SOME ISSUES AND PERSPECTIVES IN GRANULAR PHYSICS

Jean-Noël Roux

Laboratoire des Matériaux et des Structures du Génie Civil

Unité Mixte de Recherche LCPC-ENPC-CNRS

Institut Navier, Champs-sur-Marne, France

Partly inspired by (or emerged from) the ...

Recent granular trimester at Institut Henri Poincaré

- January 5–April 8, 2005. Organized by A. Barrat (CNRS, LPTHE, Orsay), Ph. Claudin (CNRS, PMMH, Paris) and J.-N. Roux
- 12 resident, invited scientists for one month at least, and many participants for shorter durations (60, outside meetings)
- Sets of lectures :
  - dense granular flows (O. Pouliquen);
  - geophysical applications (B. Andreotti);
  - granular systems and glassy dynamics (J. Kurchan, D. Dean);
  - Geometry, rigidity and stability (R. Connelly) ; quasistatic rheology and microstructure (F. Radjai) ;
  - results on granular systems in soil mechanics (F. Tatsuoka)

Recent granular trimester at Institut Henri Poincaré

- many seminars, some gathered in one day on the same theme : Isostatic structures (D. Wu); Cosserat modelling (E. Grekova)
- 3 thematic meetings (2-3 days) :
  - liquid-solid transition (F. Chevoir, O. Pouliquen) ;
  - instabilities, bifurcations, localisation (J. Sulem, I. Vardoulakis);
  - discrete numerical simulations (S. Luding, J.-N. Roux)
- See web site http://www.ihp.jussieu.fr

Some results and perspectives about *solid-like* granular materials

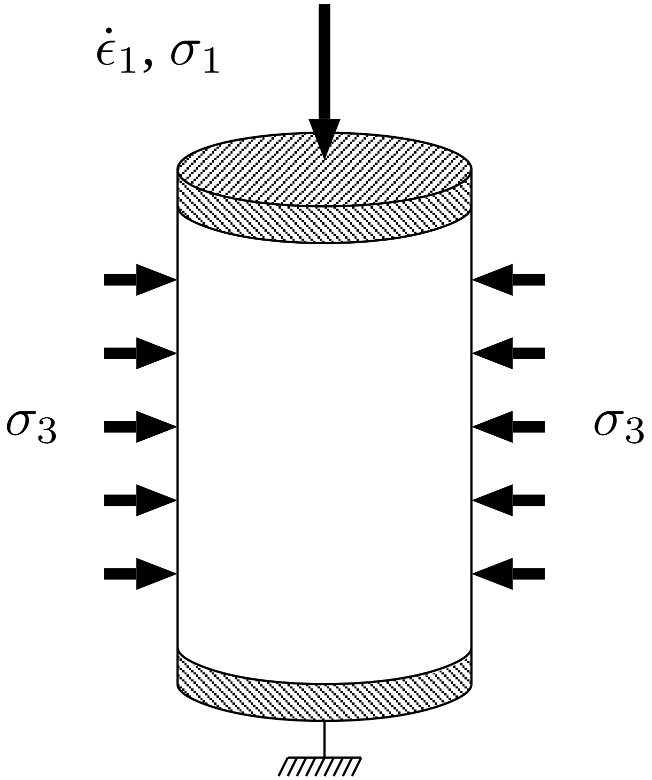
- Currently investigated and debated issues
- Presentation will hopefully provoke discussions
- Relies heavily on discrete computer simulations of granular materials
- Focus on material behavior, *i. e.*, stress/strain/internal state relationships within homogeneous samples, to be applied locally in the general, inhomogeneous case ($\Rightarrow$ boundary value problem)

Outline

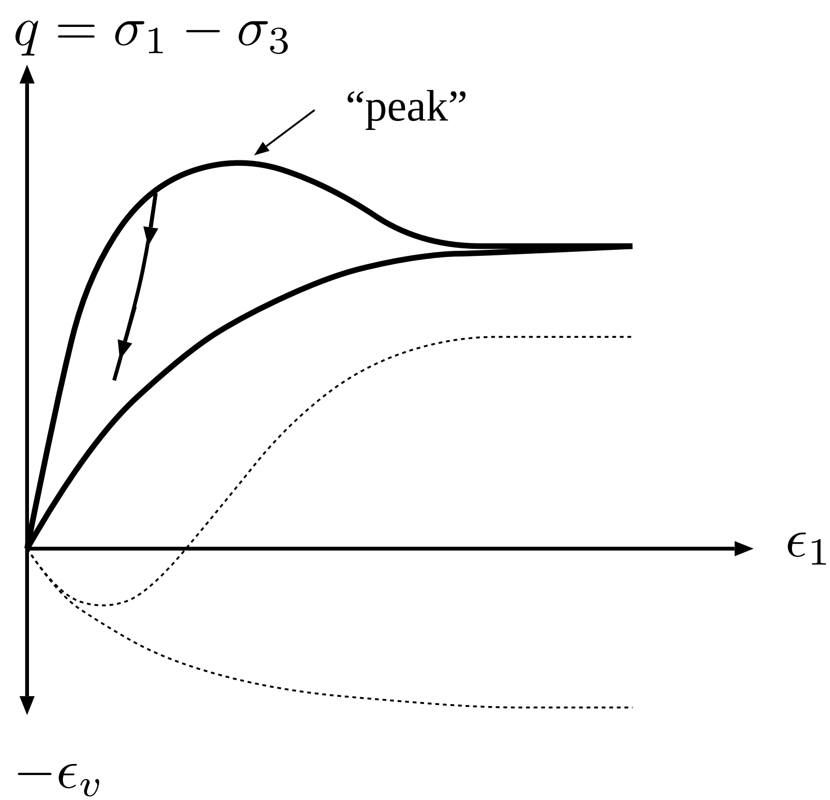
- Some basic features of macroscopic granular mechanics
- Ingredients of a microscopic model
- Grain-level approach to mechanical properties: selected topics

1. Frictionless systems: isostaticity property (in the rigid limit), minimization property... and consequences
2. Granular packings with friction: internal states, dependence on assembling procedure and micromechanical parameters
3. Elasticity : elastic domain, prediction of elastic moduli
4. Quasistatic (non-elastic) response, type I : deformation of contact network
5. Quasistatic deformation, type II : rearrangements (network continuously broken and repaired)

Rheometry of solid granular materials: triaxial apparatus

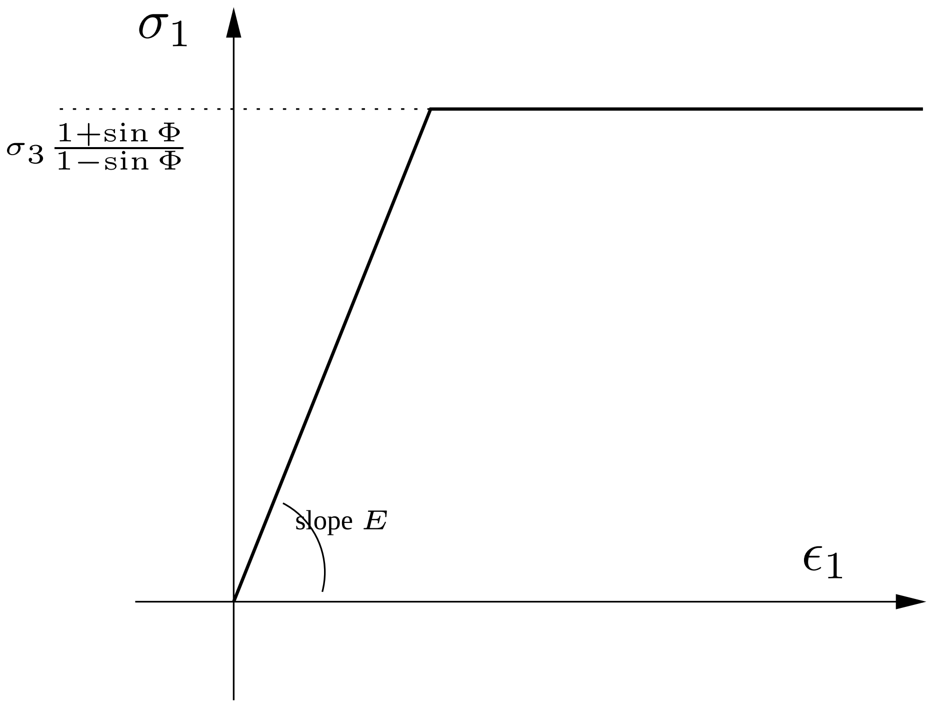


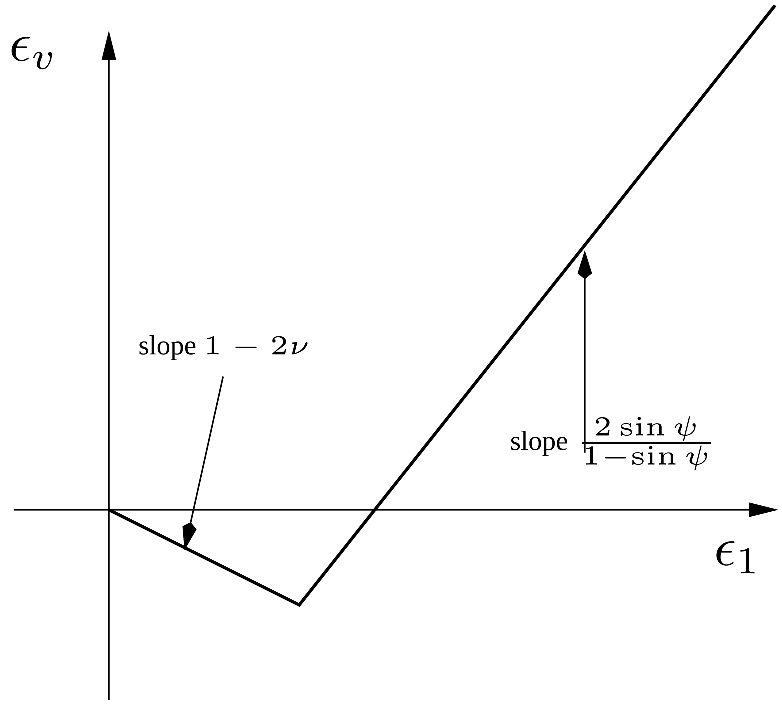
- uniform stress and strain
- $\sigma_2 = \sigma_3$
- $\sigma \sim 10 - 1000 kPa$
- $\epsilon \sim 10^{-2}$
- role of density
- $\sigma_1/\sigma_3 \leq$ maximum



- ϵ_v = "volumetric" strain (dilatancy)
- Dense and loose systems approach same "critical state" for large strains
- Irreversibility
- most accurate devices $\Rightarrow$ measurements of $\Delta\epsilon \sim 10^{-6}$

A simplified model





Linear elasticity + Mohr-Coulomb plasticity criterion, here written with principal stresses $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq 0$:

$$f(\underline{\underline{\sigma}}) = \frac{\sigma_1 - \sigma_3}{2} - \frac{\sigma_1 + \sigma_3}{2}\sin\varphi \leq 0$$

+ flow rule (dilatancy). Plastic potential ($\dot{\epsilon}_p = \lambda\frac{\partial g}{\partial \sigma}$, $\lambda \geq 0$)

$$g(\underline{\underline{\sigma}}) = \frac{\sigma_1 - \sigma_3}{2} - \frac{\sigma_1 + \sigma_3}{2}\sin\psi$$

Basic characteristics of solid material behaviour

Mohr-Coulomb model contains basic ingredients with essentially model-independent definition

- internal friction angle φ, associated with peak strength
- strain level necessary to mobilize internal friction
- dilatancy angle ($\psi < \varphi$)

$\rightarrow$ How could one obtain a prediction of those quantities ?

