Jamming of deformable foams

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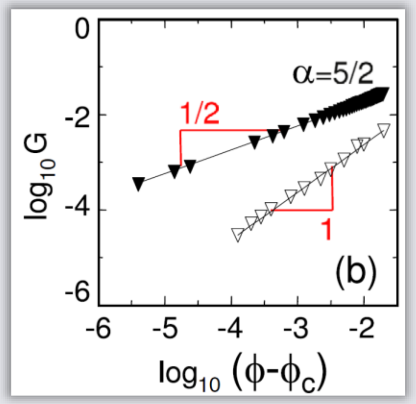
Jamming transition

- A rigidity transition of **soft athermal particles**, e.g., foams, emulsions, and granular materials, happens at **critical packing fraction, ϕ_c** [1].
- **Critical scaling near ϕ_c** has long been explored by numerical models of **soft spheres/circles** [2], where the particles are allowed to overlap!

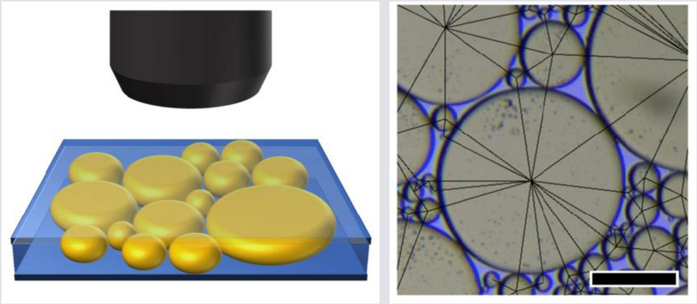


e.g., **shear modulus**

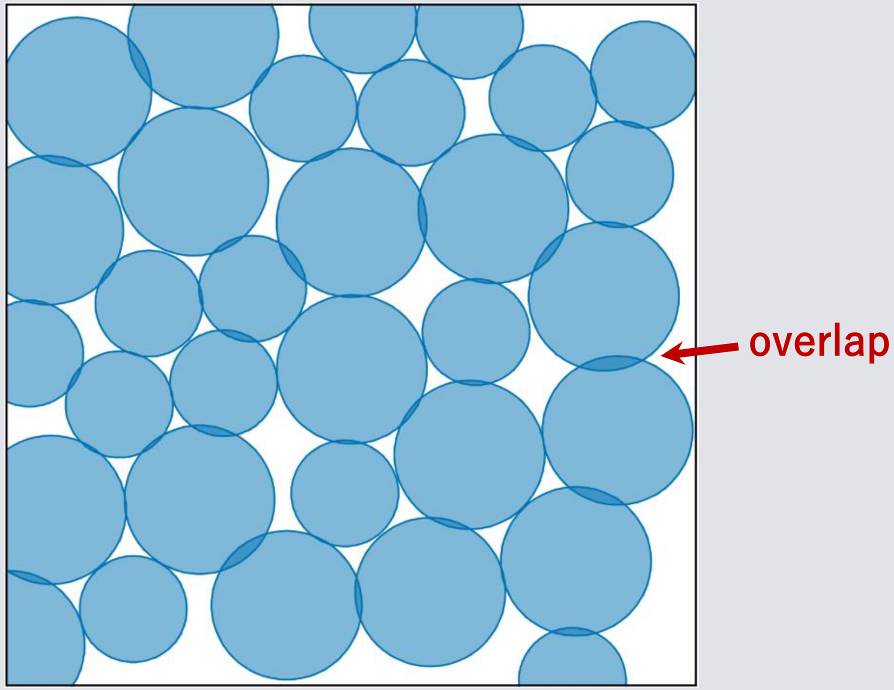
$G \propto \Delta\phi^{1/2}$

(harmonic potential)

Experiments by D. S. Shimamoto and M. Yanagisawa (2013)



Molecular dynamics (MD) simulations



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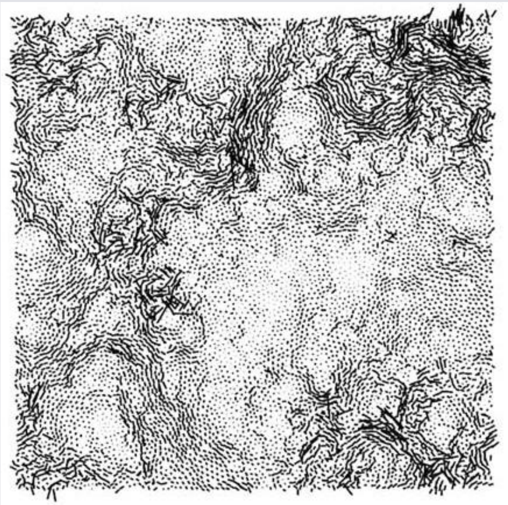
[2] C. S. O'Hern, L. E. Silbert, A. J. Liu, and S. R. Nagel, *Phys. Rev. E* **68**, 011306 (2003).

