Of Bodies Chang'd To New Forms

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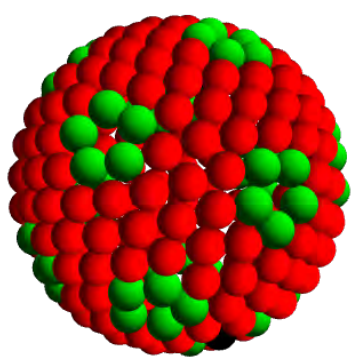
softmattertheory

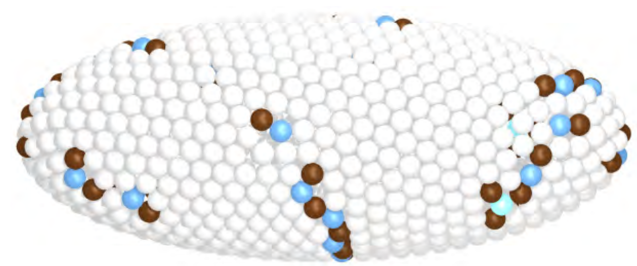
Three effects control shape-order problems

Topology



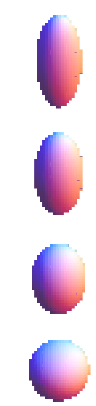
constrains the number and type of defects

Geometry



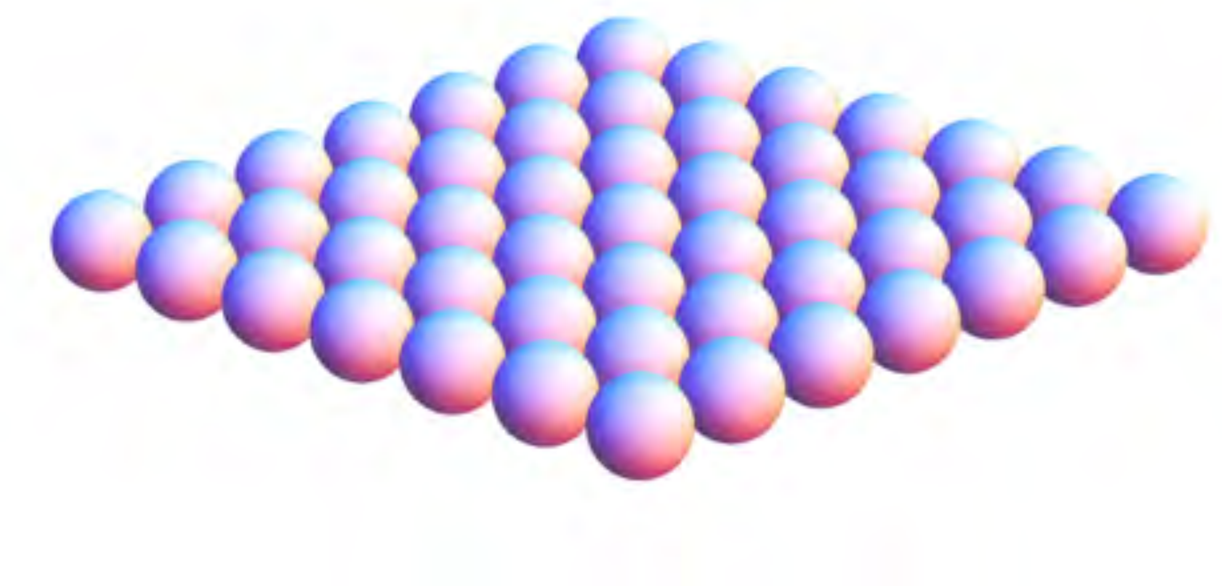
affects their arrangement

Dynamics



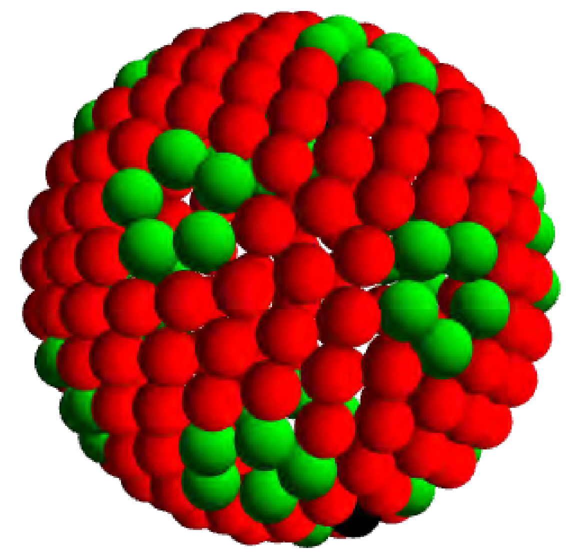
determines the range of accessible states