Insufficiencies of the Mohr-Coulomb model:

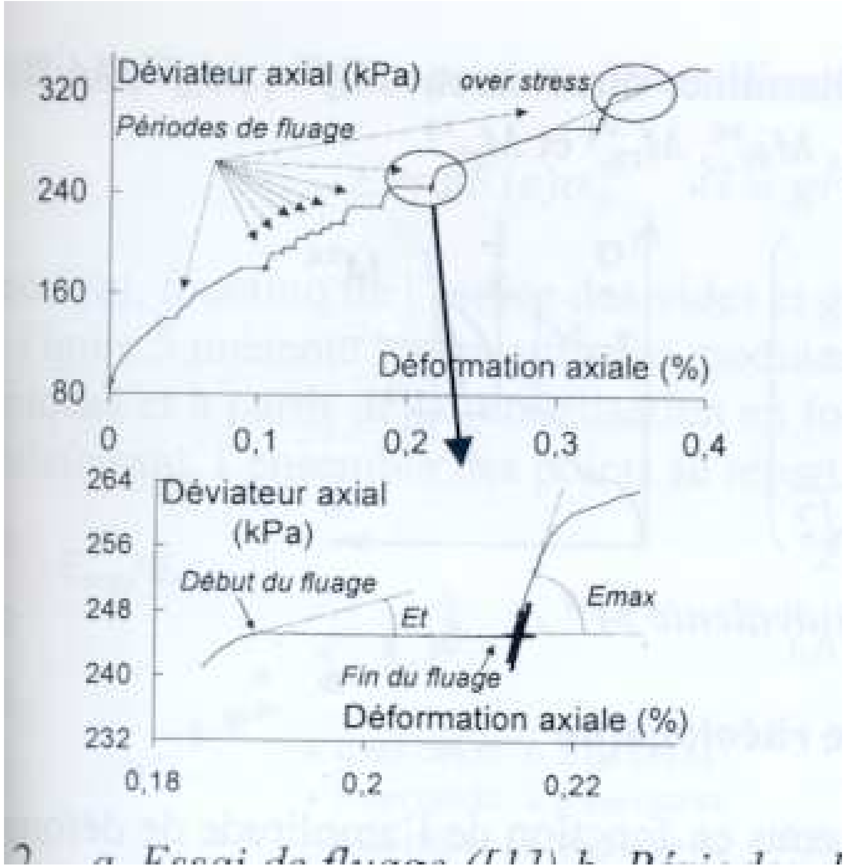
- no difference between peak and residual strength
- does not include role of initial density
- elasticity is non-linear and pre-peak response is predominantly non elastic (non reversible). “Elastic moduli” for slope of stress-strain curve = misleading term

Observations and models for sands

- Elasticity: moduli measured as slope of stress-strain curves if $\Delta\epsilon \leq 10^{-5}$ (typically). Values agree with sound propagation measurements
- Anisotropy : peak strength, pre-peak strains depend on initial (inherent) anisotropy
- effects of stress history (overconsolidation)
- Shear banding: both theoretical and experimental studies. Entails particle size effects
- Slow dynamics, creep

Well characterised and documented phenomena in soil mechanics literature. Phenomenological laws available. Practical importance (foundation engineering) established

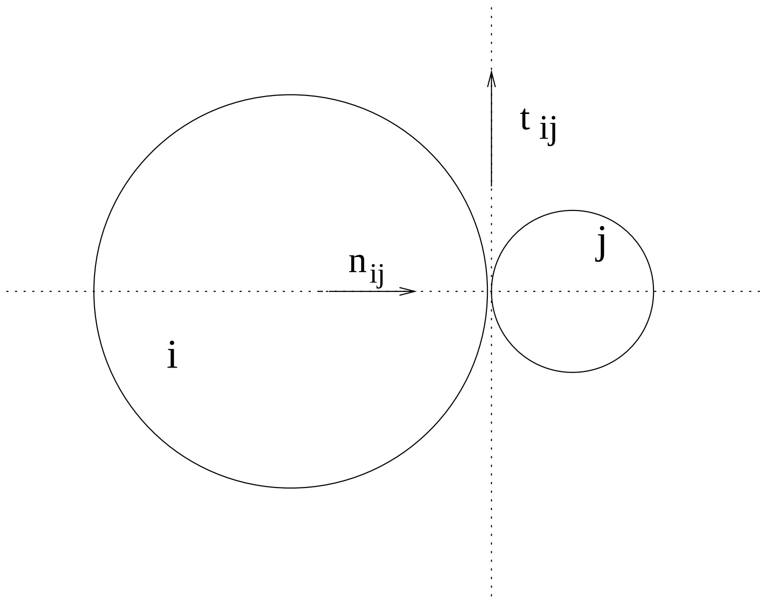
Creep and elastic domain

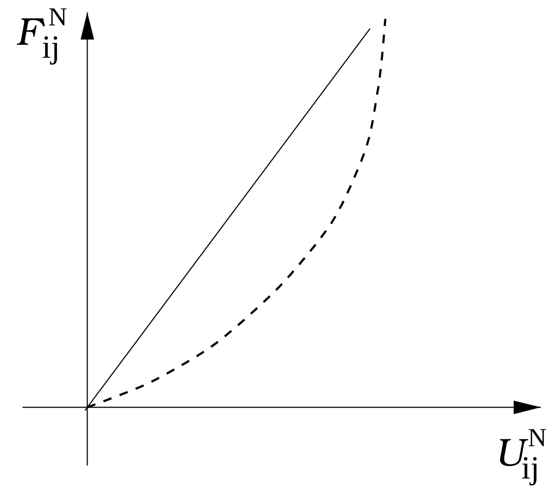


di Benedetto *et al.*

Under constant stress, samples creep (for hours, days...). Elastic moduli measures on unloading... or cycling, or reloading at constant rate after creep period

Contact laws : schematic presentation

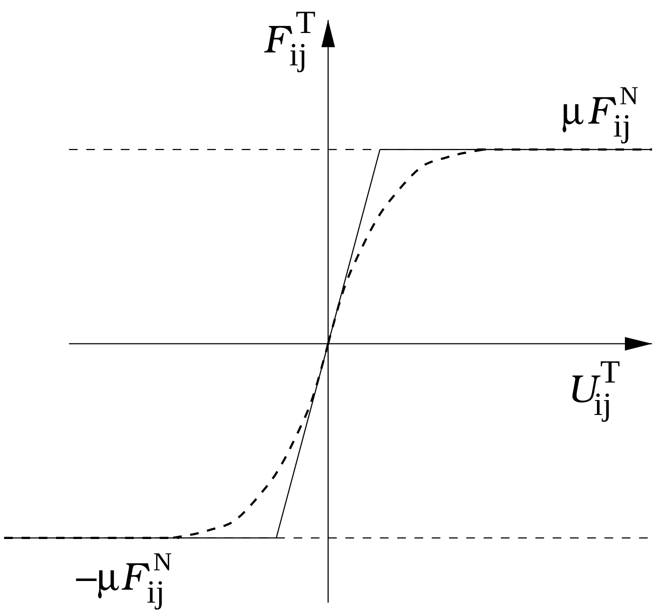




$$U_{ij}^{N} = \mathbf{n}_{ij}.(\mathbf{u}_i - \mathbf{u}_j)$$

$$U_{ij}^{T} = \mathbf{t}_{ij}.(\mathbf{u}_i - \mathbf{u}_j) + R_i \delta\theta_i + R_j \delta\theta_j$$

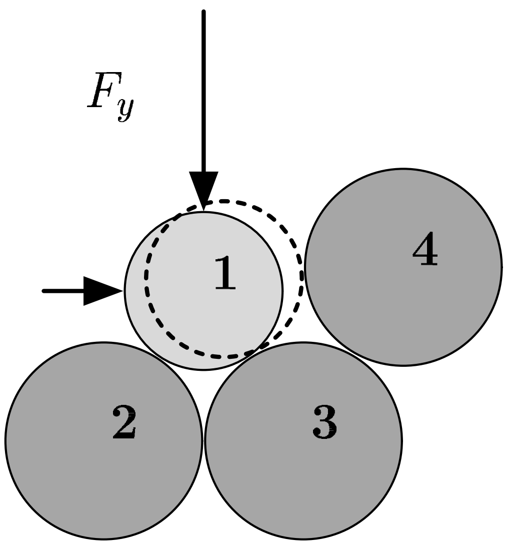
(rigidity matrix $\underline{\underline{G}}$)

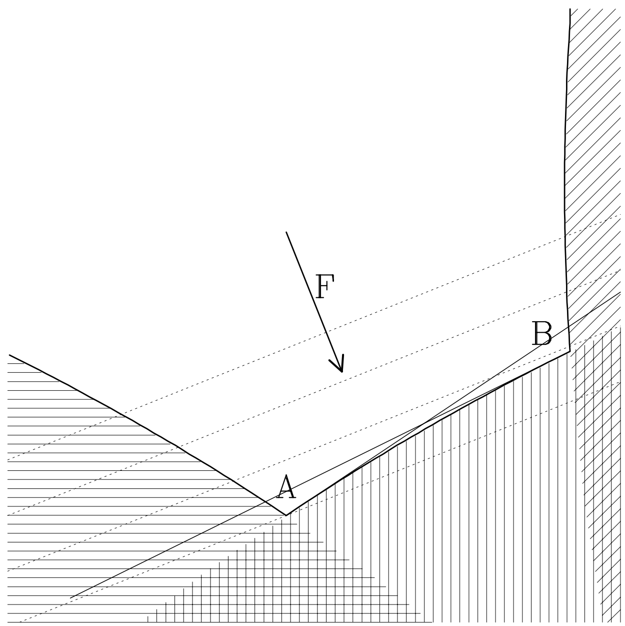


analogous to macroscopic laws, but...

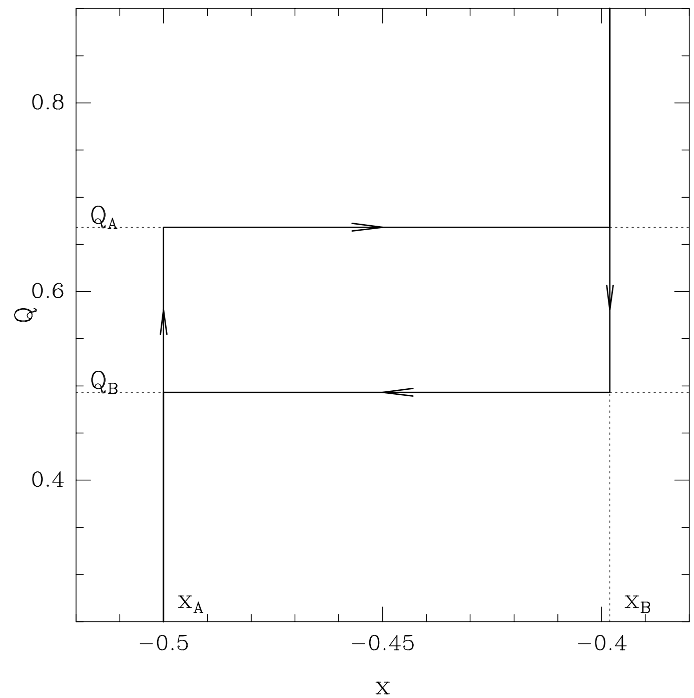
Role of geometry: rearrangements as origins of packing deformation

Example with frictionless, rigid disks, one mobile grain and two equilibrium positions





Potential energy minimization



$Q = F_x/F_y$ vs. position x.

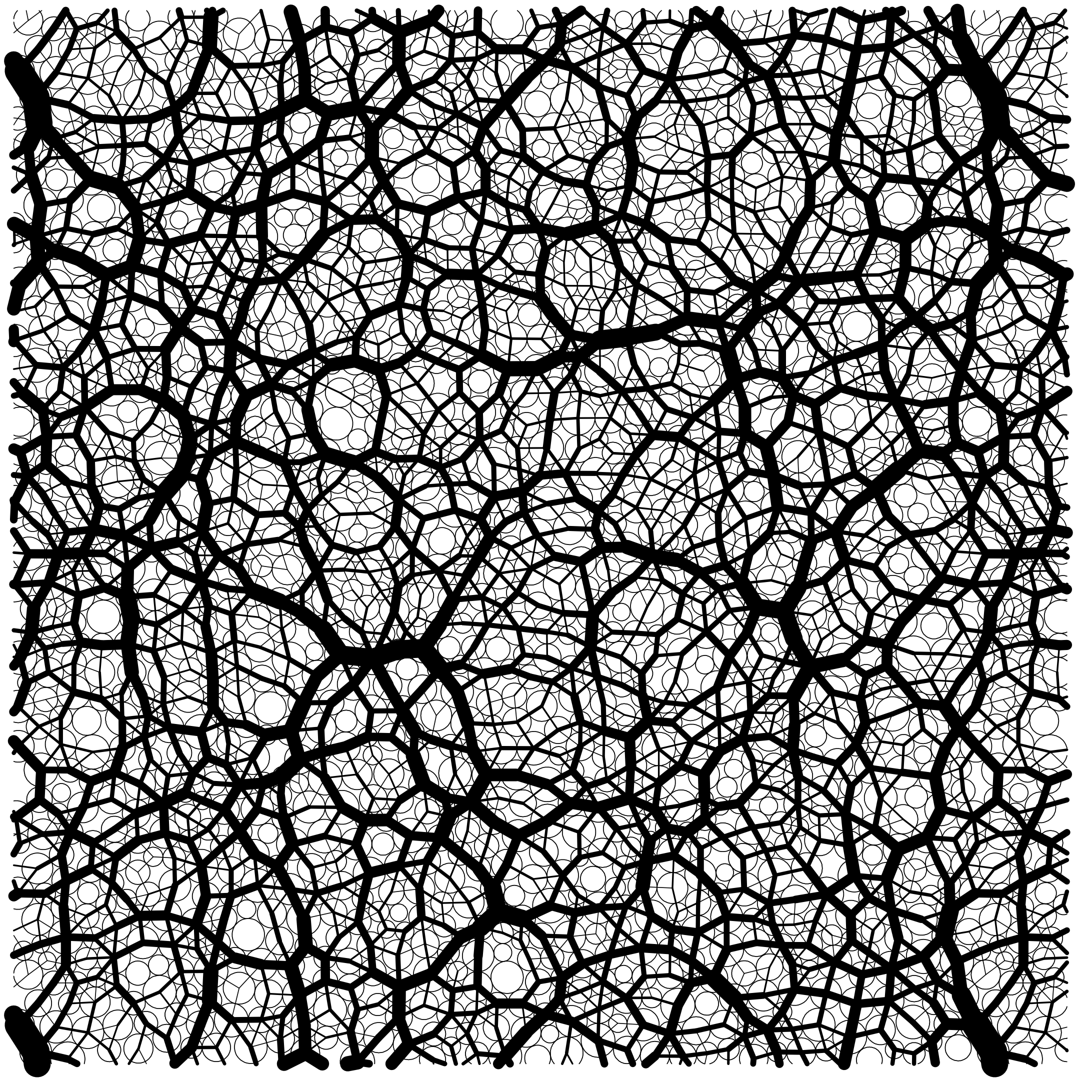
Macroscopic behavior $\neq$ naïve "average" of contact law

Ingredients of a microscopic model. Dimensionless parameters

Model involves geometry, inertia, contact law + parameters of the experiment: strain rate $\dot{\epsilon}$, pressure P.

