

# Metastable states and stochastic dynamics of granular materials

Jusqu'où peut-on calculer comme un cochon ?

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in collaboration with :

A. Martin (LMGC), F. Dubois (LMGC) and Y. Monerie (IRSN) for silo discharge

L. Staron (LMM) and J.-P. Vilotte (IPGP) for pre-avalanche instabilities



# Outline

- ▶ Introduction: Michel's criteria of convergence
- ▶ Constitutive framework and granular microstructure
- ▶ Metastable states in transition to instability
- ▶ Silo discharge as a stochastic process
- ▶ Conclusion

# Introduction

1994 in Montpellier: Michel repeated the same simulations patiently by changing the simulation parameters...

- not convinced by the **quality** of his simulations
- annoyed by the fact that slightest change in numerical parameters led to different results
- tried various **convergence criteria**

Michel's way of stating his doubts:

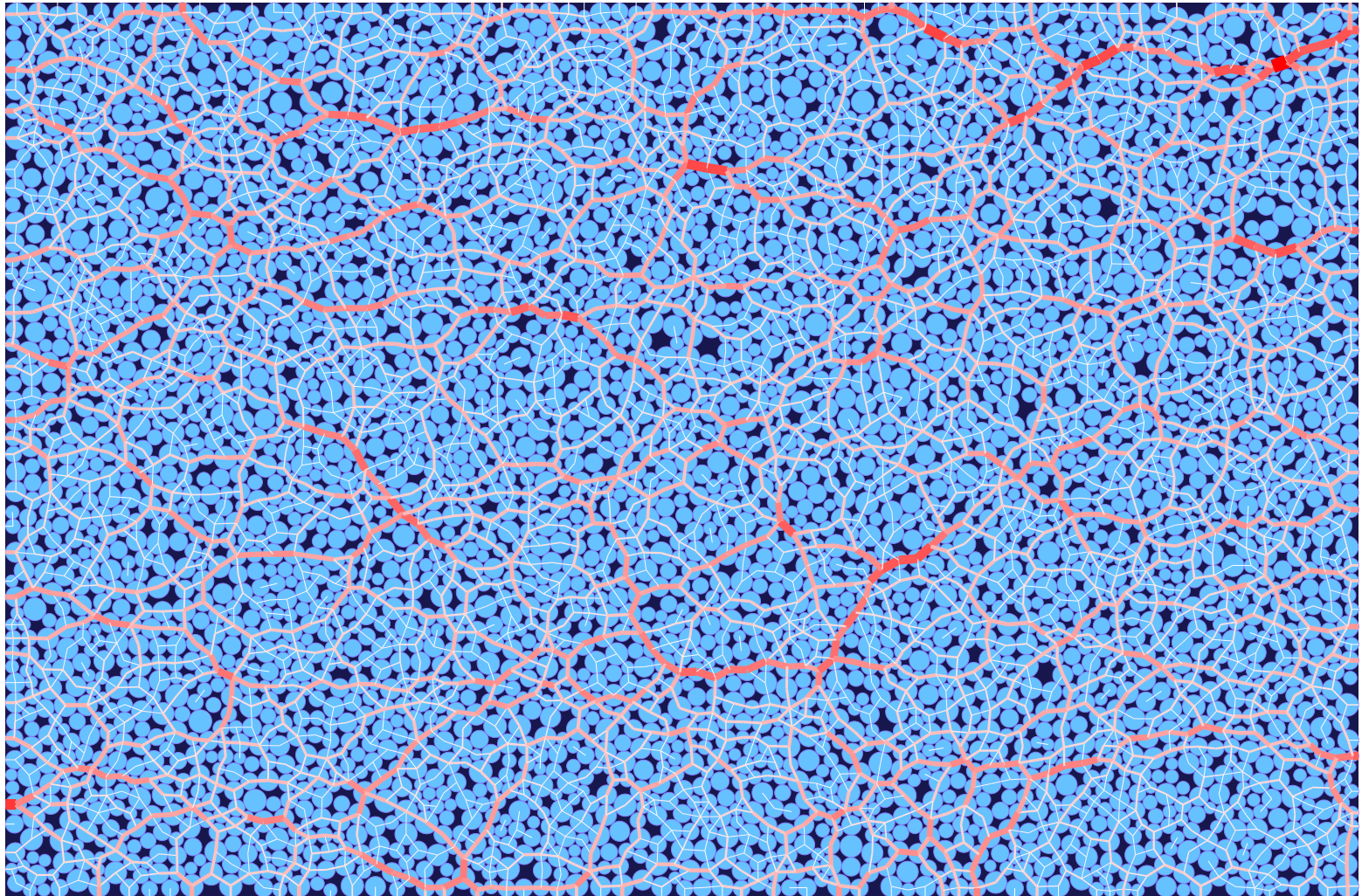
- The question is : jusqu'où peut-on calculer comme un cochon?
- When you simulate granular materials, you should take your responsibility!

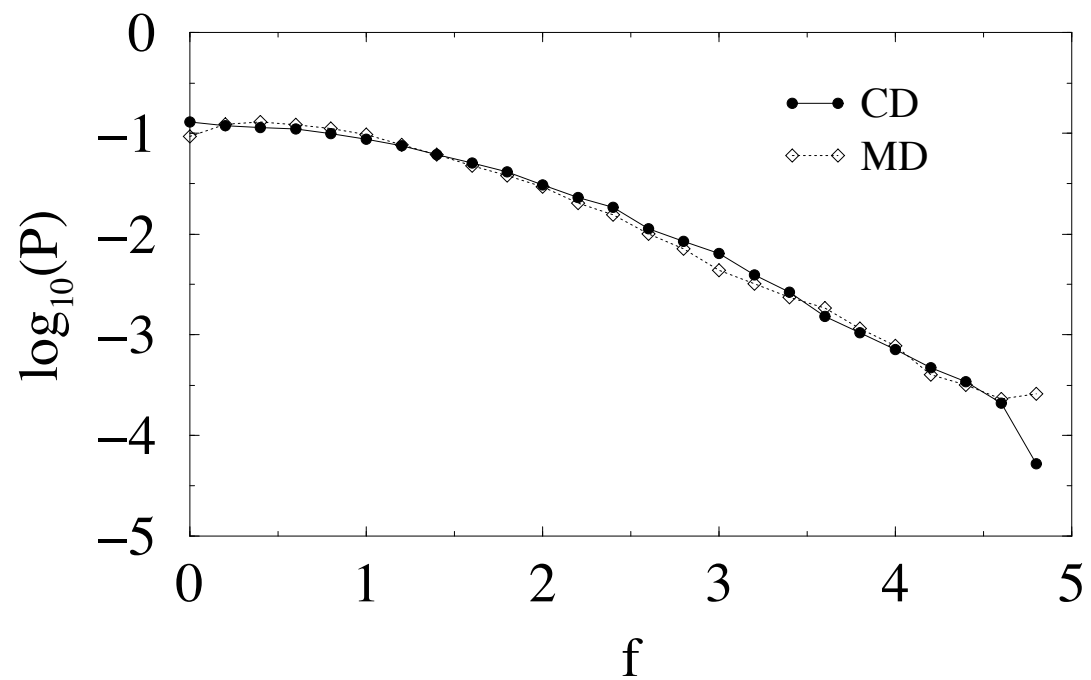
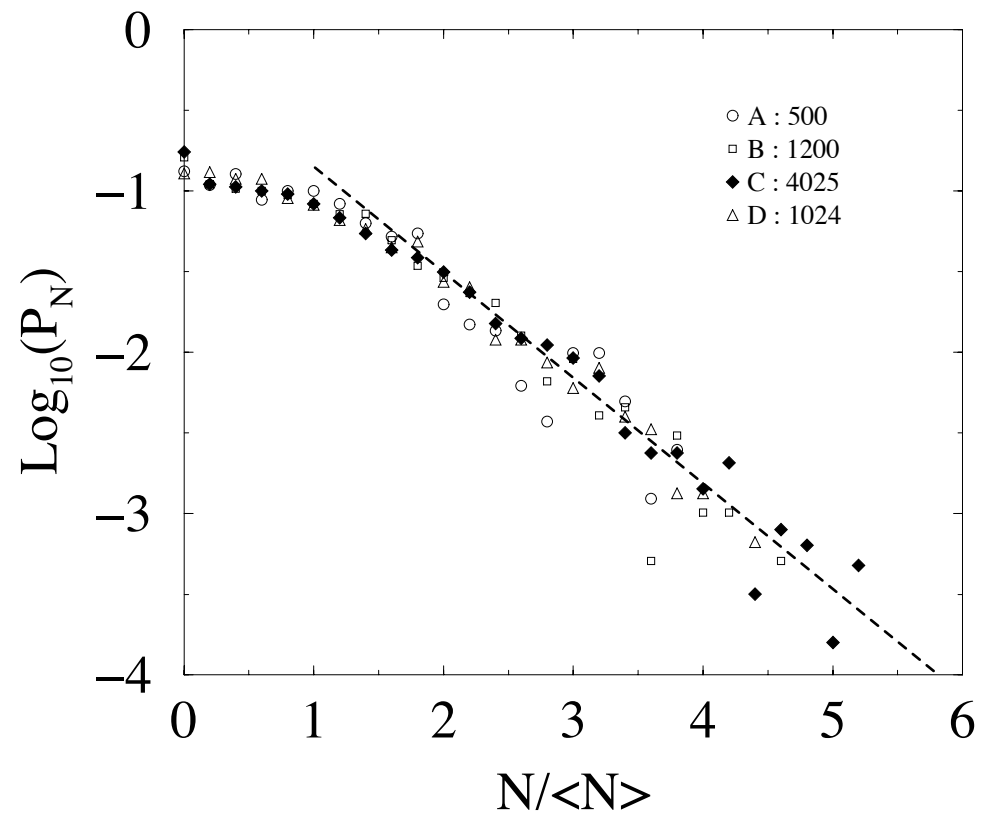
## 1996: Exponential tails

Force distributions in dense two-dimensional granular systems

F. Radjai, M. Jean, J. J. Moreau and S. Roux

Phys. Rev. Lett. 77, p.274.



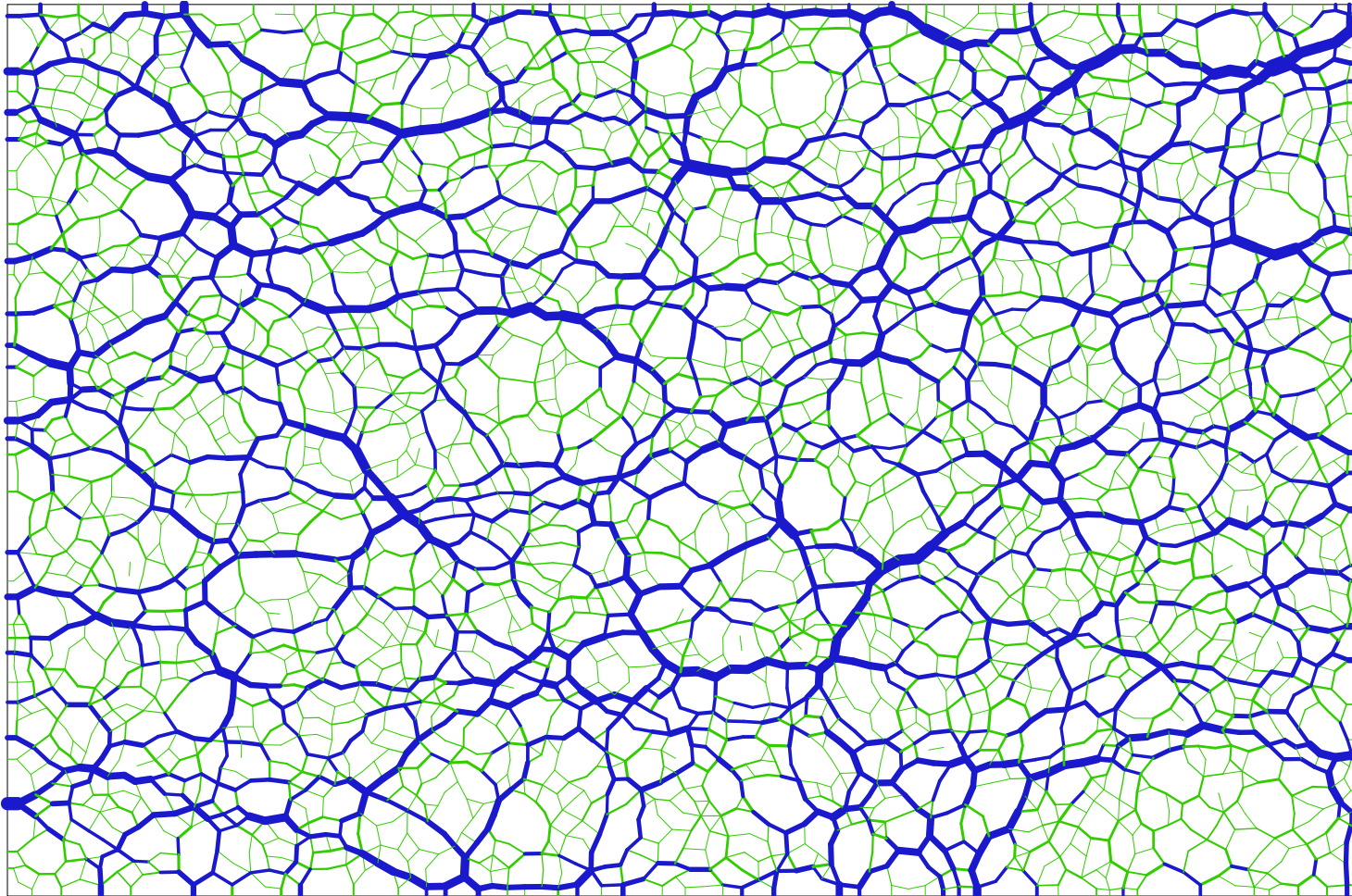


## 1998: Strong and weak networks

Bimodal character of stress transmission in granular packings,

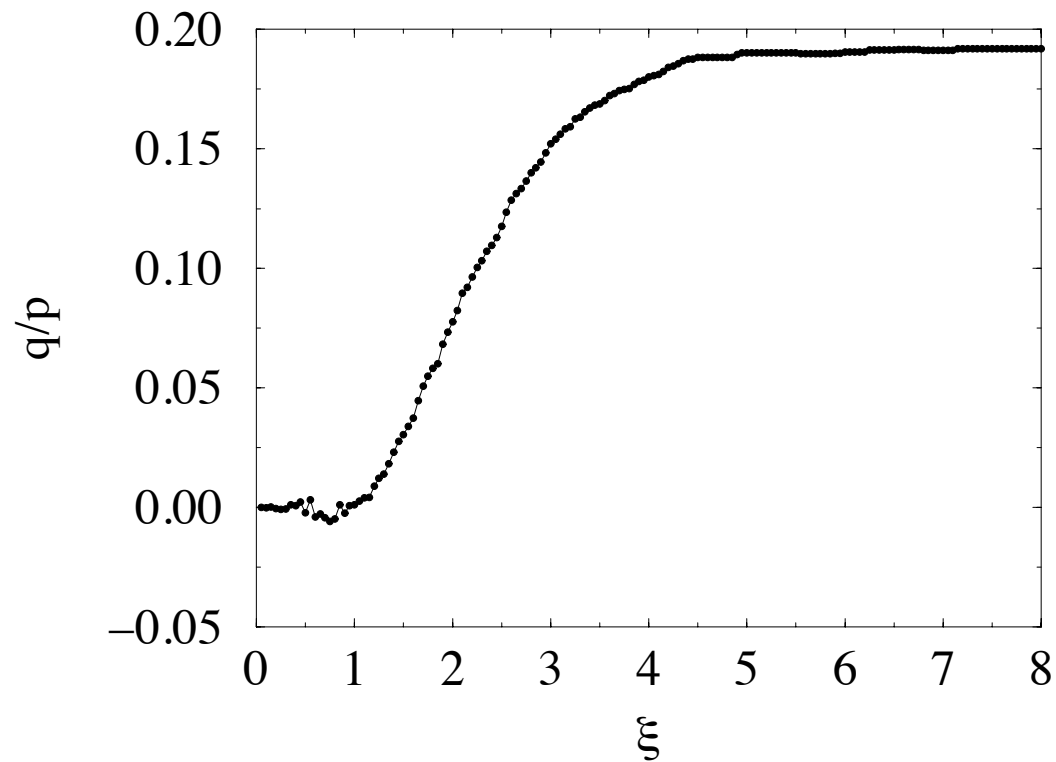
F. Radjai, D. Wolf, M. Jean, and J. J. Moreau (1998)

Phys. Rev. Lett. 90, p.61.



Shear stress sustained by contact sub-networks:

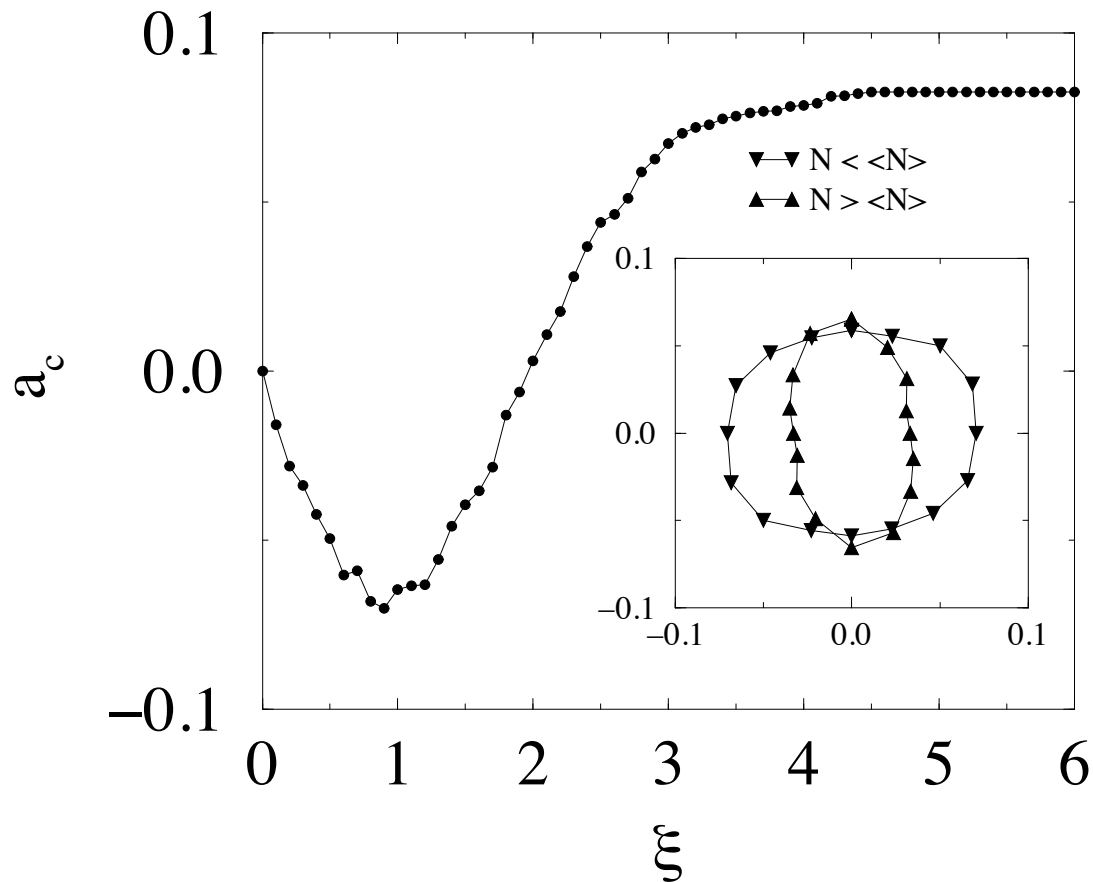
$$\mathcal{S}(\xi) \equiv \{f_n \mid f_n < \xi \langle f_n \rangle\}$$



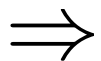
$$\boldsymbol{\sigma} = p_w \mathbf{I} + \boldsymbol{\sigma}_s$$

The shear stress is sustained by the **strong force network**.