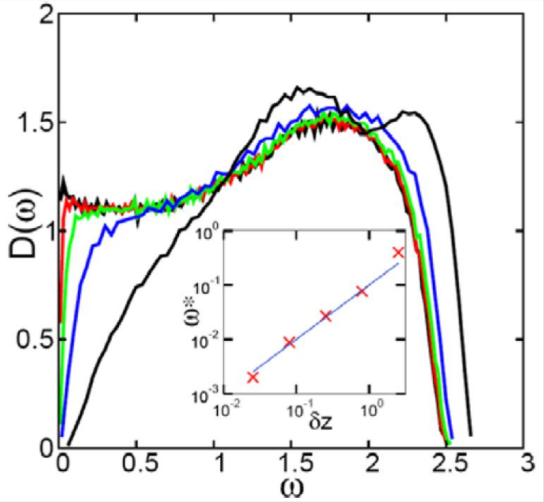
Normal modes

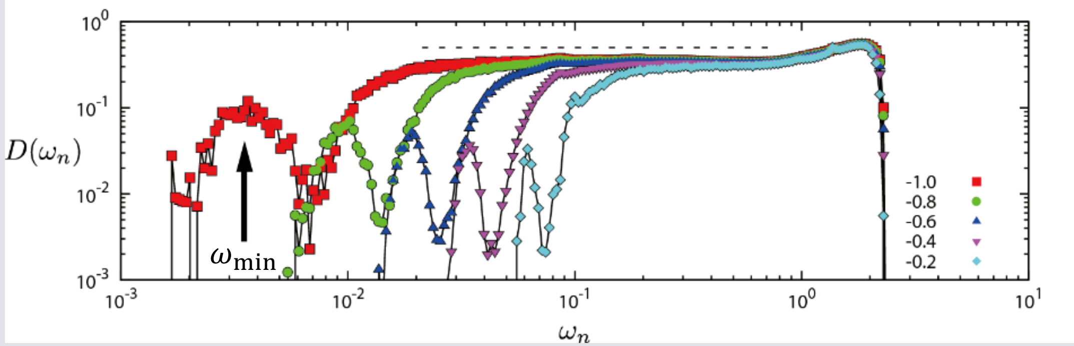
- Small vibrations of the particles around equilibrium positions are characterized by **eigen-frequencies**, ω.

- **Vibrational density of states (VDOS)** $D(\omega)$ exhibits a plateau in $\omega > \omega^*$ **above jamming**, where $\omega^* \propto \Delta z$ with **excess coordination number**, Δz [1-3], while $D(\omega)$ **below jamming** shows an isolated special mode which scales as $\omega_{\mathrm{min}} \propto |\Delta z|^{1.6}$ [4-6].

- Linear elastic and viscoelastic responses are governed by low eigen-frequencies [7, 8] as, e.g., **shear modulus**, $G = G_a - \sum_n \frac{|\langle n|\Xi\rangle|^2}{{\omega_n}^2}$.







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[5] A. Ikeda, T. Kawasaki, L. Berthier, K. Saitoh, and T. Hatano, *Phys. Rev. Lett.* **124**, 058001 (2020).
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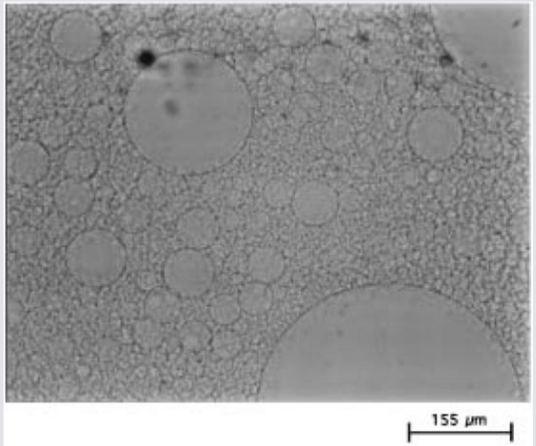
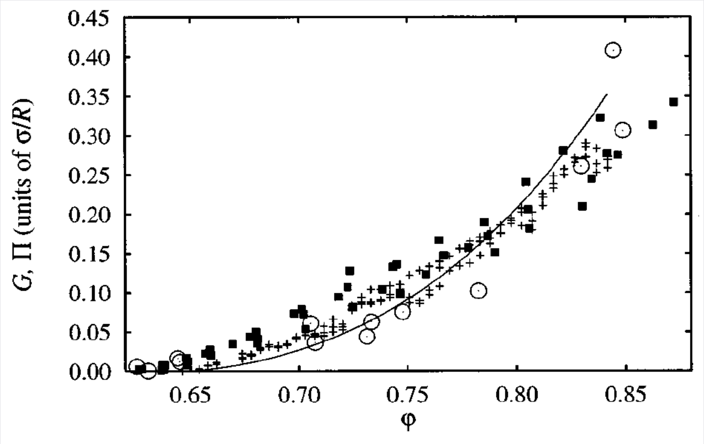
Motivation

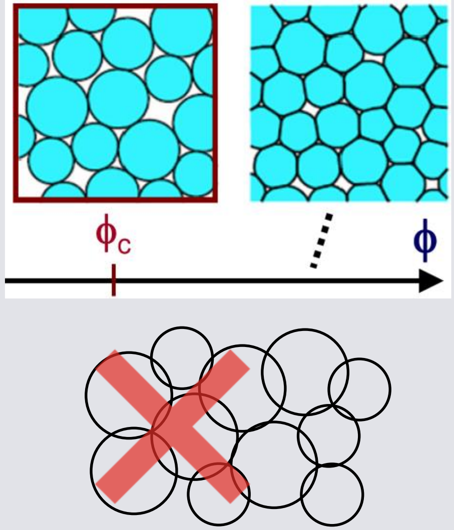
- The critical scaling, $G \propto \Delta\phi^{1/2}$, has never been validated experimentally.
- Instead, a quasi-linear scaling, $G \propto \phi\Delta\phi^{\mu}$ with $\mu \approx 1$, is favored [1, 2].