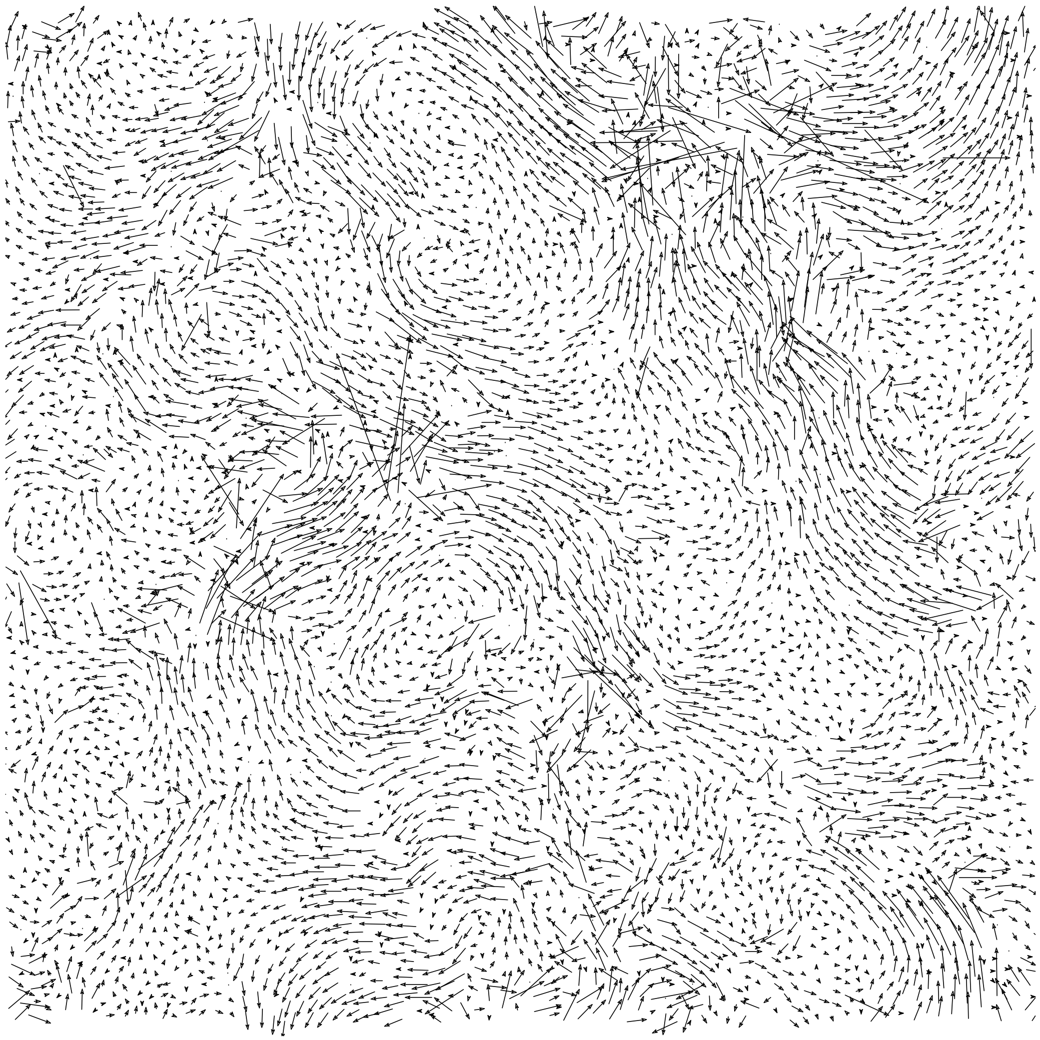
- Stiffness number κ, $\kappa = K_N/P$ (linear 2D), $\kappa = K_N/(Pa)$ (linear 3D), $\kappa = (E/(1-\nu^2)P)^{2/3}$ for Hertz contacts.
  Rigid grain limit: $\kappa \to \infty$
- K_N/K_T or Poisson coefficient ν of the grain material
- Reduced strain rate or inertia number $I = \dot{\epsilon}\sqrt{m/aP}$.
  Quasi-static limit: $I \to 0$
- ζ ratio of viscous damping to its critical value in a contact
- Friction coefficient μ

Granular disorder I : forces



Normal force intensity $\propto$ line width

Granular disorder II : displacements



Non-affine part of displacement field between two neighbouring equilibrium configurations (biaxial compression). Non negligible, often dominant

Frictionless systems

- mechanical properties are *simpler*
- statistical properties are *more complicated*
- studied by several authors (C. Moukarzel, A. Tkachenko *et al.*, R. Ball..., JNR), often attributed exotic properties
- can be dealt with by rigidity theory (bar frameworks, tensegrities... R. Connelly's lectures at IHP) $\rightarrow$ discrete maths literature
- in the $\kappa \rightarrow \infty$ limit, properties reduce to geometry

Frictionless systems: minimization property

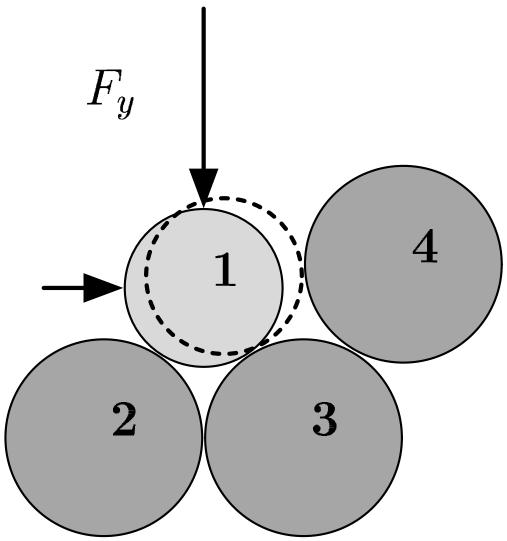
- The potential energy of external forces (+ elastic energy if deformable grains) is minimized in mechanical equilibrium.
- Applies to rigid grains ($\kappa = +\infty$), with impenetrability constraints. Normal contact forces are Lagrange multipliers
- Example: local density maximum in configuration space = stable mechanical equilibrium under isotropic pressure
- With cohesionless spheres, zero variation to first order means instability
- If minimization problem becomes convex, then the solution is unique. Happens:
  - for rigid cables
  - within the approximation of small displacements (ASD: linearize distance variations)

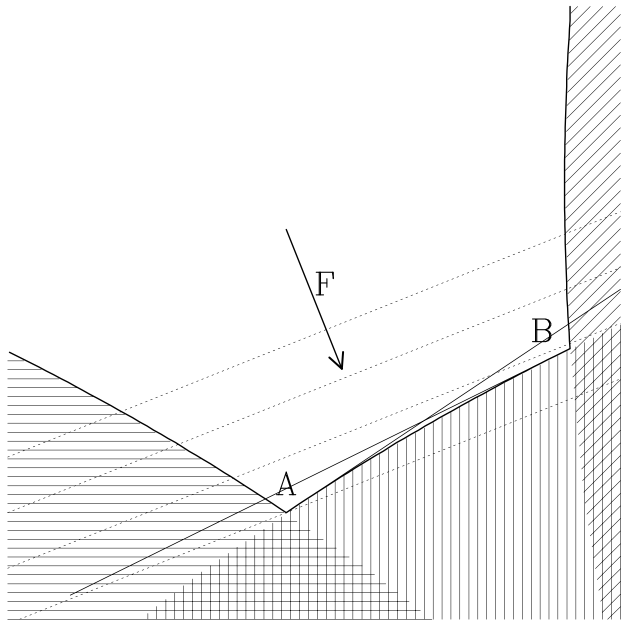
Frictionless systems, rigid grains: isostaticity property I

Isostaticity properties = properties of rigidity matrix $\underline{\underline{G}}$. Its transpose expresses mechanical equilibrium conditions as linear relations between contact forces and external forces

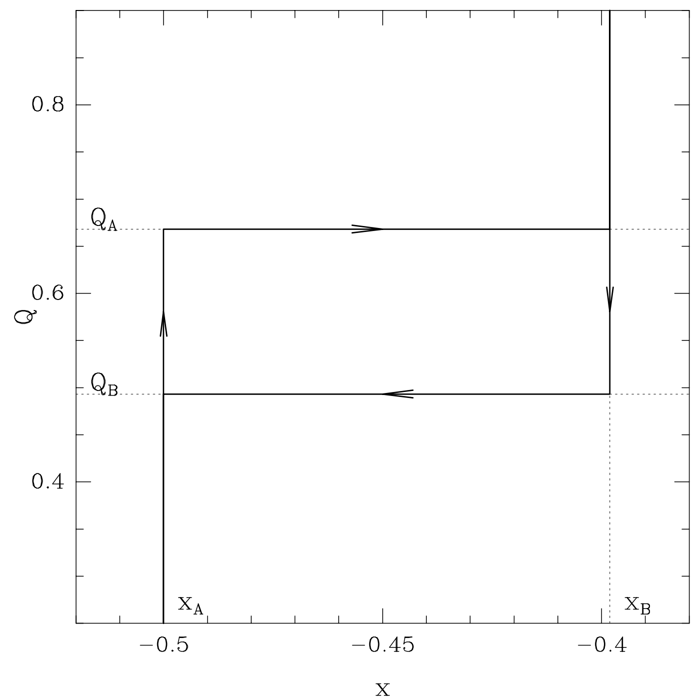
- with generic disorder, absence of force indeterminacy. Sets upper bound on coordination numbers (4 for disks and 6 for general objects in 2D; 6 for spheres, 10 for axisymmetric objects and 12 in general in 3D– see Donev *et al.* on spheroids)
- Once contacts are known, contact forces resolving the load, if they exist, are uniquely determined (isostatic *problem*)
- if *uniqueness property* holds, then the list of force carrying contacts is also determined (not true in general)

Role of geometry: rearrangements as origins of packing deformation





Potential energy minimization

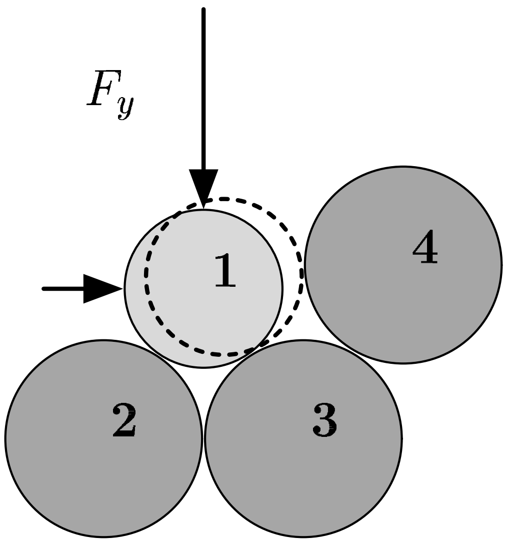


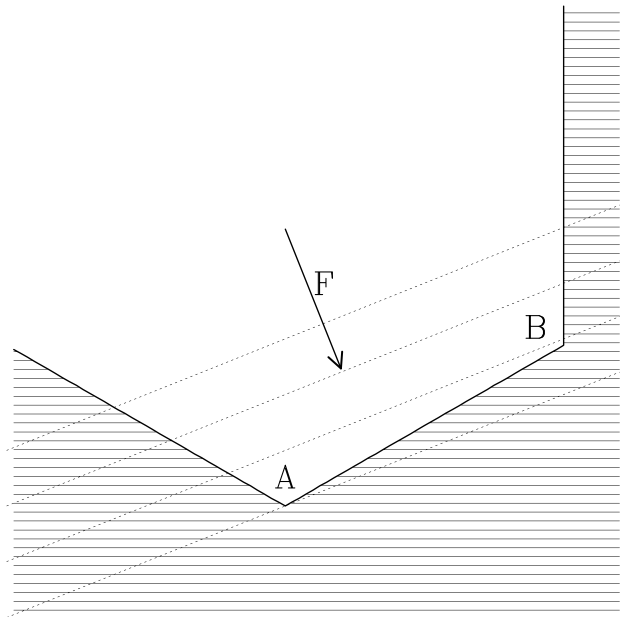
$Q = F_x/F_y$ vs. position x.