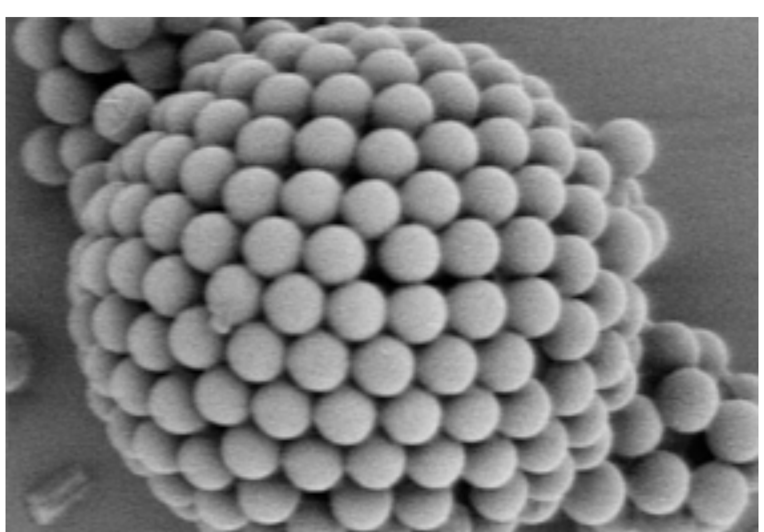
Sphere packing is a great problem to show how topology and geometry affect order



On a plane, the problem is trivial: optimal packing is the hexagonal lattice

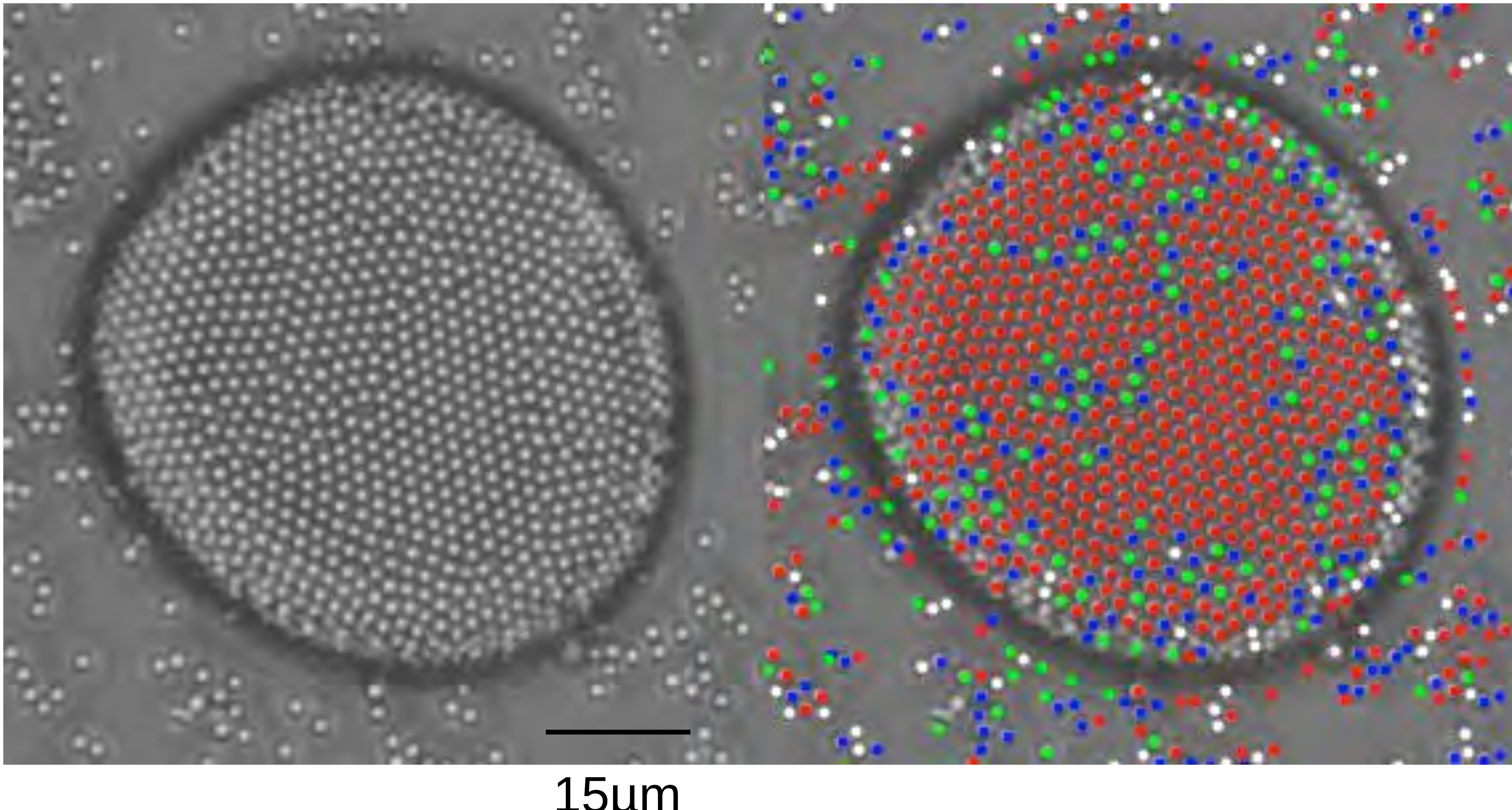
Presence of curvature necessitates introduction of defects.