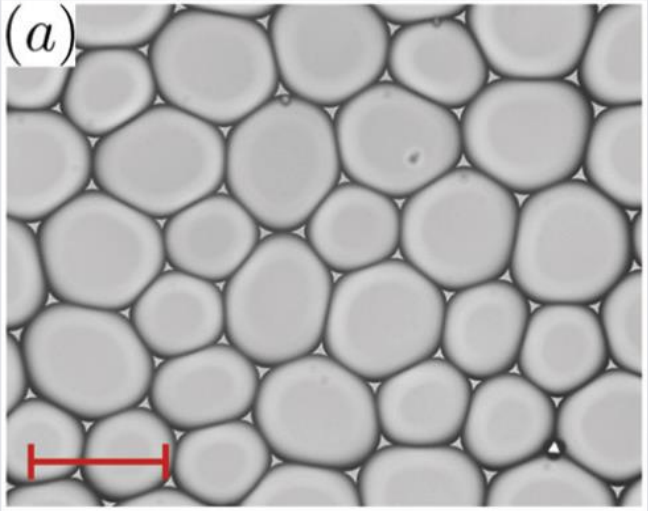
What is missing in simulations/theory:

- **Poly-dispersity?**
- **Deformability of the particles?**









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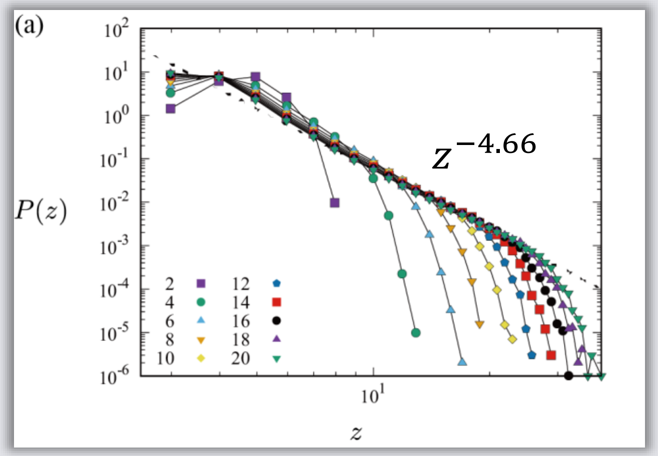
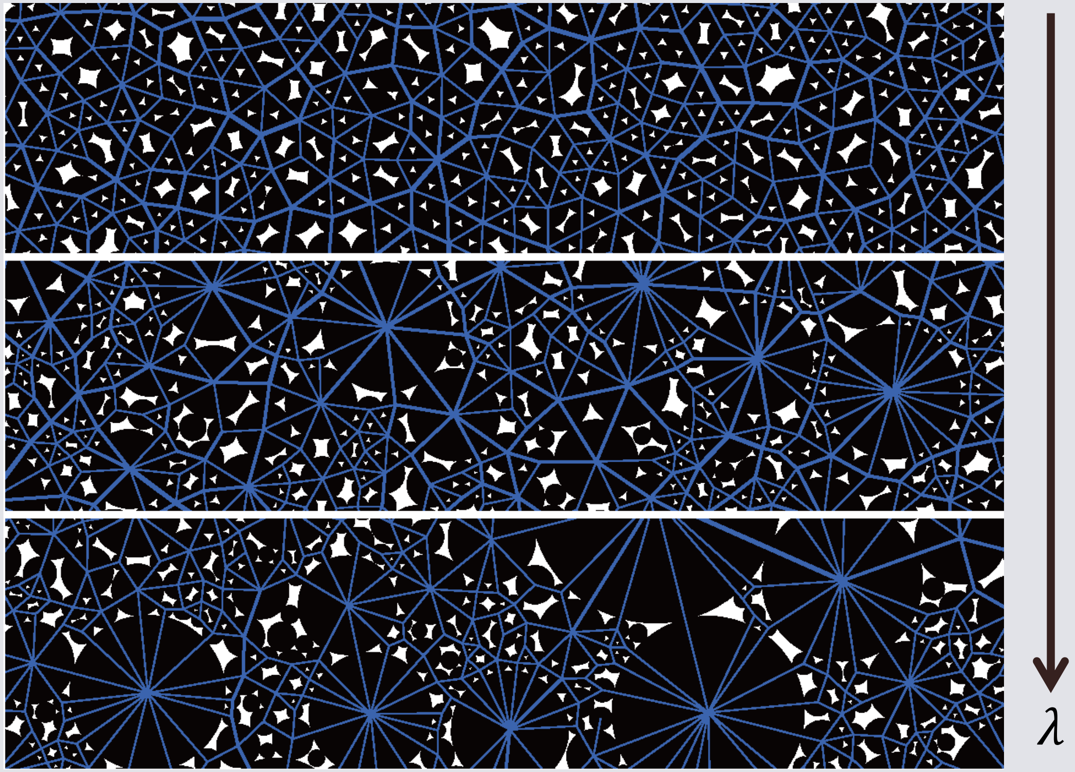
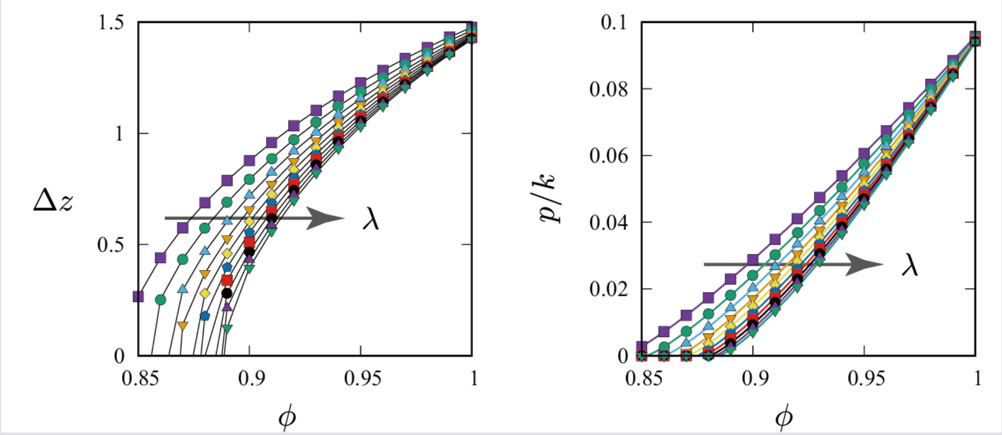
Preliminary results

