# Novel Features Arising in the Maximally Random Jammed Packings of Superballs

Yang Jiao,
Frank H. Stillinger &
Salvatore Torquato

PRINCETON UNIVERSITY

# Content

- Definition of Superballs and Superdisks
- The Donev-Torquato-Stillinger Packing Algorithm
- Maximally Random Jammed Packings
- Packing Characteristics: Density and Contact Number
- Packing Characteristics: Non-generic Local Structures
- Conclusions and Future Work

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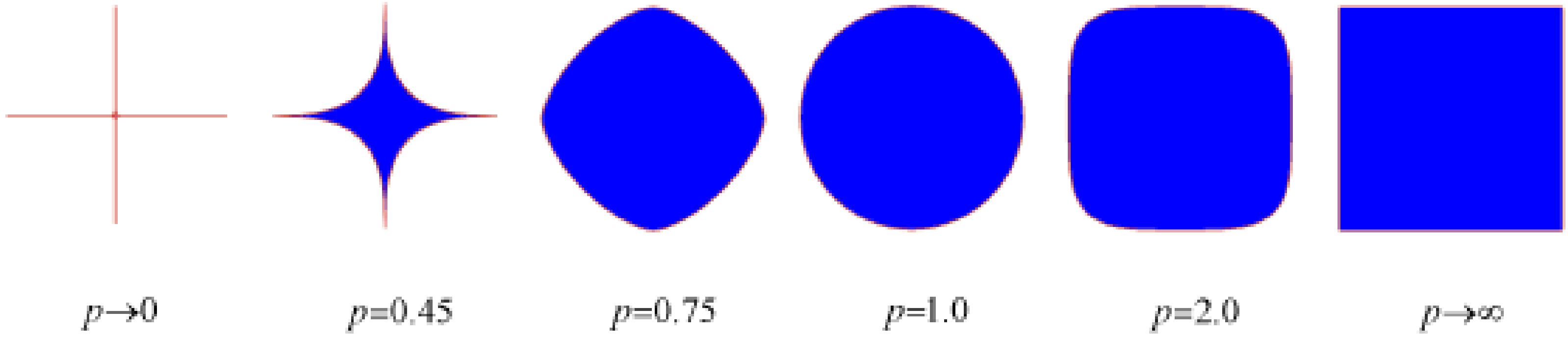
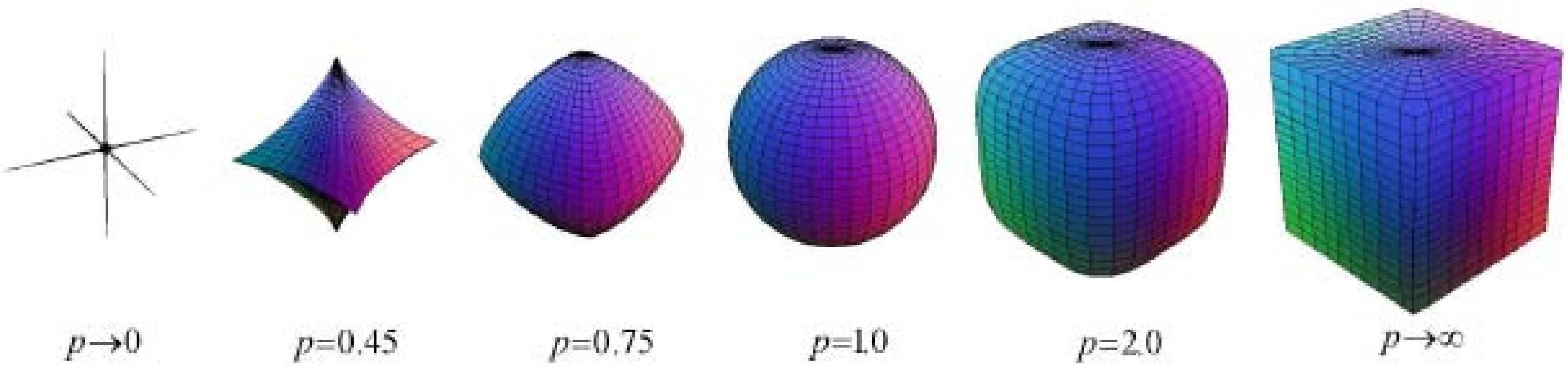
- A d-dimensional superball is a centrally symmetric body occupying the region:

$$|x_1|^{2p} + |x_2|^{2p} + \cdots + |x_d|^{2p} \le 1,$$

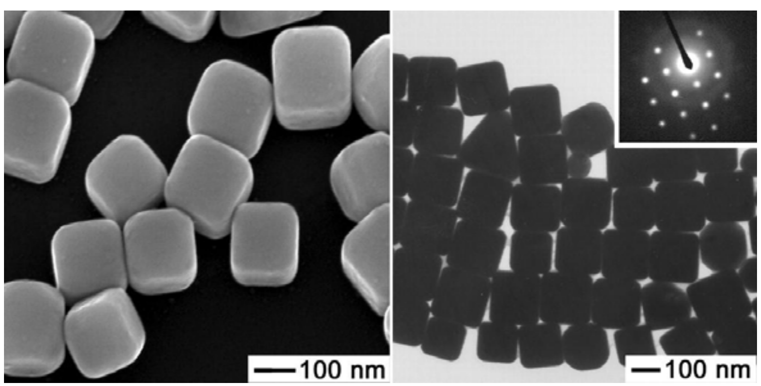
- In two dimensions, we have superdisks withs square symmetry

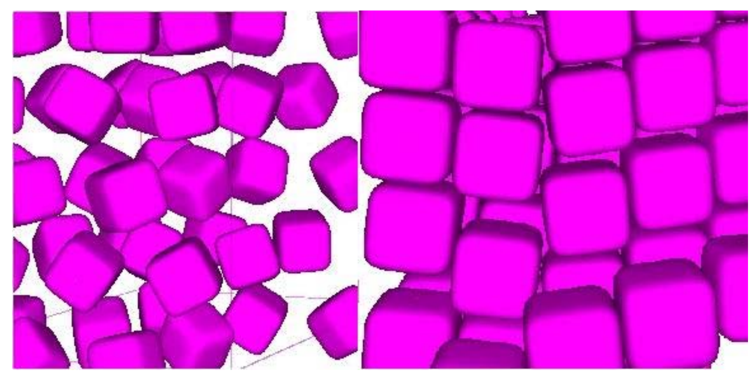


- In three dimensions, we have superballs with cubical and octahedral symmetry




- Excellent approximations for certain nanoparticles:



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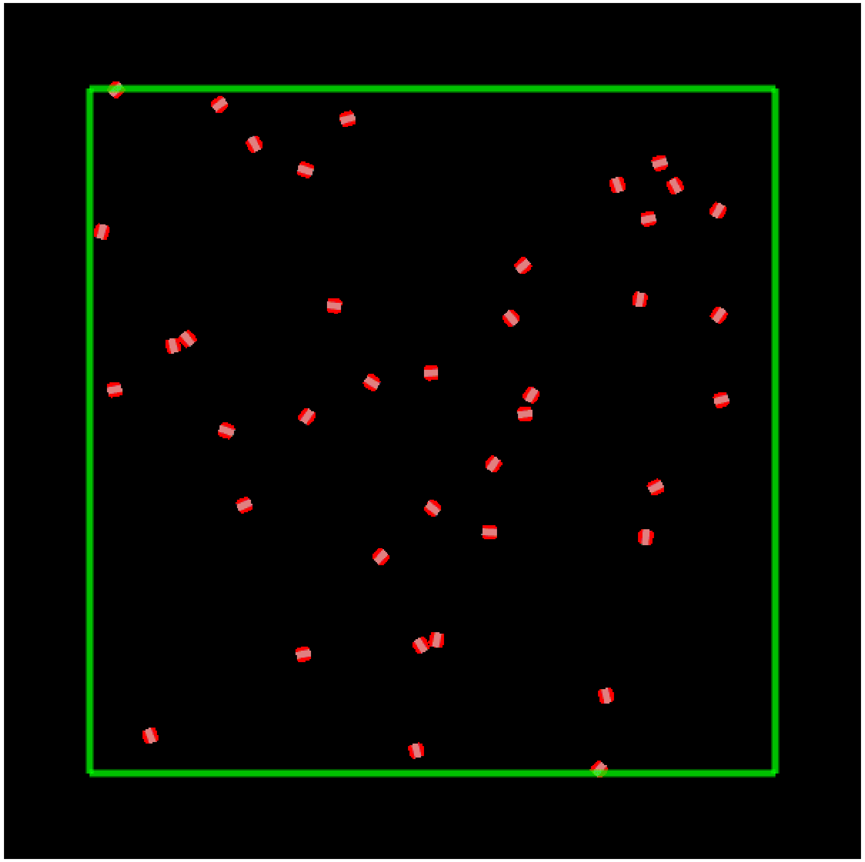
- Event-driven Molecular Dynamics --- Donev-Torquato-Stillinger Algorithm