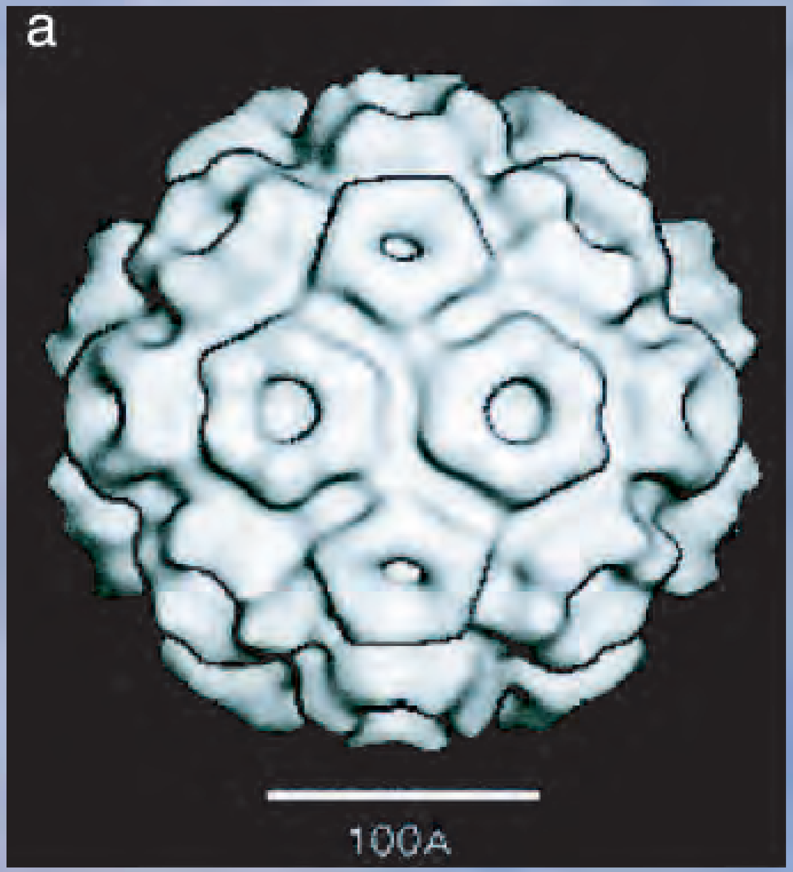


Pickering emulsions — emulsions with colloidal particles absorbed onto the fluid-fluid interface are a great model system to study this

Coloring particles by number of neighbors reveals defect structure



Also important in architecture…
… and viral structure.

