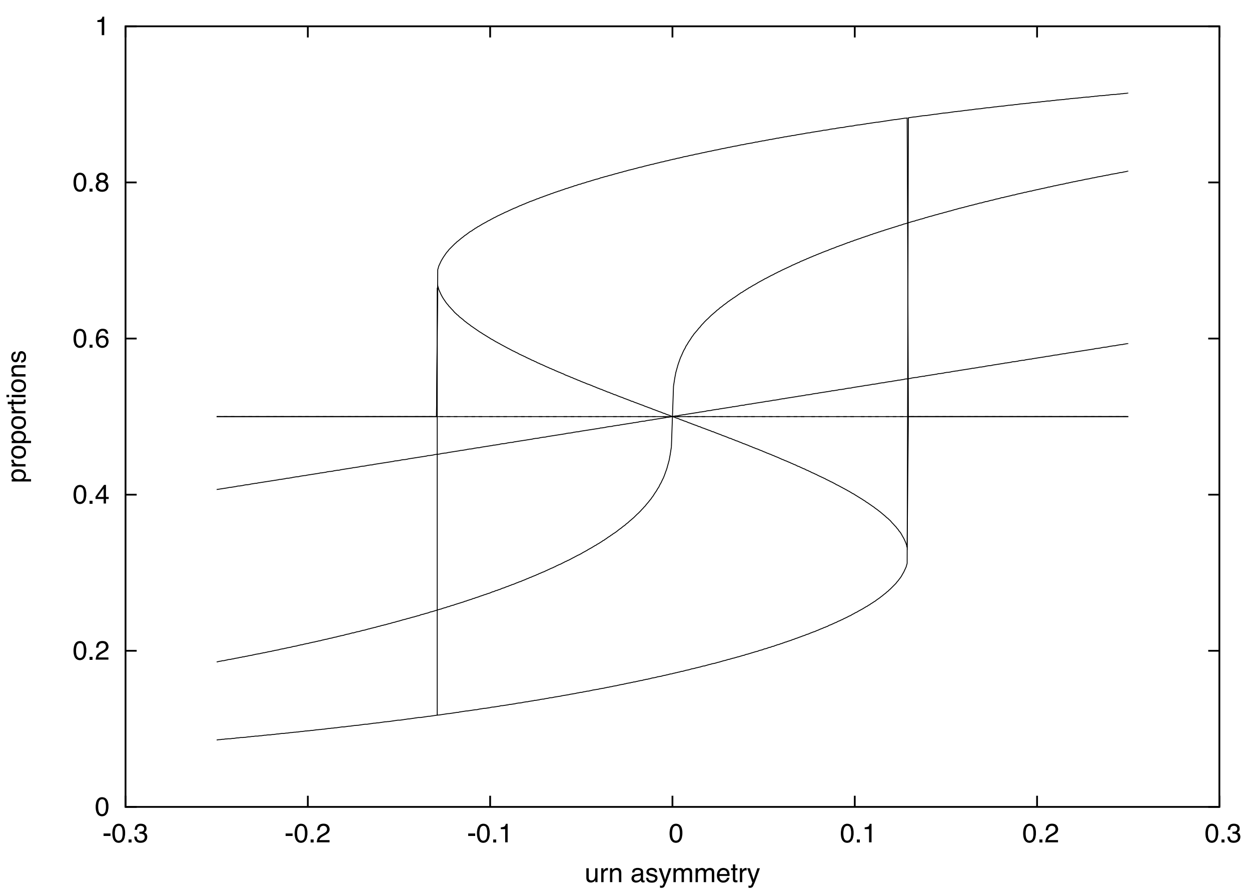
$p - 1/2$ <=> magnetization

$p - 1/2|_{h=0}$ <=> spontaneous magnetization

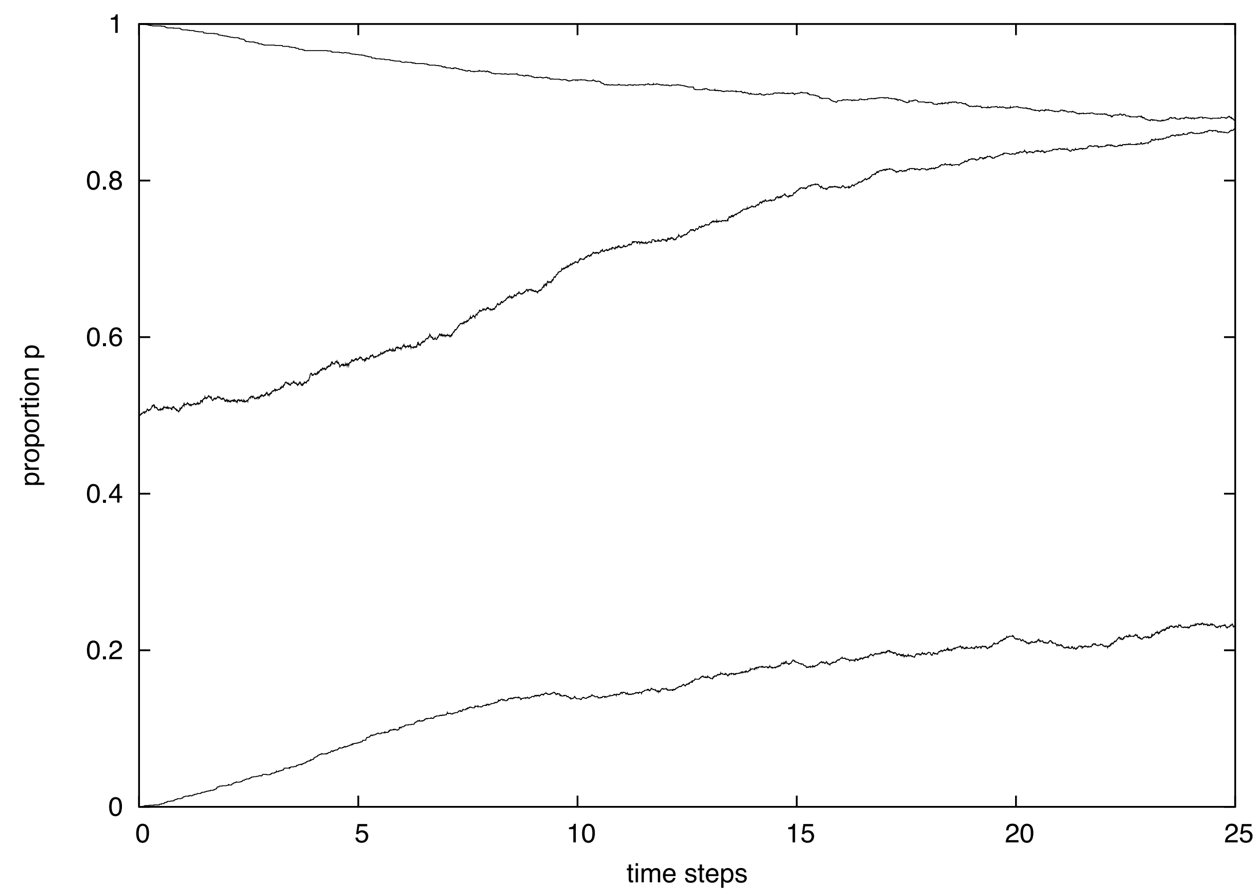
When the escape flux is that of Eggers, the Curie point is located at B=1. Metastability, hysteresis... There are two coefficients:

$$f_i(p_i) = \sqrt{B_i} p_i e^{-B_i p_i^2} \qquad B_1 = B(1+\epsilon) \qquad B_2 = B(1-\epsilon)$$

The bifurcation diagram and system evolution are:



B=0.8, 1.0, 1.2



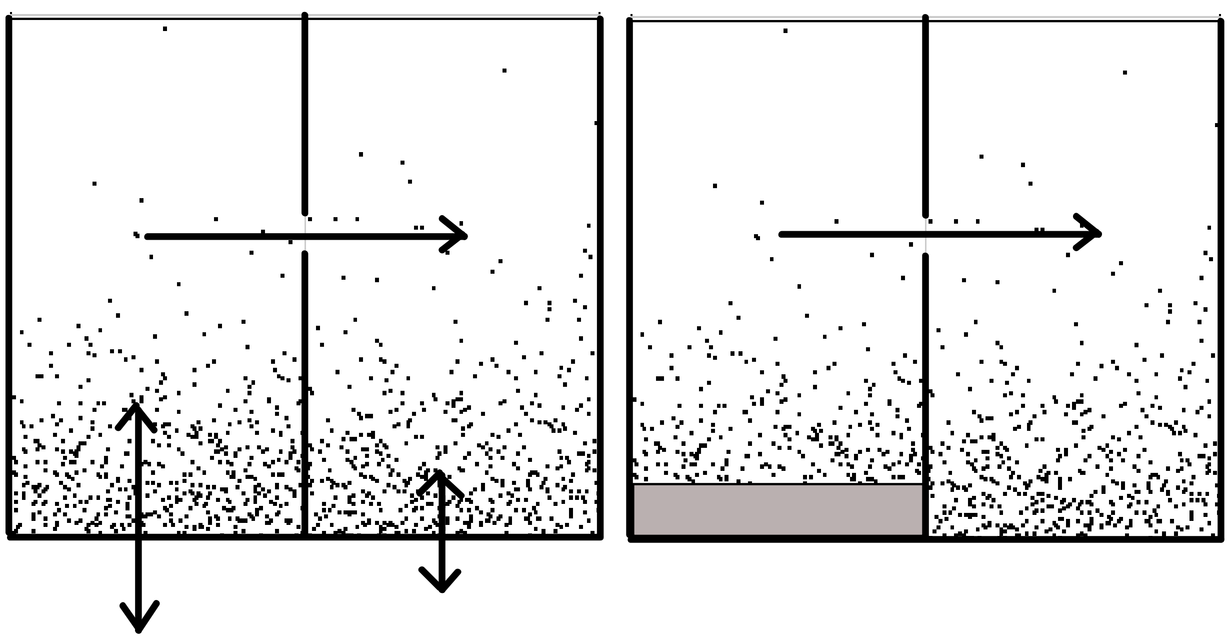
B=0.8, epsilon=0.1

How general is this behaviour?

Different choices for the escape probability lead to qualitatively equivalent behaviours