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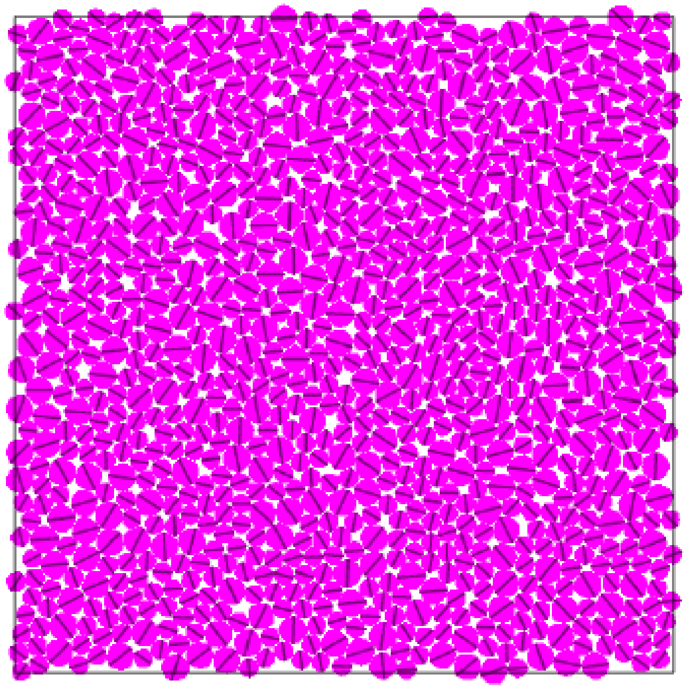
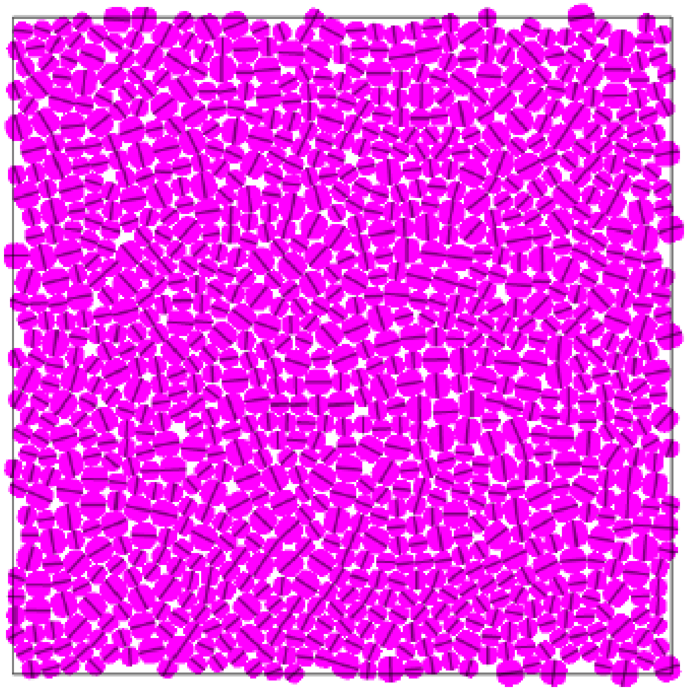
- Maximally random jammed packings of binary superdisks