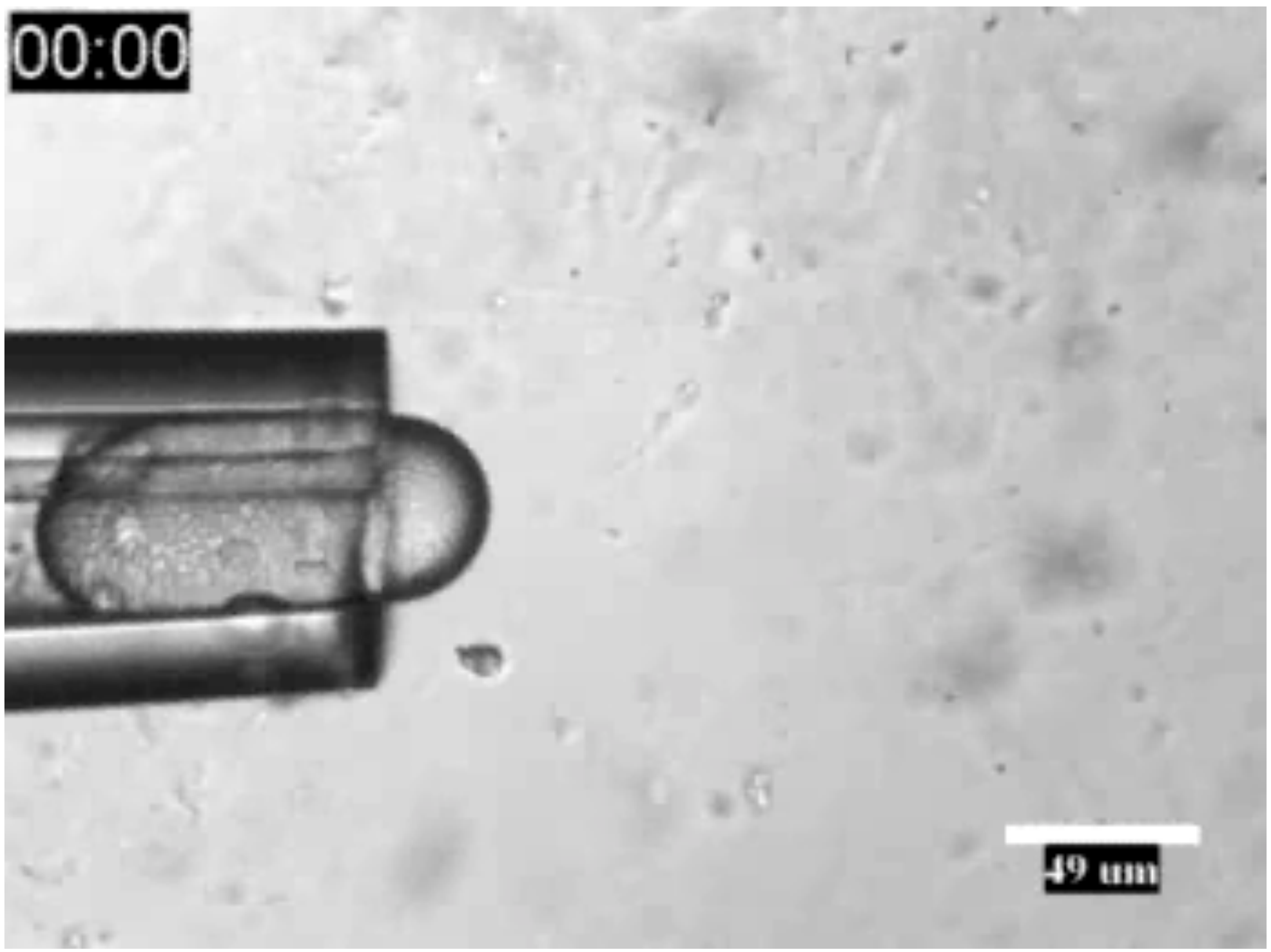


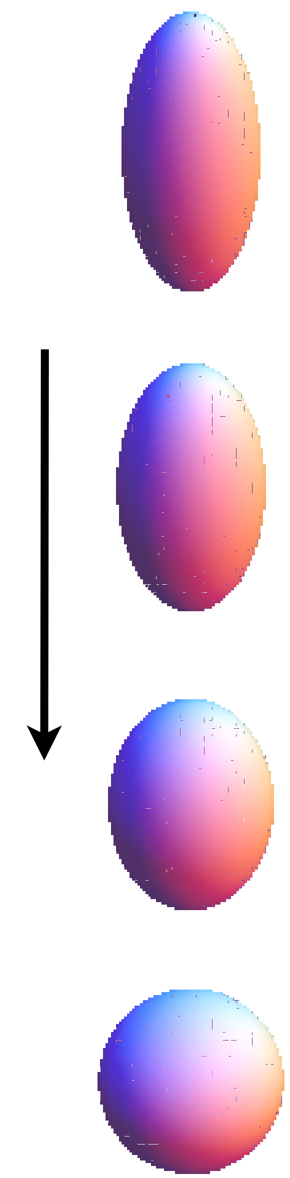
In the rest of this talk I'm going to—

1. Show how geometry controls the packing of spherical particles on a surface of nonuniform curvature.
2. Show how this can be used to stabilize non-spherical fluid droplets.
3. Characterize the relative influence of geometry and dynamics that determines the ordering.
4. Connect these systems to jamming.

