The onset of rigidity in simple particulate systems

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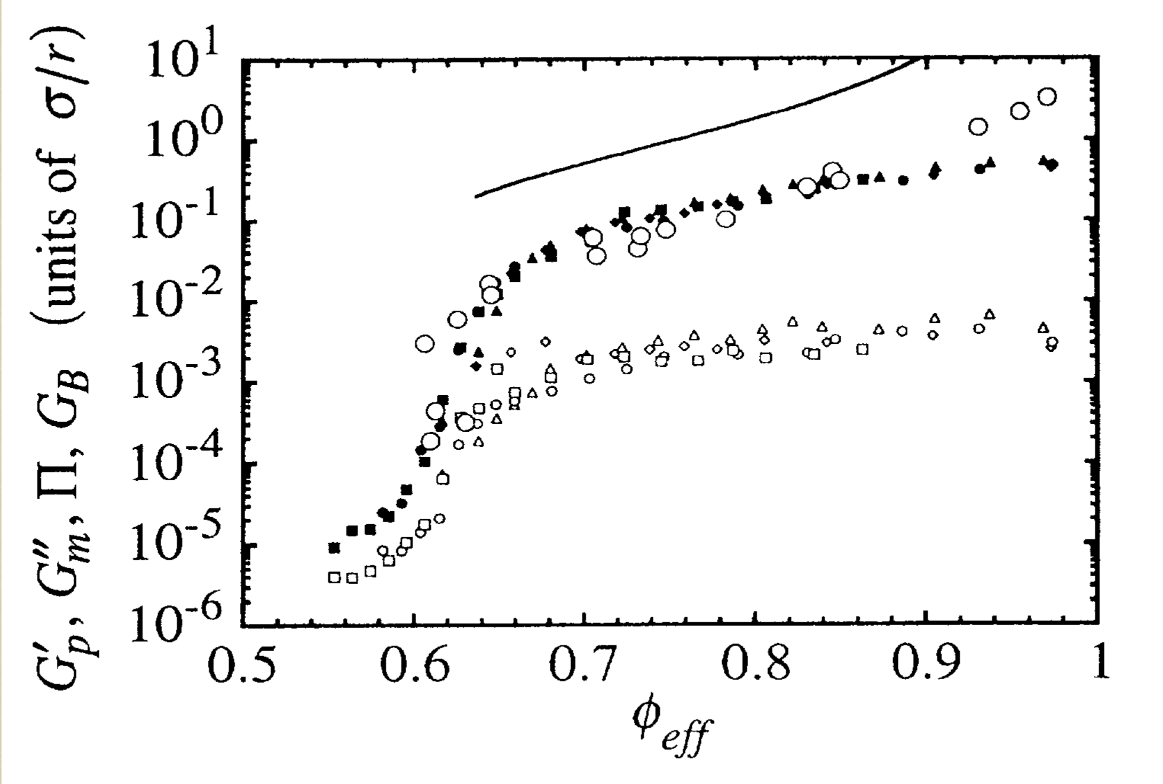
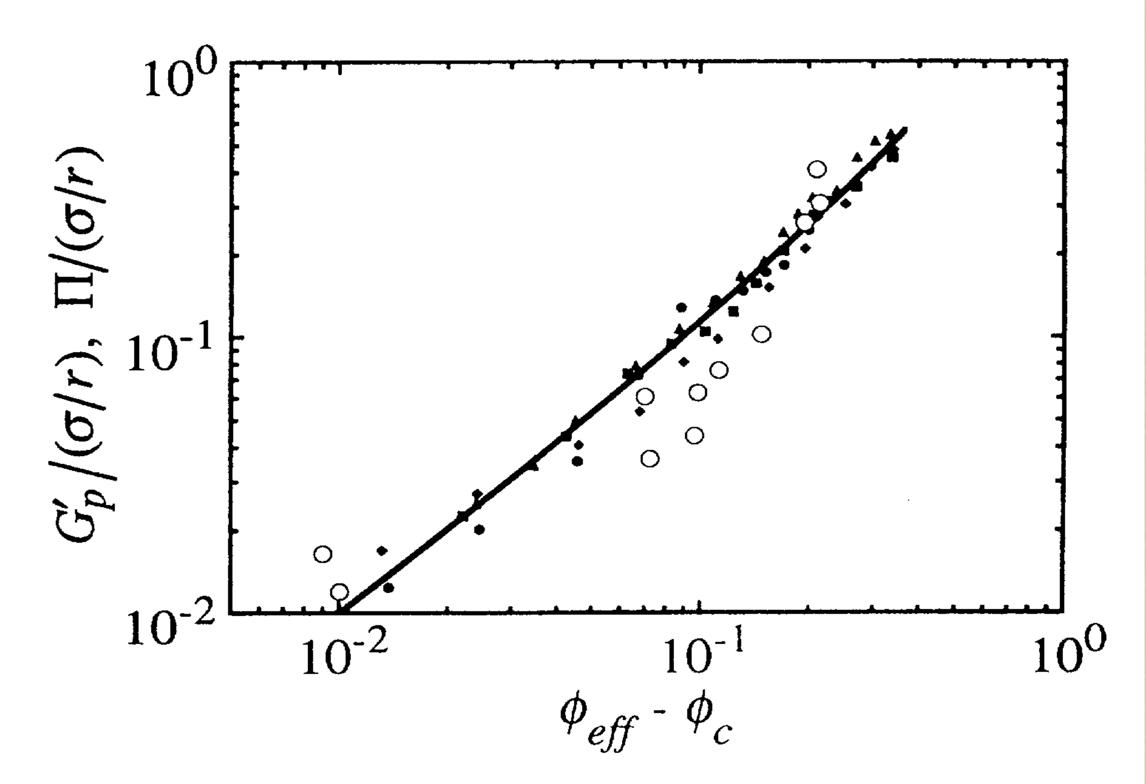
Rigidity transition

- Many systems have a rigidity transition at a finite volume fraction ϕ_c , when the elastic moduli become non-zero

- At least in some cases, the same point is reached with controlled pressure P as $P \to 0$ or (bond stiffness) $\mu \to \infty$