# Fabric anisotropy of contact sub-networks



**Weak contacts** tend to be along minor principal stress direction.



Tensorial arching effect: **Strong force chains are balanced by side-wise weak forces.**

Michel's interpretation: We might enrich purely mechanical criteria by **physical criteria** (e.g. force distributions) for the **convergence** and **quality** of calculations.

- The very weak forces are at least as frequent as the mean force; one should make sure that they are correctly calculated rather than the mean: **how many nearly zero forces are calculated within a nonzero numerical precision?!**
- Due to the broad distribution of strong forces, the representative volume element should be large enough to ensure the **statistical representativity** of strong forces.

## Michel's criteria:

- Mechanical: thick graphs and error in energy
- Physical: large systems and weak forces
- Esthetic: **simplicity and elegance** -- crucial for both the **concepts** and the code architecture, inherent in the method (Michel: I will not leave a code but a method to the next generation.)
- Human: I have my own criteria, but other choices are respectful. The NSCD has its limits, and Molecular Dynamics is (also) an intelligent method. I prefer friendly grains to smart grains.

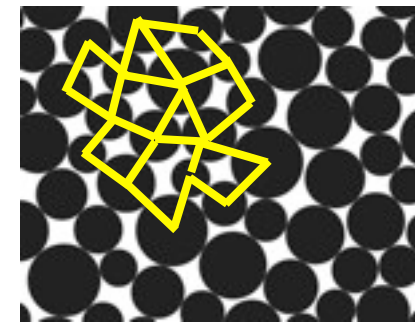
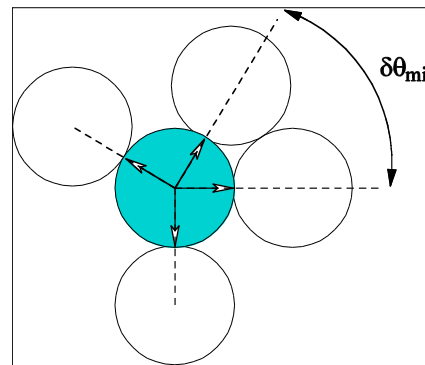
This talk: last 10 years

Michel's problem is rooted in a fundamental property of granular matter: the dynamics is **chaotic** and **multiscale** in nature. This implies:

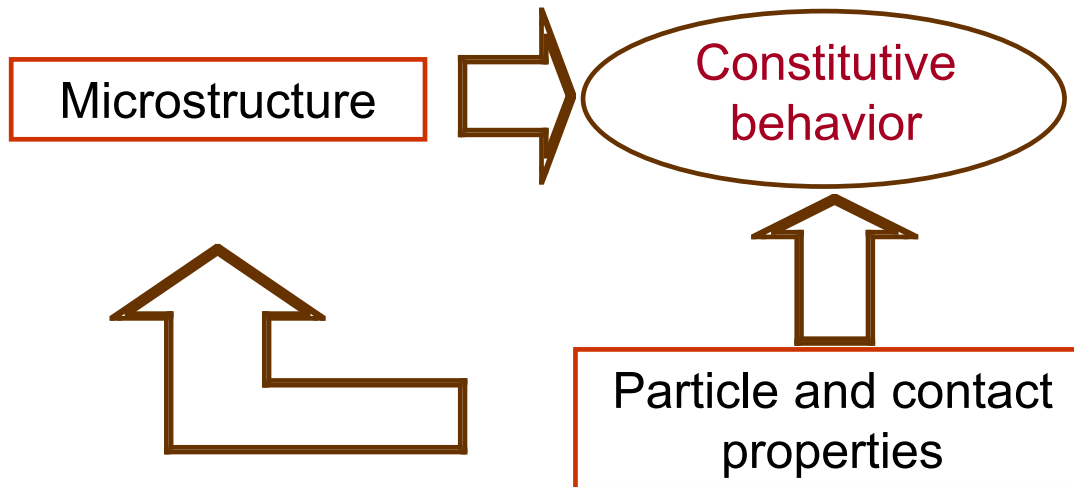
- In discrete-element calculations, we should worry about the precision of both mean values and **fluctuations** around the mean.
- However, a deterministic reproducibility is neither possible nor necessary.

# Constitutive framework and granular microstructure

- Granular matter involves discrete elements with **steric exclusions**.
- Interactions are **dissipative** (inelastic collisions, dry friction) and occur at contact.
- **Disorder** is generic and occurs both in metrics and in topology (connectivity).



There is strong analogy with **amorphous** molecular systems. But it involves **NEW** physics stemming from **nonsmooth** contact interactions.



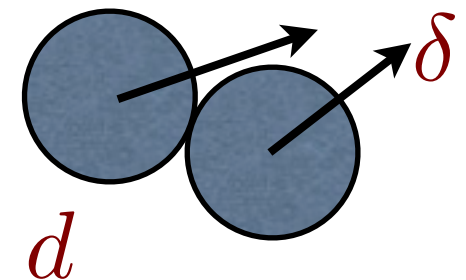
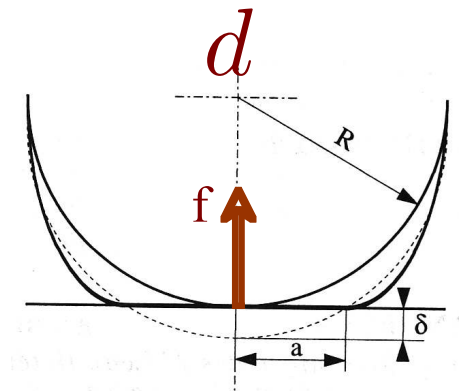
Contact elasticity  $\longrightarrow$  Elastic behavior

Particle displacements  $\longrightarrow$  Plastic behavior

$$\delta \ll d$$

Neglecting  $\delta \implies$  Rigid particles

$\implies$  Rigid-Plastic behavior




## 1) Rigid particles

No stress scale  $\rightarrow$  The domain of admissible stresses is a cone.



Yield surface characterized by a single angle

$$\sin \varphi = \frac{q}{p}$$


Macroscopic **friction angle**

## 2) Contact friction

Slip friction can be viewed as a non-associated plastic behavior.  $\longrightarrow$  The macroscopic plastic behavior is not expected to be associated.



The direction of strain rate should be specified independently of the yield surface.

$$\sin \psi = -\frac{\dot{\epsilon}_p}{\dot{\epsilon}_q}$$

**Dilatancy** angle

3) Both  $\varphi$  and  $\psi$  evolve with strain.



$\varphi$  and  $\psi$  are dependent on **state variables** pertaining to the granular microstructure.

$$\varphi(E) \quad \psi(E)$$



State variables

Candidates for  $E$  :      Coordination number  
Fabric anisotropy

**Rigid-plastic non-associated behavior** with physical state variables:

1)  $\varphi(E)$  Yield surface

2)  $\psi(E)$  Flow rule

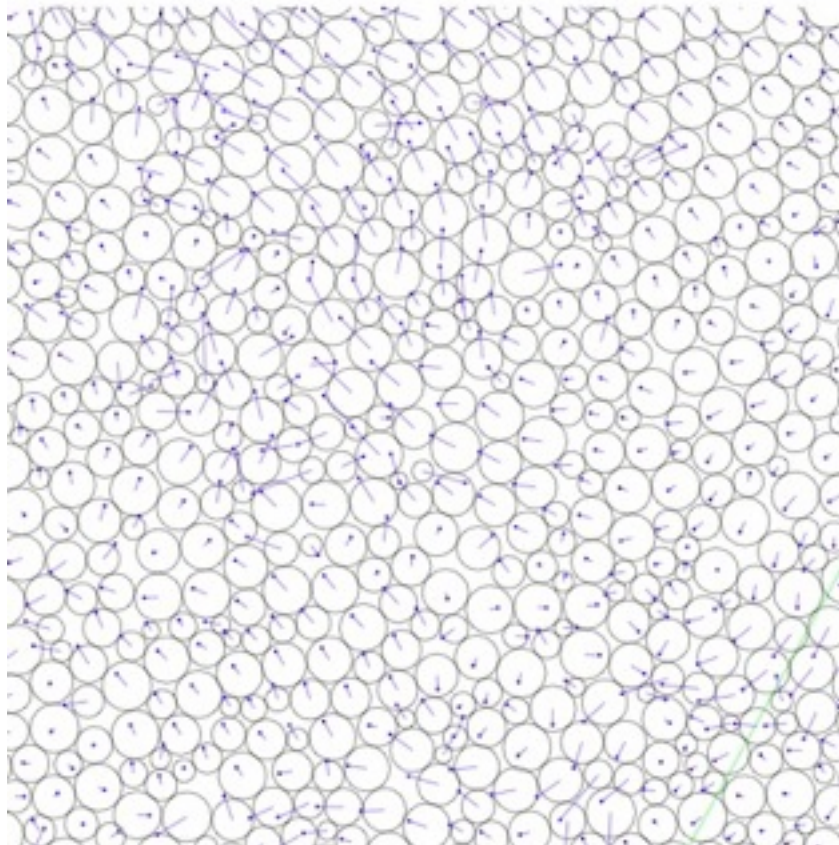
3)  $\dot{E}\{\dot{\varepsilon}, \varphi(E), \psi(E)\}$  Hardening law

**Critical state:**  $\dot{E} = 0$   $\left\{ \begin{array}{l} \psi_c = 0 \\ \varphi_c \\ E_c \end{array} \right.$

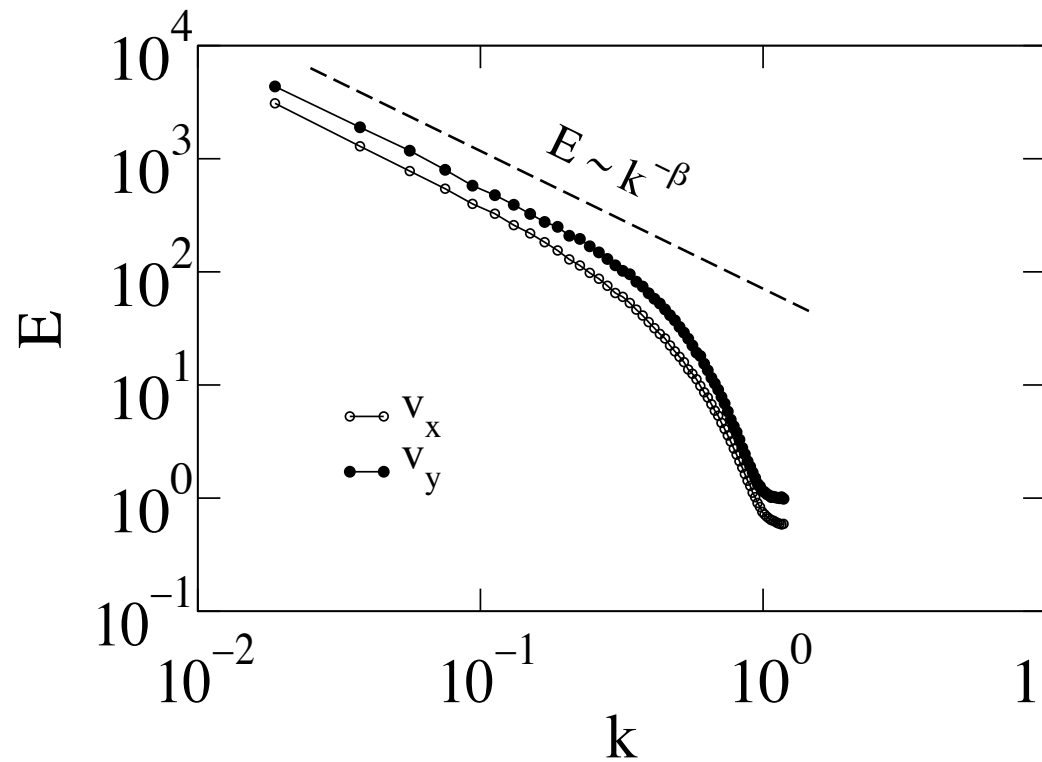
$\equiv$  Mohr-Coulomb yield criterion

**Hardening:** evolution of the microstructure due to grain motions.

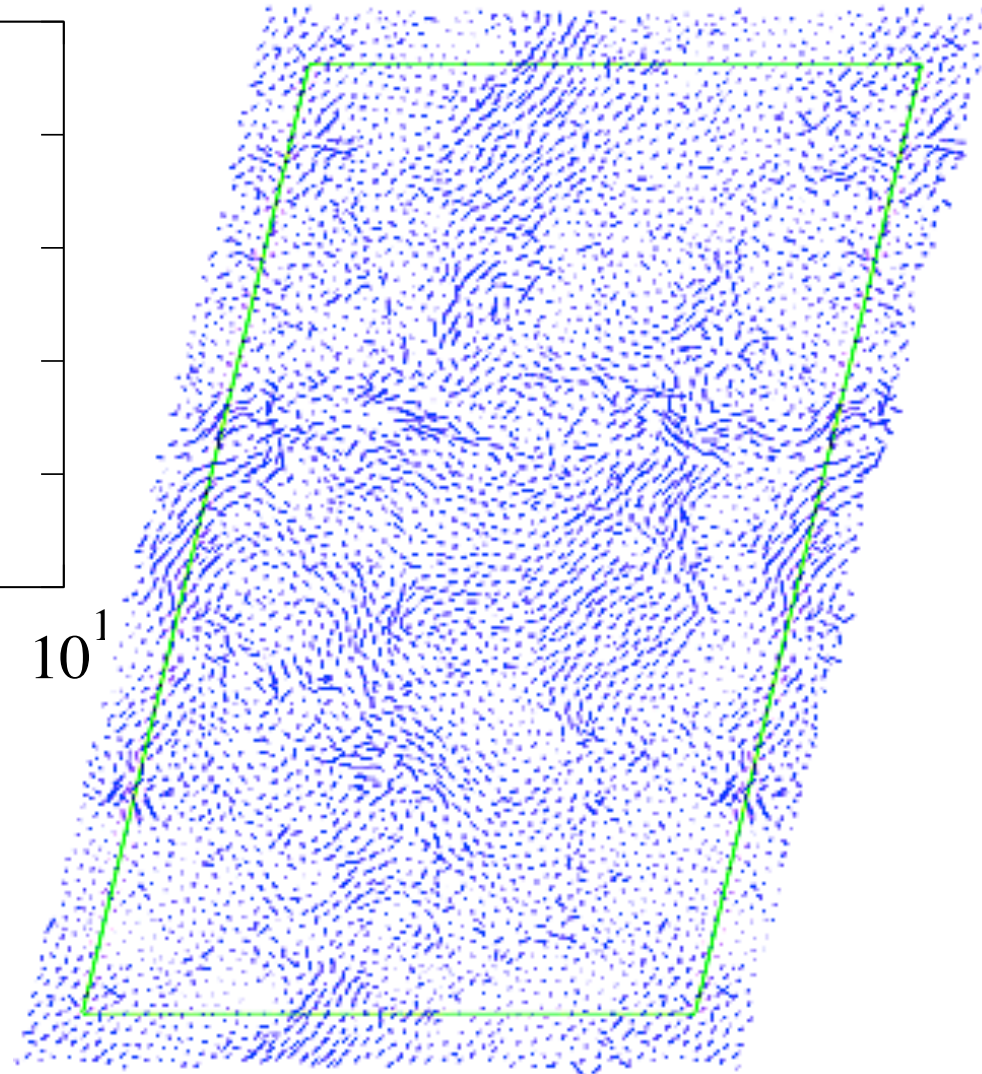
The grain motions have a **non-affine** nature.



The grain motions are strongly correlated.