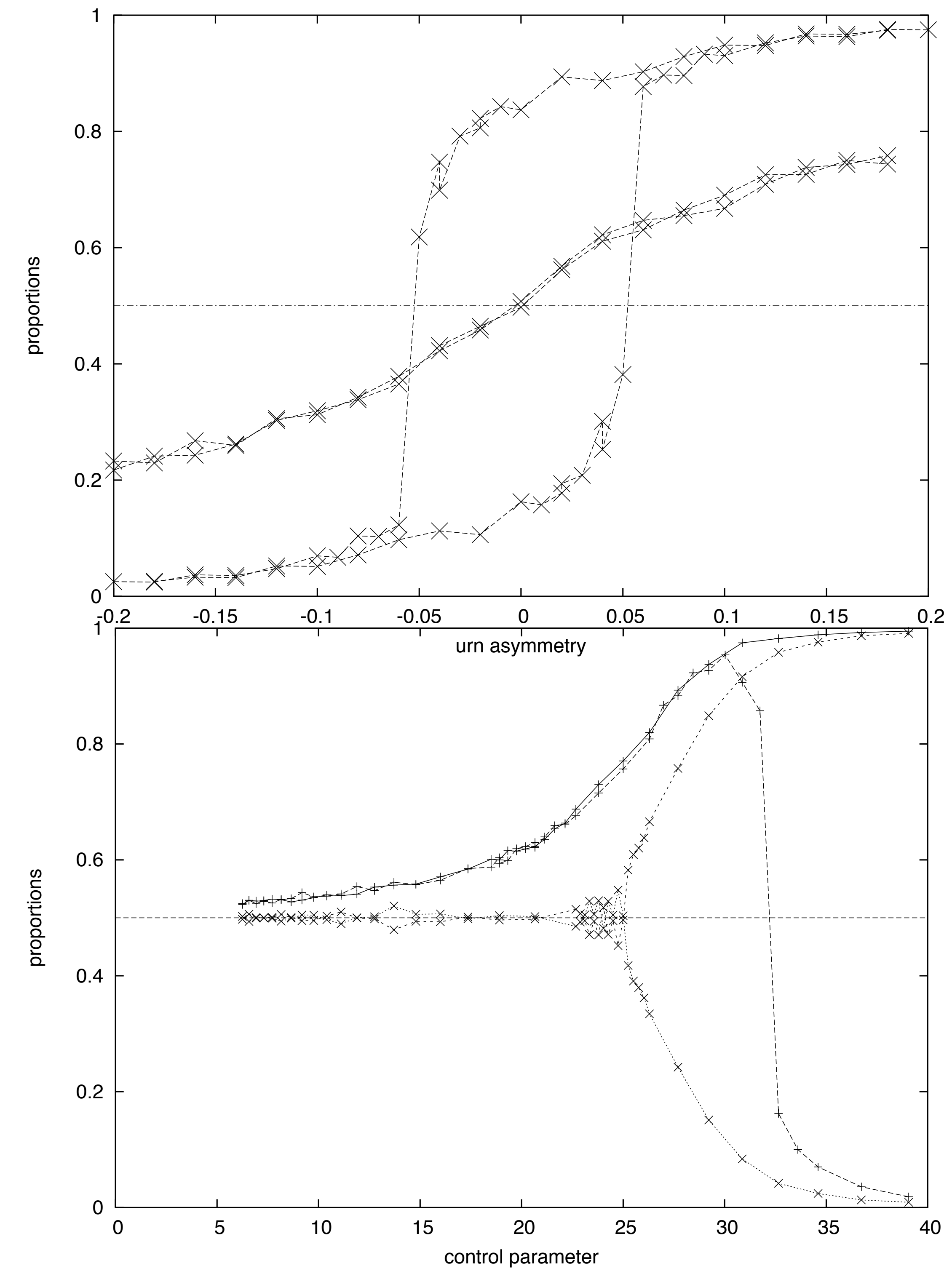
Experimental realization??

* different vibration frequency in each compartment
* different height in each compartment



Asymmetric amplitudes or frequencies

Asymmetric ground heights



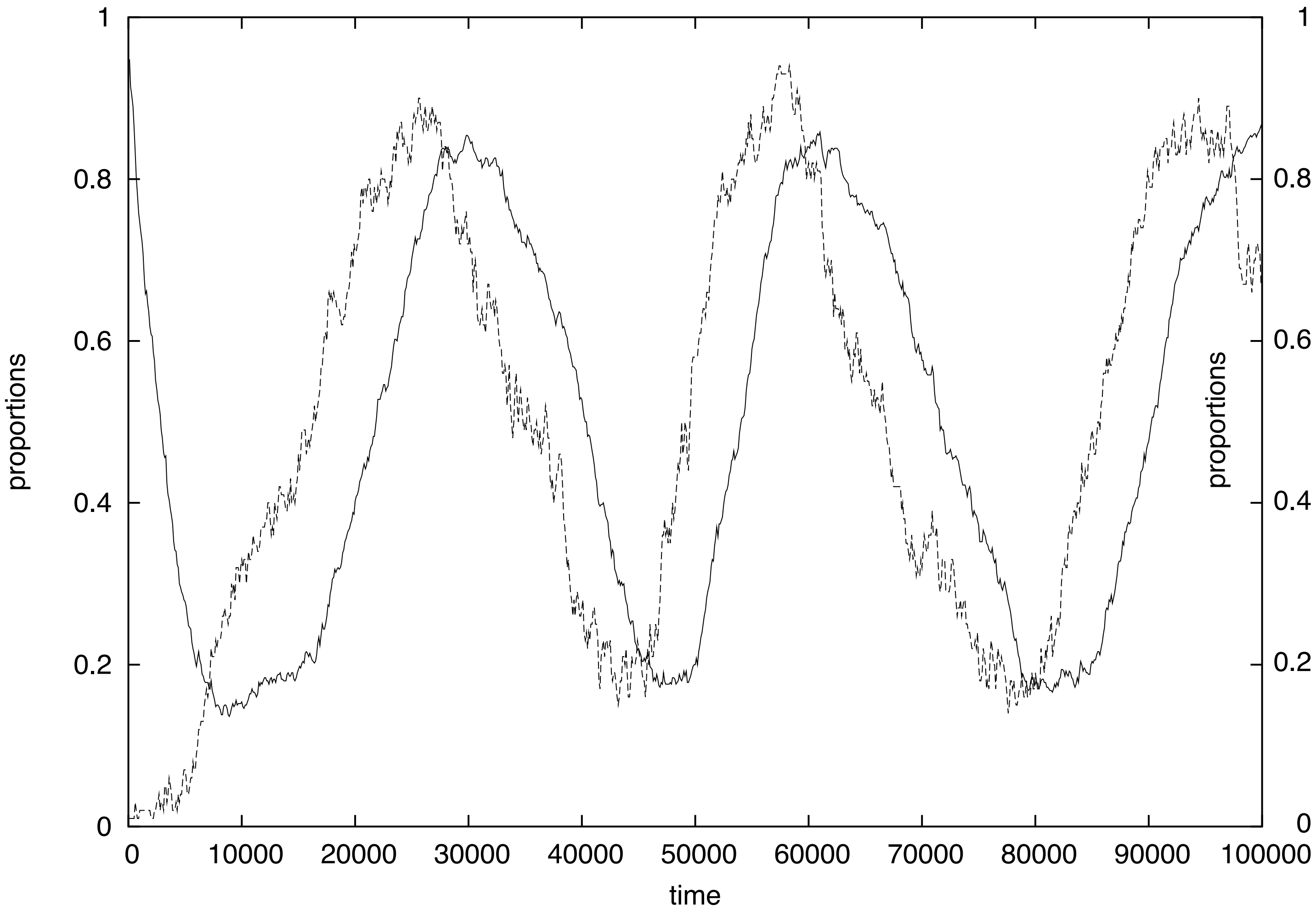
Verifications by MD of the asymmetric urn model (event-driven simulations)