Isostaticity of each equilibrium contact set, no uniqueness

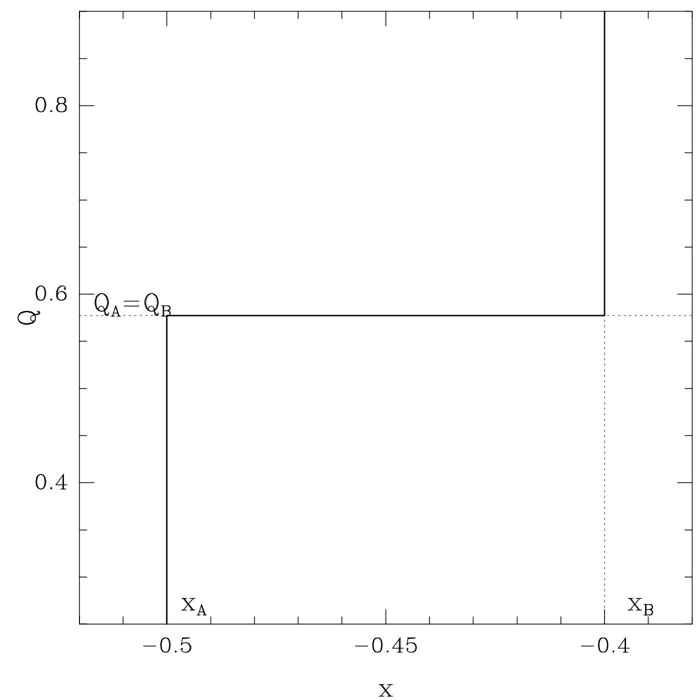
Role of the ASD

With the ASD:





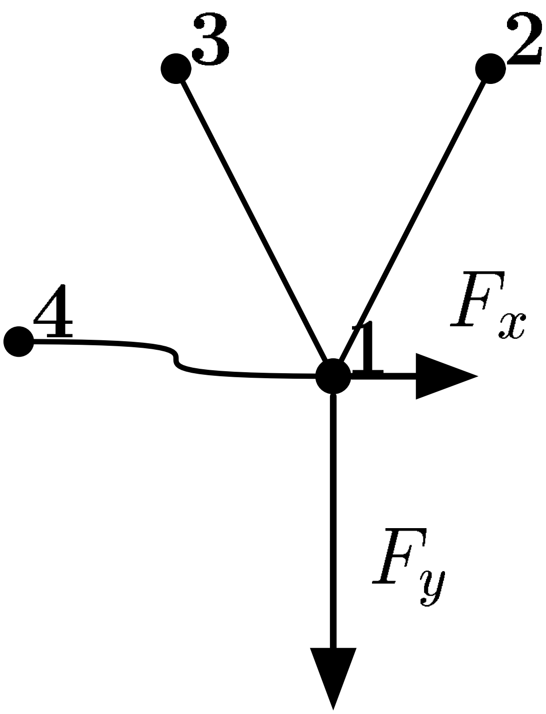
Minimization of potential energy

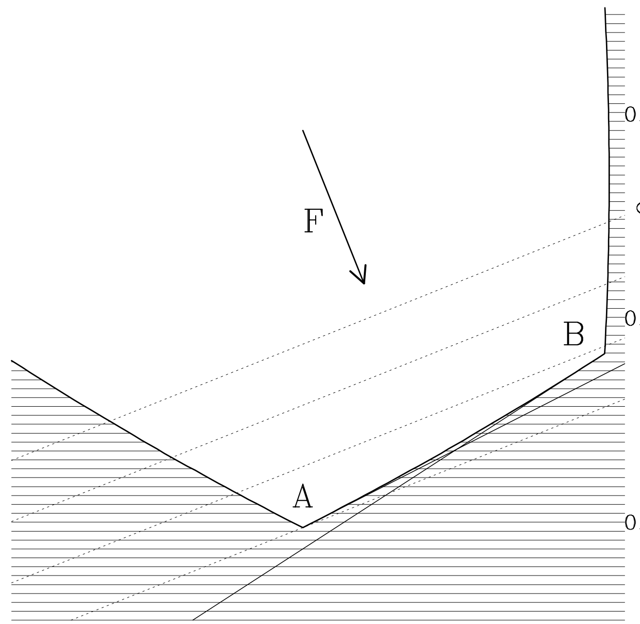


$Q = F_x/F_y$ versus position x.

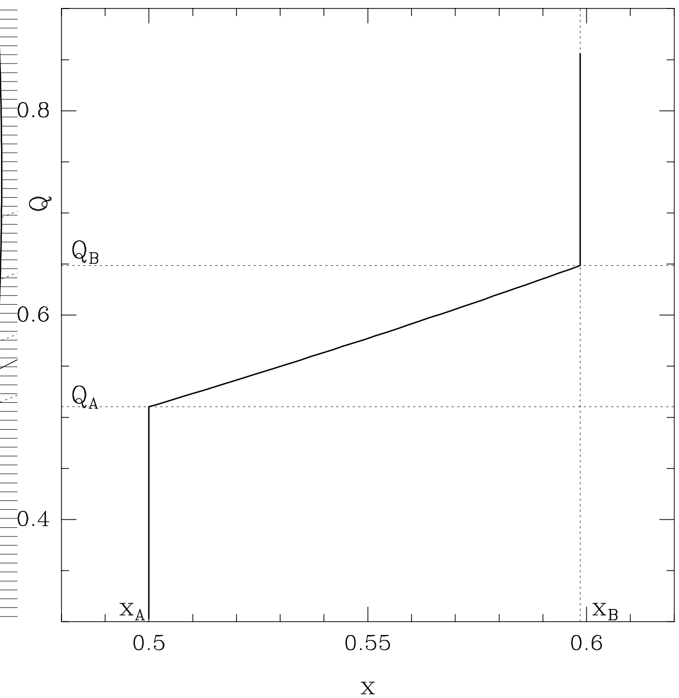
Uniqueness $\Rightarrow$ elastic behaviour

Cables versus struts





Minimization of potential energy



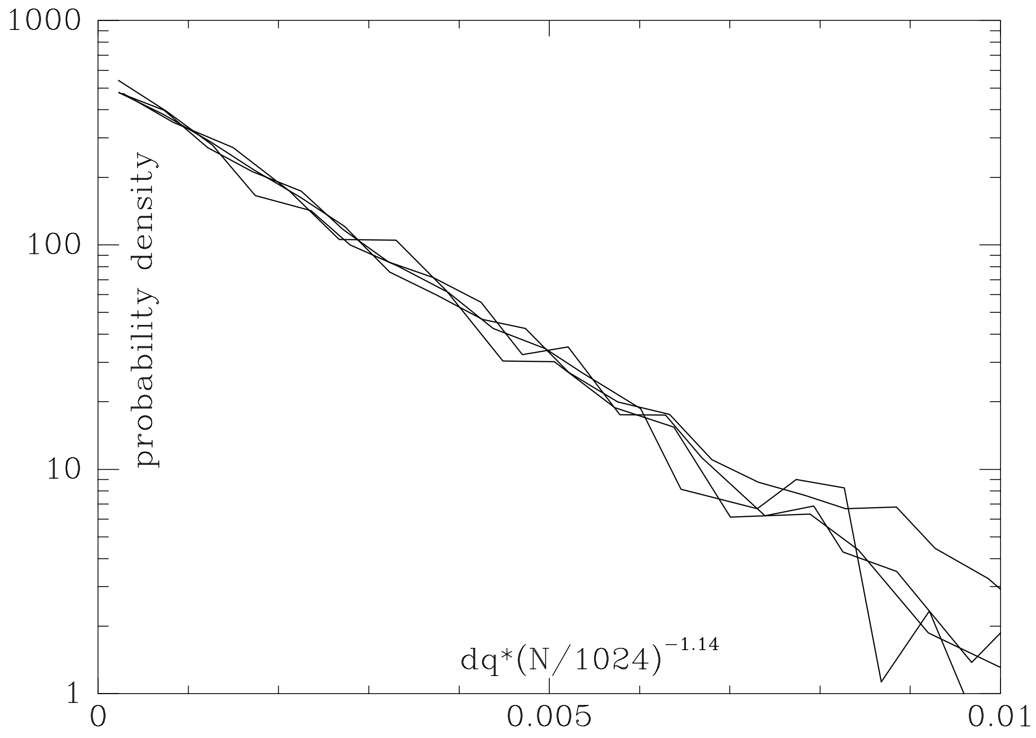
$Q = F_x/F_y$ versus position x.

Uniqueness. No force indeterminacy, but stable mechanism (kernel of $\underline{\underline{G}}$). Elastic behaviour

Frictionless cohesionless rigid spheres: isosaticity property II

- In equilibrium, the force-carrying structure is devoid of force indeterminacy and devoid of mechanisms (floppy modes). It is an *isostatic structure*
- Matrix $\underline{\underline{G}}$ is square and inversible: one-to-one correpondence between applied load and contact forces
- only true for spheres, for which there is a lower bound on coordination number z^* (excluding rattlers). $z^* = 6$ (3D), $z^* = 4$ (2D)
- Apart from the motion of rattlers, equilibrium states are *isolated points* in configuration space. Particles rearrange by jumping to different configurations with different contact network topology

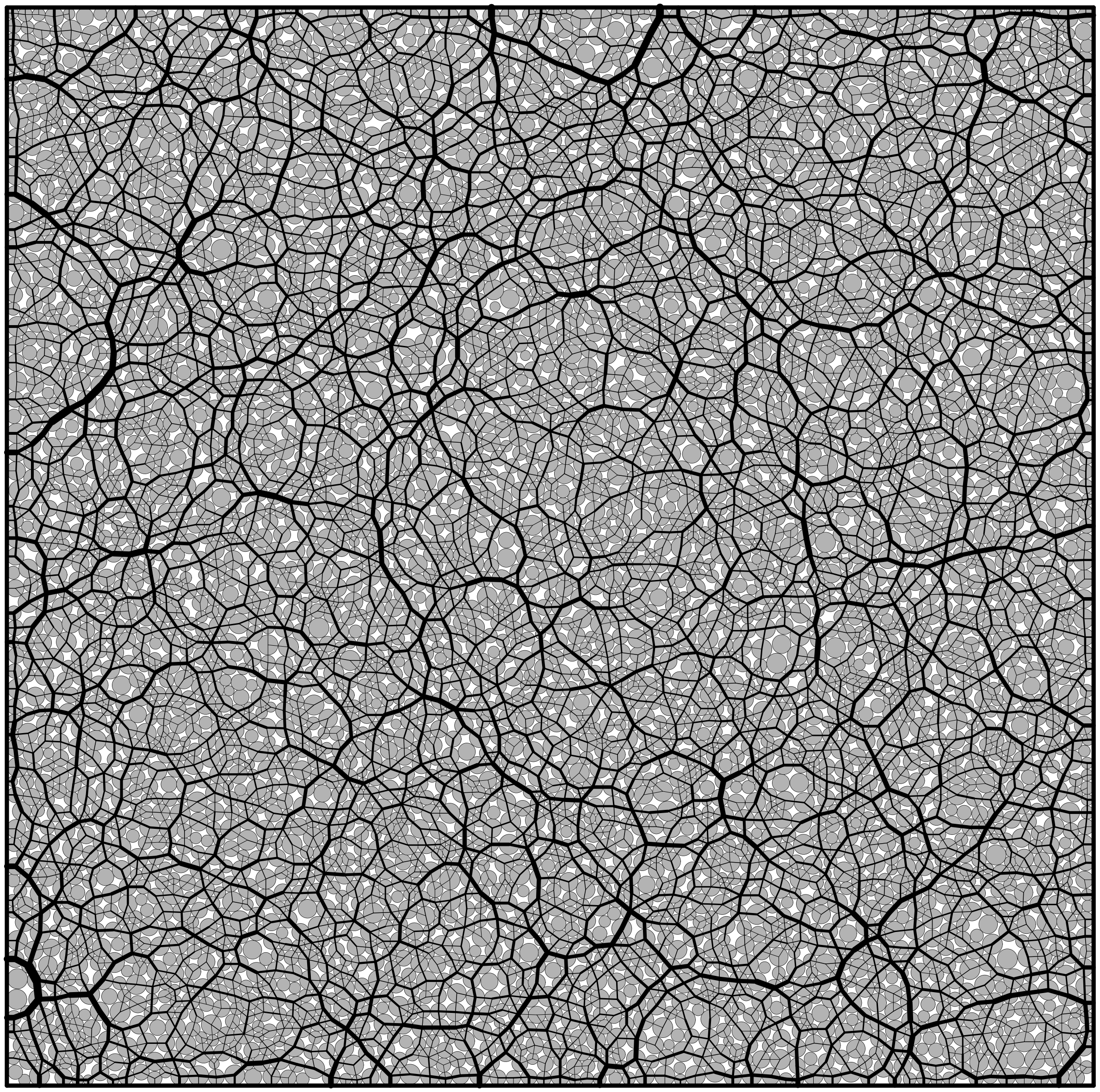
Frictionless systems, rigid grains, no cohesion: fragility property



Distribution of deviator stress intervals for which a given configuration is stable (biaxial compression of rigid frictionless disk assemblies satisfying isostaticity property in 2D), $1000 \leq N \leq 5000$ particles, Combe and Roux 2000