- Example: emulsion experiments



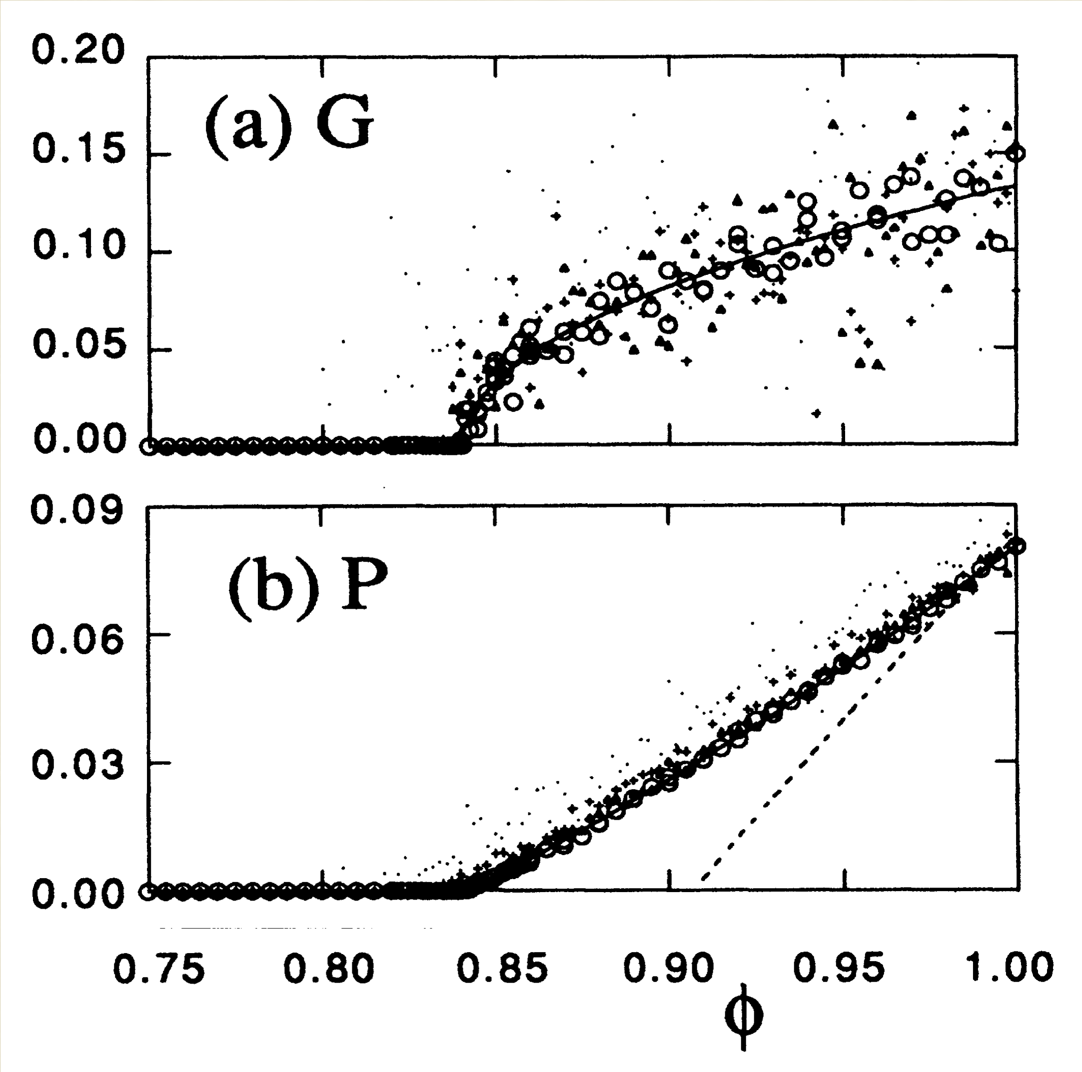


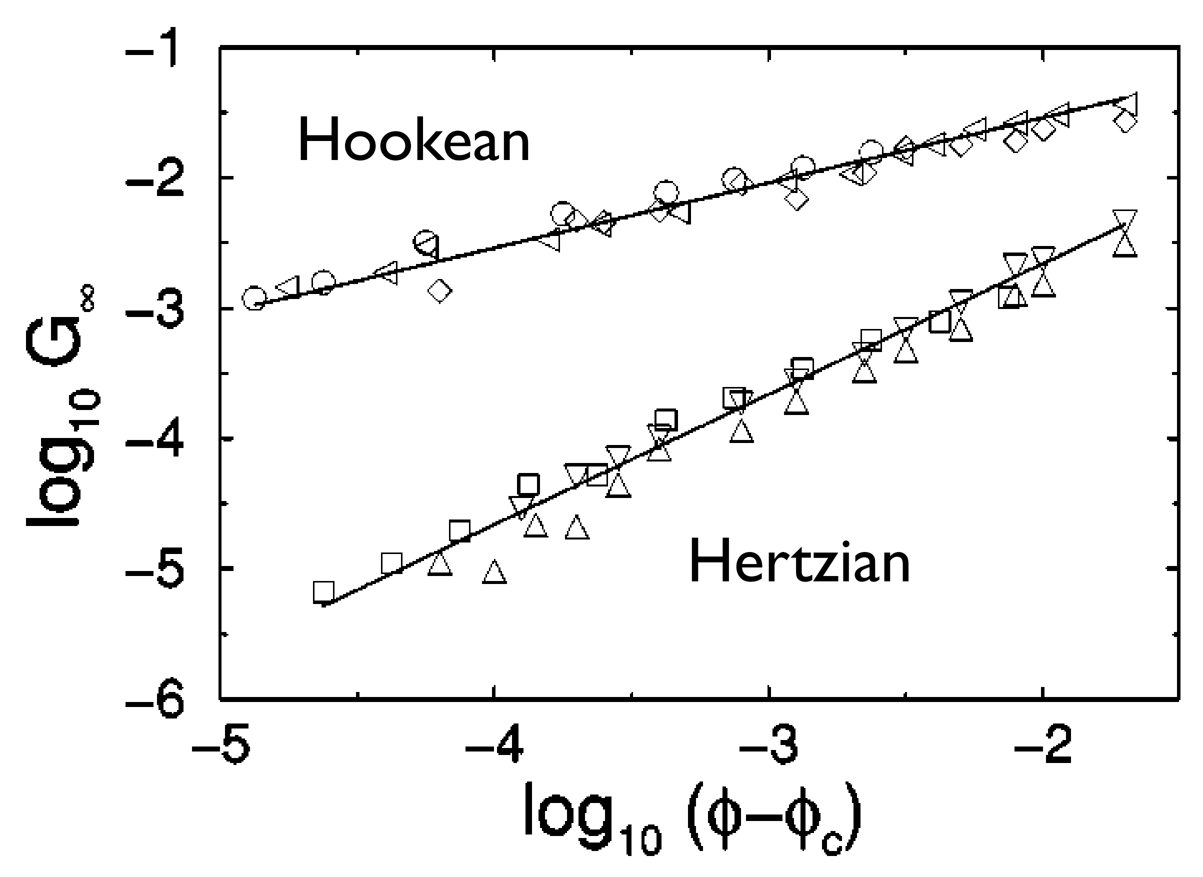
[Mason *et al.*, PRL 1995]