Segregation & oscillations

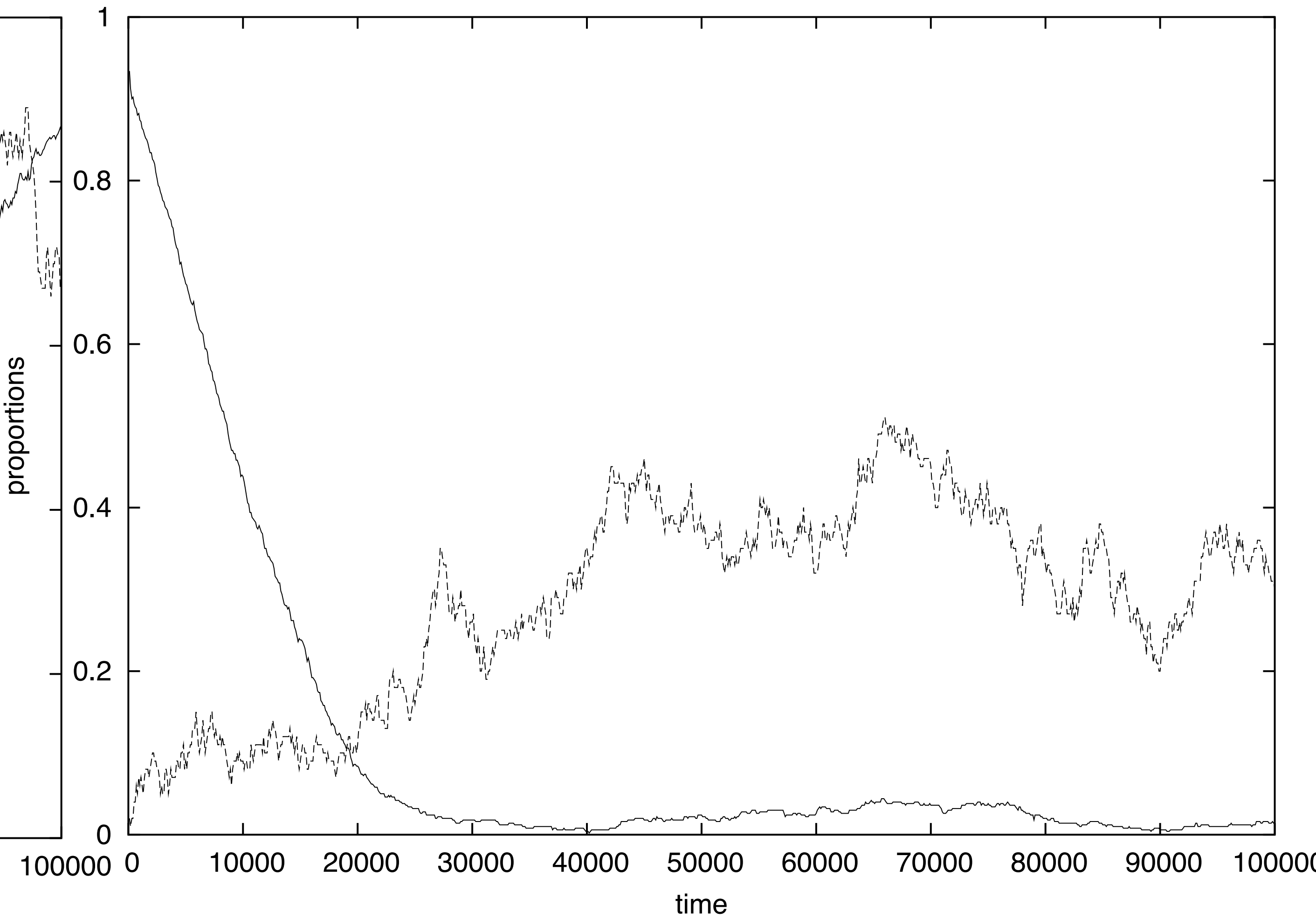
* different species <=> different dissipation rates (inelasticity parameters, masses, diameters...)

* vertical segregation phenomenon effects, such as Brazil nut effect <=> larger particles may be driven to the top