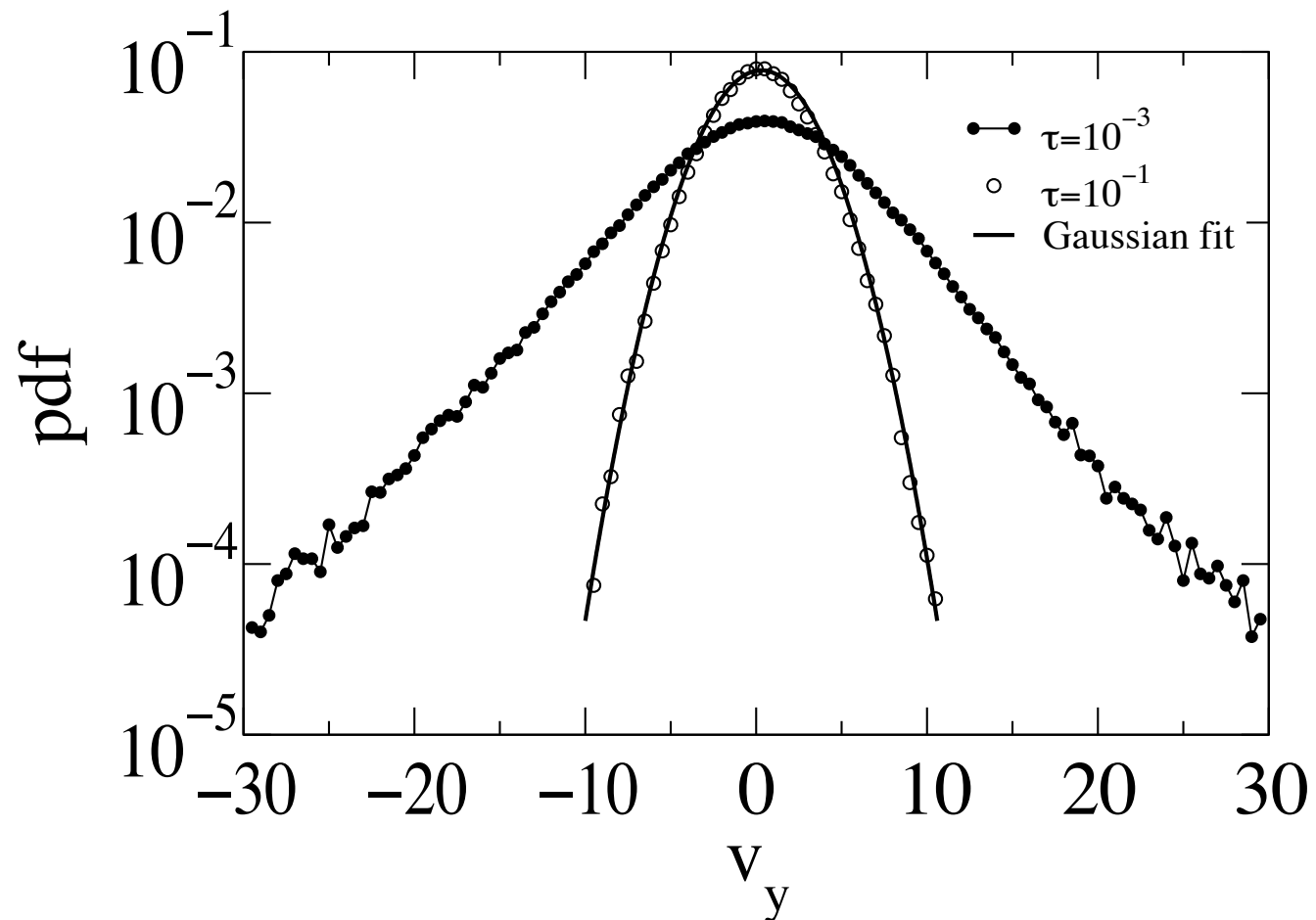
granulence



F. Radjai and S. Roux (2002)

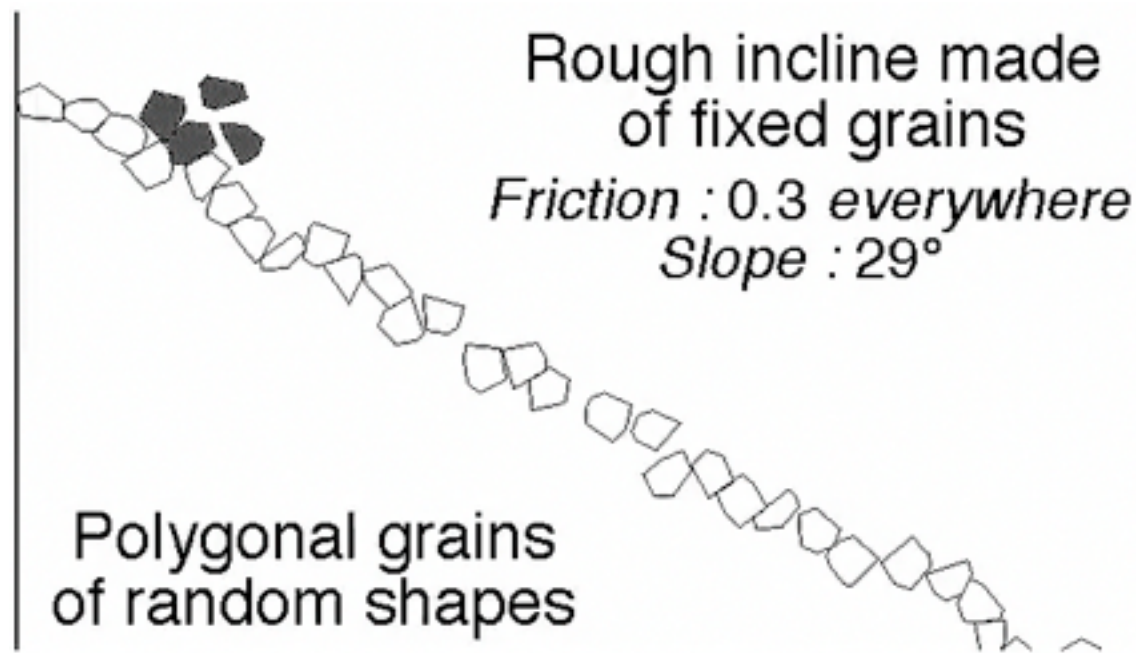
The velocity distributions depend on time resolution.

$$\vec{v}(t, t + \tau) = \frac{1}{\tau} \int_t^{t+\tau} \delta \vec{s}(t') dt'$$



In the absence of thermal agitation, the material can be found in very different **metastable states**: a partial flow of grains may occur in response to a small perturbation.

The granular flow initiated by perturbing a metastable state is **transient** and stops as the grains get jammed in a metastable state. These flows have a fluctuating behavior and the number of mobilized grains or flow lifetimes has a broad distribution.



Simulations by J. J. Moreau (1998)

## 1) individual grain movements

state:  $K(t)$  number of grain movements up to  $t$

transition:  $K \rightarrow K + 1$        $K \rightarrow K - 1$

micro-process:  $P_k(t) \equiv P\{[K(t' + t) - K(t')] = k\}$

$$\sum_{k=0}^{\infty} P_k = 1$$

## 2) jamming events

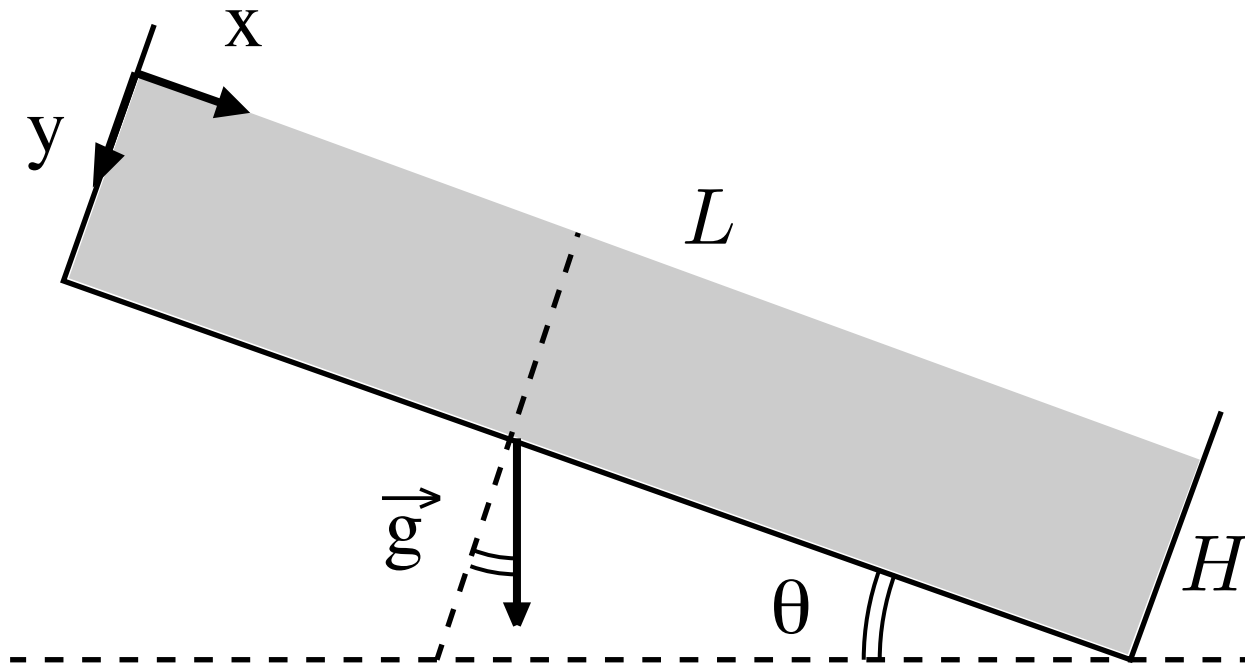
state:  $S(K)$  number of jams for  $K$  passing grains

transition:  $S \rightarrow S + 1$

macro-process:  $P_s(K) \equiv P\{[S(K' + K) - S(K')] = s\}$

$$\sum_{s=0}^{\infty} P_s = 1$$

# Metastable states

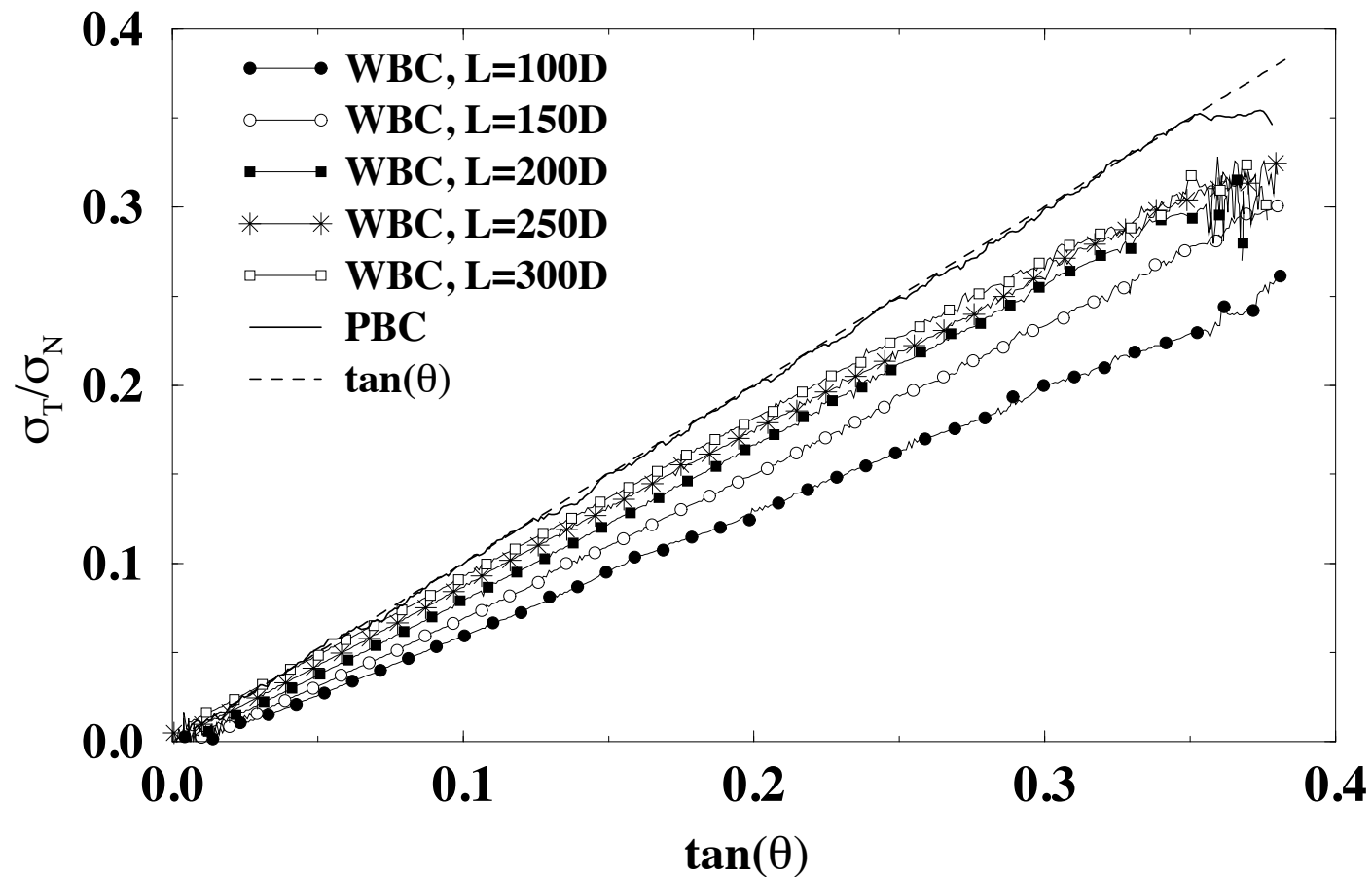


$$H \simeq 40D$$

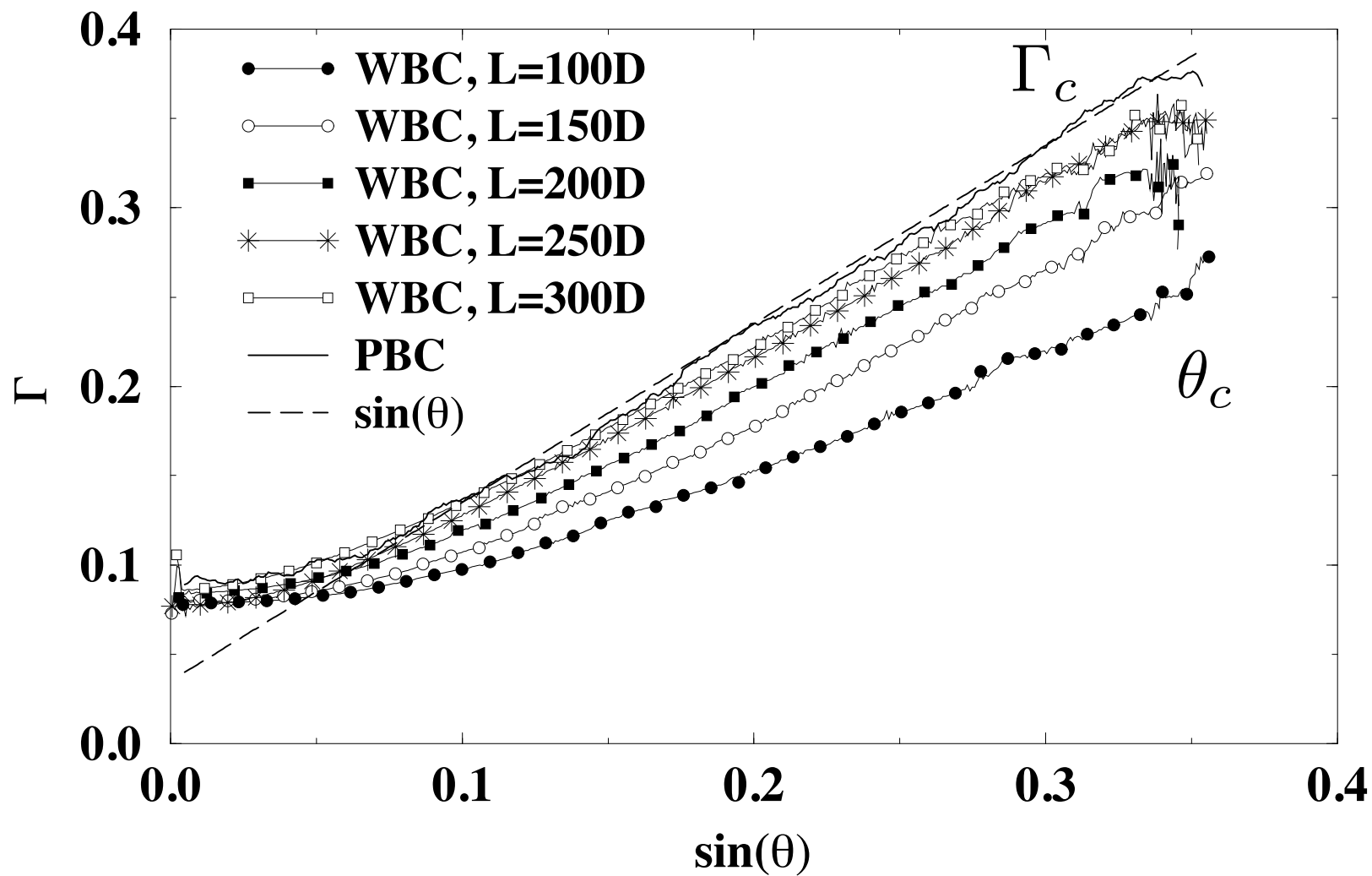
$$\omega = 1^\circ \text{s}^{-1} \quad \text{rotation}$$

## Average stresses

$$\frac{\sigma_T}{\sigma_N} = \frac{\sigma_{yx}}{\sigma_{yy}} = \tan \theta \quad \text{mechanical equilibrium + translational invariance}$$



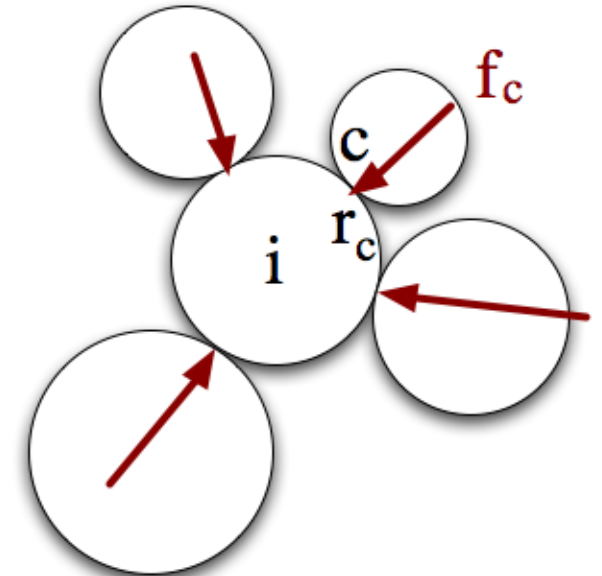
$$\Gamma = \frac{Q}{P} \quad \begin{aligned} Q &= \frac{\sigma_1 - \sigma_2}{2} \\ P &= \frac{\sigma_1 + \sigma_2}{2} \end{aligned} \quad \Rightarrow \quad \Gamma = \sin \theta$$



# Grain stresses

internal moment  
(J. J. Moreau, 1998)

$$M_{\alpha\beta}^i = \sum_{c \in i} f_{\alpha}^c r_{\beta}^c$$



Properties:

1. Symmetric

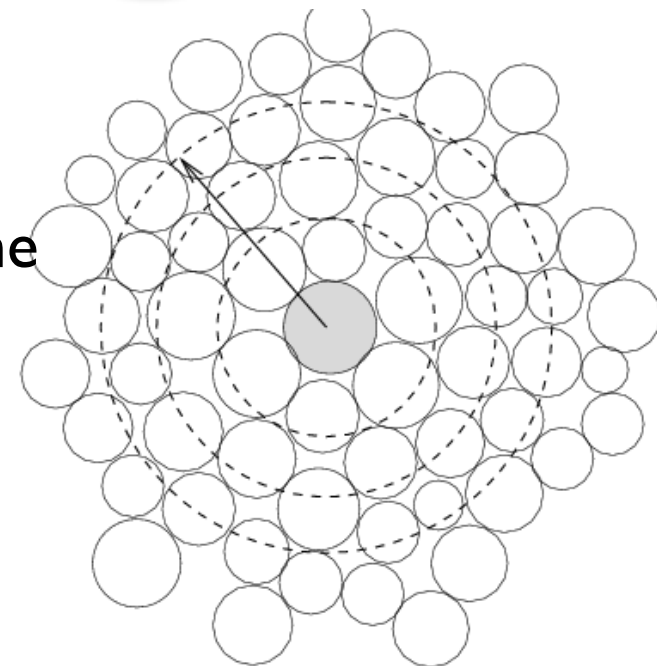
2. Independent of the choice of origin

3. Additive  $M_{\alpha\beta}^{i \cup j} = M_{\alpha\beta}^i + M_{\alpha\beta}^j$

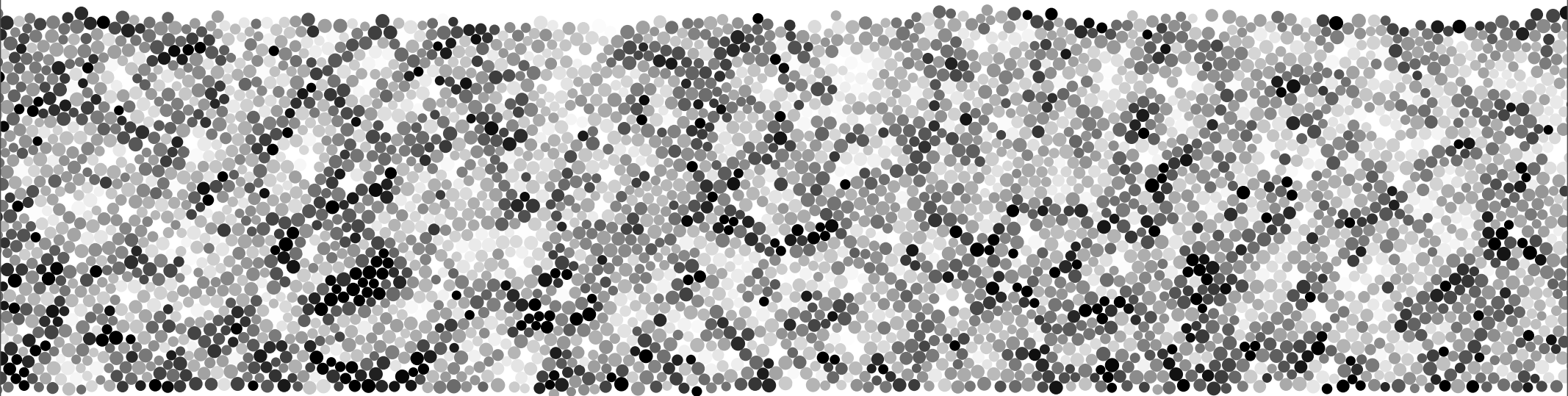
4. The density of internal moments tends to the

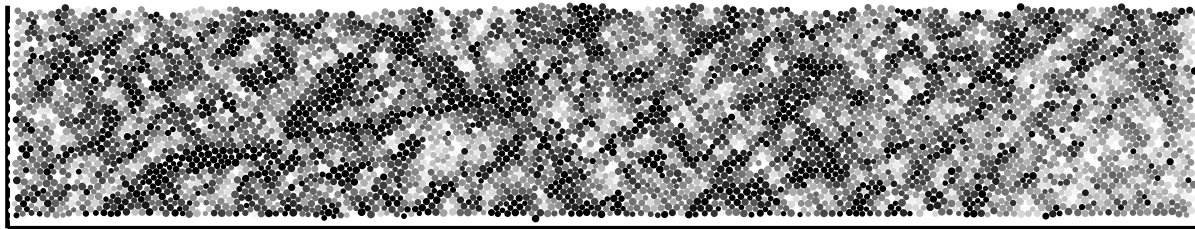
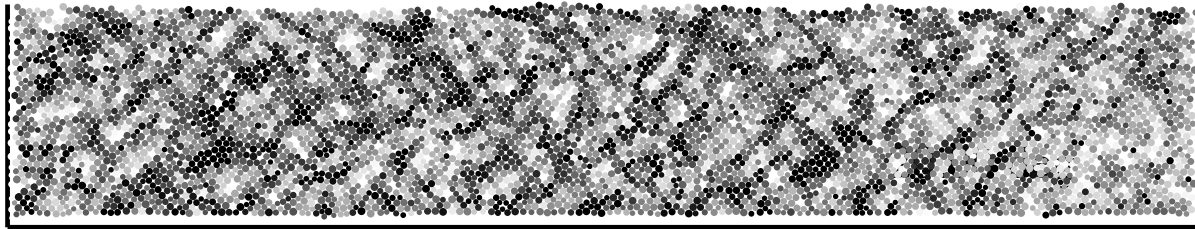
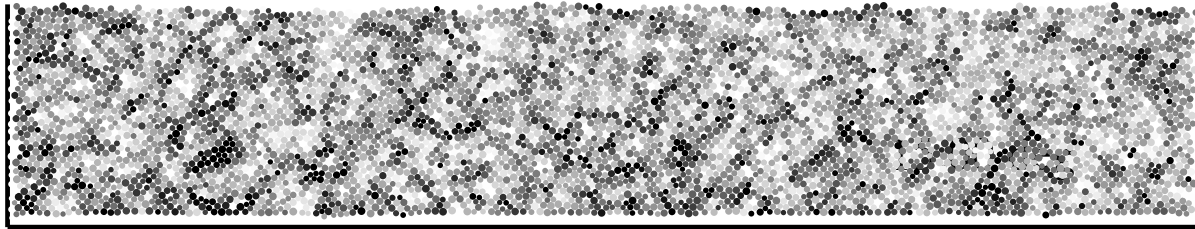
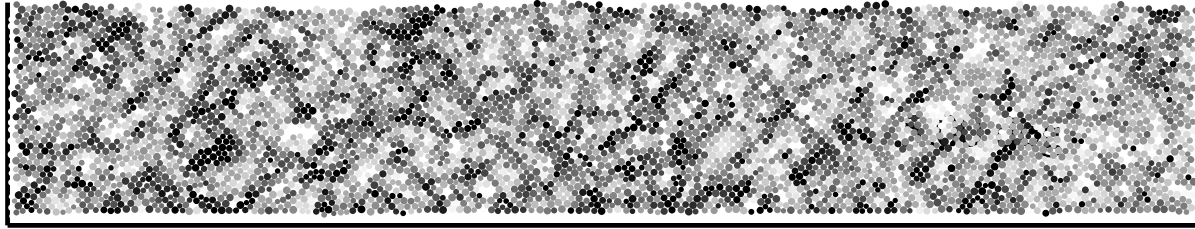
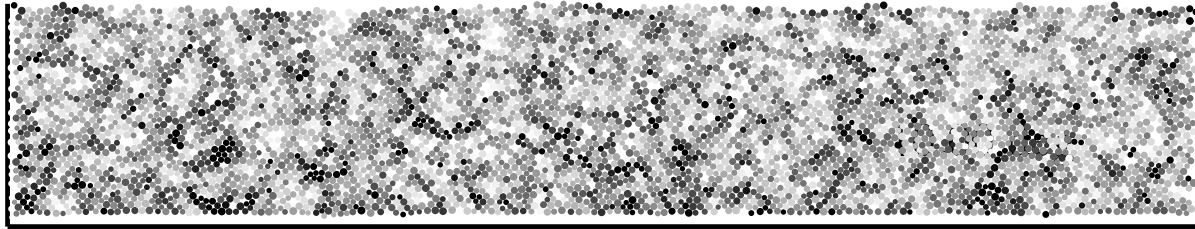
Cauchy stress tensor

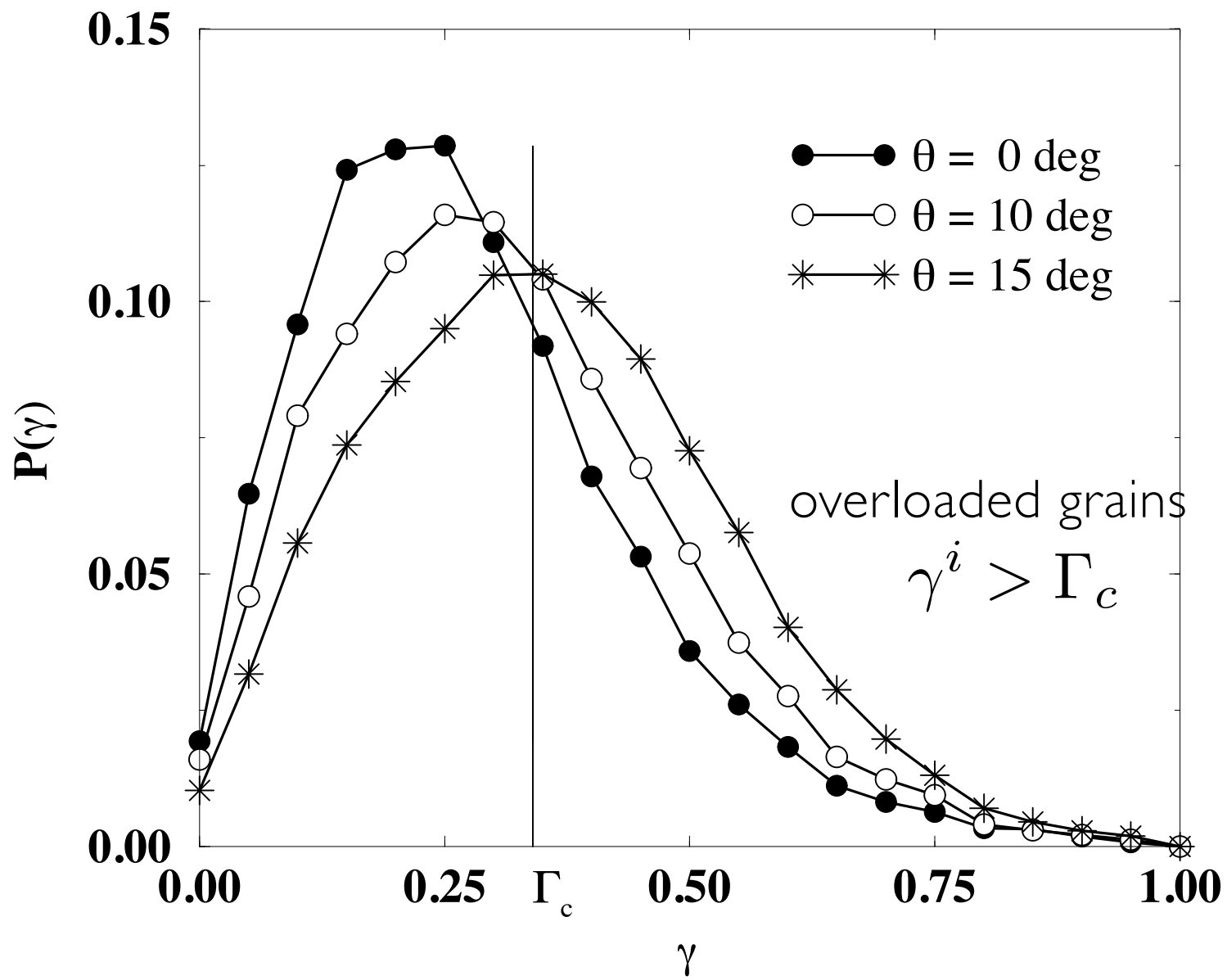
$$\frac{1}{V} \sum_{i \in V} M_{\alpha\beta}^i \rightarrow \sigma_{\alpha\beta}$$
$$V \rightarrow \infty$$

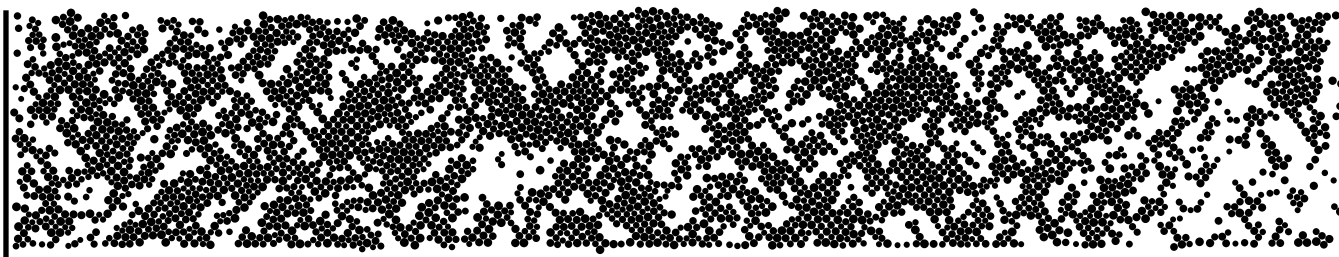
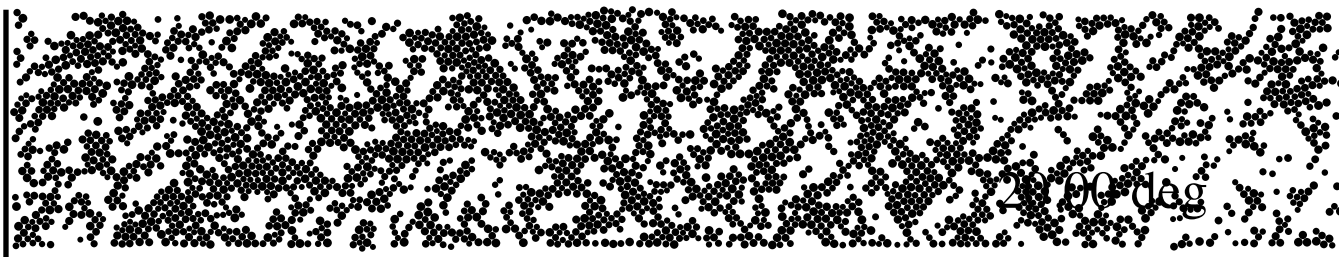
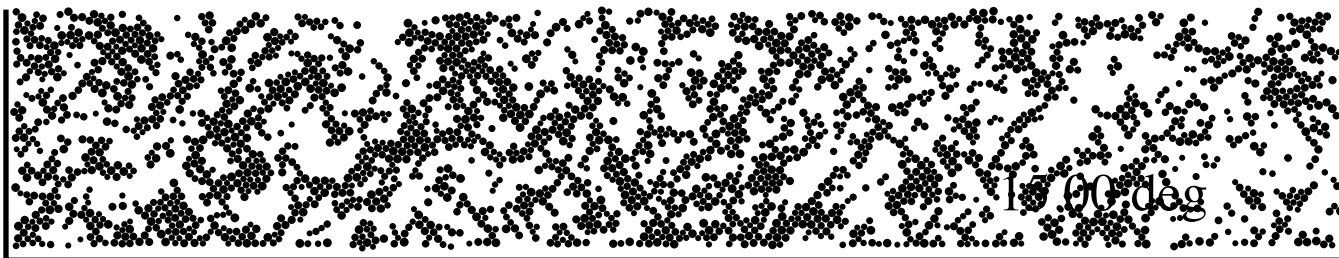
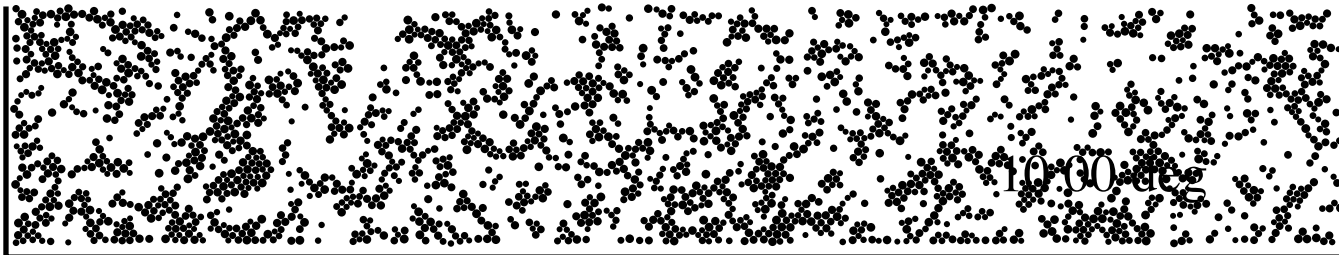
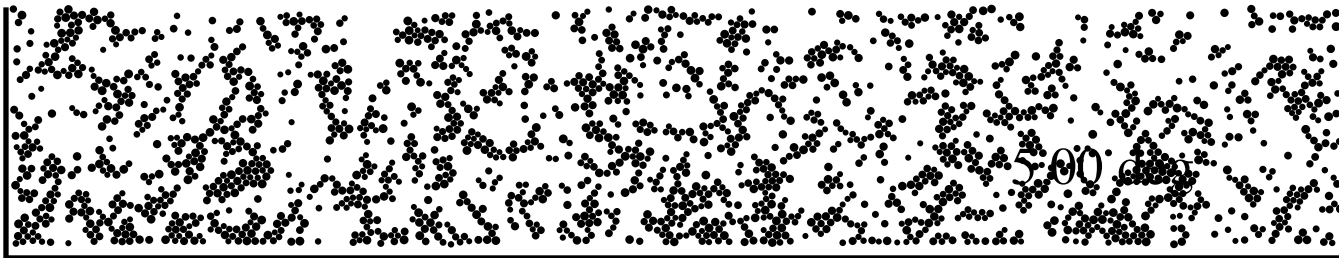