‘Bubble’ model for wet foams (d=2, molecular dynamics with viscous damping)

[D. Durian, PRL 1995]

[*cf.* Bolton & Weaire, PRL 1990]



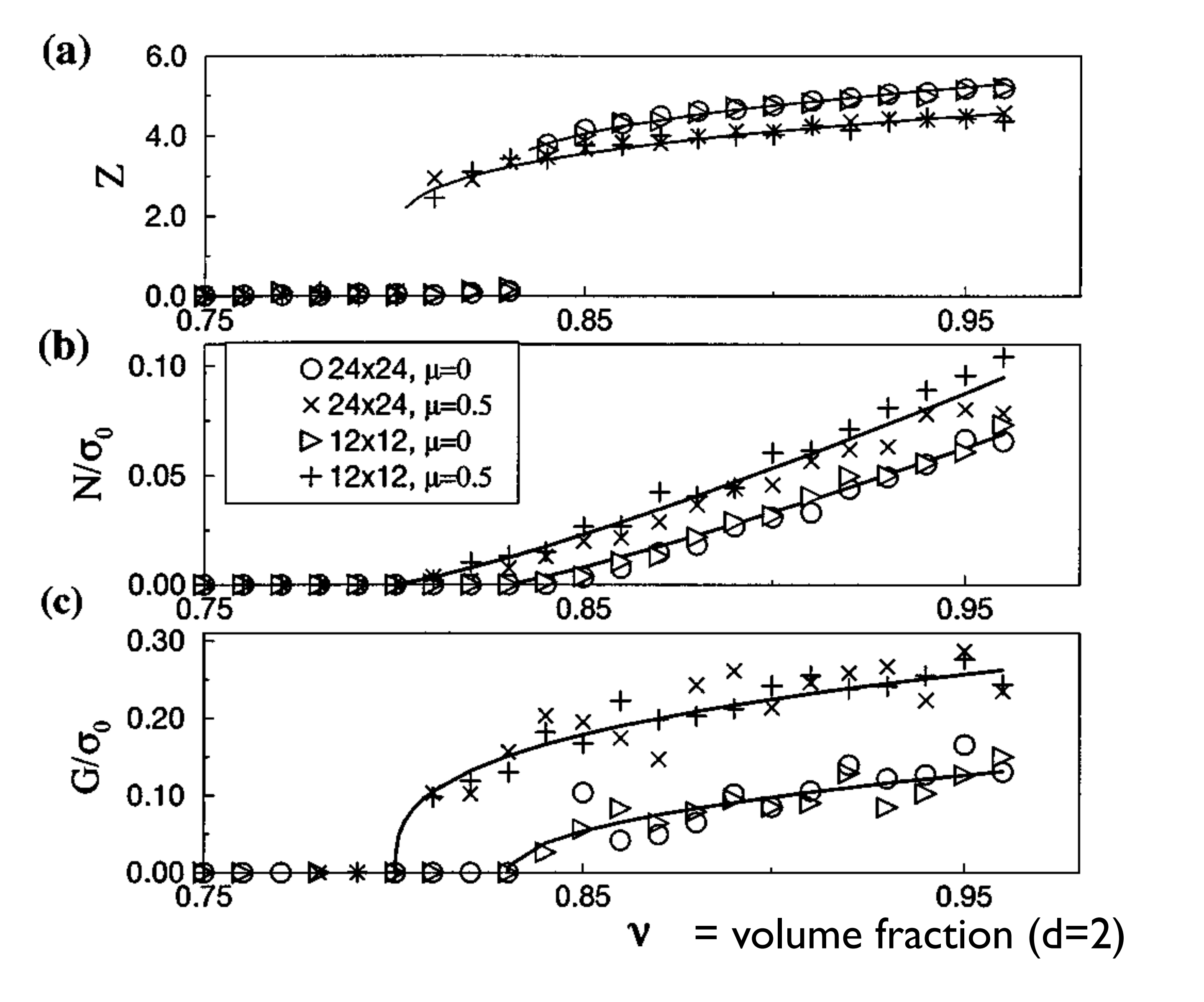


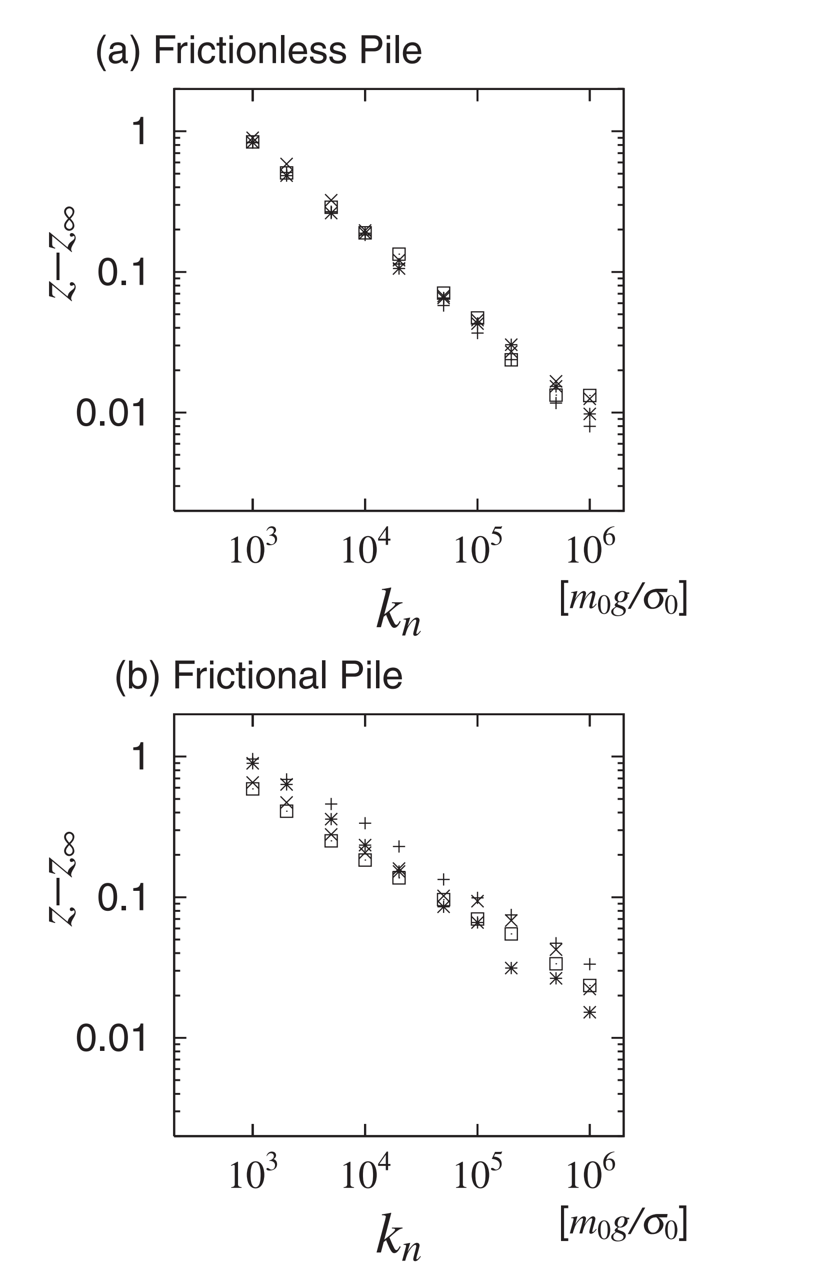
Truncated Hookean/ Hertzian contacts in d=2,3 (minimisation algorithm)