- We have studied jamming of **poly-dispersed particles** by MD simulations, where the size distribution is $P(R) \propto R^{-3}$ $(R_{\min} \leq R \leq R_{\max})$, and examined effects of poly-dispersity by changing the **size-ratio,** $\lambda = R_{\max}/R_{\min}$.

- Not only **structures**, e.g., radial distribution function, force distribution, and distribution of coordination number, $P(z)$, but also **macroscopic quantities**, e.g., Δz, pressure p, and elastic energy E, are influenced by λ.

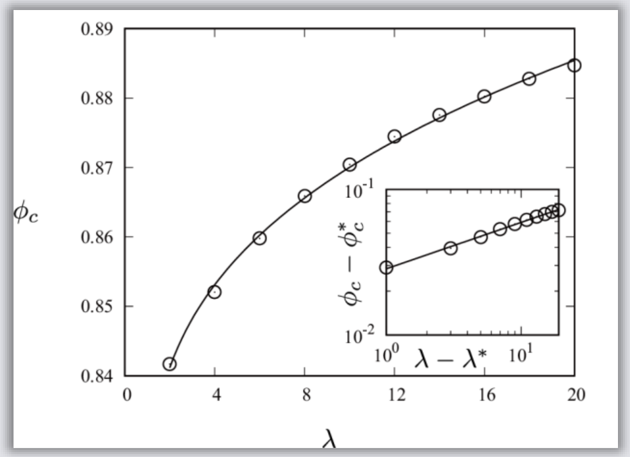


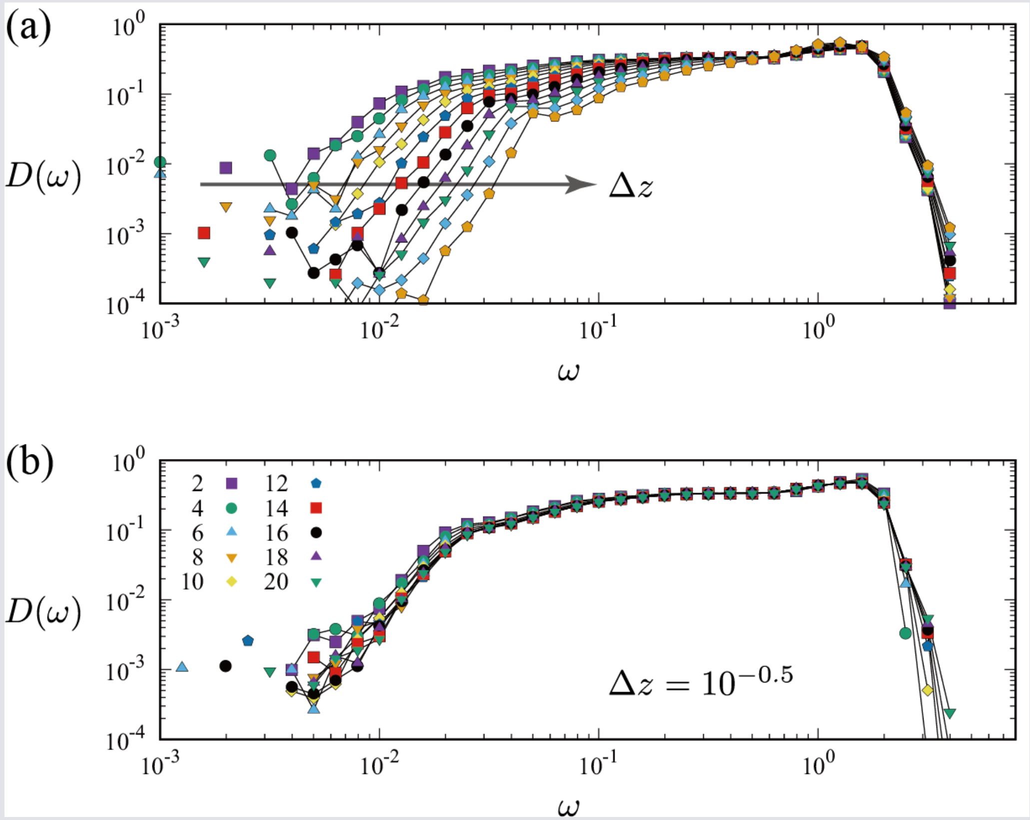