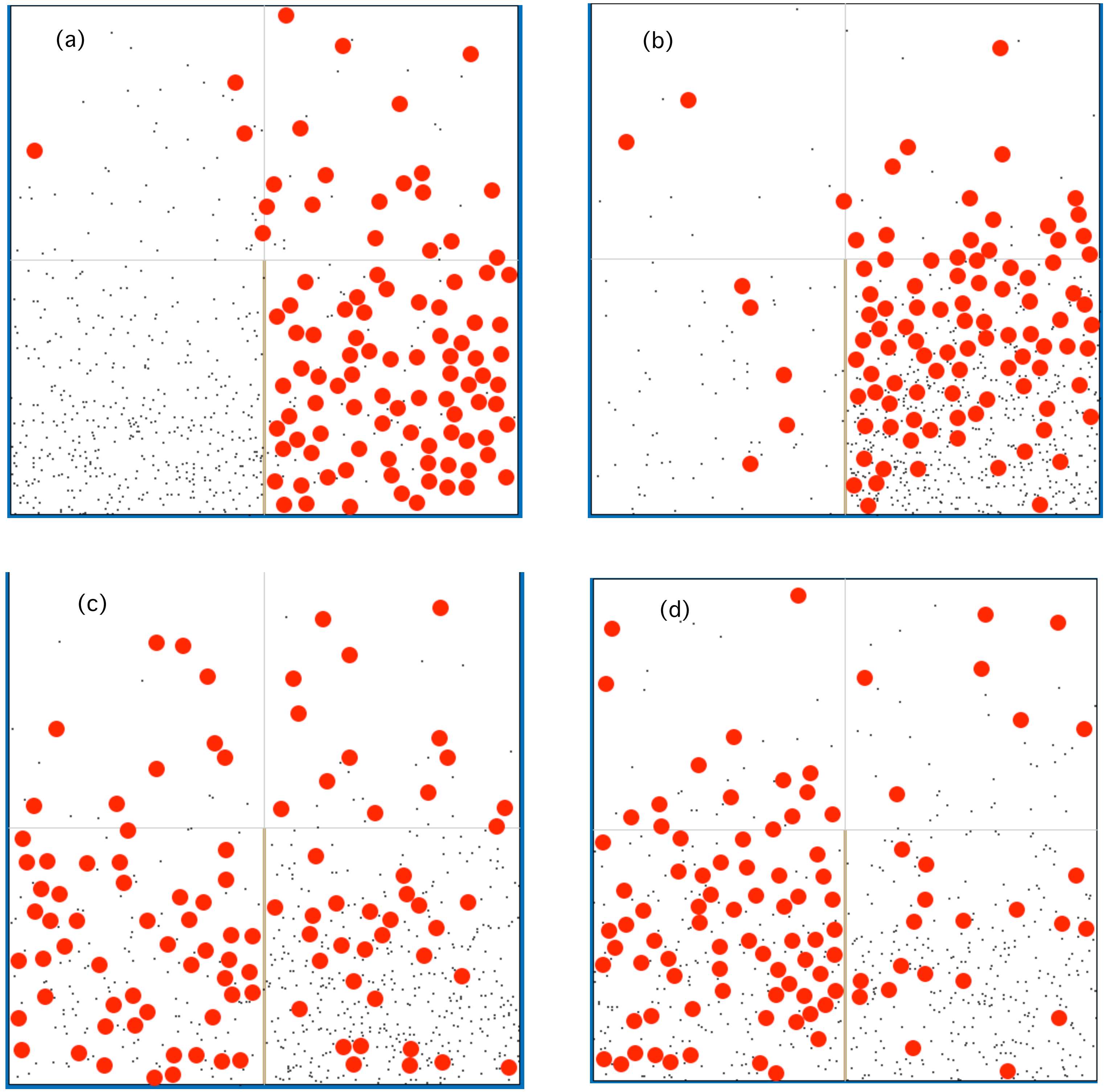
*Event-driven simulations show that the coupling of the horizontal Demon instability with vertical segregation leads to a richer phenomenology