[O’Hern *et al.*, PRE 2003]

Frictionless and frictional granular media (g=0)

[Aharonov & Sparks, PRE 1999]



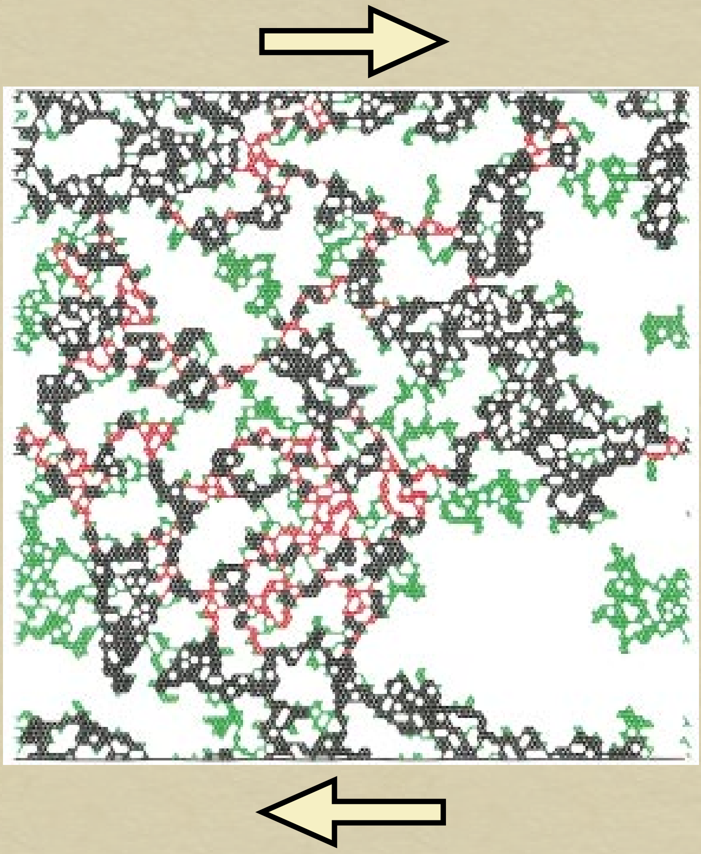


Frictionless and frictional granular media (g>0)

[Kasahara & Nakanishi, J.Phys.Soc.J. 2004]

Rigidity percolation

- Disordered lattices constructed by bond dilution
- Transport of vector quantity (force)
- Exhibits **rigidity percolation** when a rigid cluster first spans the system
- e.g. d=2 Hookean springs: $z_c = 3.961(2)$, $D_f = 1.86(2)$, $D_b = 1.80(3)$ [Jacobs&Thorpe, PRL 1995]
- Typically start from unstressed networks, although prestresses are important [Alexander, Phys. Rep. 1998]
- Dynamics-inspired dilution rules have been devised [Thorpe *et al.*, J. Non-Cryst. Sol. 2000; Schwarz *et al.*, *cond-mat/0410595*]



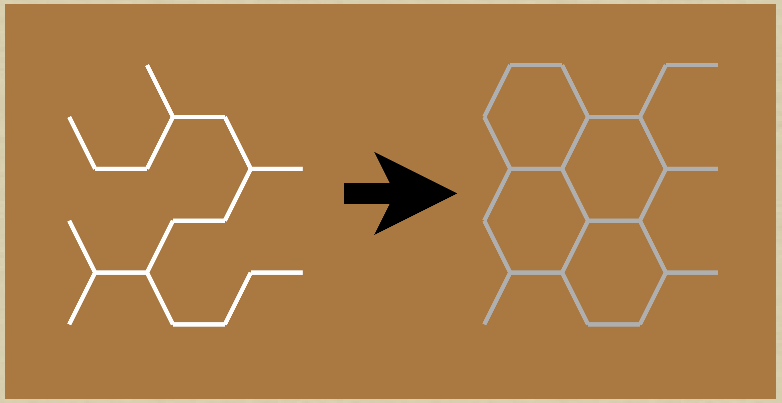
[C. Moukarzel *et al.*, PRL 1997]
(Black - stressed; green - rigid but unstressed; red - 'cutting')

Approximation schemes

Effective medium approximation (EMA)

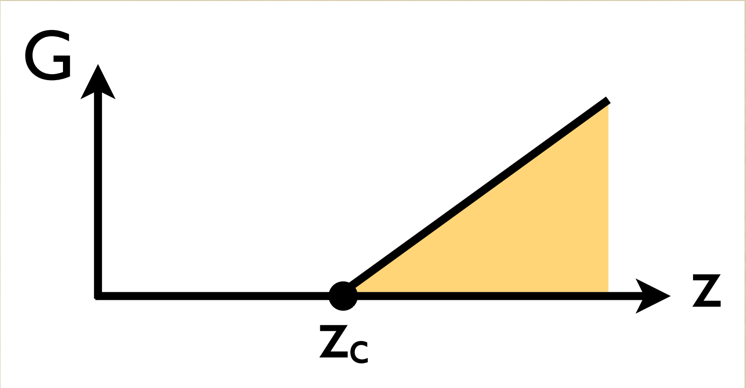
[S. Feng *et al.*, PRB 1985]