$$\gamma^i = \frac{q^i}{p^i}$$

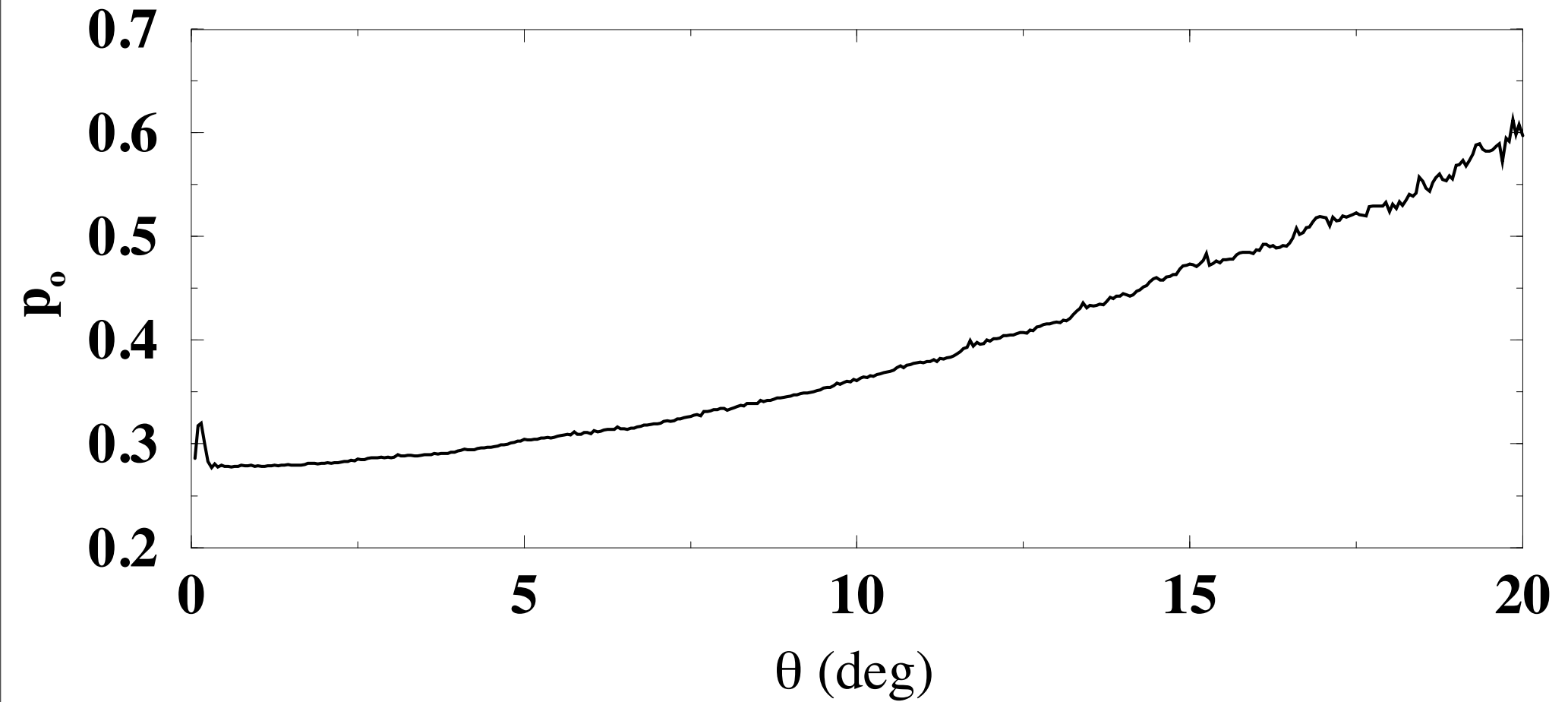








# proportion of overloaded grains



Stress ratio for a circular volume of radius  $l$  centered on the particle  $i$

$$\gamma^i(l)$$

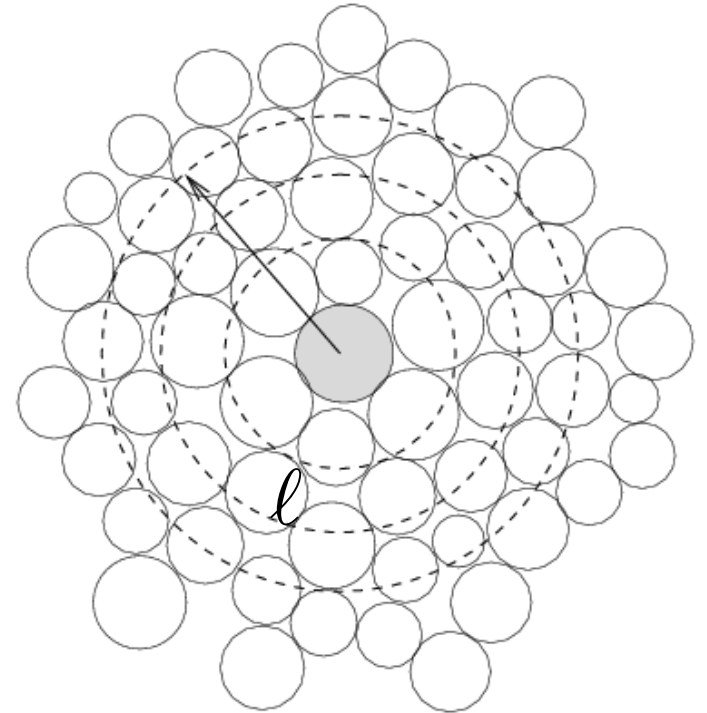
coarse-graining length  $l_c^i$

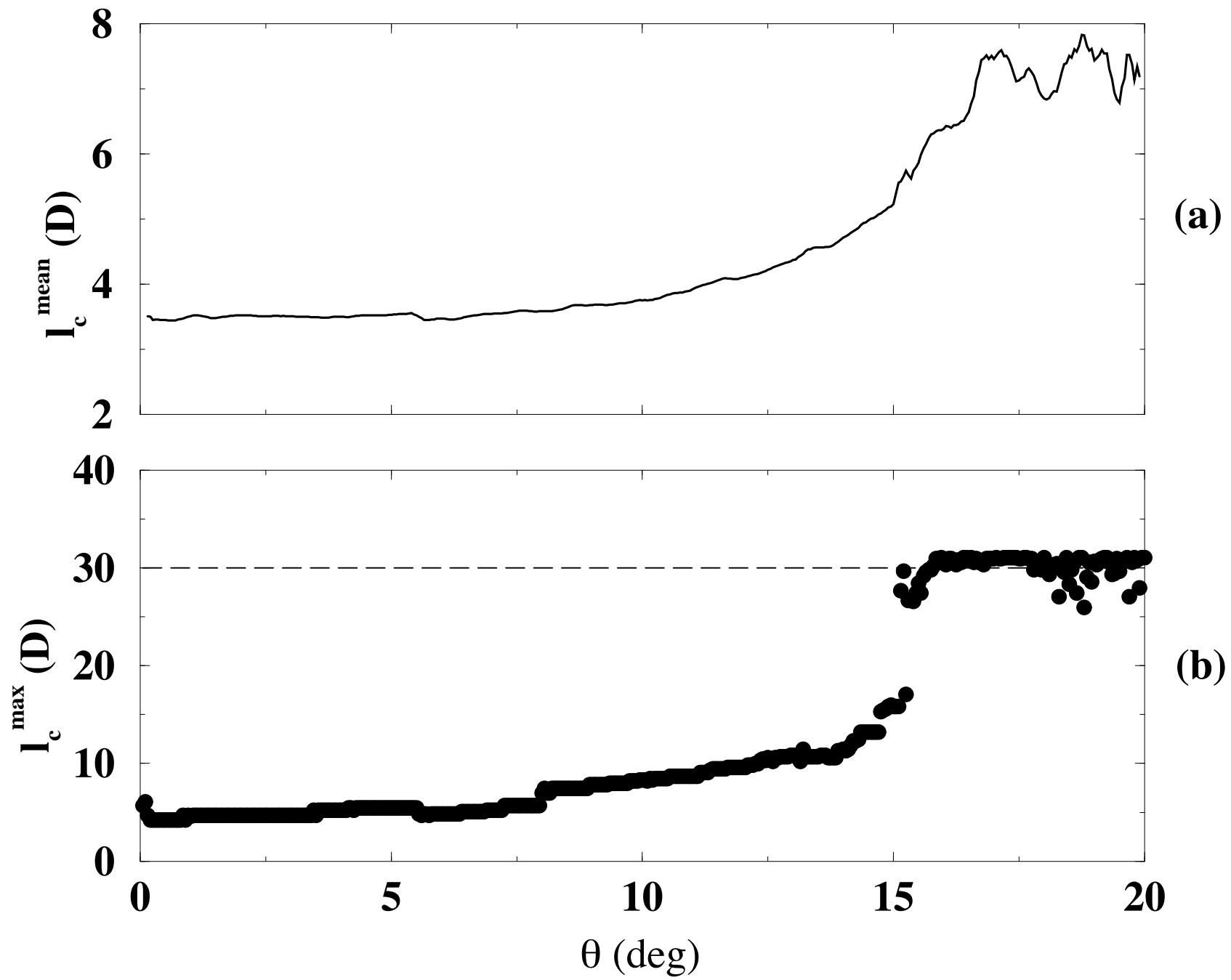
$$\gamma^i(l_c^i) = \Gamma_c$$

$\Rightarrow$

$$l_c^{max} = \max\{l_c^i\}$$

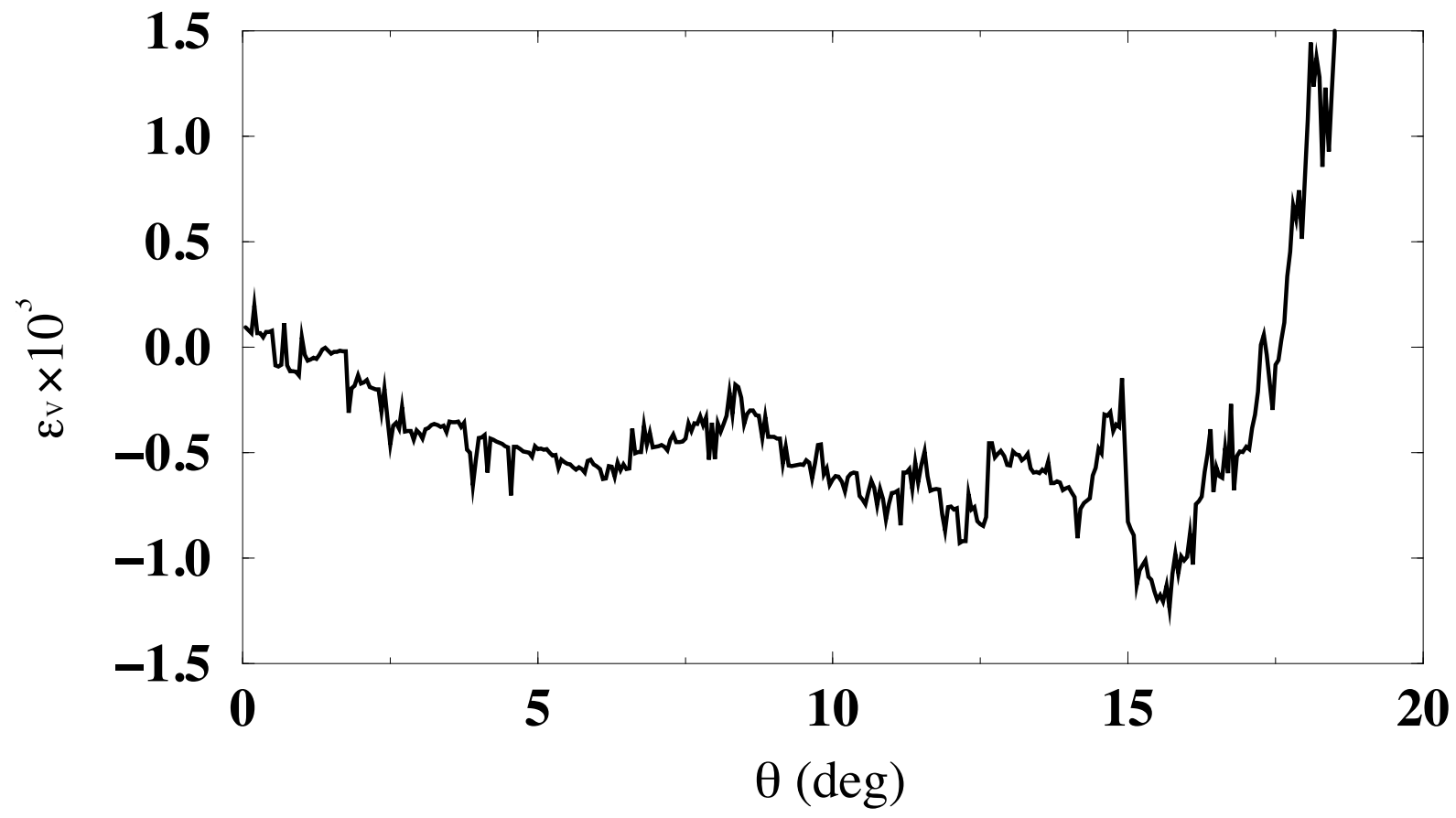
$$l_c^{mean} = \frac{1}{N_c} \sum_1^{N_c} l_c^i$$



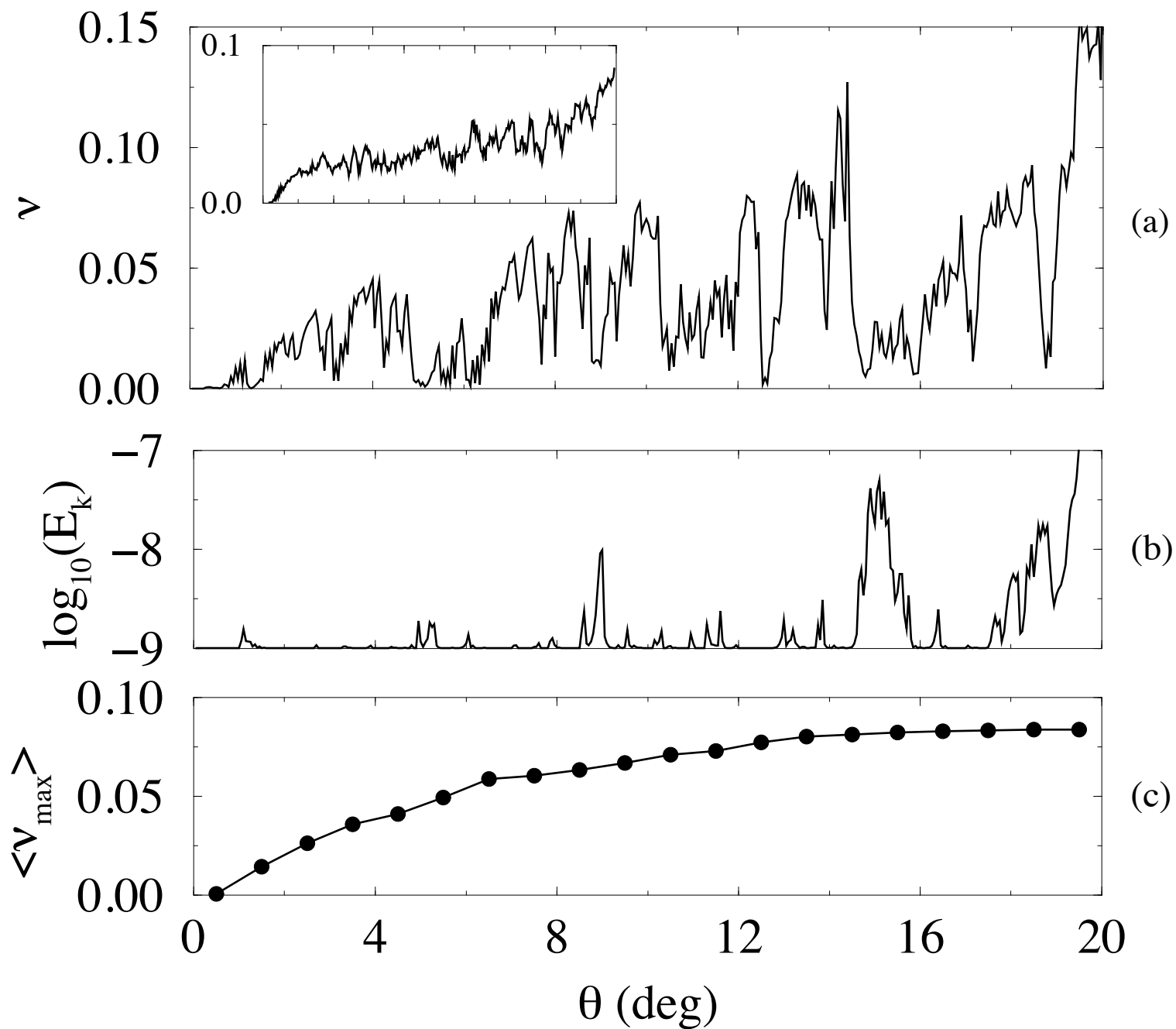


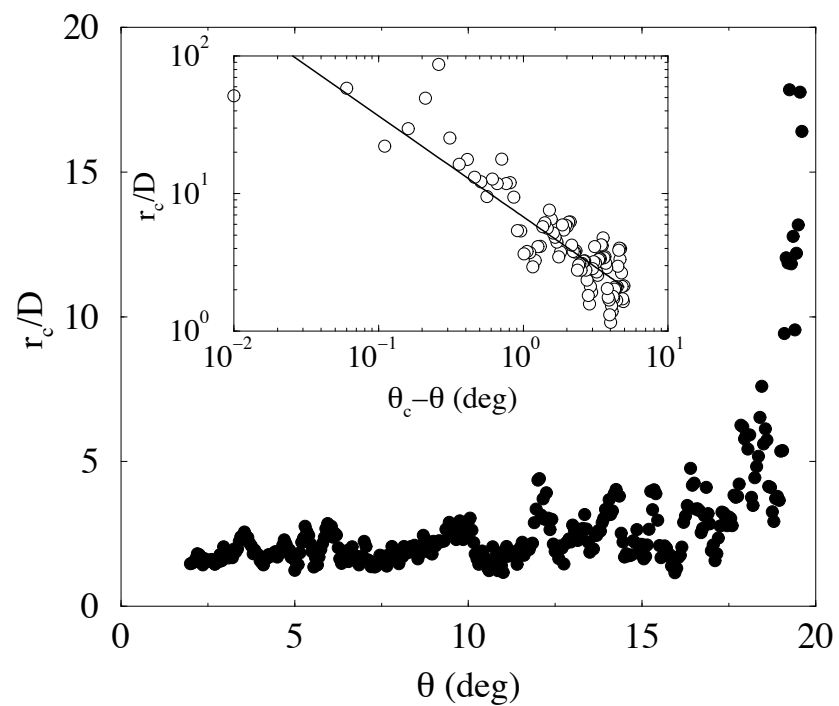
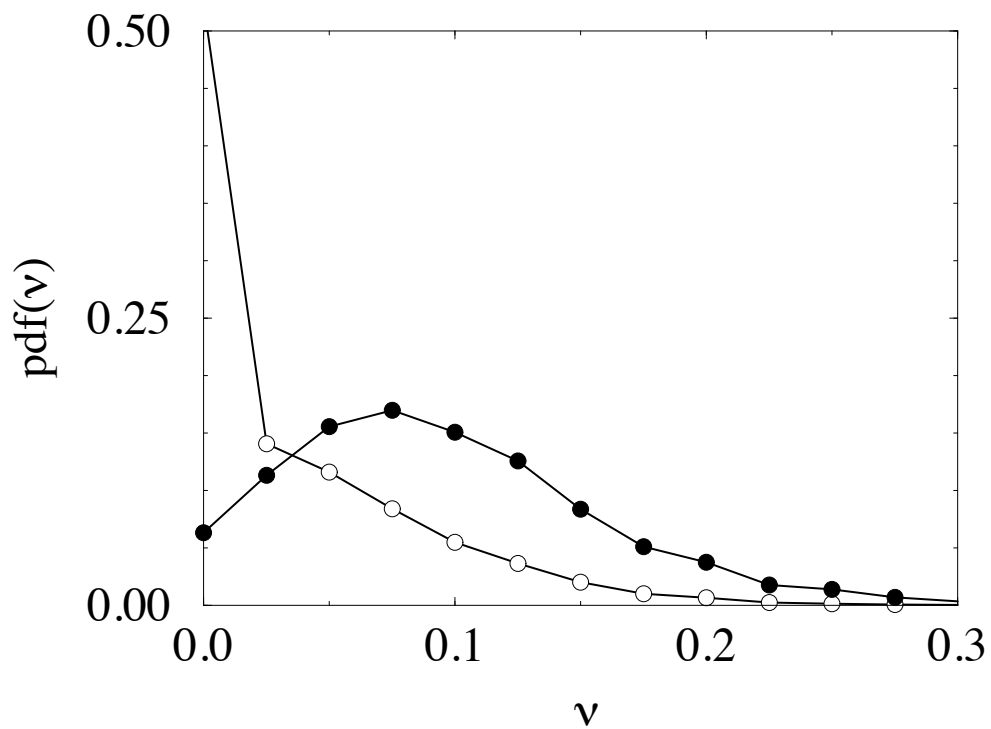
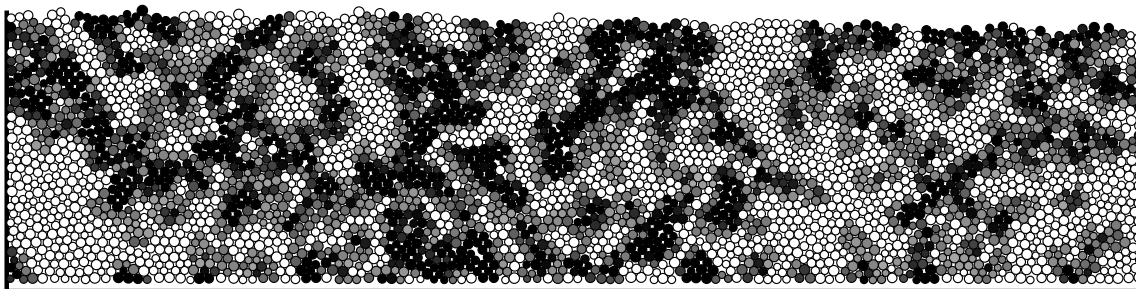
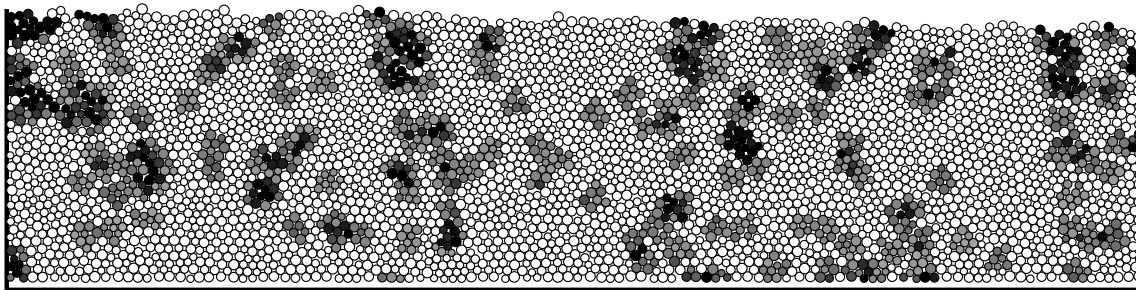
L. Staron, F. Radjai and J.-P. Vilotte (2004)