Consequences

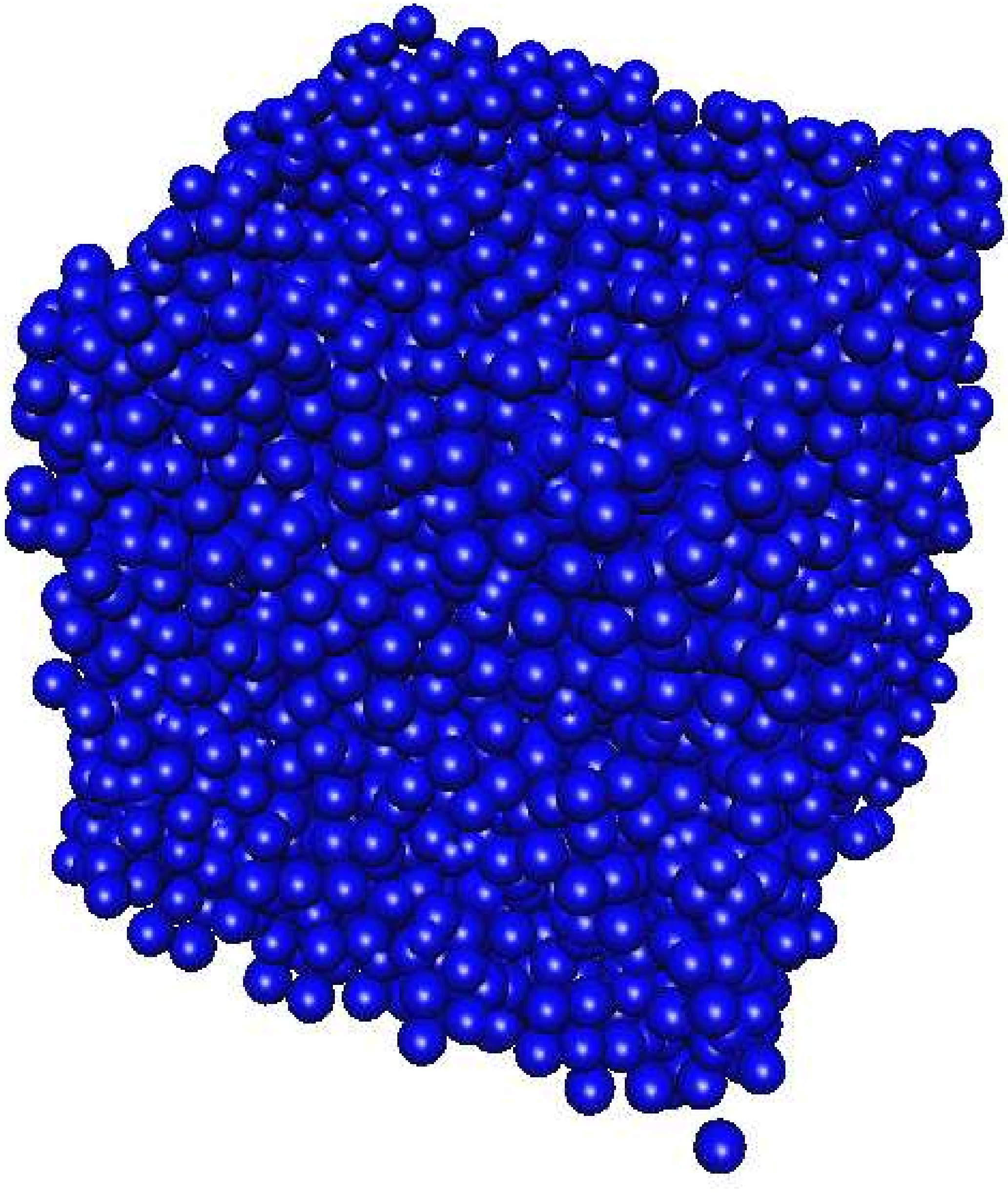
- Response to stress increments involves rearrangements (except if $\delta\underline{\underline{\sigma}} \propto \underline{\underline{\sigma}}$)
- how forces distribute on isostatic network (ignoring sign conditions) : still open question (depends on fabric ?)
- isostaticity is compatible with elastic behaviour (cable networks). Arguments predicting exotic properties should not apply to cable networks
- what about soft grains ?



4900 disks in equilibrium (isotropic stress state, two wall d.o.f.). $n^* = 4633$ disks and $N^* = 2n^* + 2 = 9268$ contacts carry forces. Isostatic force-carrying structure

Generically disordered assemblies of spheres

(nearly) rigid, frictionless, cohesionless contacts



Triaxial tests on frictionless spheres

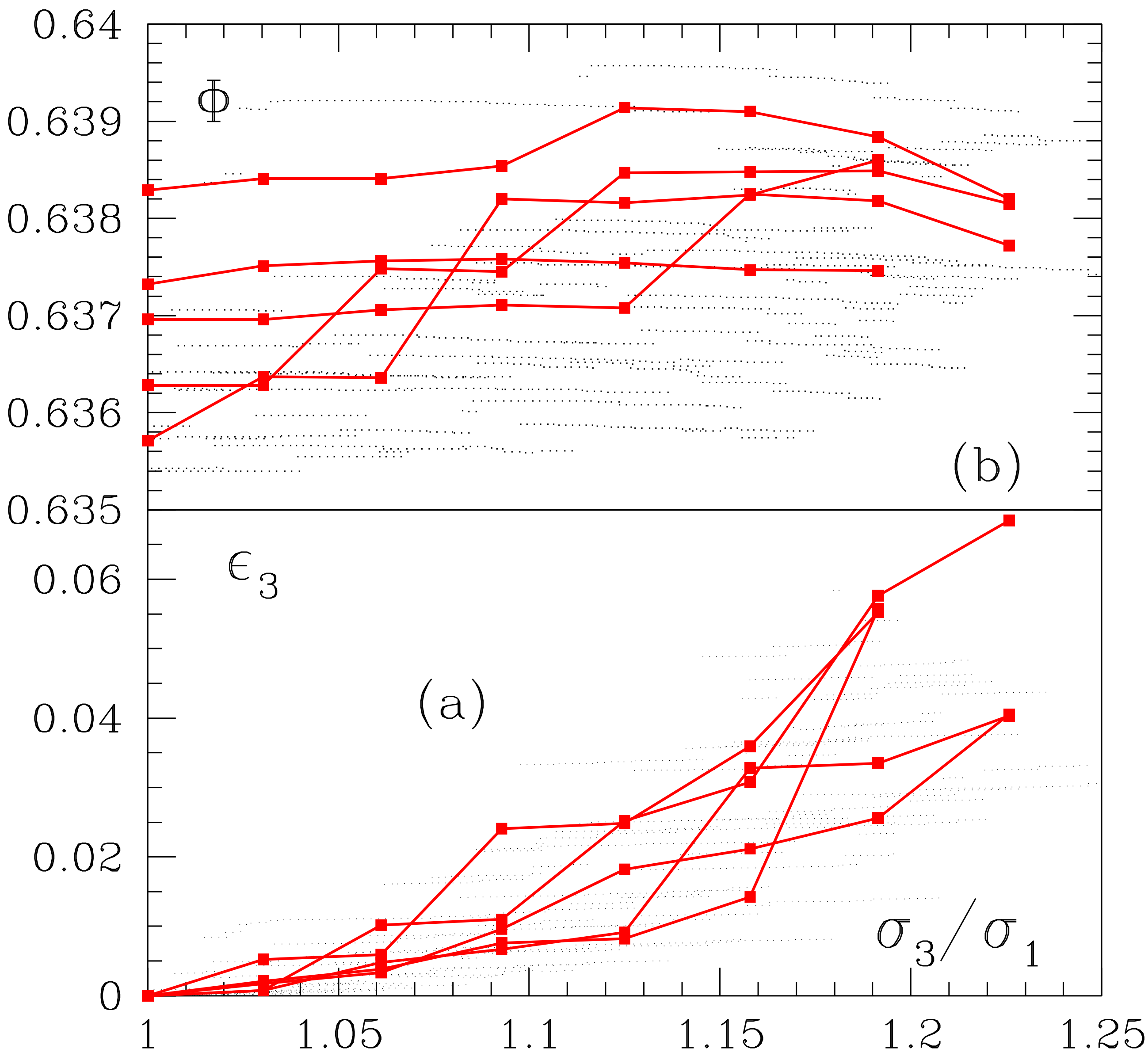
From initial isotropic state, apply:

$$\begin{cases} \sigma_1 & = p - q/2 \\ \sigma_2 & = p - q/2 \\ \sigma_3 & = p + q \end{cases}$$

increasing stepwise q/p by 0.02, waiting for equilibrium

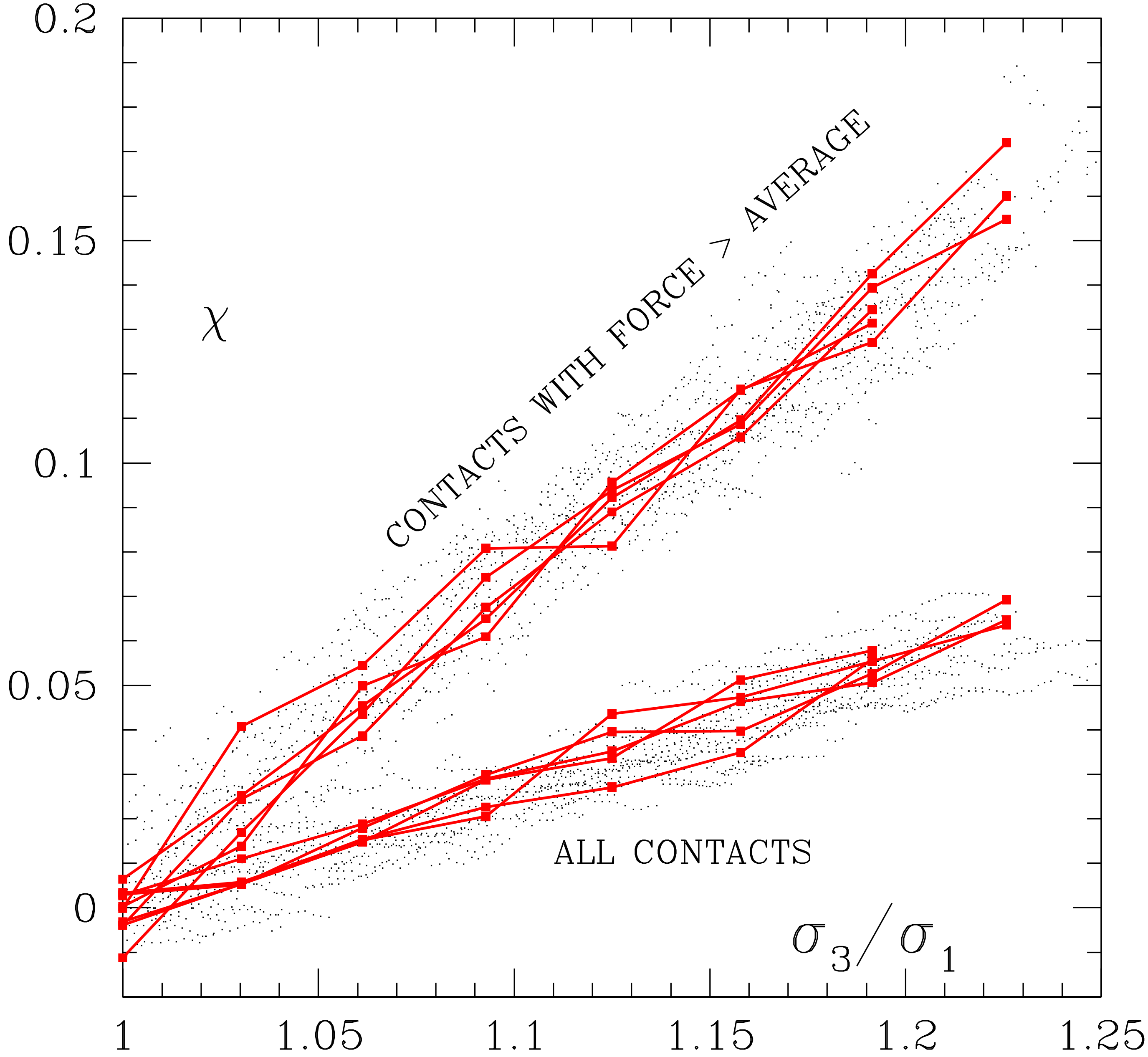
Triaxial tests on frictionless spheres

Packing fraction Φ and axial strain ϵ_3 vs. principal stress ratio. $n = 1372$ (small symbols), $n = 4000$ (connected dots)