Disordered lattice,
known stiffness μ



Homogeneous lattice,
unknown effective stiffness μ^{eff}

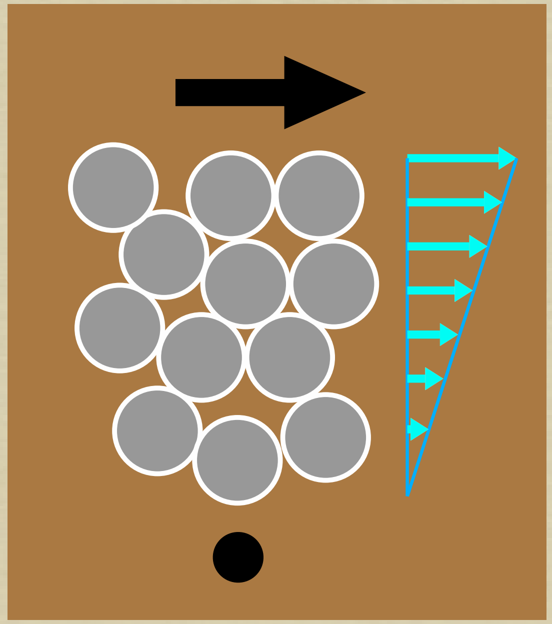
Rigidity transition at $z = z_c = 2d$:



Affine deformation

[K. Walton, J. Mech. Phys. Solids 1987;
H. Makse *et al.*, PRL 1999]

Impose microscopic
displacement field



No transition at finite
volume fraction ϕ

More complex theories reduce G;
still no clear transition

[F. Trentadue, Int. J. Sol. Struct. 2001;
N. P. Kruyt *et al.*, Int. J. Eng. Sci. 1998]

Maxwell counting

- A cluster is rigid when any non-trivial deformation mode increases the elastic energy, *i.e.* the elastic moduli are non-zero
- A system at the onset of rigidity can be called e.g. ***isostatic***, ***marginally rigid*** or at the ***rigidity percolation threshold***.
- Can determine *via* constraint counting; **in its *simplest* form** :

Contact forces are the degrees of freedom	d.o.f.	Force/torque balance	z_c
Particle position/ orientation are the d.o.f.	Geometric constraints	d.o.f.	z_c
Frictionless spheres	$\frac{Nz}{2} \cdot 1$	$N \cdot d$	2d
Frictionless non-spheres	$\frac{Nz}{2} \cdot 1$	$N \cdot \frac{1}{2} d(d+1)$	d(d+1)
Friction (any convex shape)	$\frac{Nz}{2} \cdot d$	$N \cdot \frac{1}{2} d(d+1)$	d+1

- Constraint counting is *not* exact
  - “Rattlers” or other independent subsystems should not be counted
  - Rigid body translation/rotation of the entire cluster should be subtracted off
  - ... ?
- Frictionless sphere systems appear to agree with the predicted value if the two corrections above are included

[A. Donev *et al.*, cond-mat/0408550;
C. O’Hern *et al.*, PRE **68**, 011306 (2003)]

- Not clear if extra corrections are required for transverse forces
- Only considers mechanical *equilibrium* (*i.e.* force/torque balance); says nothing about mechanical *stability*

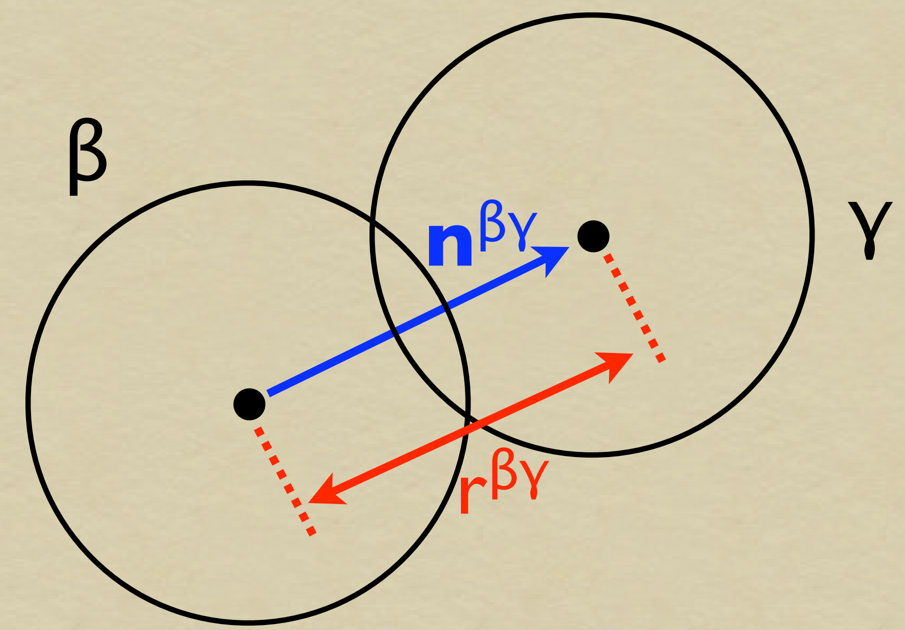
ii. Statics: the MMA

- Determination of mechanical stability by an approximation scheme (the ‘mean mode approximation’, or MMA) which:
  - Requires no mapping to analogous system with known Green’s function
  - Can incorporate prestress
  - Has a finite z transition