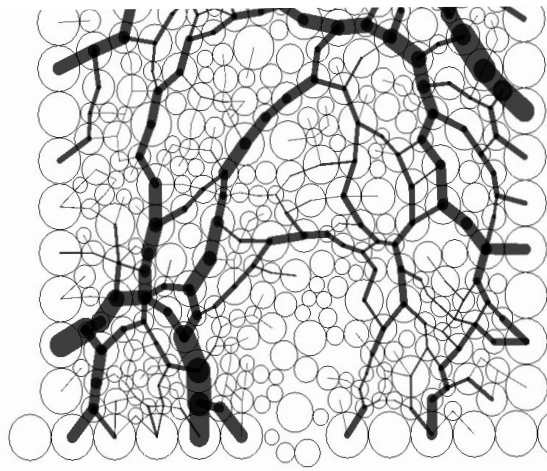
# critical contacts



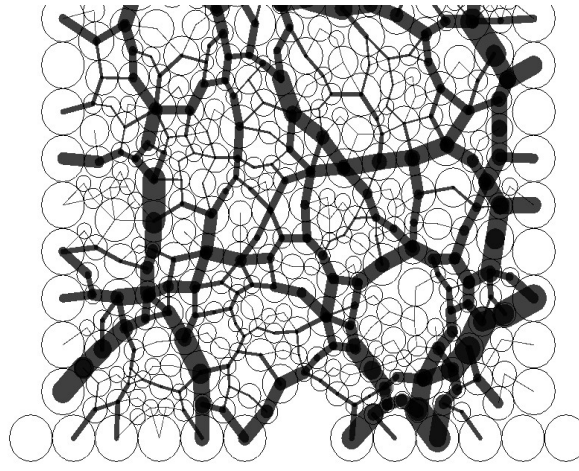


# Silo discharge

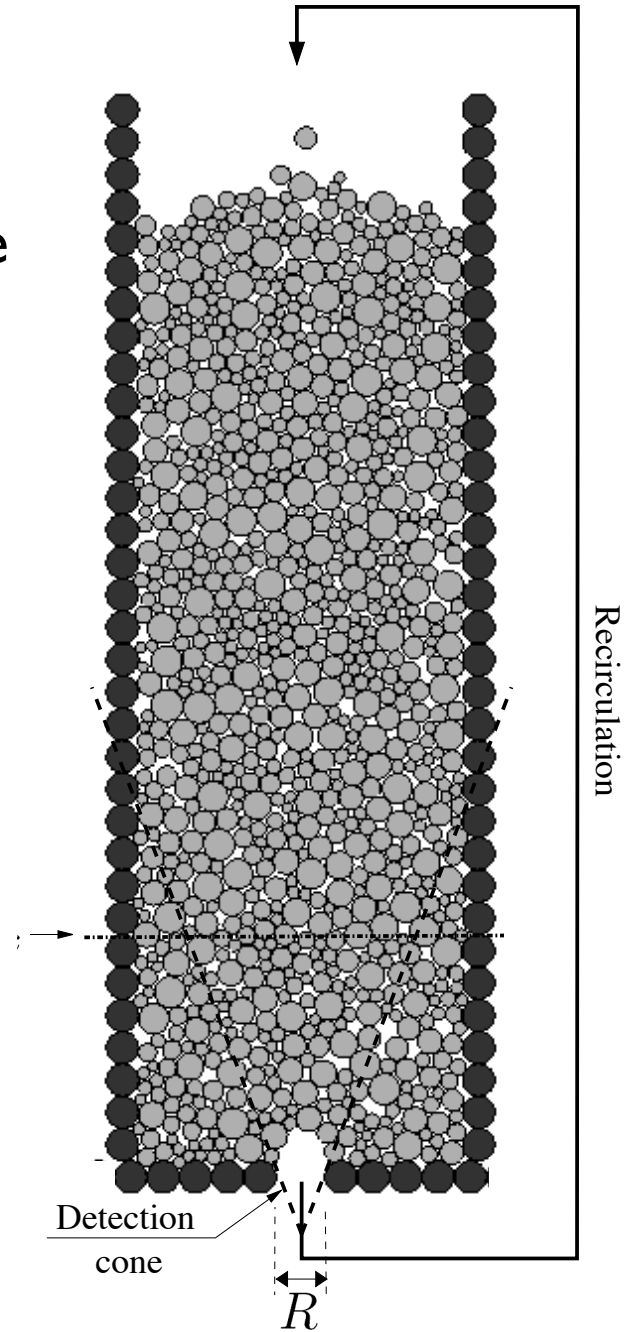
For a narrow outlet, the flow stops in finite time.



flow

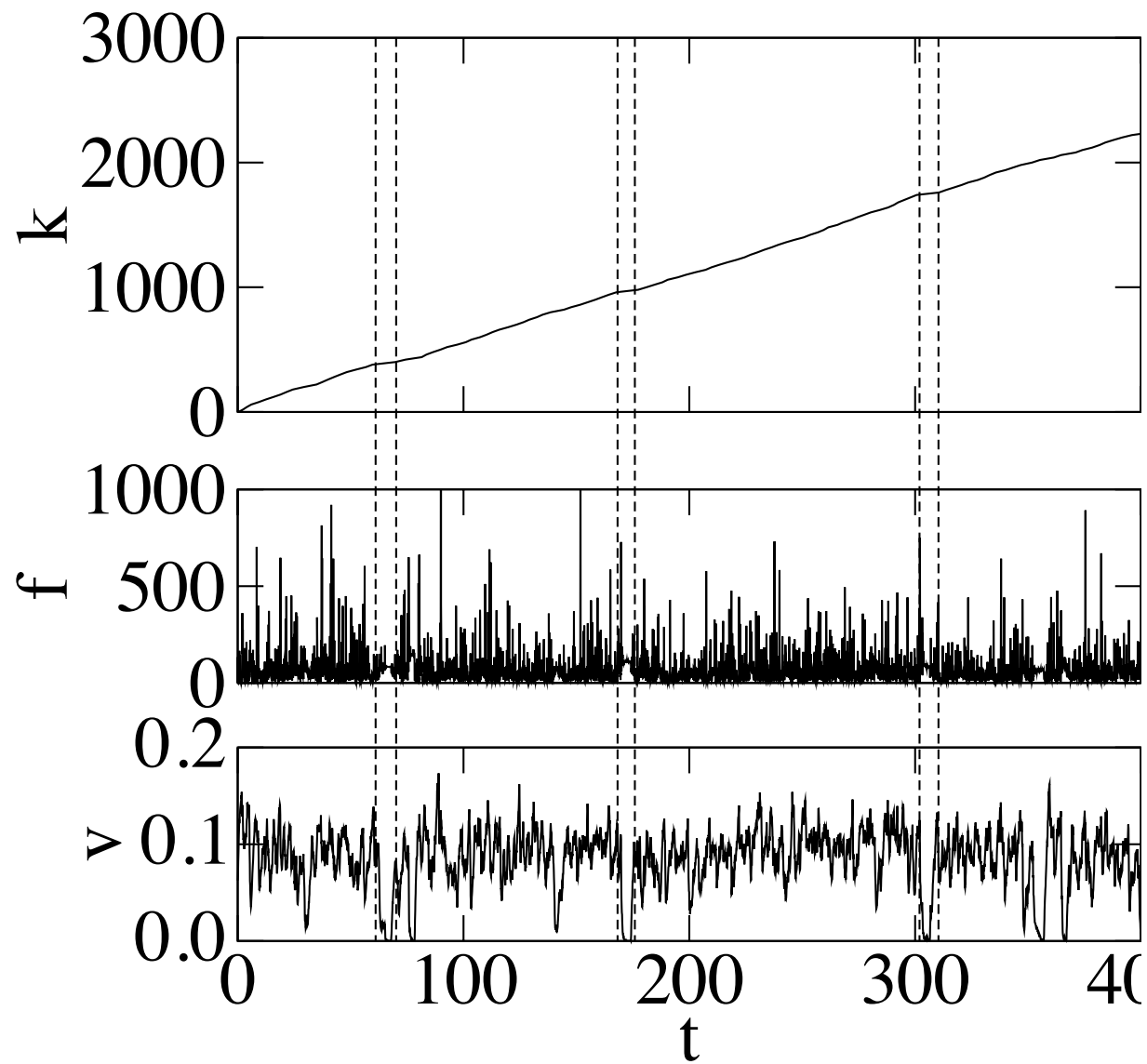


stop

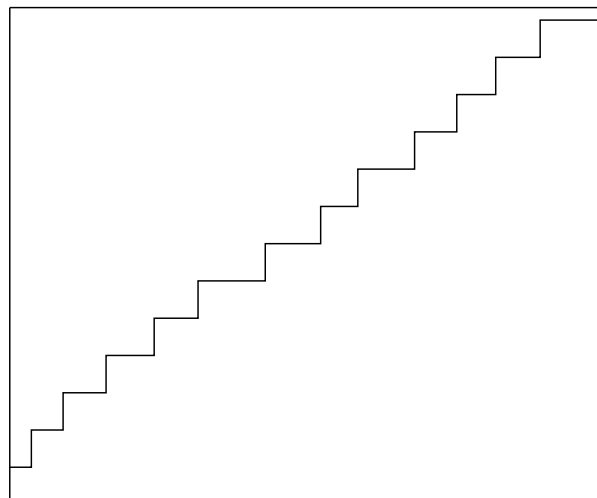
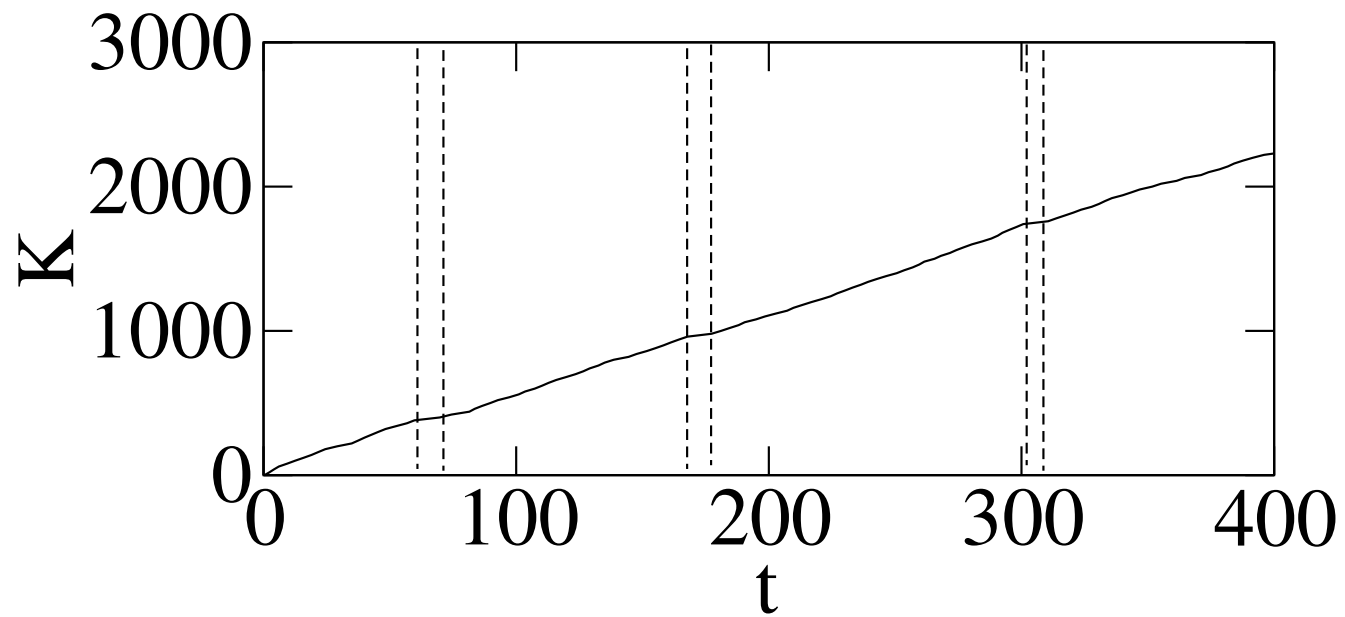


- What is the discharge rate?
- How many grains will pass?
- How long does it last?

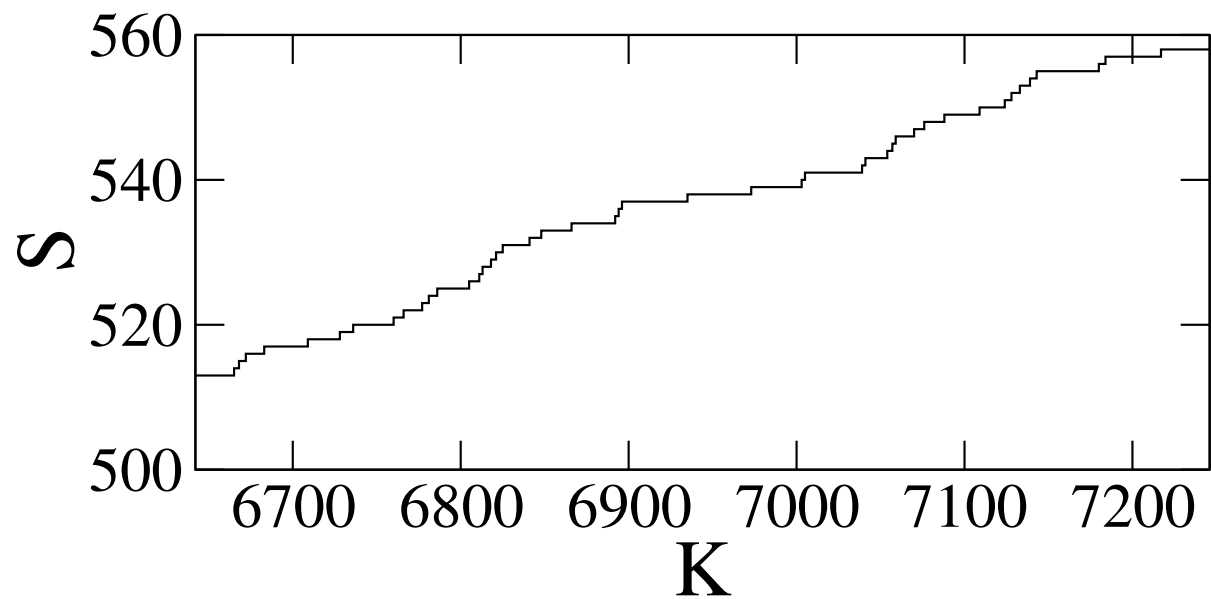
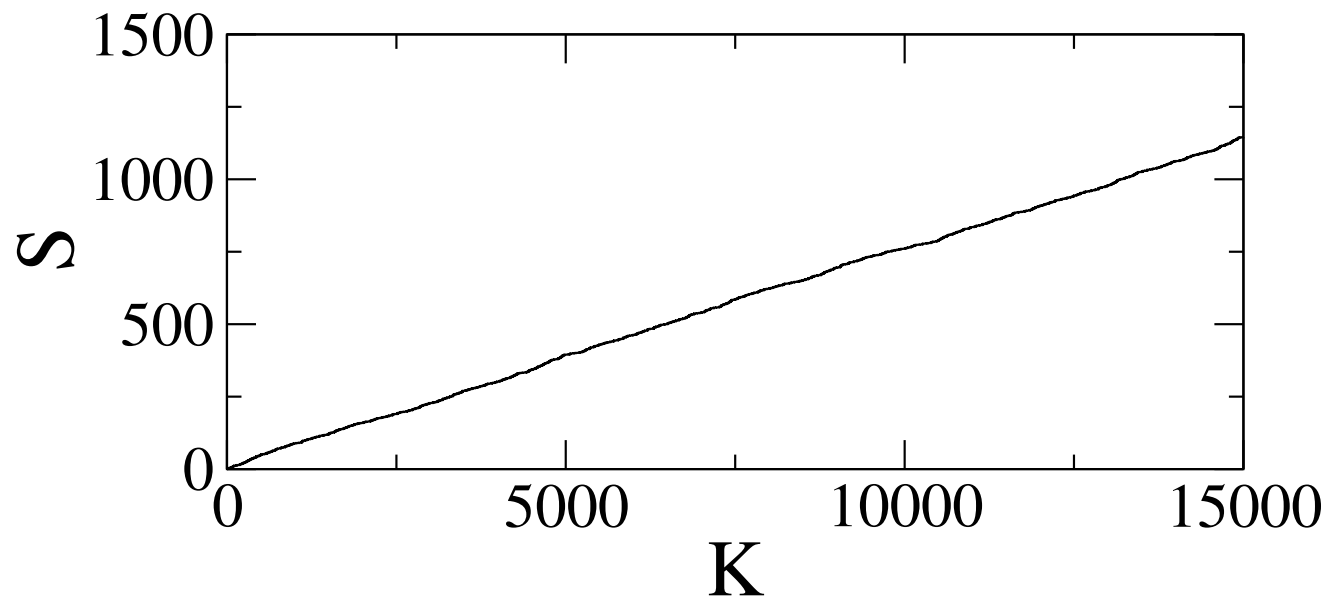
Martin, Dubois, Monerie, Radjai, soumis (2010)