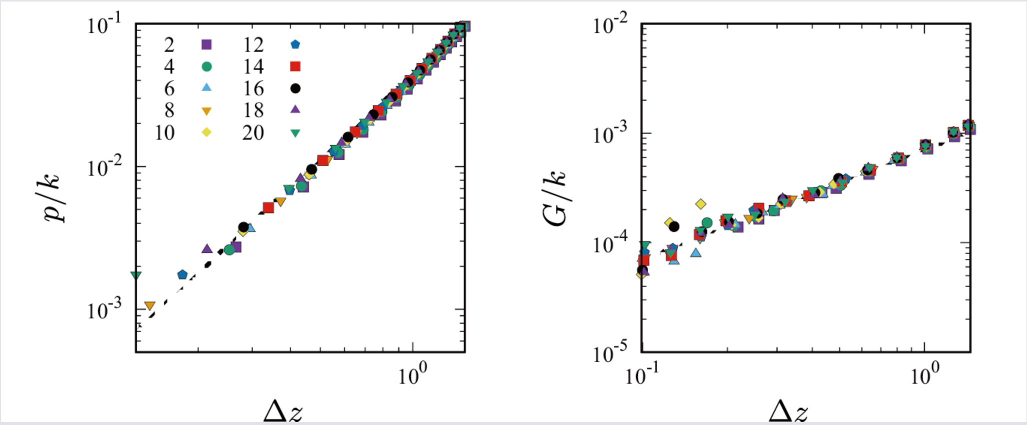


Preliminary results

- ϕ_c increases with λ!
- Vibrational properties, i.e., $D(\omega)$ and $\omega^* \propto \Delta z$, are insensitive to λ.
- Scaling exponents, i.e., $p \propto \Delta z^2$ and $G \propto \Delta z$, are not affected by λ.
- Discussion: size-dependent stiffness, k_{ij}

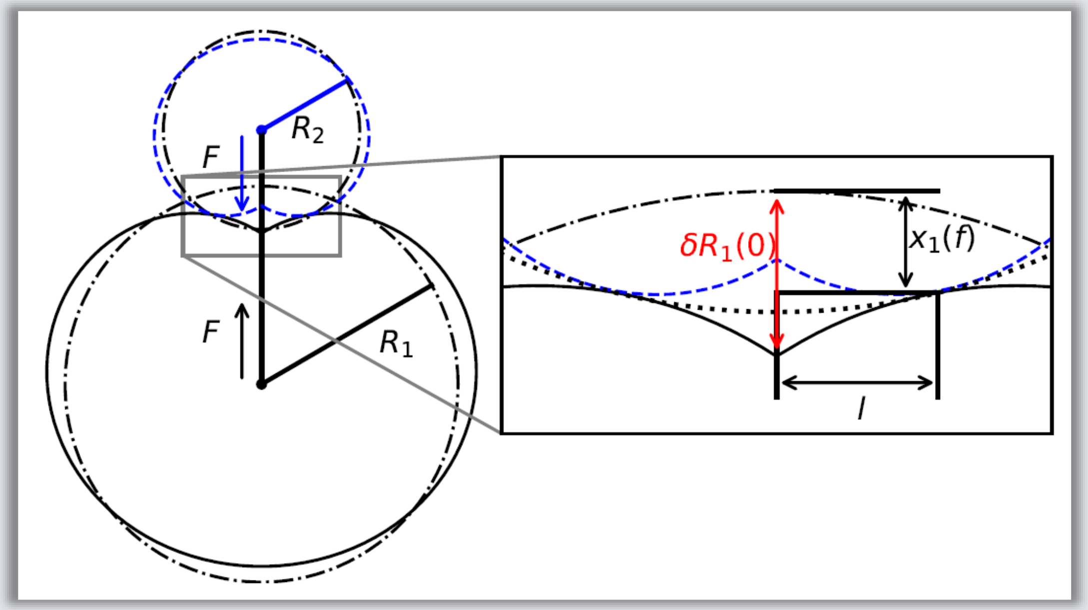






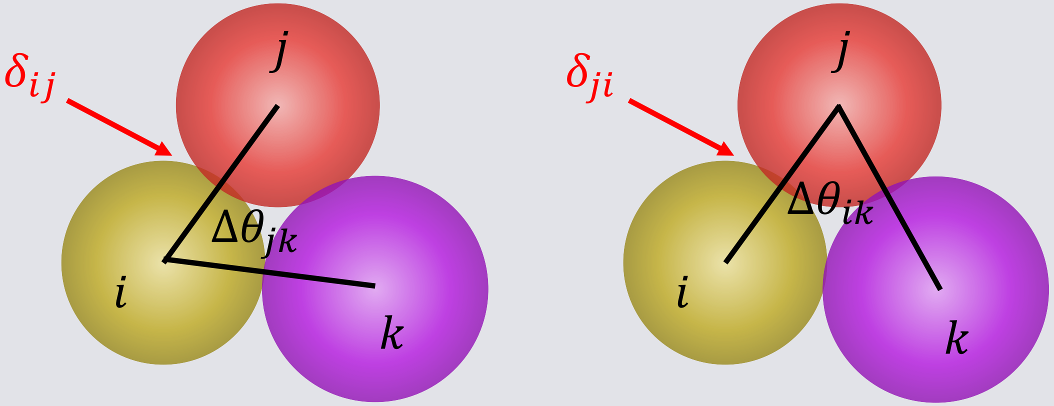
Morse-Witten theory

- A model of **deformable foams** in 2D: (i) the force law is derived from the Young-Laplace equation and (ii) non-spherical shapes are given by an analytical expression [1].