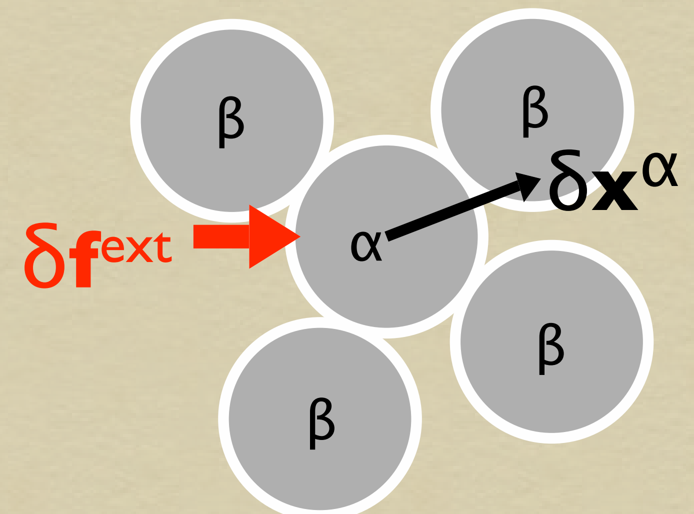
Start from a static configuration $\{\mathbf{x}^\beta\}$ of soft spheres β with contact forces

$$\mathbf{f}^{\beta\gamma} = f(r^{\beta\gamma})\hat{\mathbf{n}}^{\beta\gamma}$$

$$f(r) = \begin{cases} \mu\left(1 - \frac{r}{r_0}\right)^\alpha & : \ r < r_0 \\ 0 & : \ \text{otherwise} \end{cases}$$



Apply a small external force $\delta\mathbf{f}^{\text{ext}}$ to α



Ensemble average over configurations with macroscopic quantities fixed; force balance on α:

$$\delta\mathbf{f}^{\text{ext}} - \left\langle \sum_{\beta\sim\alpha} \delta\mathbf{f}^{\alpha\beta} \right\rangle = 0$$

with

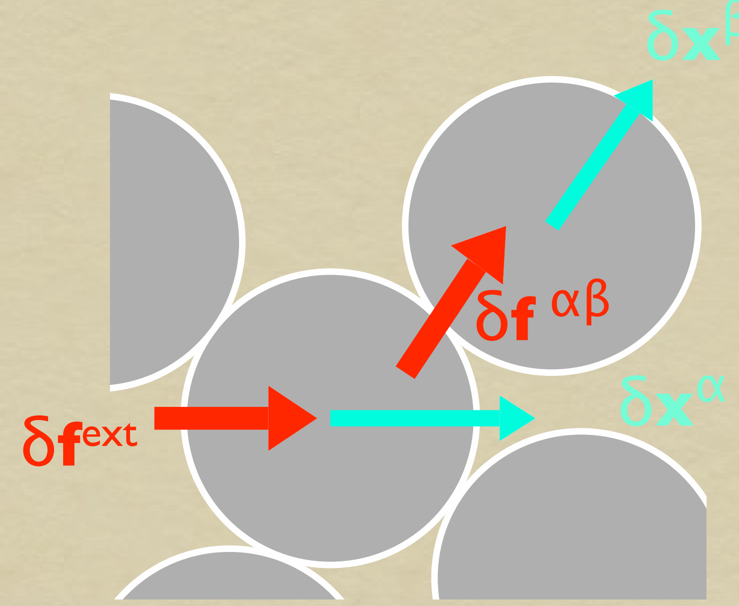
$$\delta f_i^{\alpha\beta} = A_{ij}^{\alpha\beta}\left(\delta x_j^\beta - \delta x_j^\alpha\right)$$

$$A_{ij} = \frac{f(r)}{r}(\delta_{ij} - \hat{n}_i\hat{n}_j) + f'(r)\hat{n}_i\hat{n}_j$$

(sum over all β in contact with α)

[Tanguy *et al.*, PRB 2002]

Mean mode approximation



- Mean response of α follows from symmetry,

$$\langle \delta \mathbf{x}^\alpha \rangle = \lambda \delta \mathbf{f}^{\mathrm{ext}}$$

  - Impose this form *before* averaging
  - Further impose an intuitive form on the β:

$$\delta \mathbf{x}^\beta = \lambda \delta \mathbf{f}^{\alpha\beta}$$

- Can now determine each contact force from the external force:

$$\begin{aligned} \delta f_i^{\alpha\beta} &= S_{ij}^{\alpha\beta} \delta f_j^{\mathrm{ext}}, \\ S_{ij}^{\alpha\beta} &= \left[1 + (\lambda |f'(r^{\alpha\beta})|)^{-1}\right]^{-1} \hat{n}_i^{\alpha\beta} \hat{n}_j^{\alpha\beta} \\ &\quad + \left[1 - \left(\frac{\lambda f(r^{\alpha\beta})}{r^{\alpha\beta}}\right)^{-1}\right]^{-1} \left(\delta_{ij} - \hat{n}_i^{\alpha\beta} \hat{n}_j^{\alpha\beta}\right) \end{aligned}$$

- To perform final averaging, make simplest choices:
  - z independent of f
  - contact angles uniformly, independently distributed
  - Monodisperse overlaps, so all f, f′ equal