number of passing grains  $K(t)$



number of jams  $S(K)$



## Measurements

$P_\tau(\tau)$  Distribution of waiting times between consecutive passing events

$P_N(N)$  Distribution of the number of passing grains between consecutive jams

## Normalization $\{g, d, \rho\}$

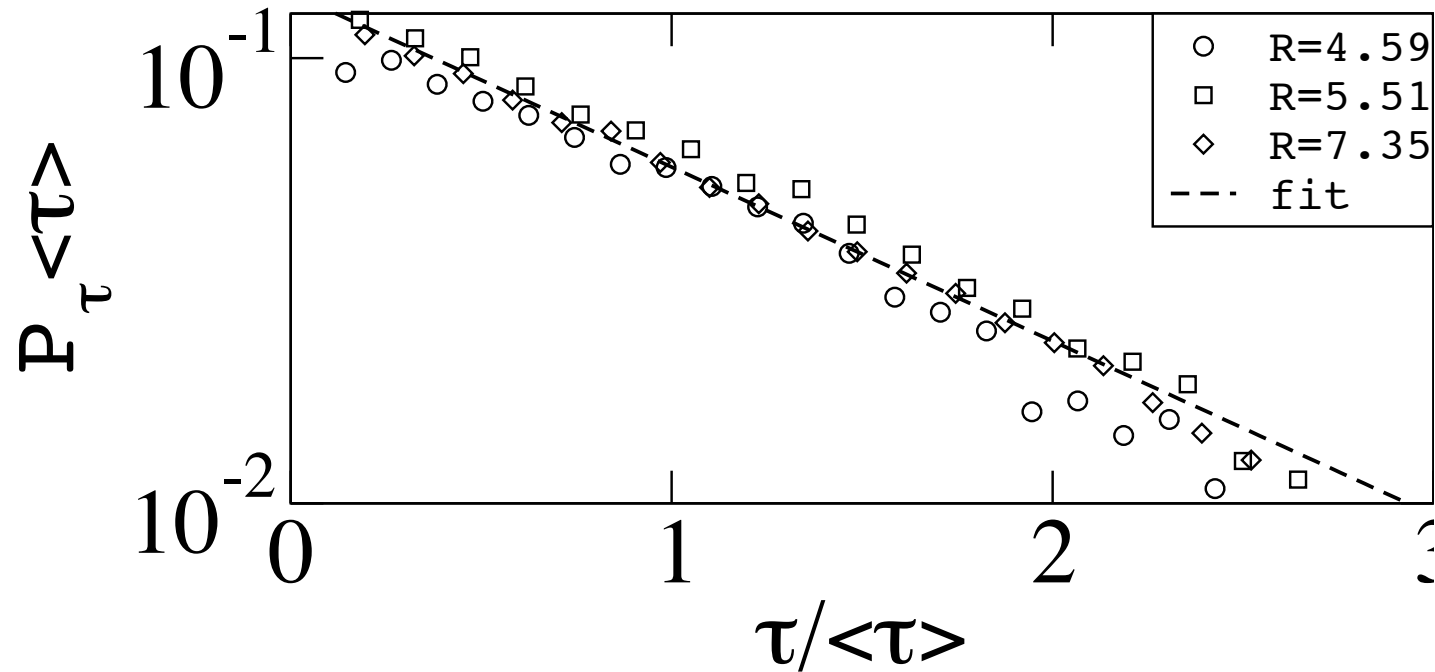
$R = \frac{\phi}{d}$  normalized orifice size

$t \sim \sqrt{\frac{d}{g}}$  time

$v \sim \sqrt{dg}$  velocity

$f \sim \rho d^2$  force

$$P_\tau(\tau) = Qe^{-Q\tau} \quad \text{memoryless process}$$



$$P_0(t) \equiv P\{[K(t) - K(0)] = 0\}$$

The probability that the first passing grain occurs after time  $t$

$$P_0(t) = \int_t^\infty P_\tau(\tau) d\tau = e^{-Qt}$$

The probability that no grain will pass in the time interval  $(0, t]$

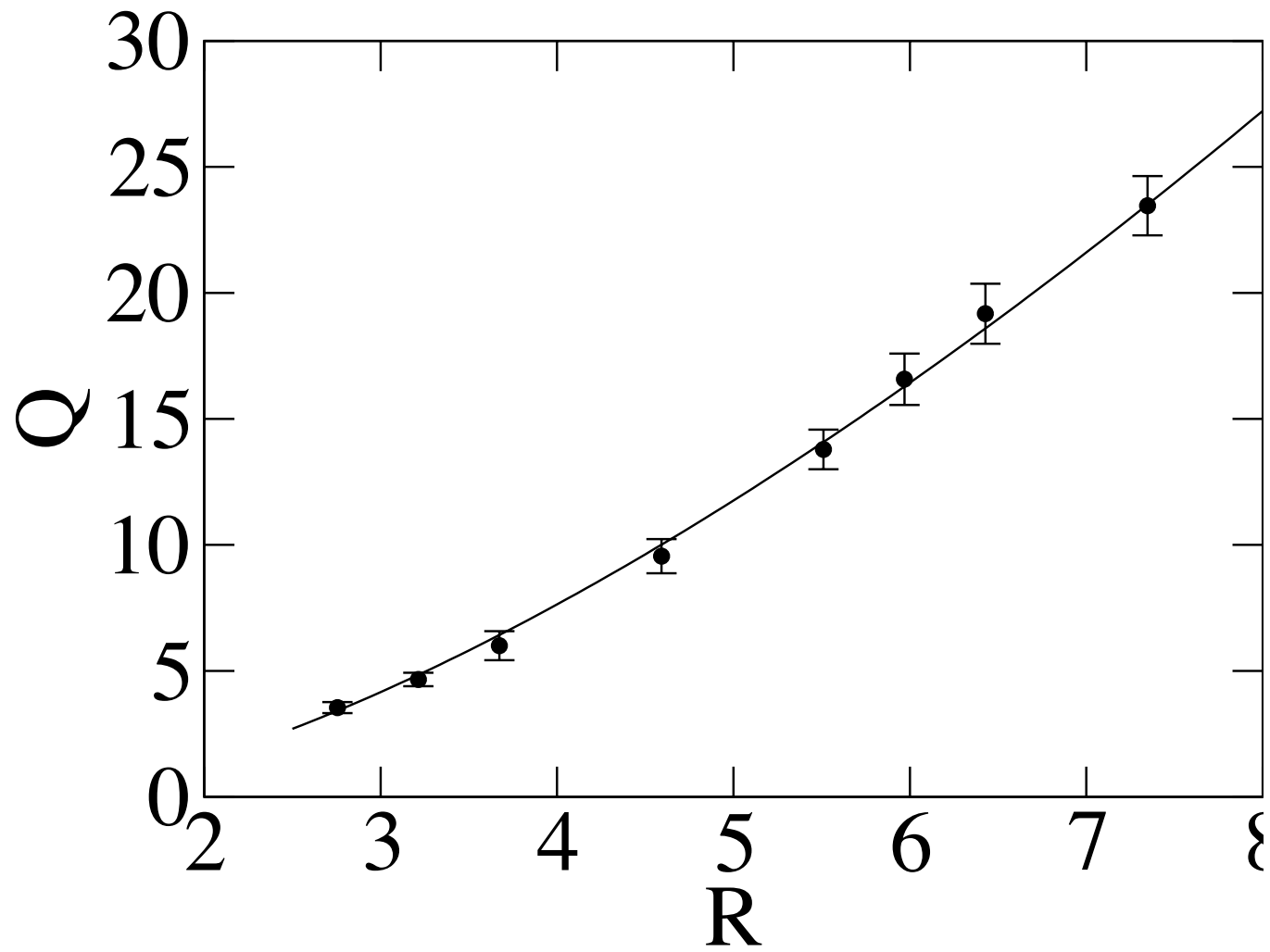
1) The number of passing events in any bounded interval of time after a given time is independent of the number of passing grains before.

2) The processes is time-homogeneous: the mean discharge rate is the same in different periods of flow.

3) Passing grains occur almost never simultaneously.

⇒ The discharge flow is a **Poisson process**.

$$P_k(t) = \frac{(Qt)^k e^{-Qt}}{k!}$$



$$Q = C(R - R_e)^{3/2}$$

Beverloo law

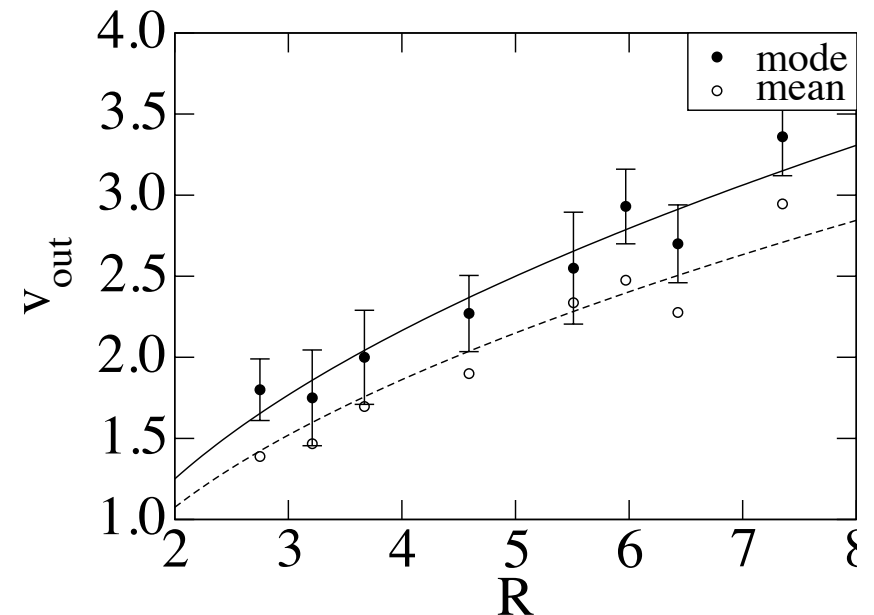
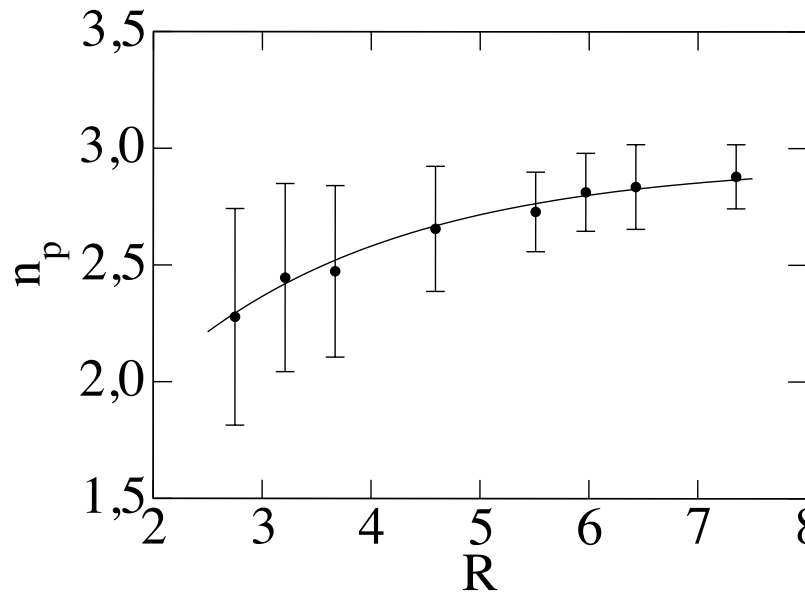
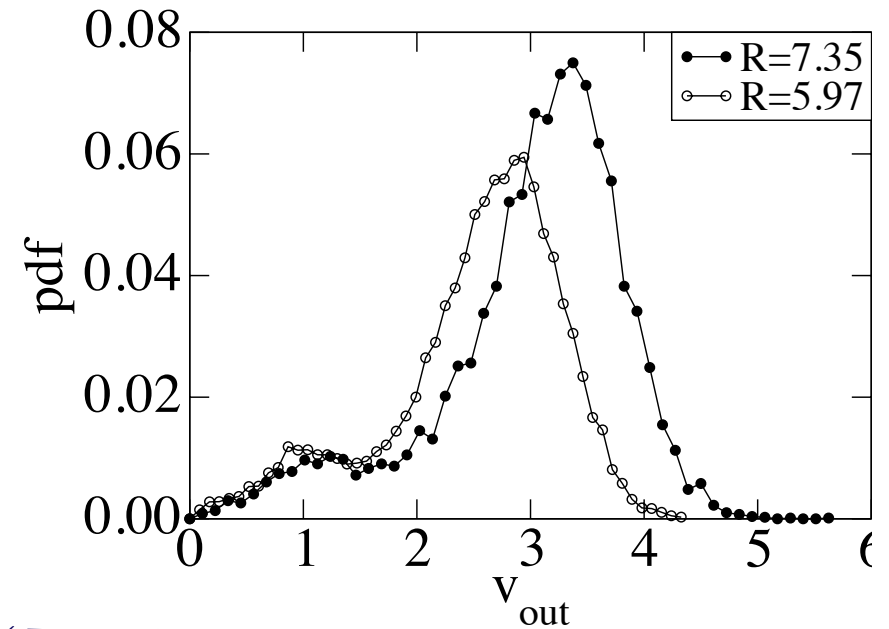
$$R_e \simeq 1$$

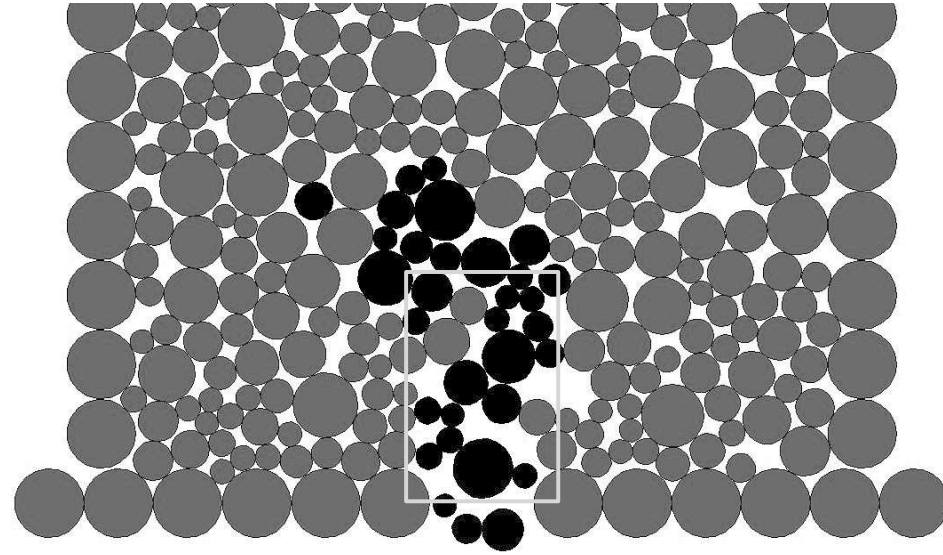
$$Q = n_p v_{out} s(R - R_e)$$

$$v_{out} = C_v (R - R_e)^{1/2}$$

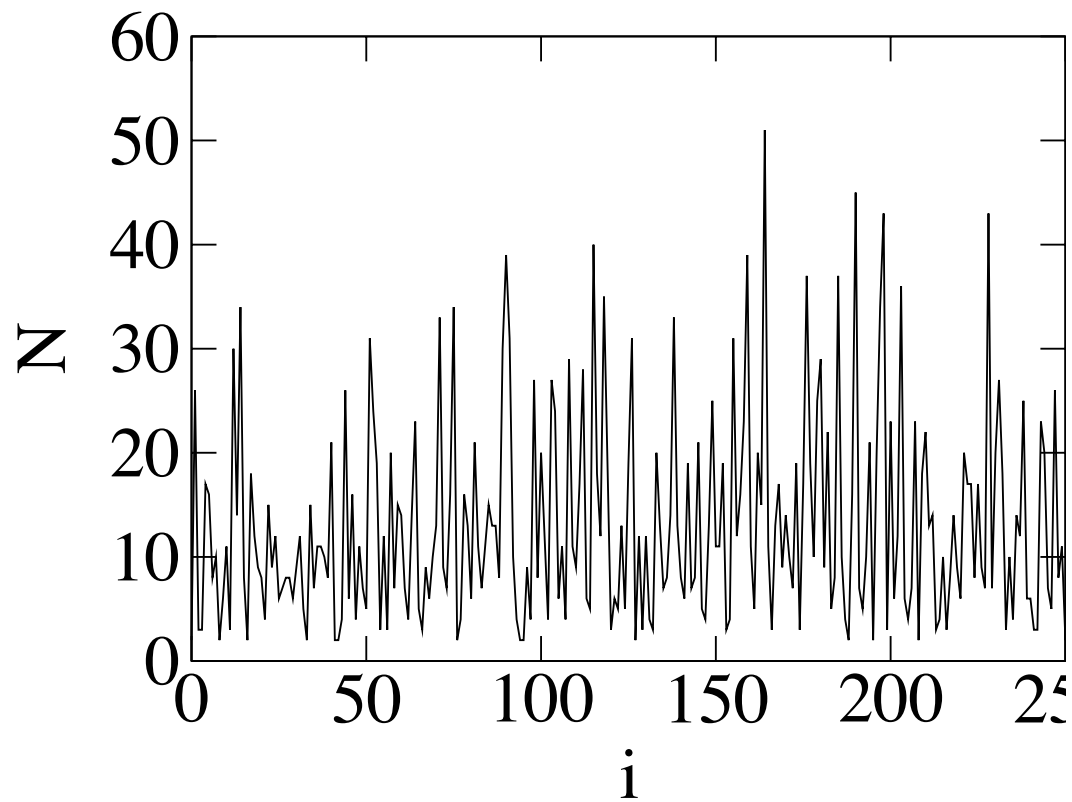
$$n_p = C_n \{1 - \alpha e^{-\beta(R - R_e)}\}$$