Triaxial tests on frictionless spheres

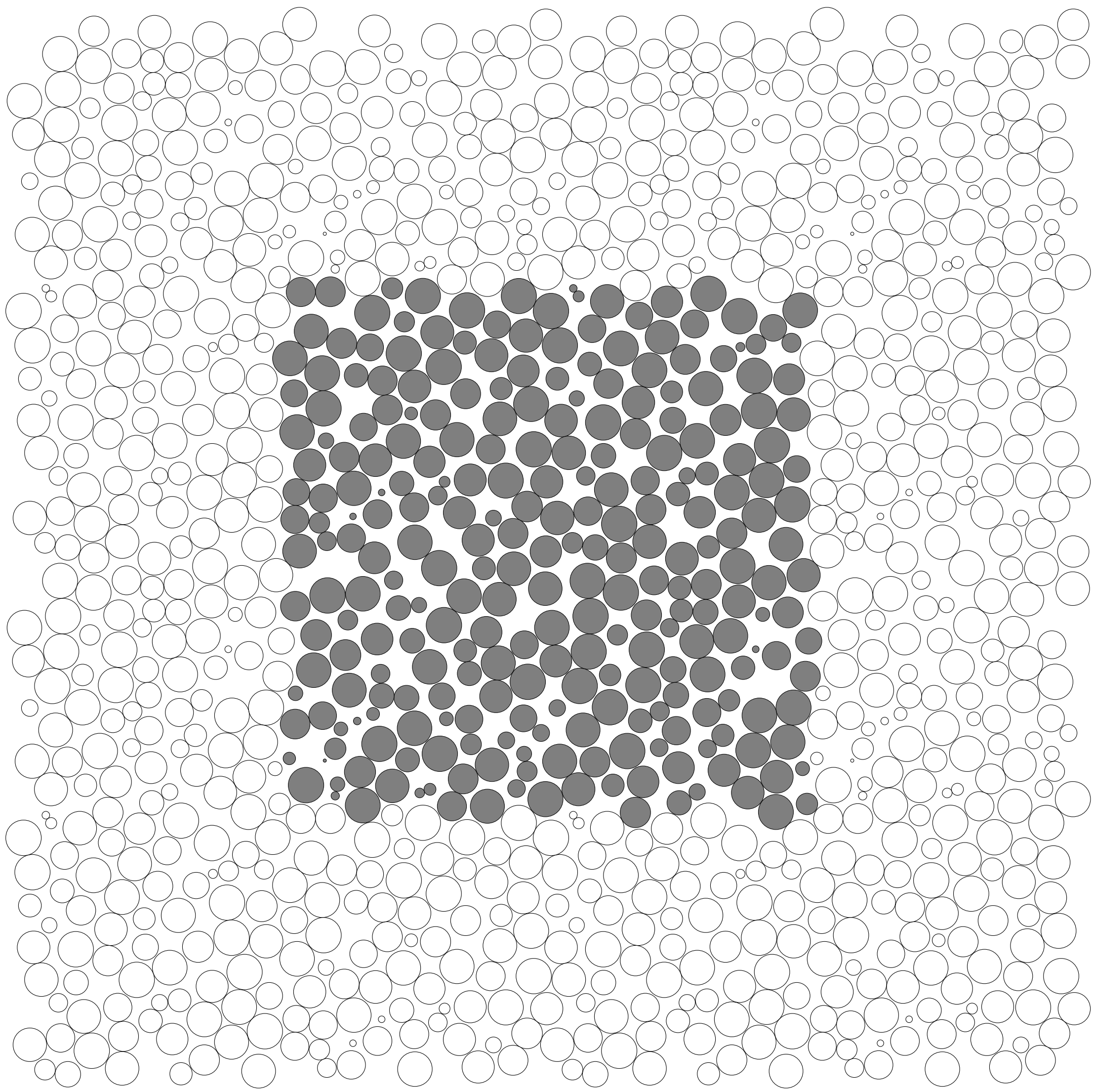
Fabric parameter $\chi = 3\langle n_z^2 \rangle - 1$ versus principal stress ratio.



Triaxial tests on frictionless spheres: conclusions

- Apparently, no clear approach to stress-strain curve (it was concluded before that no such curve existed, Combe 2000)
- evidence for a fabric/stress ratio relationship
- internal friction angle $\sim$ 5 or 6 degrees
- no dilatancy, RCP density for different stress states

Cut through dense sphere packing

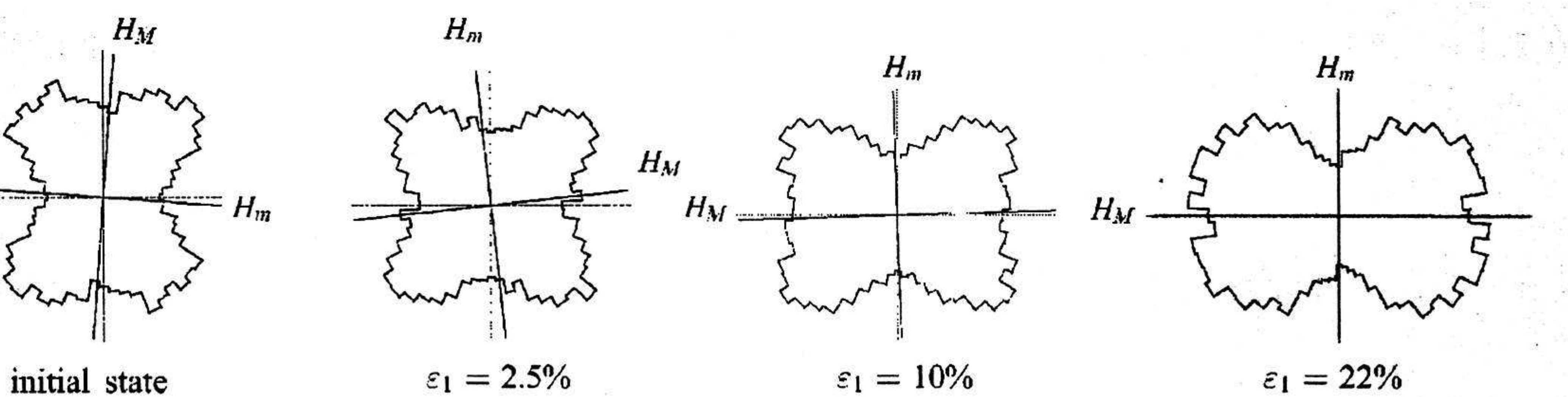


Difficult to obtain coordination number from direct observations

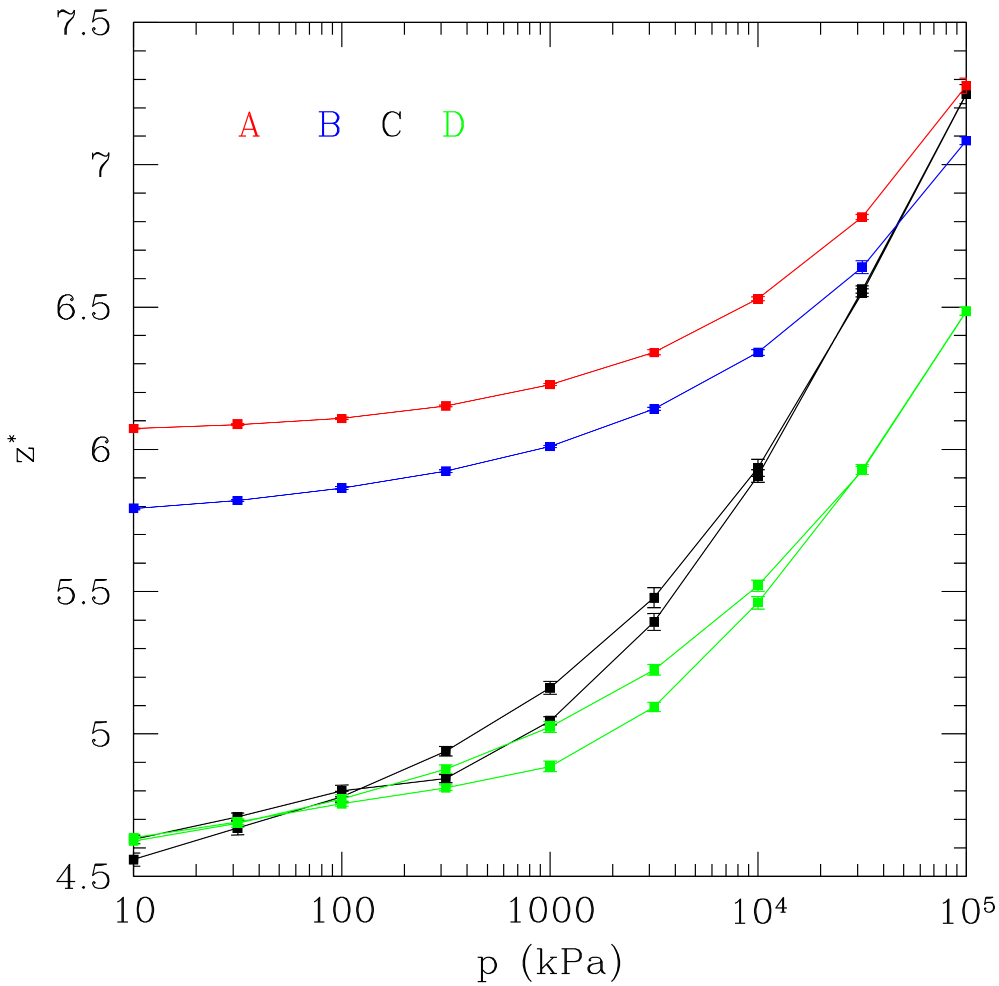
Microstructures of frictional packings

Much wider variety than with frictionless ones:

- different solid fractions Φ possible (while disordered frictionless packs never below RCP density)
- deposition anisotropy
- independence between density and coordination number. Example: Numerical procedure (C) designed to mimic vibration compaction produces high density ($\Phi \simeq 0.635$), low coordination number ($z^* \simeq 4.5$), high rattler fraction (13%) isotropic sphere packings under low pressure with $\mu = 0.3$



Initial states, coordination number and packing fraction



Simulated glass bead packs ($E = 70$GPa), assembled in isotropic states by different procedures. Packing fractions (at 10 kPa):

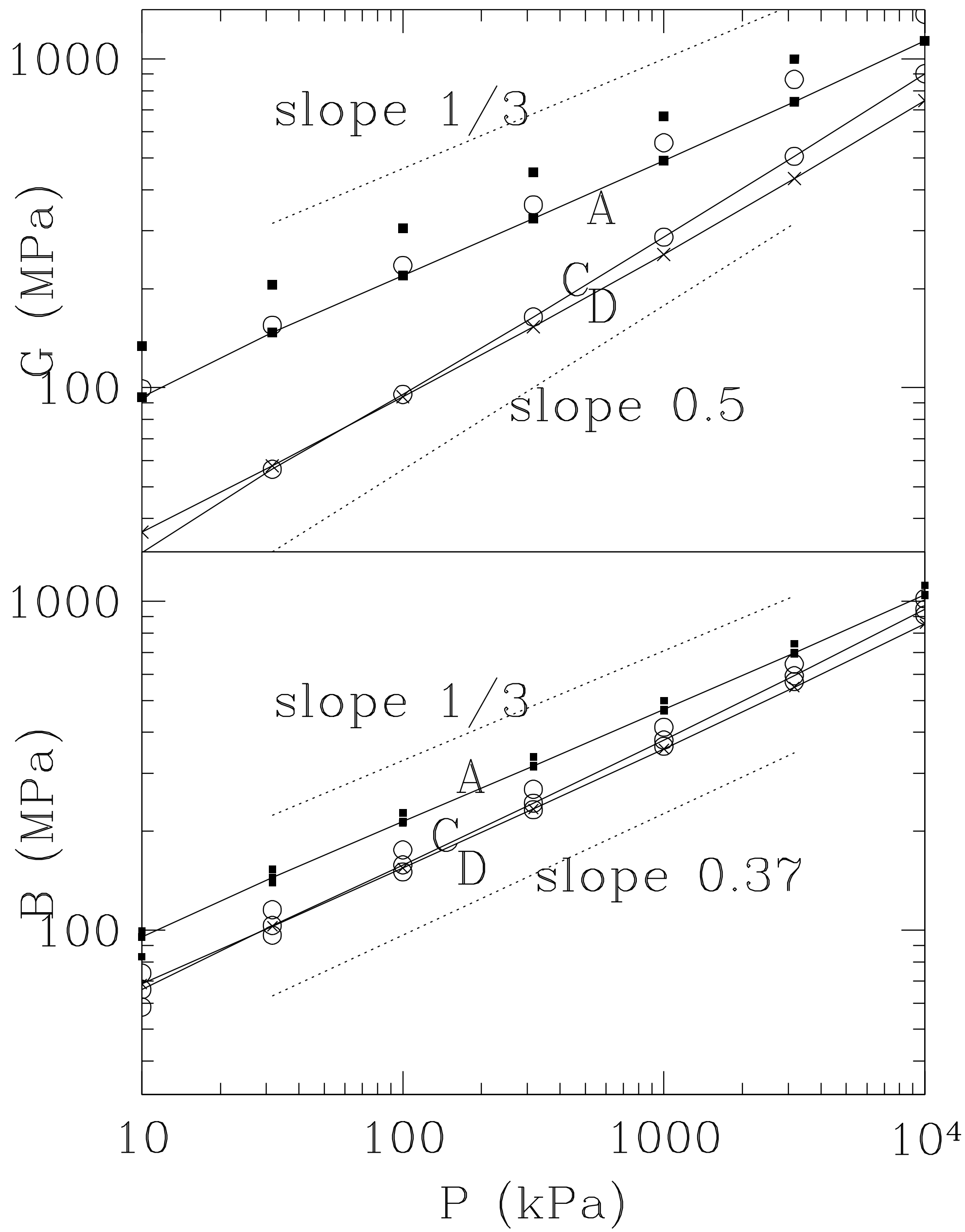
$\Phi_A = 0.637 > \Phi_C = 0.635 > \Phi_B = 0.625 > \Phi_D = 0.606$

- Effect of pressure increase on coordination number relatively moderate in most usual experimental range (no more than a few MPa)
- Both μ and ζ have influence (see e.g., Silbert *et al.*) on result of assembling process, while dense flow or quasi-static deformation are not sensitive to viscous dissipation
- More studies needed: incomplete experimental or numerical knowledge, no theory for the sudden arrest of flow and compression of a granular gas into a quiescent solid

ELASTICITY OF GRANULAR PACKINGS

- Elasticity of contact network (= spring network if friction not mobilized, which is usually the case at equilibrium)
- Effect of confining pressure on moduli
- Deviation from expected behaviour (e.g., from affine approximation) predicting growth as $P^{1/3}$ for Hertz contacts

Simulated glass beads: pressure-dependent elastic moduli



A = square dots

C = open circles

D = crosses

B not shown (close to A)

Moduli are shown with connected symbols

Estimates (bounds) are shown as symbols (not connected) for A and C

Elasticity of sphere packings under isotropic pressure

- bulk modulus B satisfactorily bracketed by simple approximations (Voigt-Reuss type bounds)
- Shear modulus exhibits more anomalous behaviour, especially in low-z systems
- pressure increase faster than expected not due to z increase (would affect B as well as G)
- related to anomalous distribution of eigenvalues of stiffness matrix in systems with low force indeterminacy (see O'Hern *et al.*, Wyart *et al.*) ?
- elastic moduli related to coordination number (rather than density)

ANELASTIC BEHAVIOUR OF CONTACT NETWORKS

- Emerging theme... see publications on set of possible contact forces, force indeterminacy... (McNamara *et al.*, Snoeijer *et al.*...)
- Static problem, can be dealt with regarding contact set as network of springs and plastic sliders
- in the recent literature, focus on forces rather than (small) displacements.