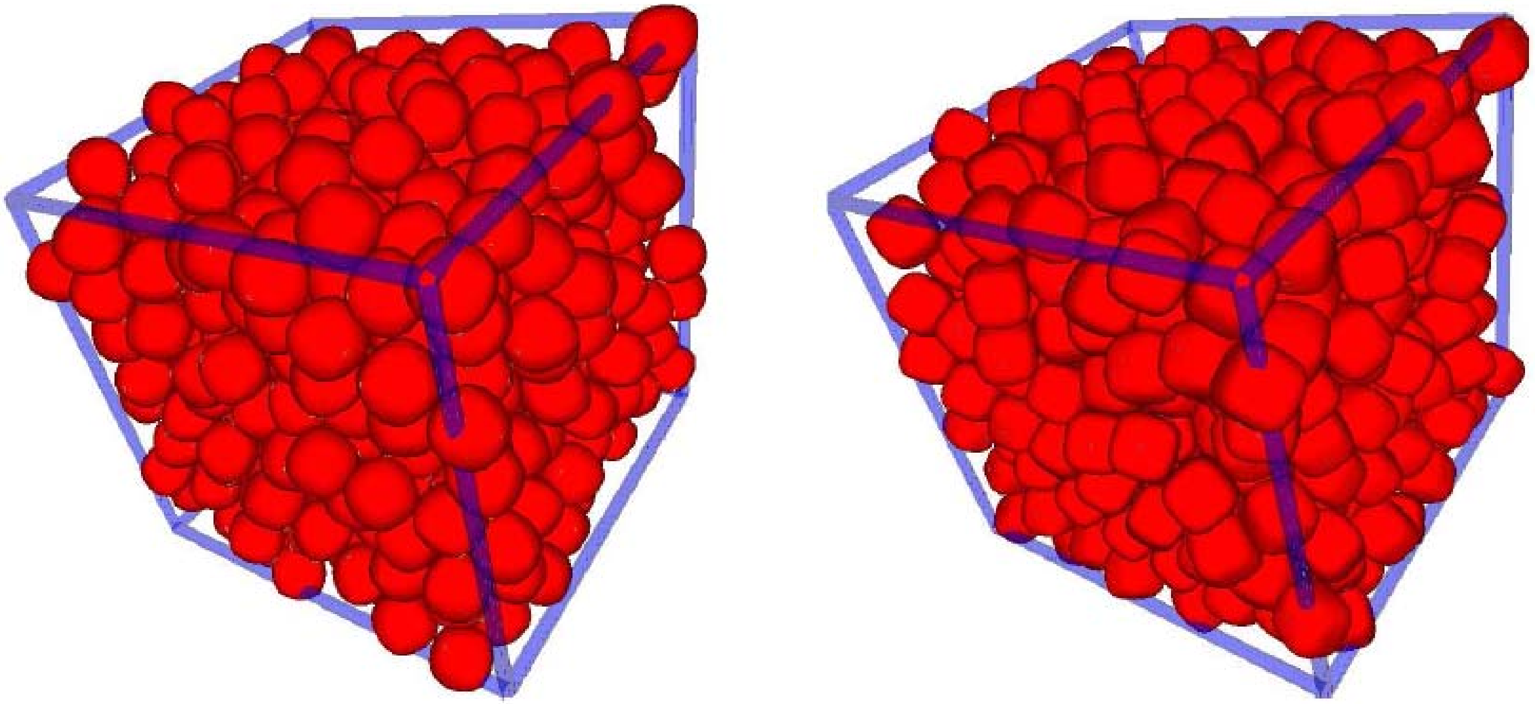


(a) $p = 0.85$



(b) $p = 1.5$

- Maximally random jammed packings of congruent superballs



(a) $p = 0.85$ (b) $p = 1.5$