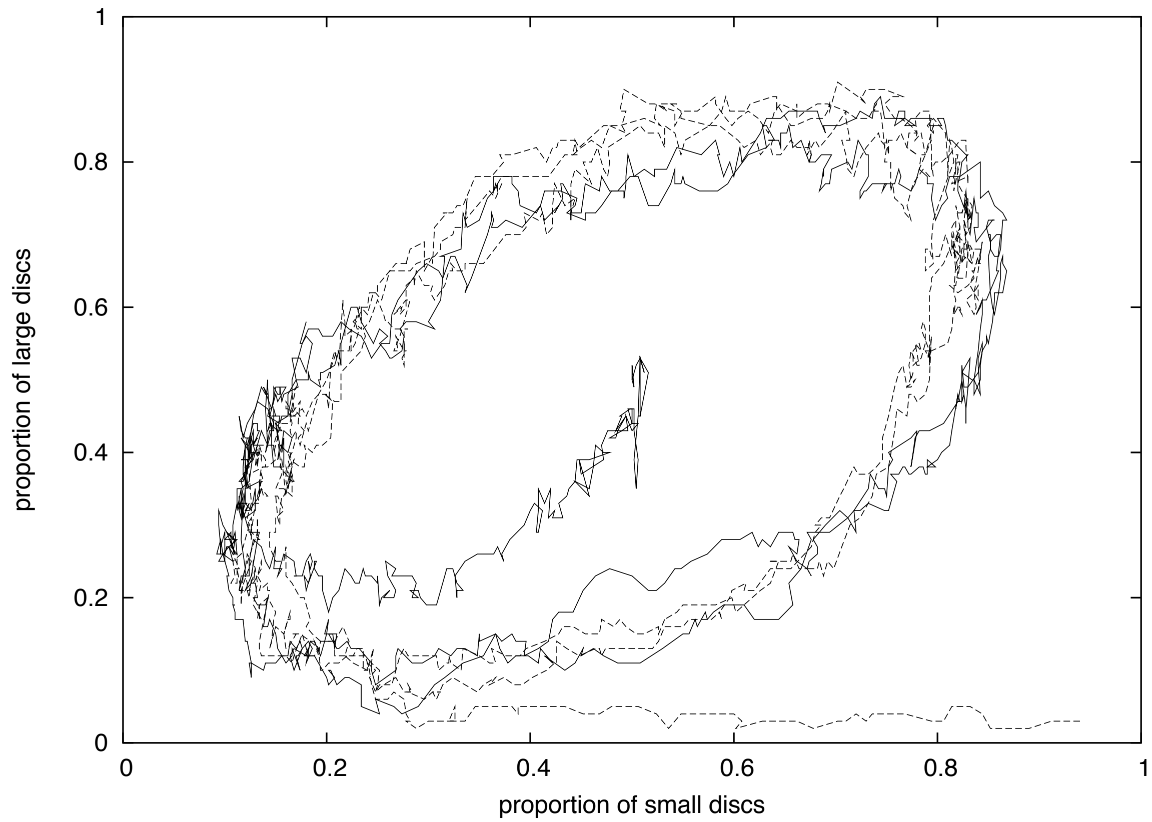
Oscillations with time delay

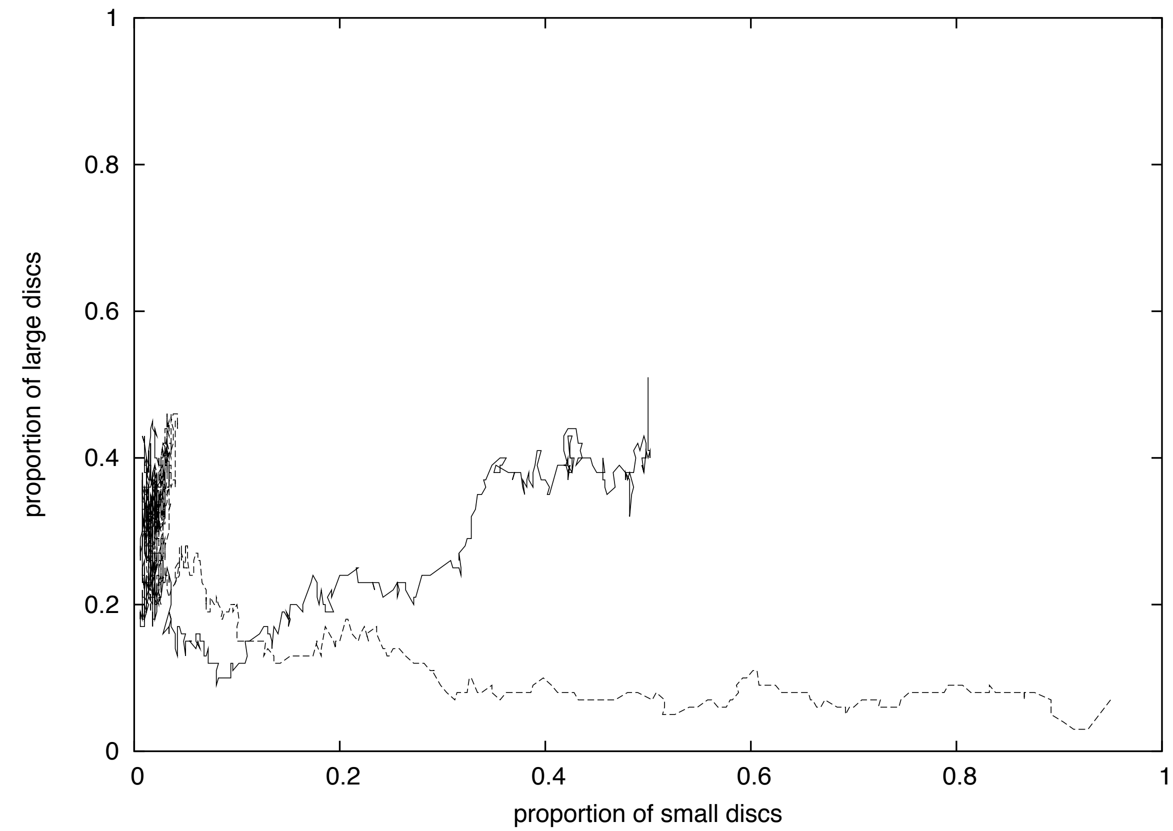


Horizontal segregation

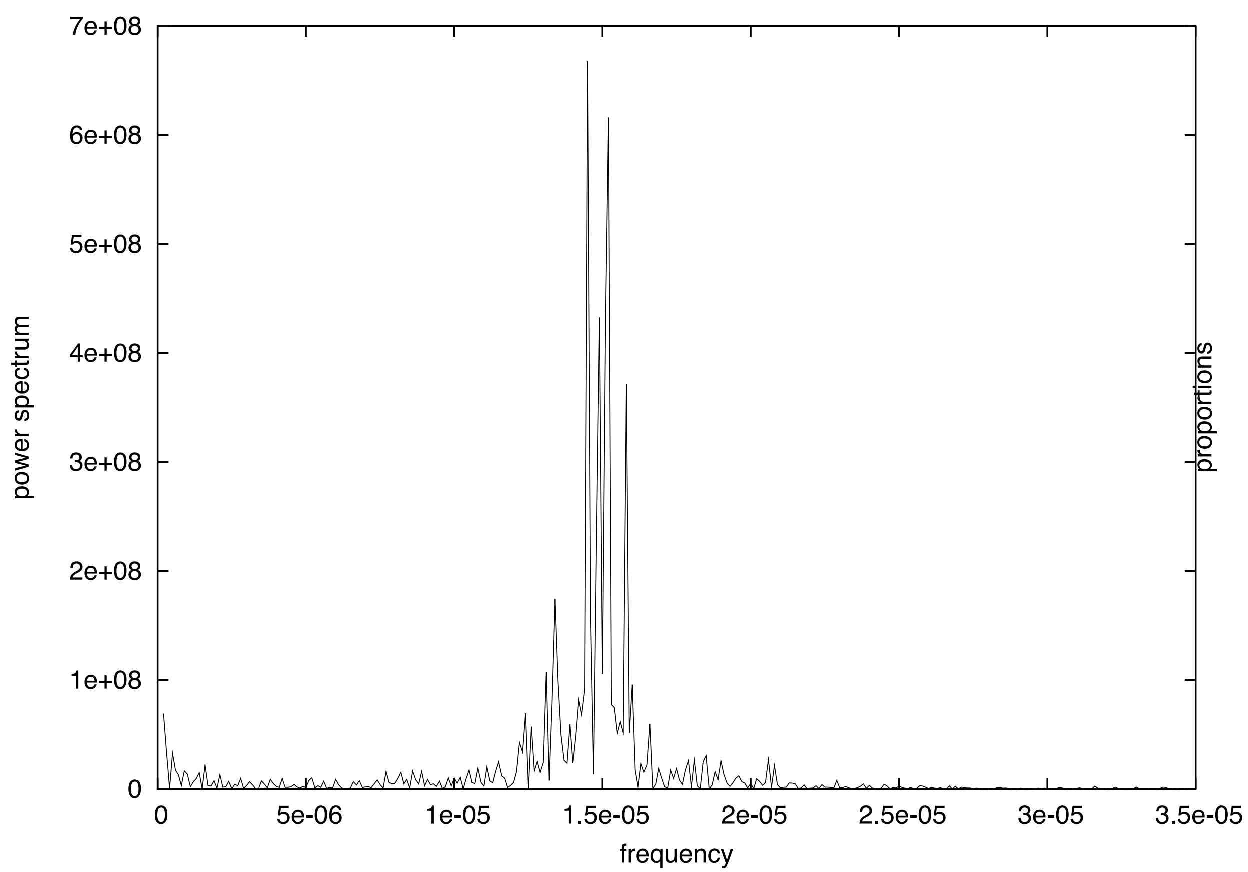

(a)
(b)
(c)
(d)