$$\Rightarrow Q = C_v C_n s(R - R_e)^{3/2} \{1 - \alpha e^{-\beta(R - R_e)}\}$$

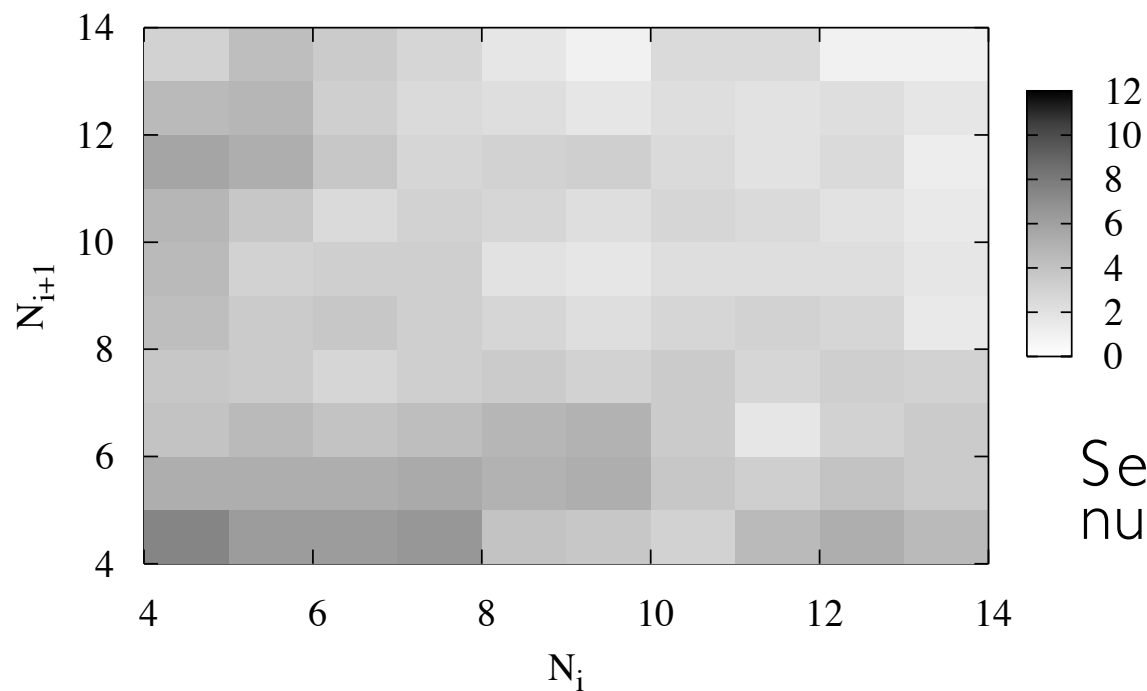




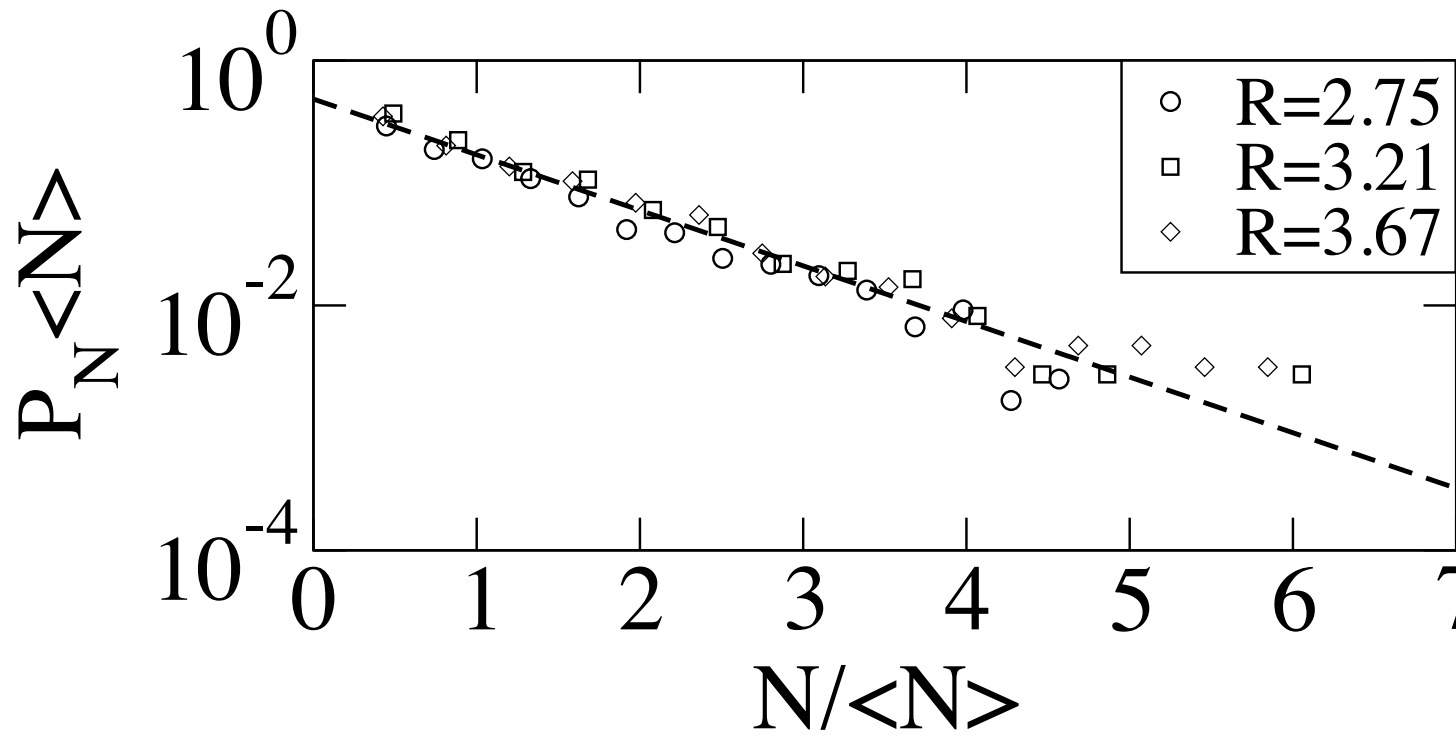
fluidized zone



number of passing grains  
between jams



Self-correlation of the  
number of passing grains



$$P_N(N) = \lambda e^{-\lambda N}$$

$$\langle N \rangle = \sum_{N=0}^{\infty} N P_N(N) = 1/\lambda \quad \langle T \rangle = \langle N \rangle / Q = \langle \tau \rangle \langle N \rangle$$

Since jamming is a consequence of arching, the macro-process is a way of sampling the collective dynamics of grains above the outlet. This is a Poisson process:

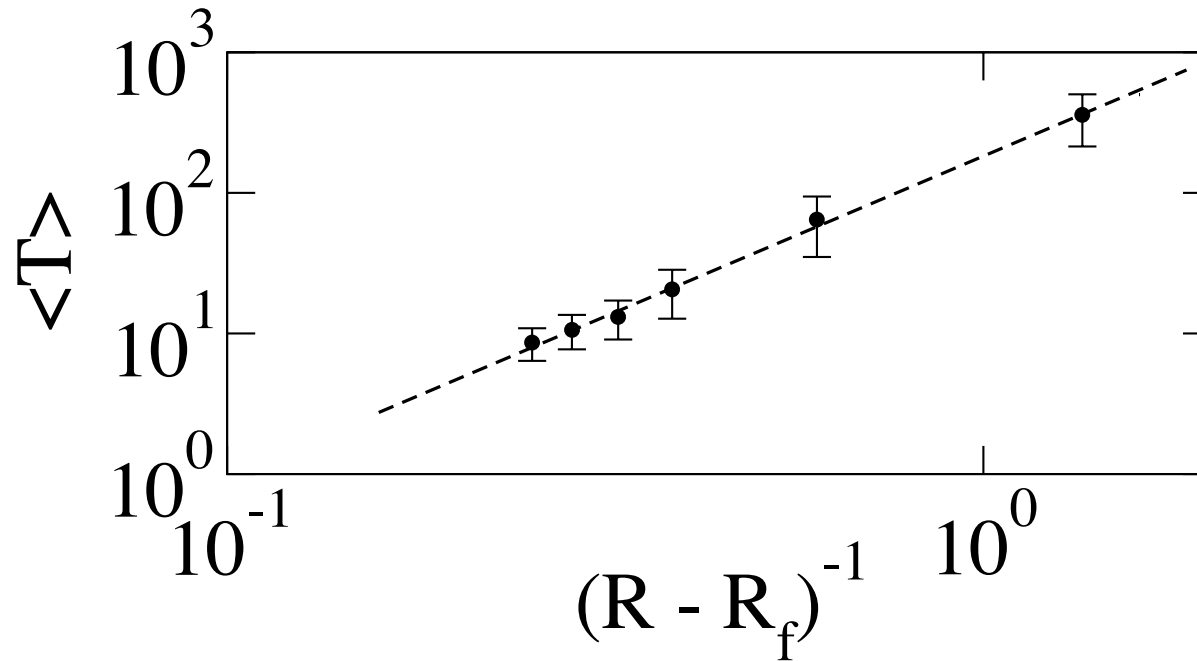
$$P_s(K) = \frac{(\lambda K)^s e^{-\lambda K}}{s!}$$

### Probability of jamming

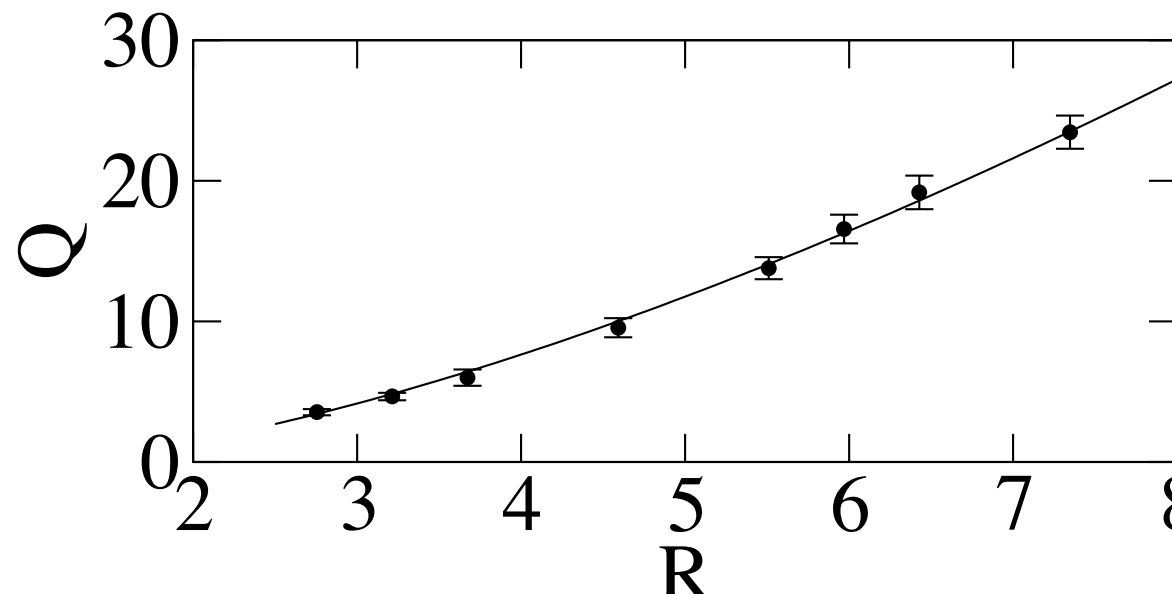
$$J_K = 1 - P_0(K) = 1 - e^{-K/\langle N \rangle}$$

probability that the flow gets jammed before the passing of  $K$  grains

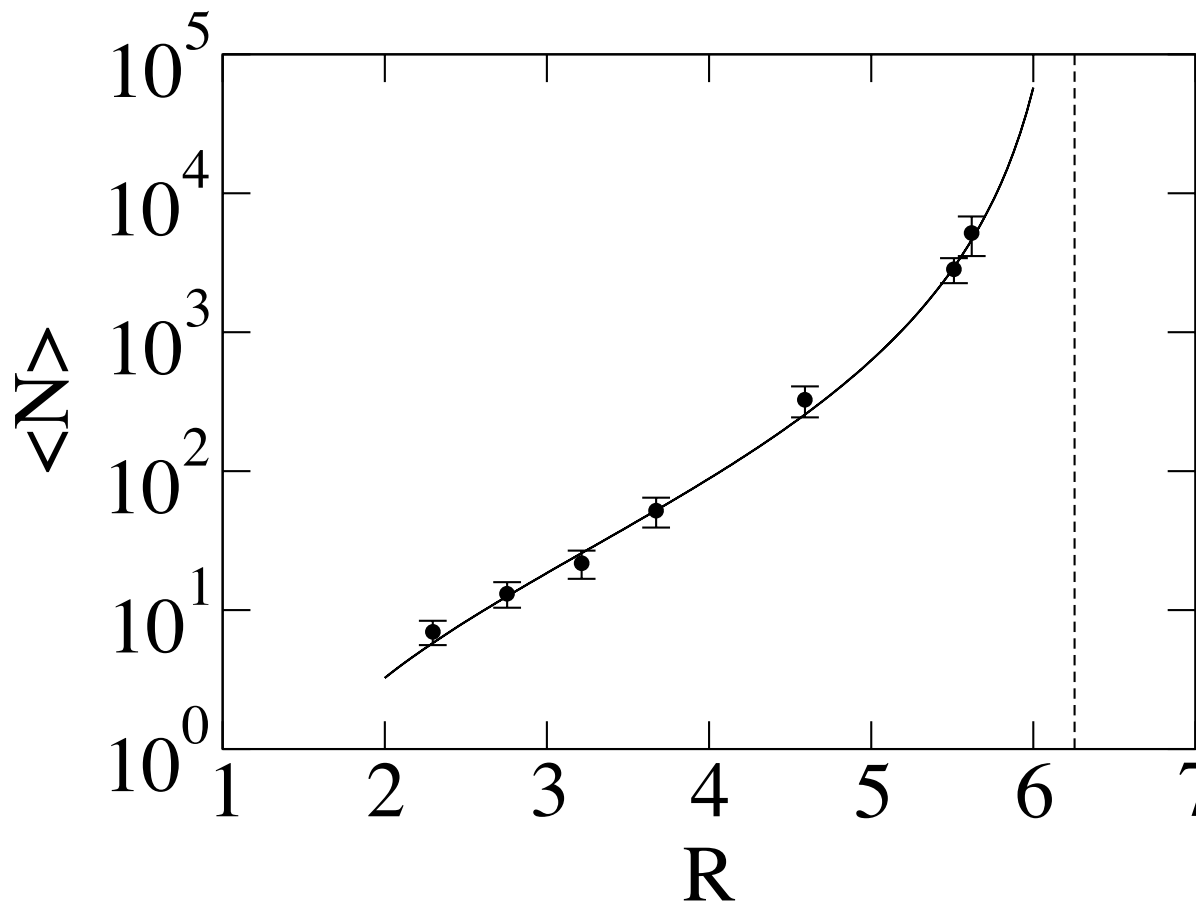
$$\langle N \rangle = Q \langle T \rangle$$



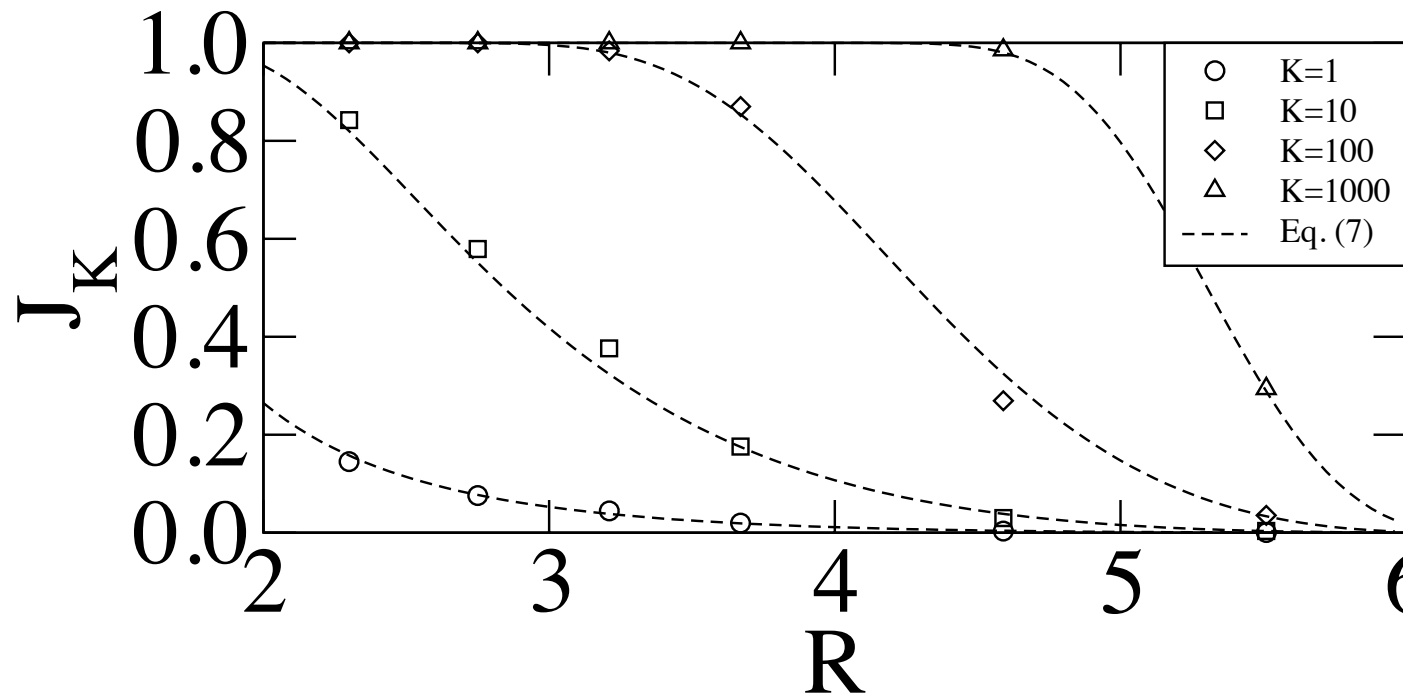
$$\langle T \rangle \propto (R_f - R)^{-\gamma}$$



$$Q = C(R - R_e)^{3/2}$$



$$\langle N \rangle = Q T = C_N (R - R_e)^{3/2} (R_f - R)^{-\gamma}$$



$$J_K(R) = 1 - \exp \left\{ -\frac{K}{C_N} (R_f - R)^\gamma (R - R_e)^{-3/2} \right\}$$

# Conclusions

- A granular system can be found in very different packing and flow states. The transitions between these states are unstable and of stochastic nature.
- The time fluctuations and dynamic inhomogeneities (cochoneries?) are intrinsic (generic) to granular motion.
- The numerical precision does not seem to alter the nature of the dynamics but only the scale at which we resolve the motion.