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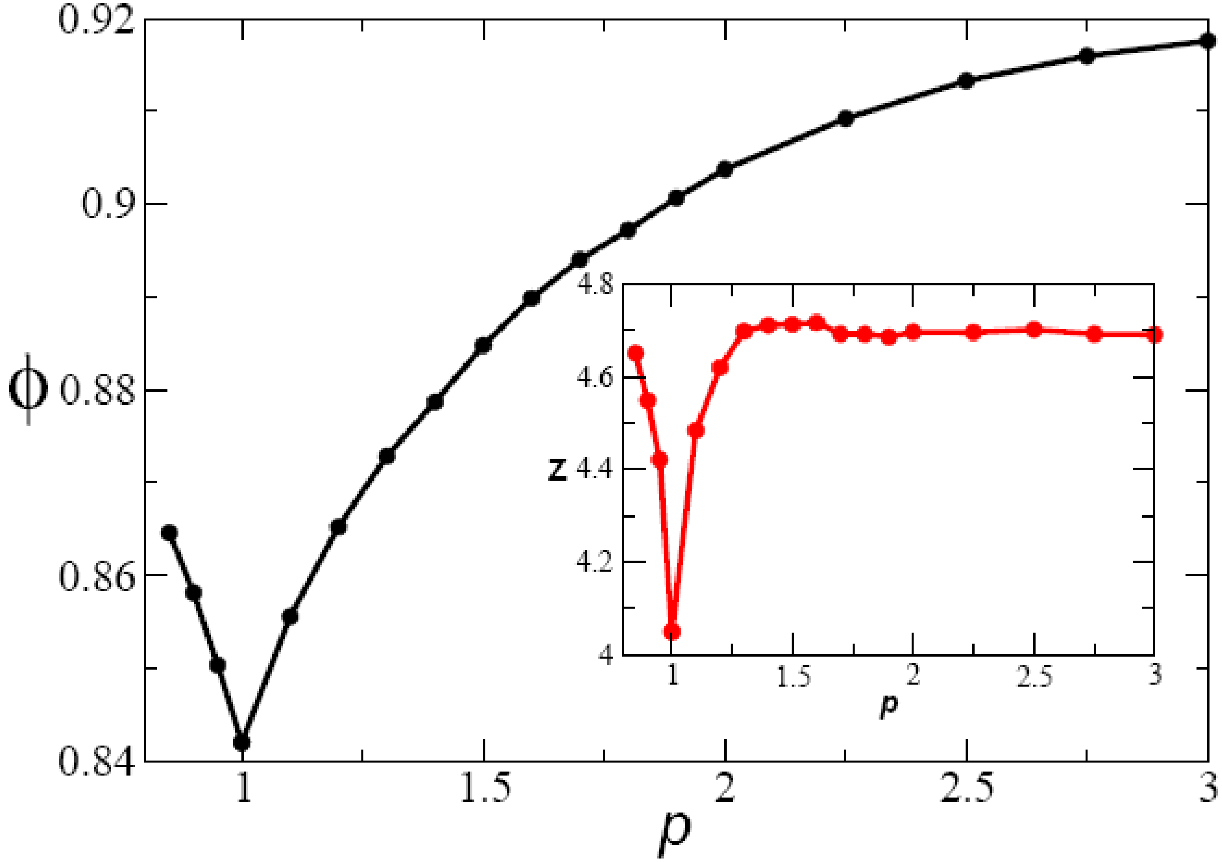
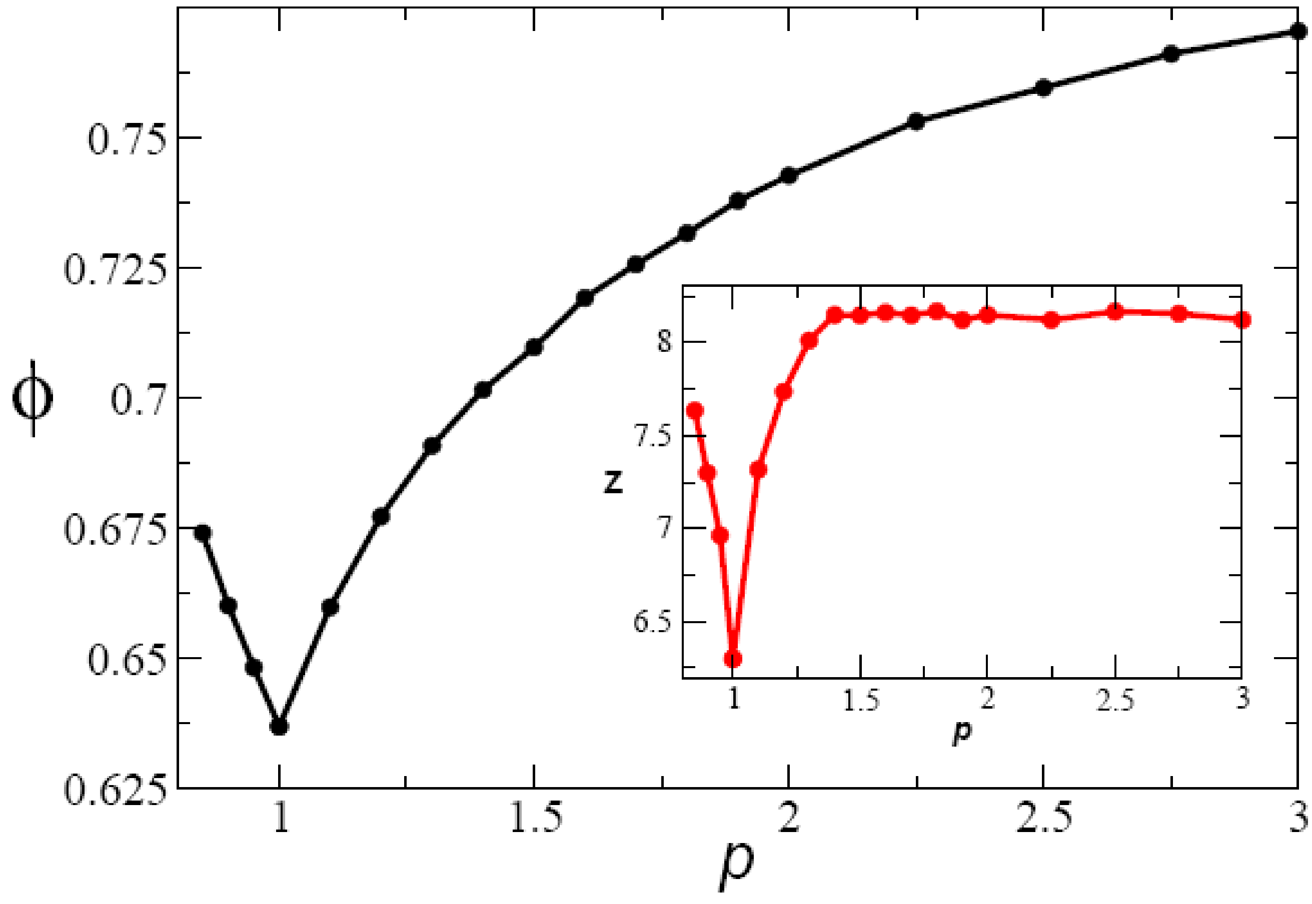
- Density and average contact number for binary superdisks