"Critical yield analysis" formulation: consider *e.g.* an equilibrium state in 2D under $\sigma_1 = \sigma_2 = p$, apply $\sigma_1 = p + q$, $\sigma_2 = p$, by increments of q (biaxial compression). For which q value does the initial contact network become unstable ?

$\rightarrow$ Ask whether contact forces exist that are both *statically admissible* (they balance the load), and *plastically admissible* (they satisfy Coulomb inequalities).

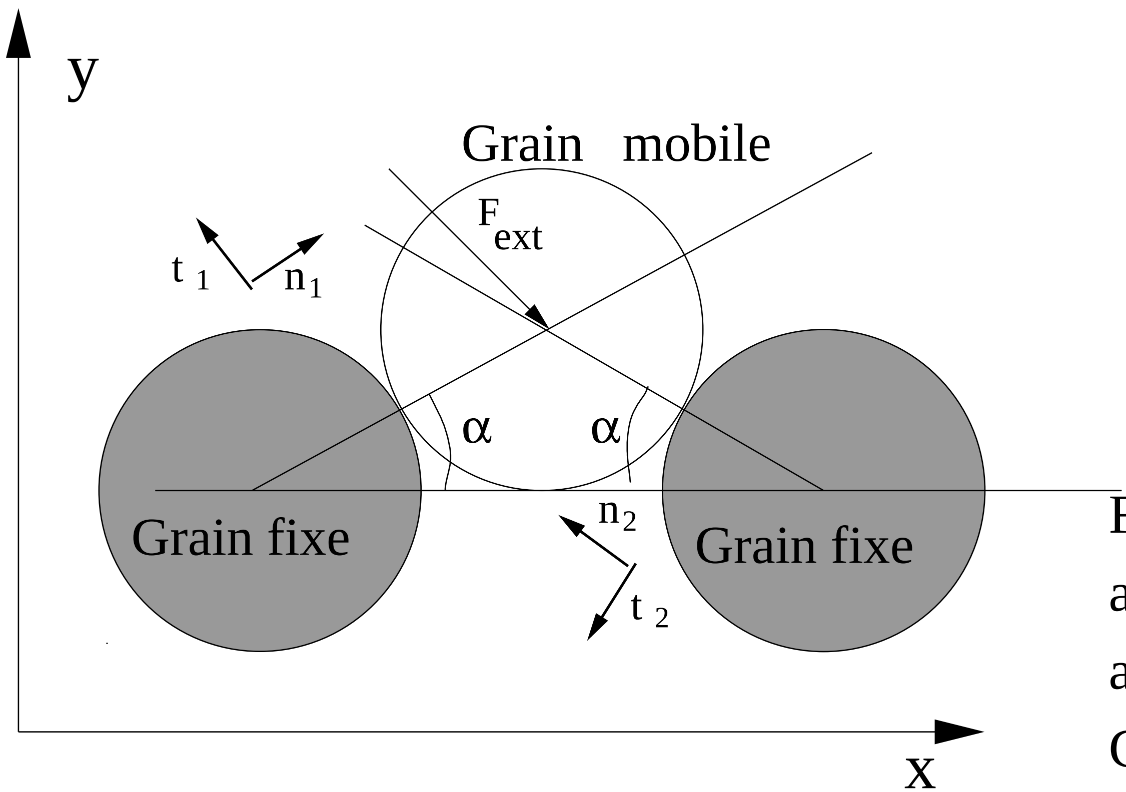
This is a *necessary* condition for stability (supported load)

Is it sufficient ?

Some bad news

For a solution to exist, it is necessary that contact forces both plastically and statically admissible exist.

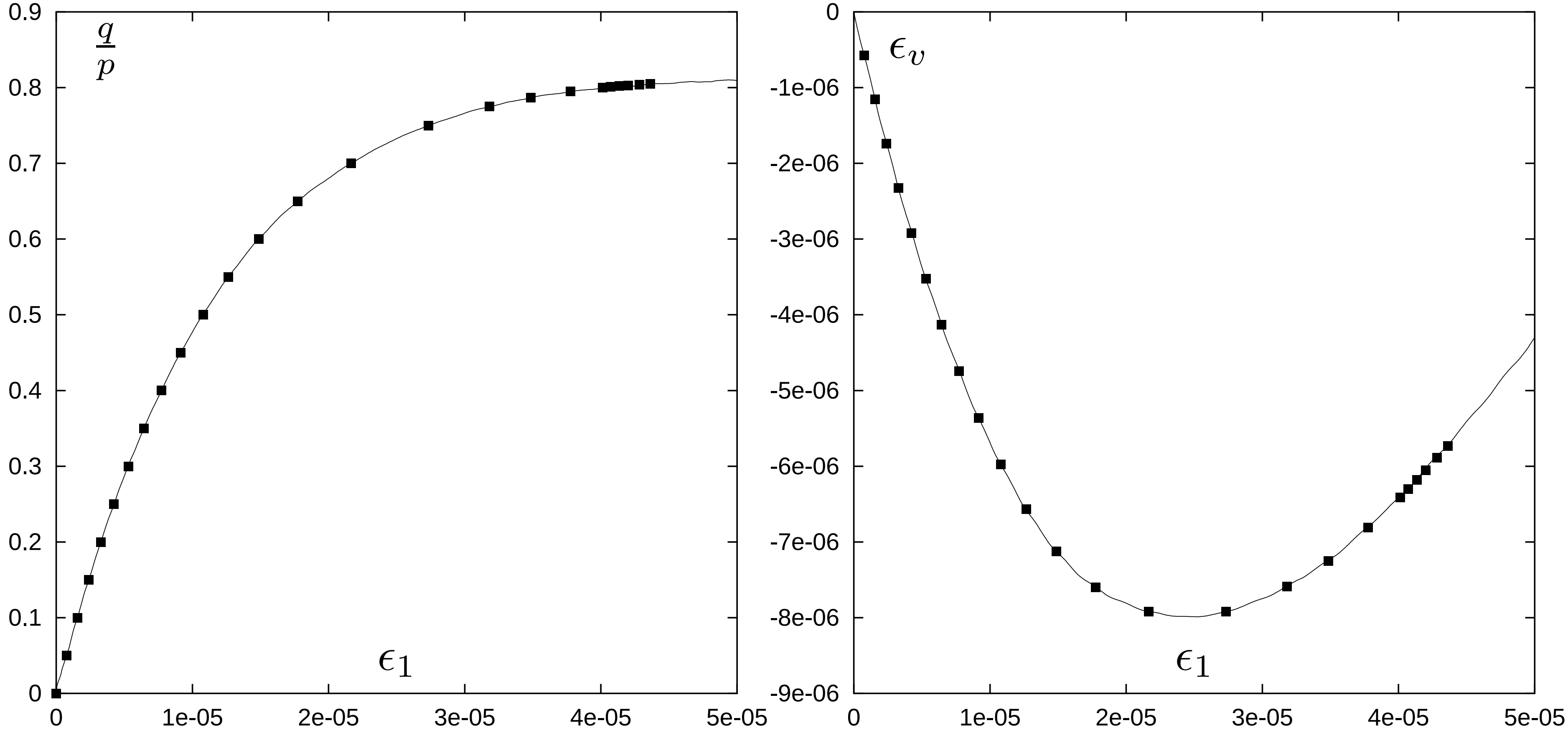
For grains with Coulomb friction this is not sufficient. Example:



For $\alpha < \varphi$ (friction angle) all external forces can be balanced by contact forces in Coulomb cone

(Halsey-Ertas "ball in a groove" system, See study by S. McNamara, R. García Rojo and H. Herrmann)

Biaxial compression test: static elastoplastic calculation vs. MD



4900 disks. Identical results for static (dots) and MD (curves) calculations.

Results with G. Combe (2001,2002)

Biaxial compression: other results and remarks

- Strains are inversely proportional to K_N (normal stiffness of contacts)
- Detailed comparisons show that static and dynamic methods *locally* give identical results (small systems)
- Static method applicable as long as initial network carries deviator (*type I strains*)
- It fails as soon as the network has to rearrange
- Contacts open, others yield in plastic sliding... non-elastic and non-linear behaviour
- Upper q limit of static method range appears to have finite limit q_1 as $n \to \infty$, even for $\kappa\infty$. Granular systems with friction are not "fragile"
- q_1 is **strictly smaller** than the deviator maximum