- Effective overlap between the particles i and j, i.e., $\delta_{ij} = R_i + R_j - |\boldsymbol{r}_i - \boldsymbol{r}_j|$, is formulated as

  - Line tension, γ
  - Geometrical factor, $g(\theta) \equiv (\pi - \theta)\sin\theta - \frac{\cos\theta}{2} - 1$

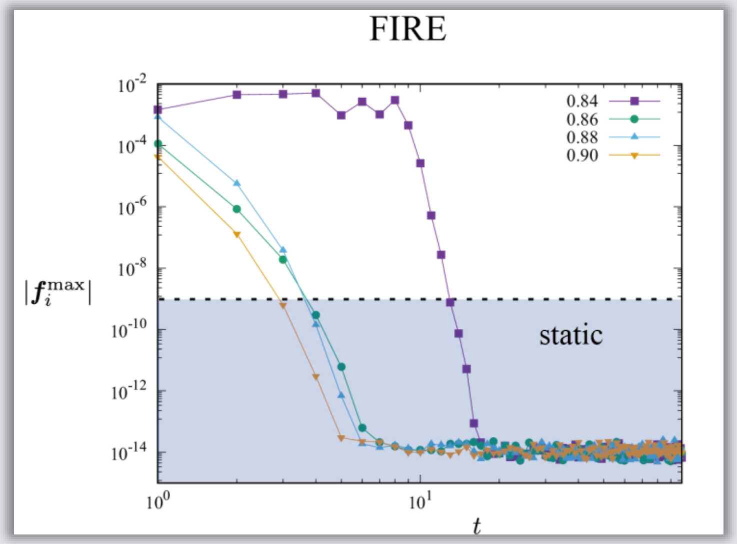


- The magnitude of contact force, f_{ij}, is obtained by solving the **simultaneous linear equations.**

[1] D. Morse and T. Witten, *EPL* **22**, 549 (1993).

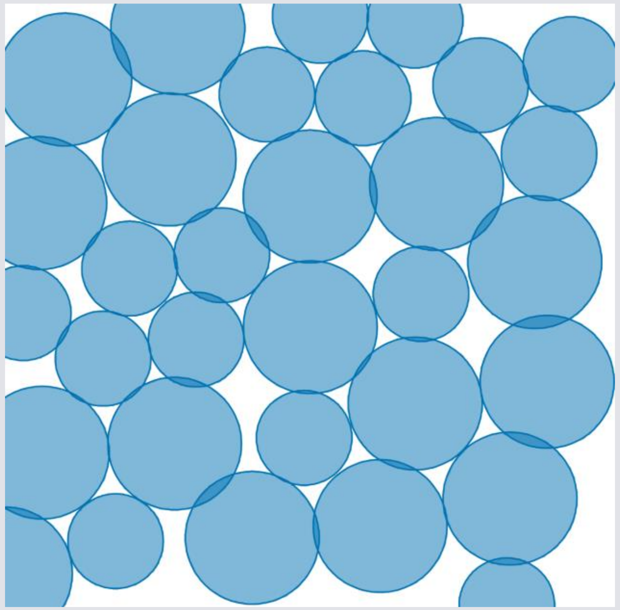
Energy minimization

- **Initial state** is static packing of undeformed circles with ϕ.
- We numerically solve the simultaneous linear equations (to obtain contact forces, f_{ij}) and integrate equations of motion by the **FIRE algorithm**.
- The system is assumed to be **static** if every magnitude of total force, $|\boldsymbol{f}_i| = \left|\sum_j \boldsymbol{f}_{ij}\right|$, drops below a threshold.

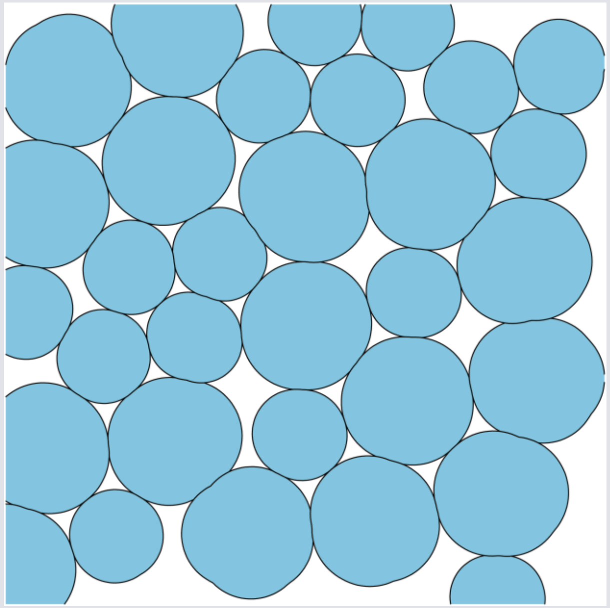


- Initial $\phi = 0.84 \sim 0.90$
- $N = 32$ particles (6.4×10^4 samples)
- $N = 128$ particles (1.6×10^4 samples)
- Units; m, σ_0, and $t_0 \equiv \sqrt{m\sigma_0/\gamma}$

initial state (undeformed circles)