- Density and average contact number for congruent superballs



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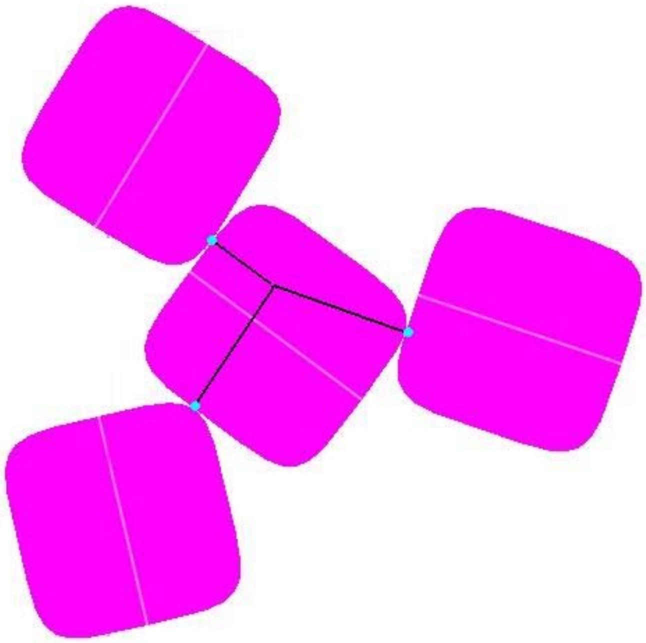
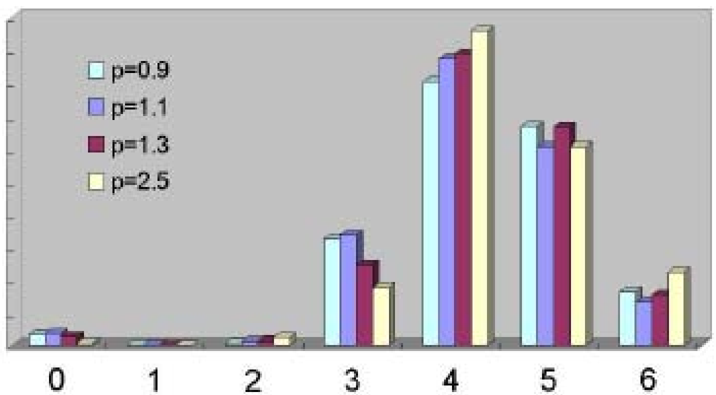
- **Isostatic** hypothesis: In a large maximally random jammed packing, the number of average contacts per particle is approximately **equal to** twice the total number of degrees of freedom.
- **Hypoconstrained** packing: jammed packing with average contact number **less than** twice the total number of degrees of freedom.
- Isostatic random packings of **non-spherical** particles are **difficult to realize**: the required maximal contact number necessarily increases the translational order.
- Hypoconstraining implies **non-trivial correlations** within the local arrangements of jammed packings.
- We term such local arrangements "**non-generic**" in light of their correlations.