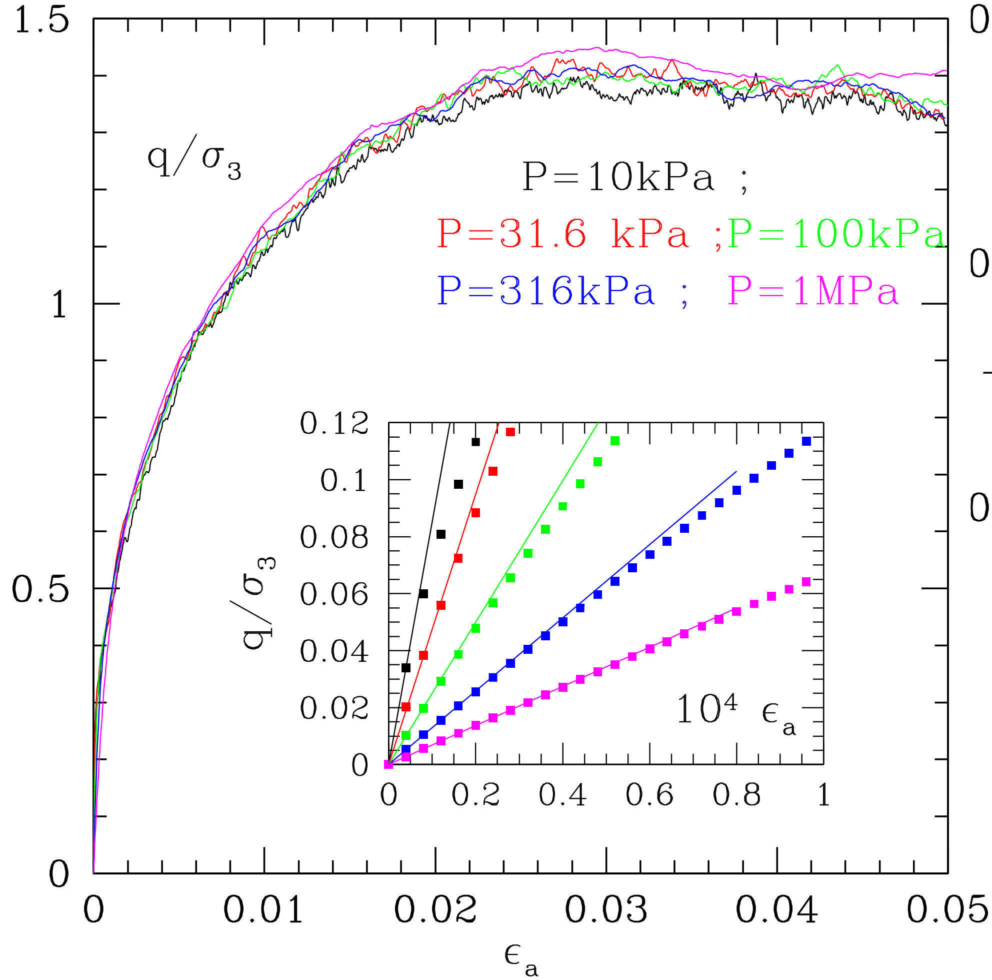
Properties of quasi-static regime I

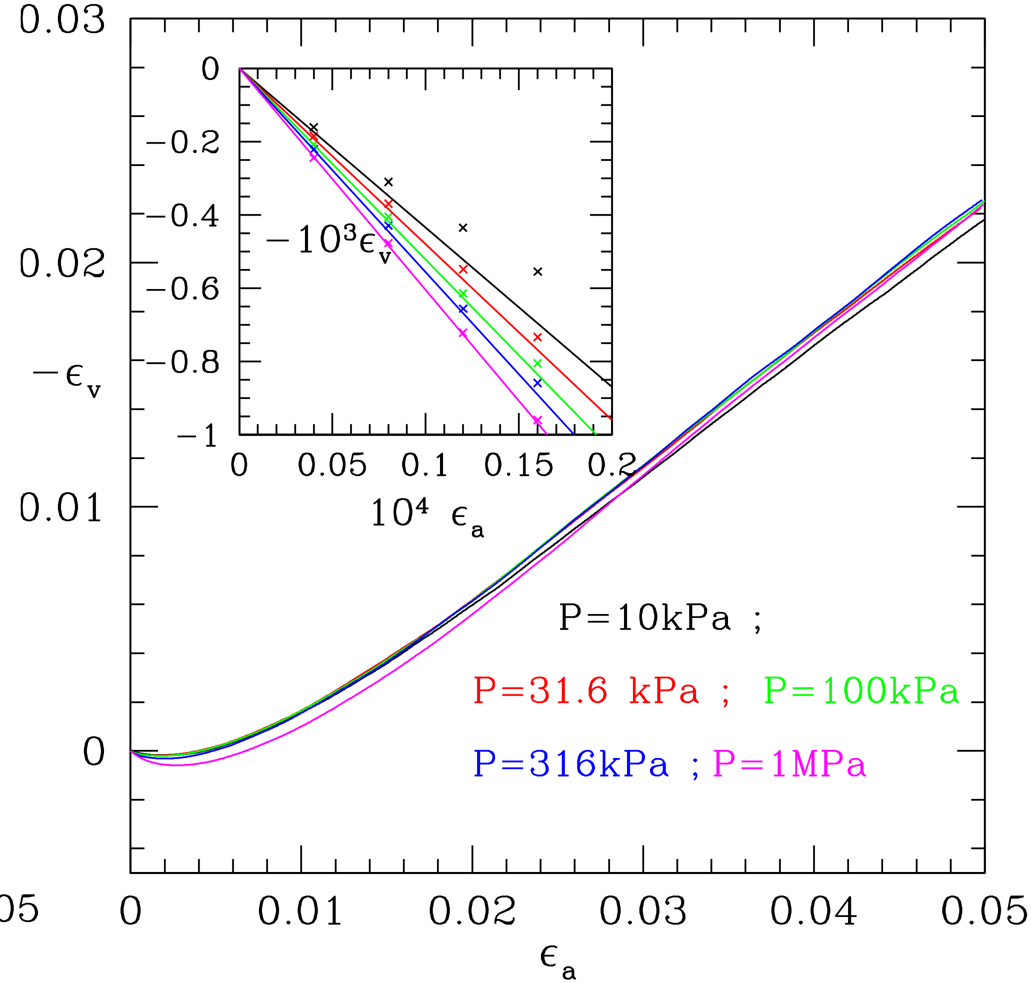
- strains inversely proportional to κ (hence small), non reversible (plastic), but contained by contacts staying in elastic regime
- evolution *via* a continuous set of equilibrium states in configuration space (quasistatic in the strictest sense)
- little sensitivity to perturbations, return to equilibrium easy
- regime extends to large stress intervals when coordination number is high (large force indeterminacy), or upon unloading (friction being mobilized in the direction associated with loading)

Regime II

- Beyond stability of initial network,
- strains not sensitive to stiffness level κ
- larger fluctuations, slower approach to large system limit
- successive equilibrium states do not form continuous trajectory in configuration space: system has to evolve by dynamic crises. “Quasistatic” evolution in an extended sense (if details of the dynamics statistically irrelevant)
- Characteristic of quasistatic response of granular assemblies with low force indeterminacy

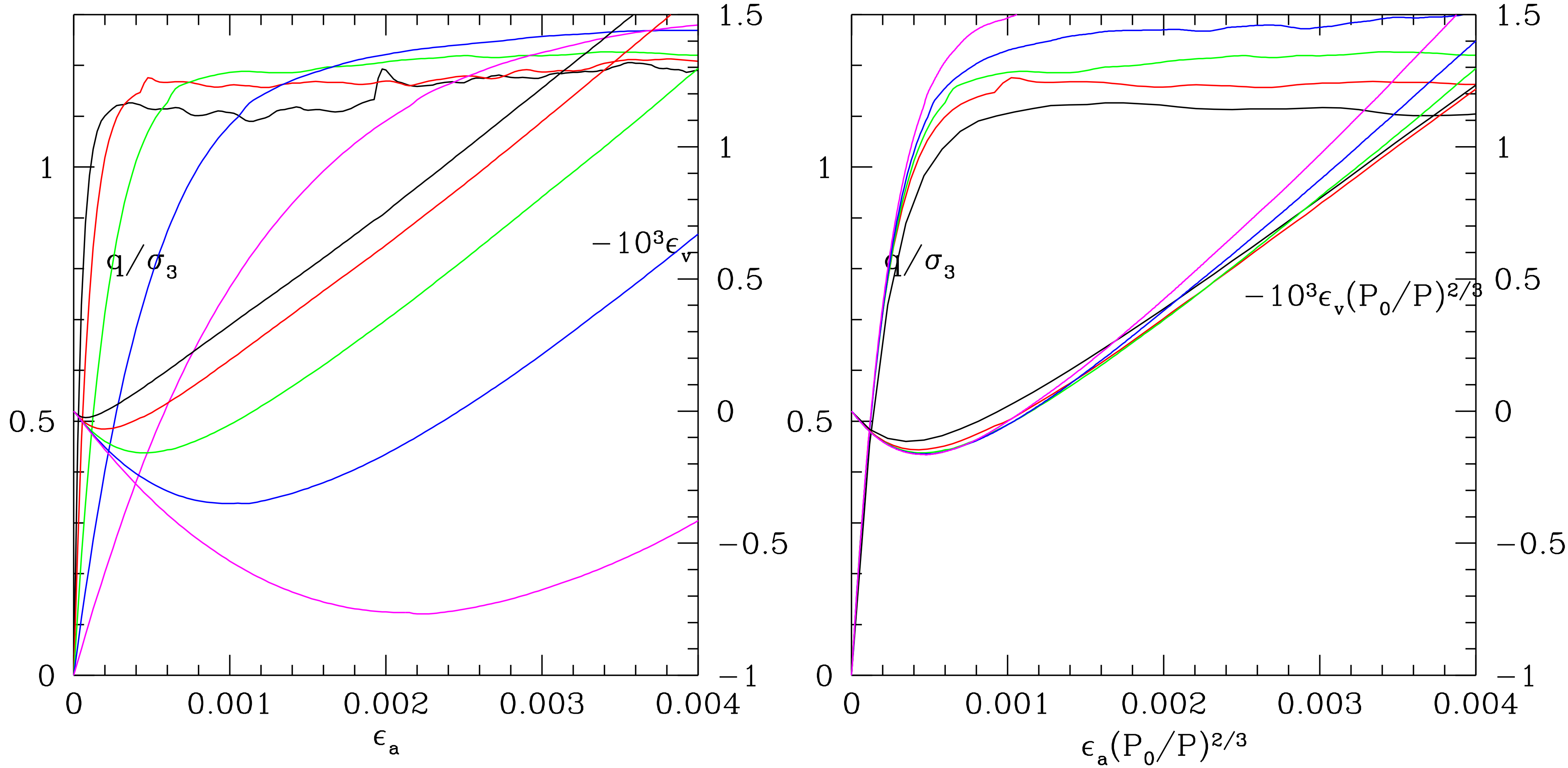
Triaxial compression, from isotropic initial state: influence of κ





Dense state ($\Phi \geq 0.635$ for large κ), coordination number $z^* \simeq 4.6$ if $\kappa \geq 10^4$ (10 kPa). Strain independent on κ (type II) except at very low ϵ_a (inset : slope = elastic modulus) **Assembling method mimics compaction by vibration**

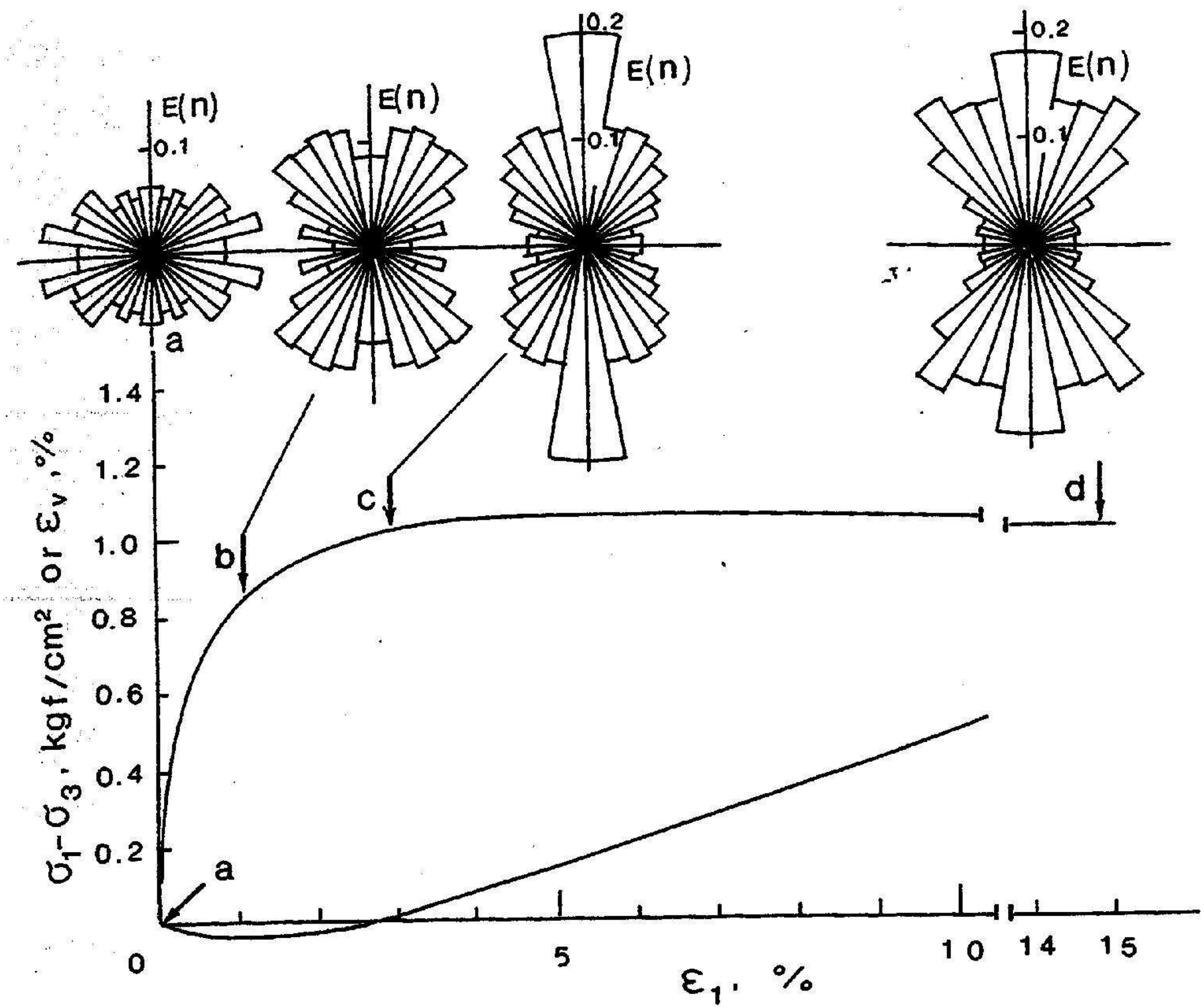
Triaxial compression, from other isotropic initial state:



Dense state ($\Phi \simeq 0.637$ for large κ), coordination number $z^* \simeq 6$ if $\kappa \geq 10^4$ (10 kPa). Strain of order κ^{-1}.

Assembling method with $\mu = 0$ (perfect lubrication). **Type I strain regime**

Internal state evolution in quasistatic deformation: contact orientations



Rothenburg ($\sim$ 1990), Radjai, Kruyt and Rothenburg...

Microscopic theoretical approaches, attempted predictions

- Homogenization ideas (from continuum mechanics of disordered media): bounds, self-consistent estimates... → limited to regime I. (Jenkins & La Ragione...)
- ⇒ important to delineate regimes I and II !
- Attempts to describe internal state (complete list of state variables)... in other words : define an “ensemble”
- Variables include density, coordination number and fabric tensors (contact anisotropy)... Critical state = stationary state for such variables
- Neglect of specific geometry of granular packings, and of its variability... = pitfalls of modelling attempts