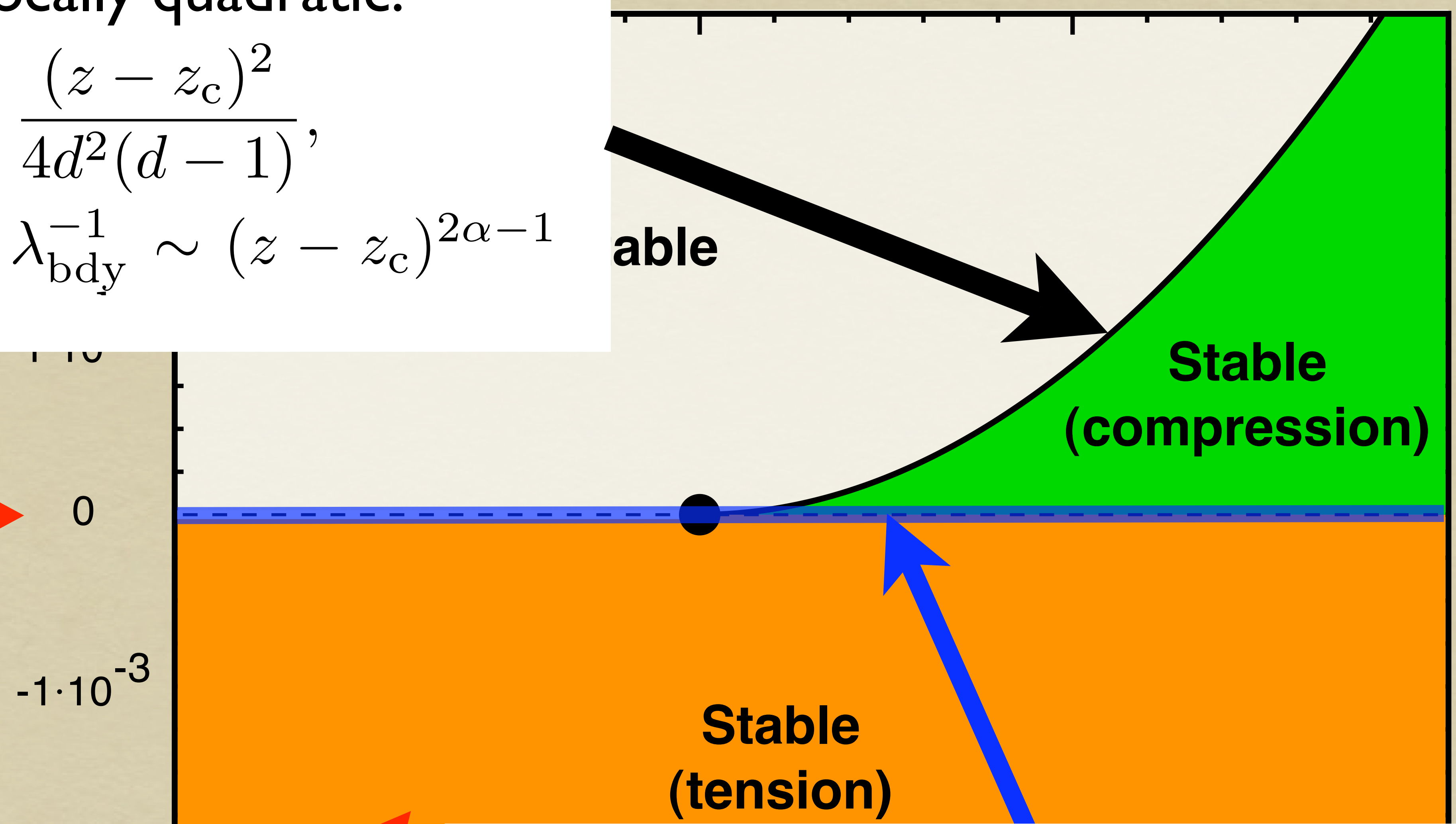
Can now solve for λ, G, K ~ λ^{-1}

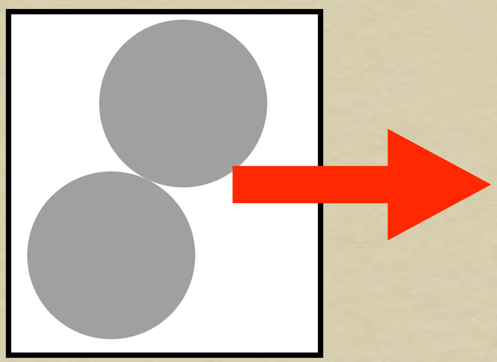
$$\omega = \frac{f(r)/r}{|\,f'(r)\,|} \sim \frac{1}{\alpha}\left(1 - \frac{r}{r_0}\right)$$

Boundary is locally quadratic:

$$\omega_{\rm bdy} \approx \frac{(z - z_{\rm c})^2}{4d^2(d-1)},$$

$$G_{\rm bdy}, K_{\rm bdy} \sim \lambda_{\rm bdy}^{-1} \sim (z - z_{\rm c})^{2\alpha - 1}$$

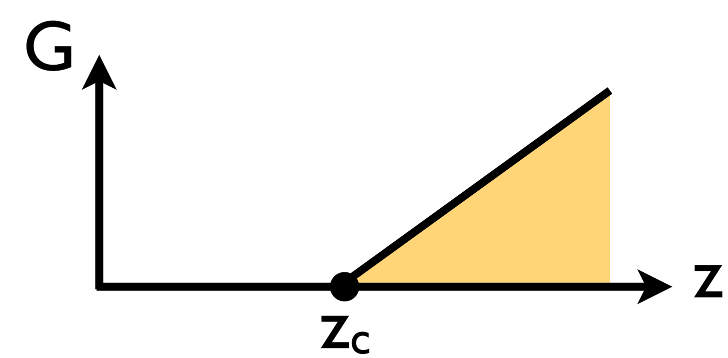




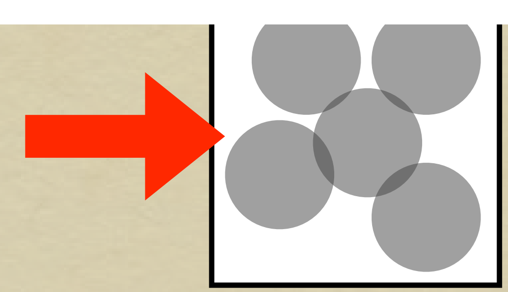
$$\lambda|f'| = (z/d - 1)^{-1},$$

$$G, K \sim (z/z_{\rm c} - 1)^f,$$

1



Lattice models under tension also show an extended stable regime; cf. [Tang&Thorpe, PRB 1988; Zhou *et al.*, PRE 2003]



(z = mean coordination number)

iii. Dynamics

- One-particle description of dynamical phase as the excited system relaxes
- Overdamped motion (kinetic energy is ignored)
- Spontaneous evolution cease when a stable regime has been reached (*coupling to statics*)

Energy potential

- Suitable energy potential depends on whether volume V or pressure P is being controlled (overdamped limit):