We can use microfluidics to produce nonequilibrium droplet shapes

Fluid droplet ejected from pipette relaxes to spherical ground state:



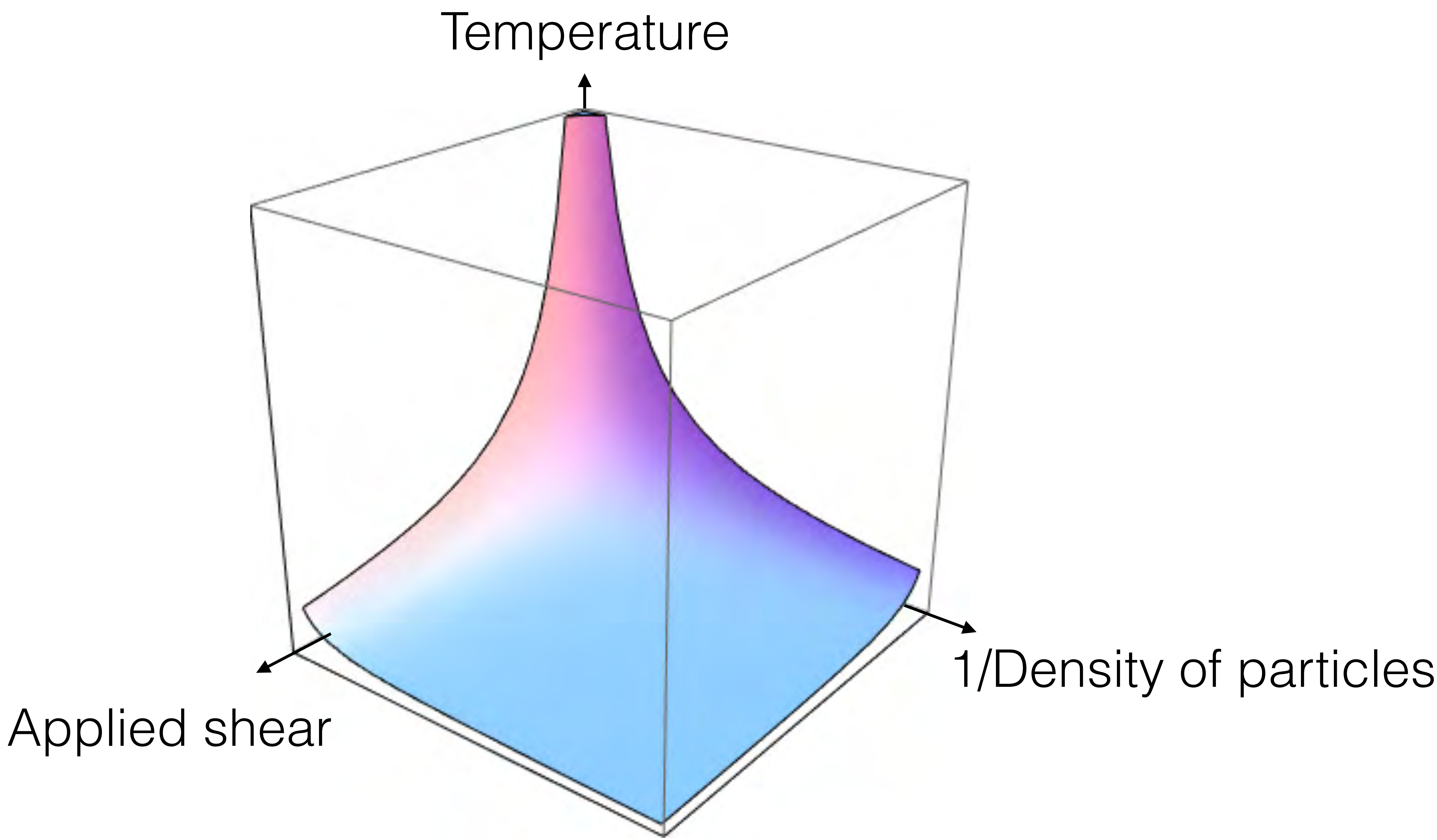


Volume conserved, but surface area decreases as a function of time.