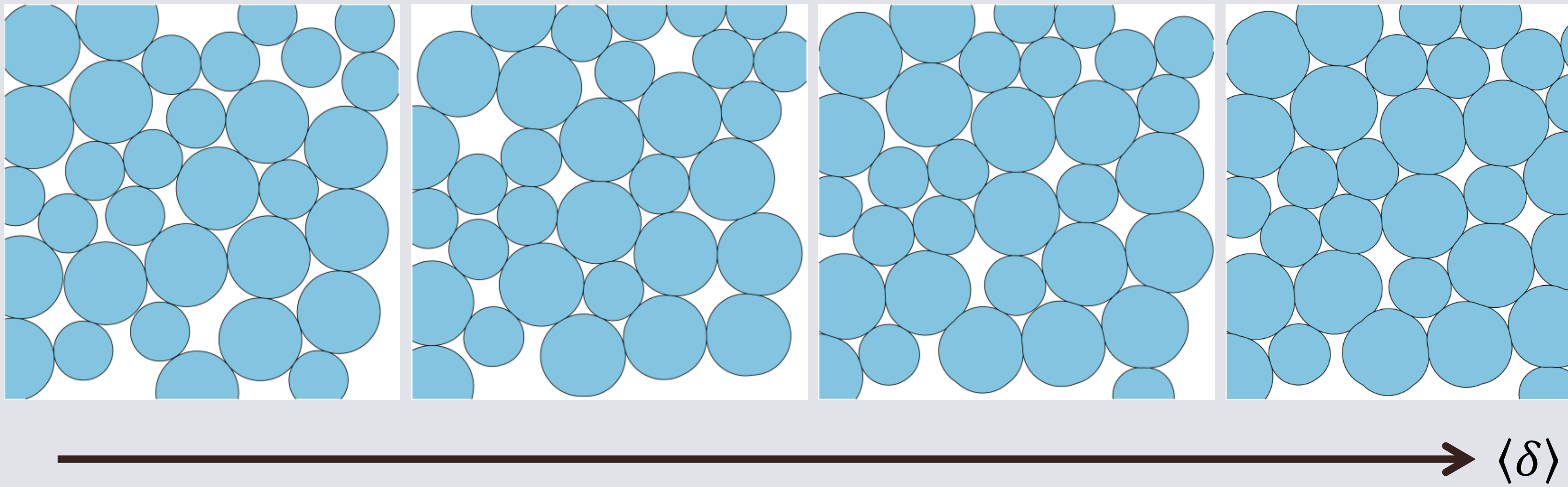
final state (deformable foams)

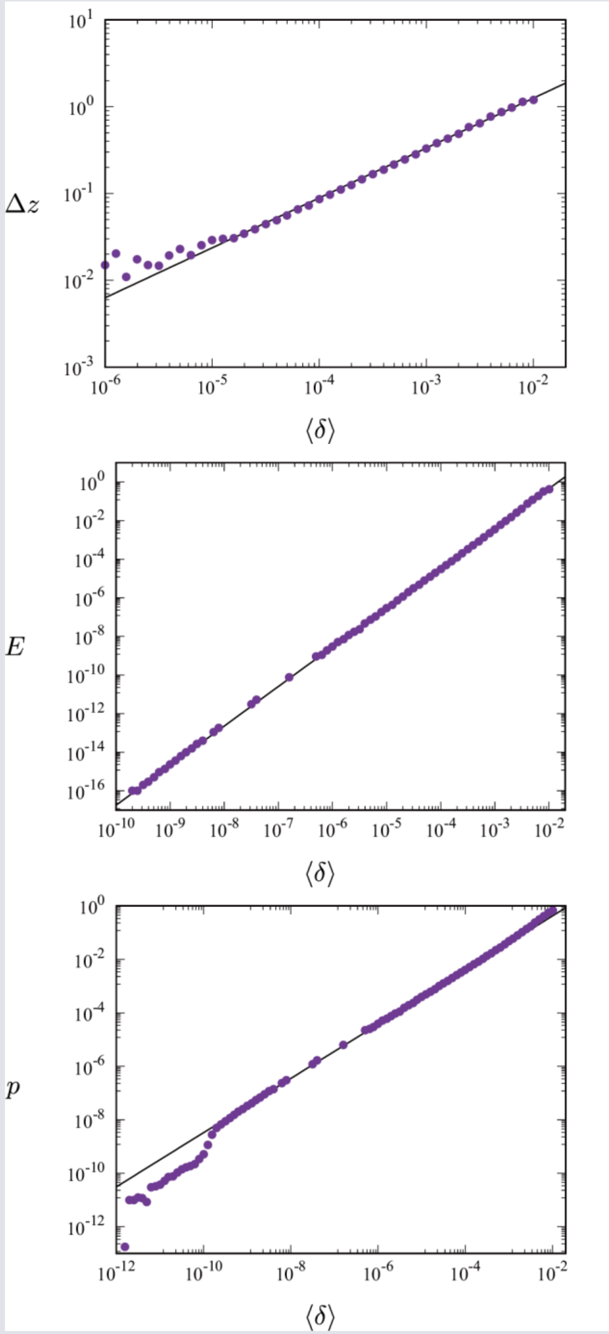


Critical scaling

- At the onset of unjamming, **mean effective overlap, $\langle\delta\rangle$**, goes to zero, i.e., $\langle\delta\rangle = \frac{1}{N_c}\sum_{ij}' \delta_{ij} \to 0$. Note that **mean overlap, $\bar{\delta} \propto \phi - \phi_c$**, of undeformed circles is equivalent to the distance from ϕ_c.

- Numerical data indicate $\Delta z \propto \langle\delta\rangle^{0.57}$, $E \propto \langle\delta\rangle^{2.05}$, and $p \propto \langle\delta\rangle^{1.01}$.