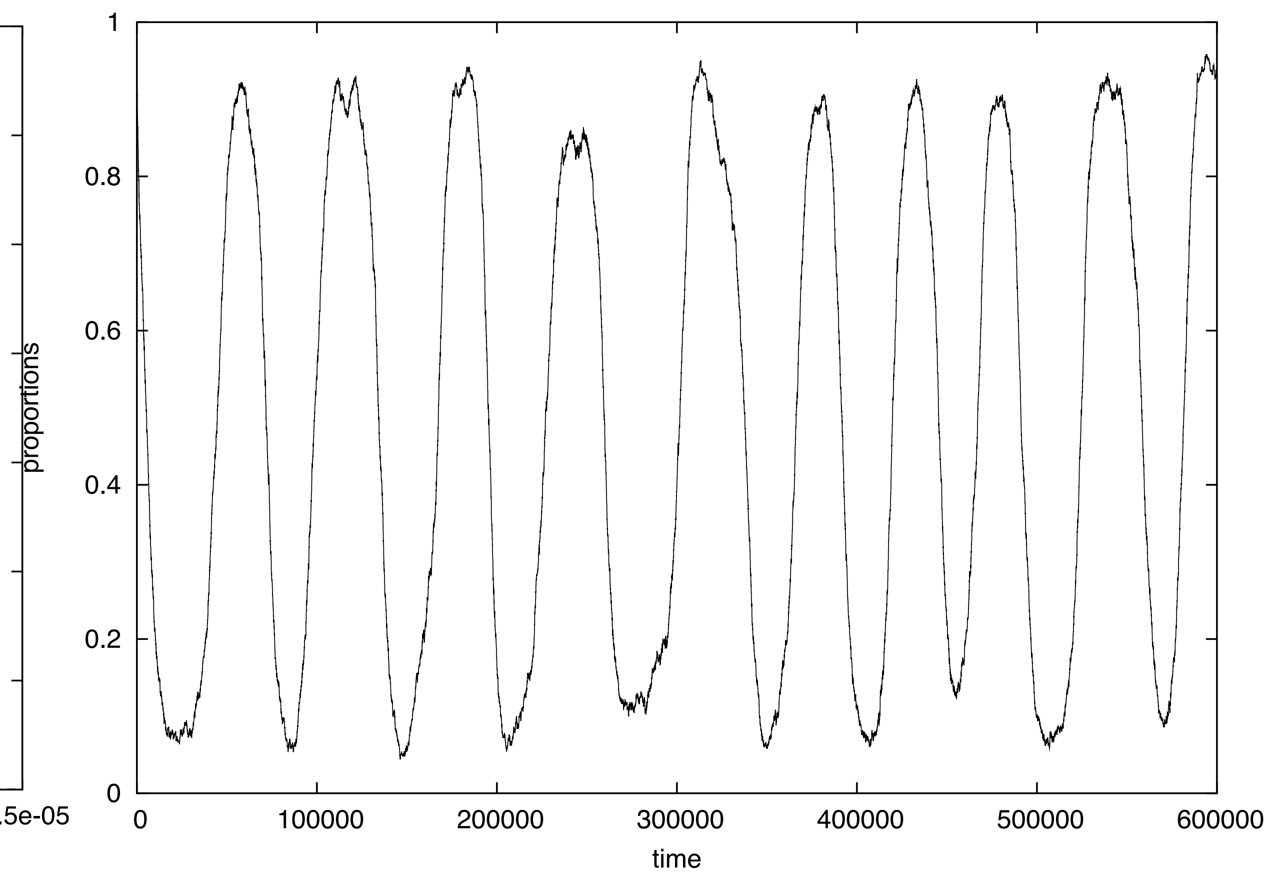
No metastability





Well-defined Oscillations



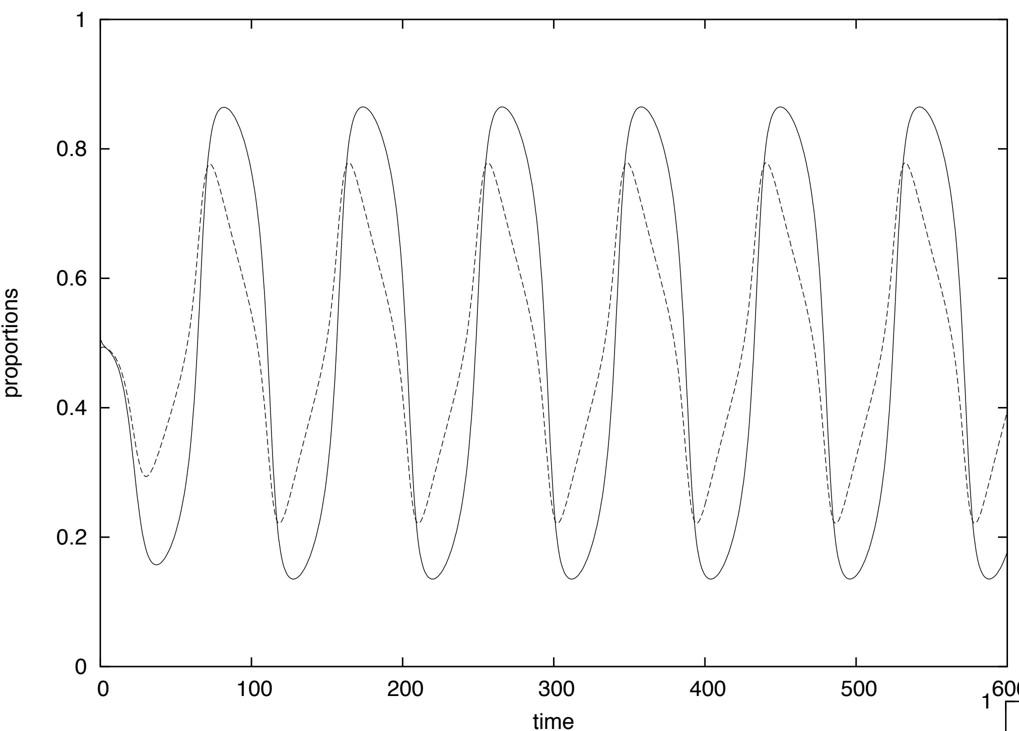


Qualitative model, which tries to relevant phenomena, based upon the Eggers theory:

$$\frac{\partial n}{\partial t} = -nF(n,m)(1-s_L) + (1-n)F(1-n,1-m)(1-s_R)$$

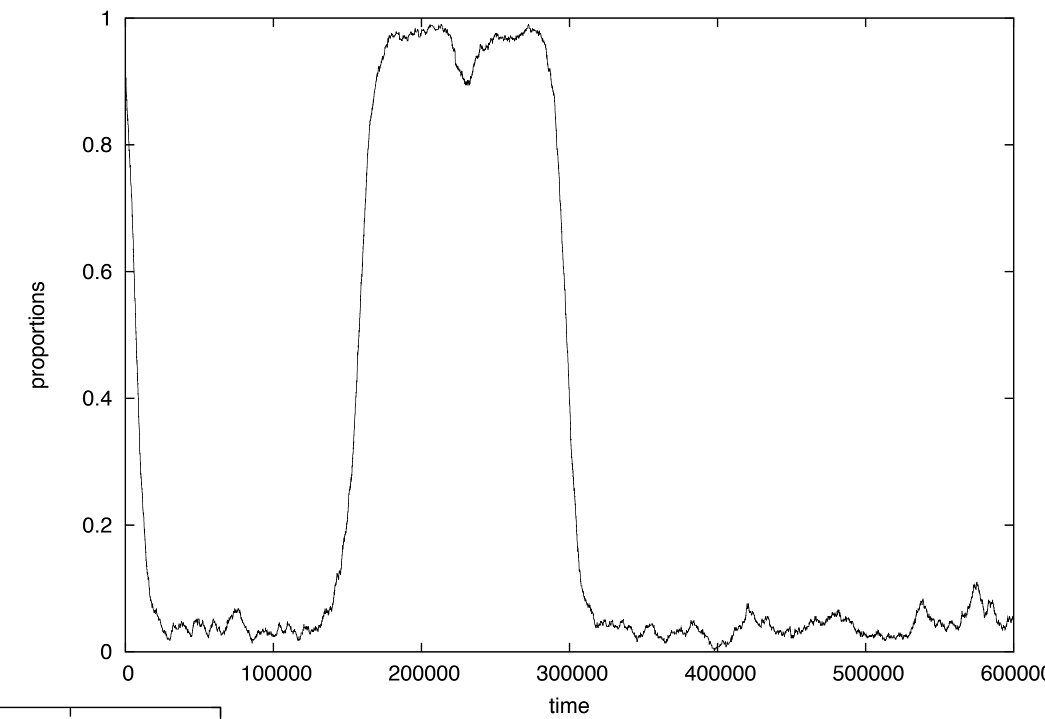
$$\frac{\partial m}{\partial t} = -mF(n,m)(1+s_L) + (1-m)F(1-n,1-m)(1+s_R)$$

$$\frac{\partial s_L}{\partial t} = -\lambda(nm - s_L) \qquad \frac{\partial s_R}{\partial t} = -\lambda((1-n)(1-m) - s_R)$$

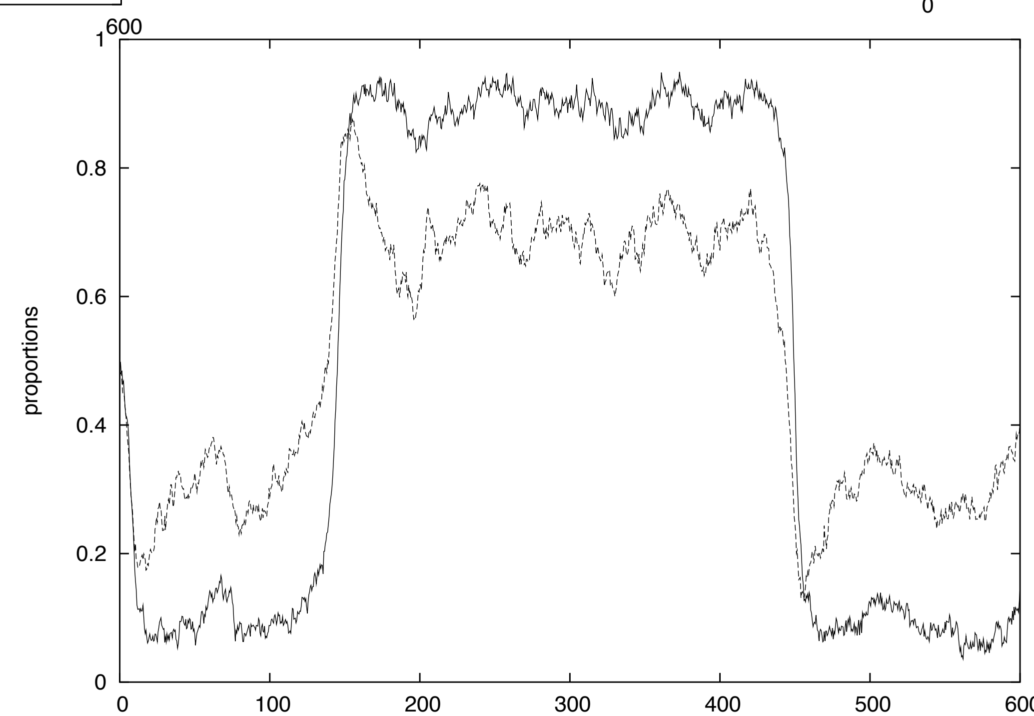


Model

Model + noise



MD



Conclusion

- Anomalous velocity distributions: formation of non-Maxwellian tails + *infinite* energy solutions (truncated Lévy distributions)

→ Links with a non-linear random walk + infinite energy solutions for arbitrary cross sections

- Non-equipartition of energy: mean field models + MD and DSMC simulations + predictions for K components

→ Comparison with real experiments + MD simulations

- Granular Demon model: order-disorder transitions + complex behaviours (oscillations, metastability)

→ Real experiments of the asymmetric model and of the mixture model + detailed MD simulations of the systems