Constant V	Constant P
Internal energy U	Enthalpy H=U+PV

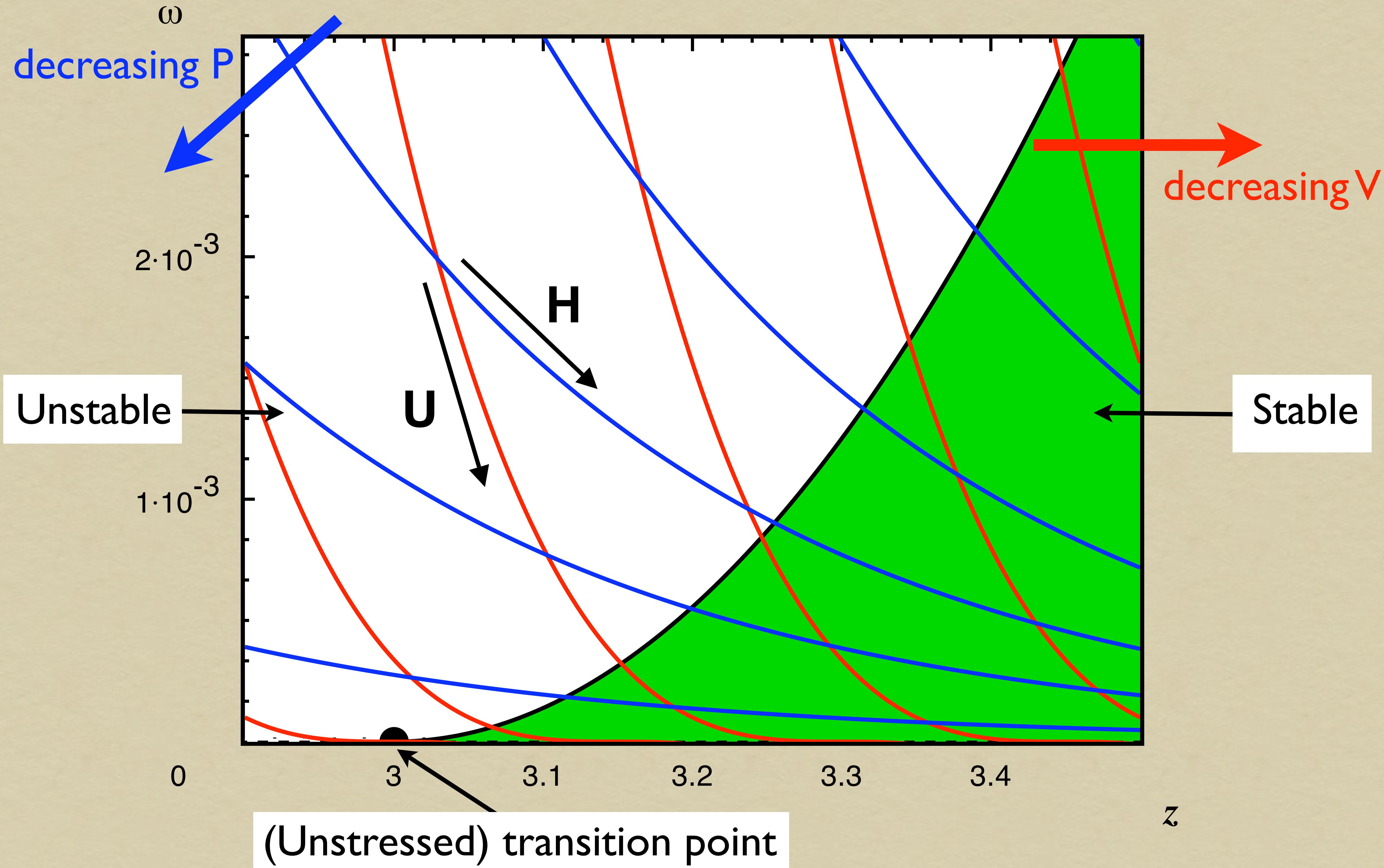
- Using same simplifications as for the statics,

$$U = \frac{Nz}{2}\frac{r_0\mu}{\alpha+1}(\alpha\omega)^{\alpha+1} \qquad PV = \frac{Nz}{2}\frac{r_0\mu}{d}(\alpha\omega)^{\alpha} \qquad (\alpha\omega \sim 1 - r/r_0)$$

- Simple choice for V: decreasing function of z and ω that obeys

$$\frac{V_{,z}}{V_{,\omega}} = D\omega^b \quad \text{as} \quad \omega \to 0$$

so that V barely changes with z when particles are 'just' overlapping



Red lines : constant volume (minimising the internal energy U)
Blue lines : constant pressure P (minimising the enthalpy H=U+PV)

Exponents

Model	$G, K \sim \Delta z^c$	$P \sim \Delta z^e$	$\Delta V \sim \Delta z^g$
MMA $\alpha > 0,\ d \geq 2$	$2\alpha - 1$	2α	2
Wet foam [9] $\alpha = 1,\ d = 2$	$\approx 1^a$	2 ± 0.4	2 ± 0.4
O'Hern *et al.* [29] $\alpha = 1,\ d = 2, 3$	1.01 ± 0.1^a	2.1 ± 0.2	2.04 ± 0.1
$\alpha = 3/2,\ d = 2, 3$	2.08 ± 0.1^a	3.15 ± 0.3	2.08 ± 0.1
Zhang *et al.* [12] $\alpha = 1.28,\ d = 3$	-	≈ 2.45	≈ 1.96
Makse *et al.* [32][b] $\alpha = 3/2,\ d = 3$	-	3.3 ± 0.5	2.1 ± 0.6

[a]Result for shear modulus shown.
[b]Only frictionless data shown.

[c.f. Schwarz *et al.*, *cond-mat/0410595* for a scalar lattice treatment]

Prospects

- Still many issues:
  - Evolution after the first arrest by *e.g.* shaking/tapping
  - Taking the dynamics away from the overdamped limit
- Not yet a model for granular media
  - No friction or particle asphericity
  - No gravity, or any form of anisotropy (including shear)

Distributed contact forces

- Distribution of overlaps $P(\delta)$, $\delta = r_0 - r$
- Assume system approaches a (stressless) rigidity transition
- Make the following *ansatzes* for $\varepsilon = (z - z_\mathrm{c})/z_\mathrm{c} > 0$
  - λ vanishes near transition as $\lambda = \lambda_0 \varepsilon^{-\nu}$
  - Distribution scales uniformly, $P(\delta) = \varepsilon^{-\gamma} q(\varepsilon^{-\gamma}\delta)$
- Perform integration to get $$\begin{aligned} 1 - \frac{d}{z} &= (d-1)\frac{\lambda_0 \mu}{r_0}\varepsilon^{-\nu+\alpha\gamma}\left\langle x^\alpha \right\rangle_{q(x)} \\ &+ \frac{1}{\lambda_0 \mu \alpha}\varepsilon^{\nu-\gamma(\alpha-1)}\left\langle x^{1-\alpha}\right\rangle_{q(x)} \end{aligned}$$
- Stability boundary corresponds to λ_0 real
- Self-consistency demands get $\gamma=2$, $\nu=2\alpha-1$ as in the monodisperse case

Equation for λ

$$d\left(\frac{1}{z}-1\right)=(d-1)\frac{1}{\frac{\lambda f(r)}{r}-1}-\frac{1}{1+\lambda\mid f'\mid}$$

- d : dimension
- z : mean coordination number
- λ : compliance
- r : interparticle separation
- f(r) : interparticle potential
- $f'(r)<0$ assumed

Pressure scaling

$$\frac{P}{\mu} \sim \frac{N r_0}{2V_0} \left\{ \frac{\alpha (z - z_\mathrm{c})^2}{4d^2(d-1)} \right\}^\alpha$$

- μ : contact stiffness (units of force)
- V_0 : volume at transition
- N : Number of particles