Vibrational properties

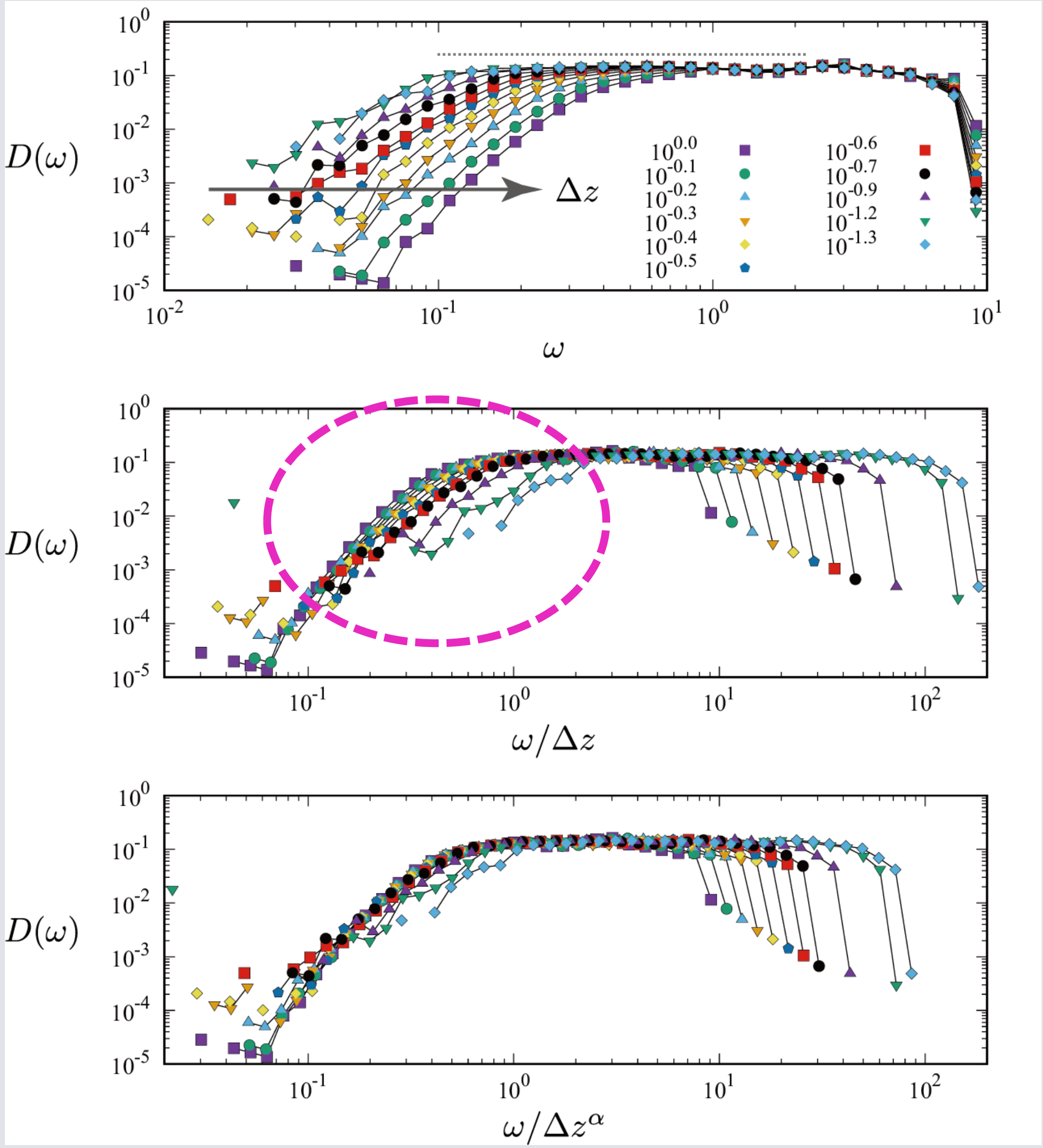
- **Dynamical matrix (Hessian), $\mathcal{H}$**, can be formulated as

$$\Delta E = \frac{1}{2}\langle f|\delta\rangle \equiv \frac{1}{2}\langle \boldsymbol{u}|\mathcal{H}|\boldsymbol{u}\rangle$$

  - effective overlaps, $|\delta\rangle \equiv (\cdots, \delta_{ij}, \cdots)^{\mathrm{T}}$
  - contact forces, $|f\rangle \equiv (\cdots, f_{ij}, \cdots)^{\mathrm{T}}$
  - displacements, $|\boldsymbol{u}\rangle \equiv (\cdots, u_i, \cdots)^{\mathrm{T}}$

- The VDOS $D(\omega)$ exhibits a plateau in $\omega > \omega^*$, where the **crossover frequency** scales as $\omega^* \propto \Delta z^\alpha$ with $\alpha = 0.75$ rather than $\alpha = 1$.

- **Discussion**: the shear modulus, G



Summary

We have examined the effects of

- poly-dispersity
- deformability of the particles

on **vibrational properties** and **critical scaling** near jamming.

- The $D(\omega)$ and critical exponents for ω^*, p, and G are not affected by the **poly-dispersity**, λ.
- Jamming of deformable foams are successfully simulated by the **Morse-Witten model**.
- The critical exponents for Δz, E, and p are close to those of undeformed circles.
- There is no band-gap in $D(\omega)$ but ω^* scales differently from that of undeformed circles.

Deformable polygons by
J. D. Treado et al., *Phys. Rev. Materials* **5**, 055605 (2021).