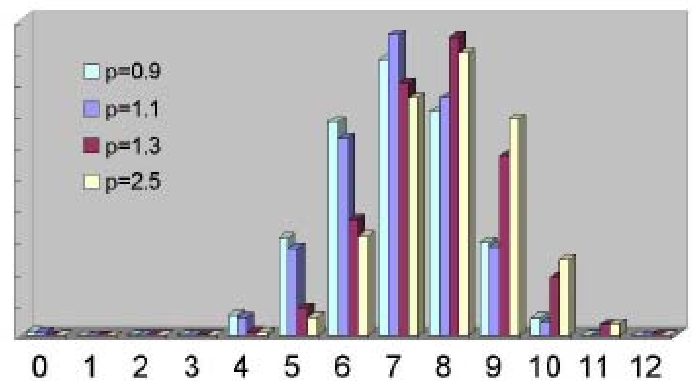
- Non-generic locally jammed superdisk configuration: the curvature at contacts plays an important role.

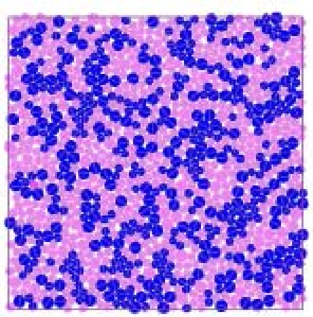


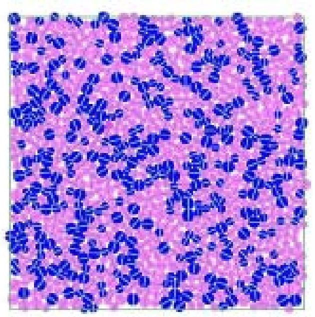
- Four degrees of freedom, only three contacts. To jammed the central particle, torque balance has to be considered, which introduce correlation.

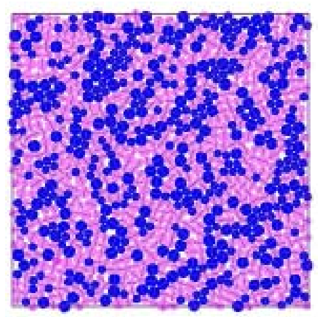
- Measure the degree of “non-genericity”: Png the fraction of local configurations with less contacts than average.
- For p close to unity Png ~ 0.65 and 0.78 for d=2 and 3
- For large p, Png ~ 0.6 and 0.68 for d=2 and 3

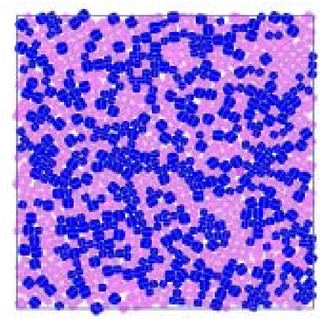




$p$=0.9


$p$=1.1


$p$=1.3


$p$=2.5

- Non-generic configurations are not rare
  a. **competition** between translational and rotational jamming
  b. relative **small asphericity** makes translational D.O.F plays a more important role, i.e., translational jamming comes in first
  c. towards the jamming limit, rotational jamming can be also achieved, with the neighboring particles orientationally correlated in a way such that the torque is balanced.

- Such jamming mechanism necessarily leads to **non-vanishing orientational correlation** in the maximally random jammed packing, as measured by the cubatic order parameter P4 (plateaus at 0.32 and 0.21 for d=2 and 3 respectively).

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- Conclusions:

  a. Packing density increases dramatically and non-analytically as p moves aways from unity

  b. The packings remain highly hypoconstrained even for large deviation $|p-1|$

  c. Competition between translational and rotational D.O.F. leads to “non-generic” jammed configurations, which are not rare events.

- Future Work

  a. Better characterization of the jammed packing

  b. Generalize to the family of super-ellipsoids

Thank You!

Questions?