Video courtesy of Patrick Spicer and Marco Caggioni

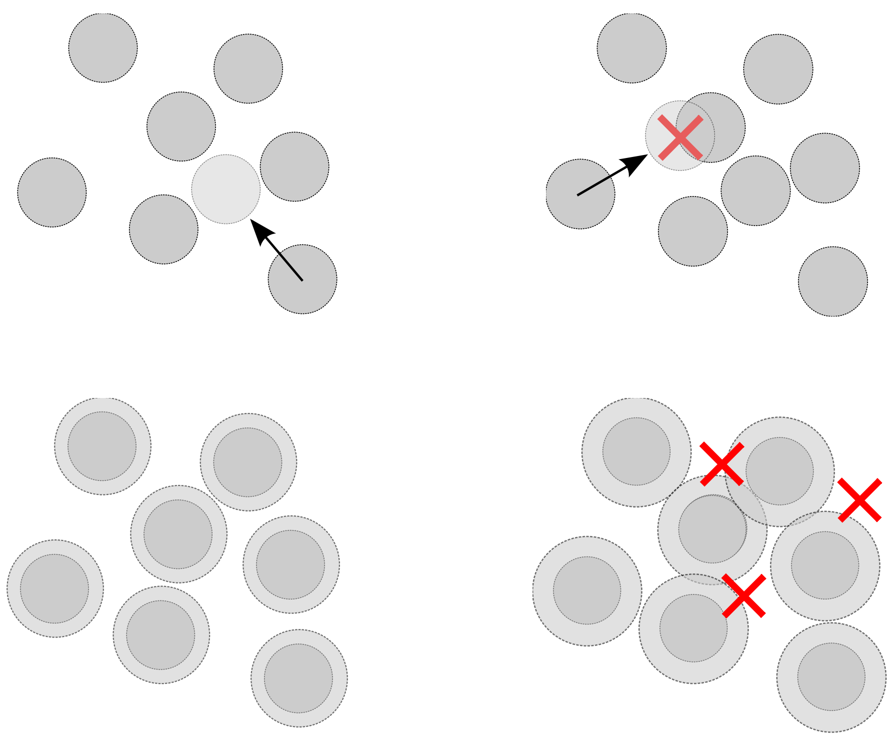
Jamming

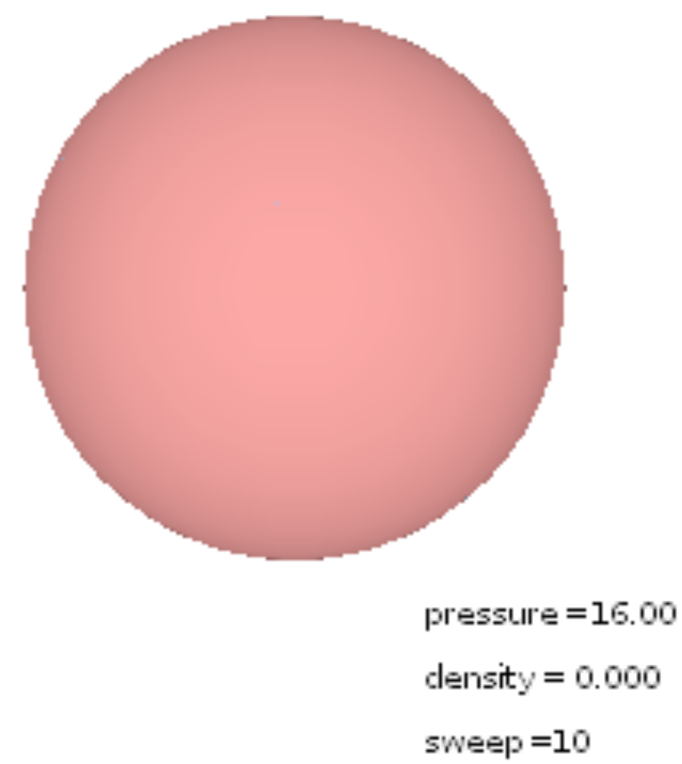
Jamming is described by a phase diagram as a function of the influences on the system



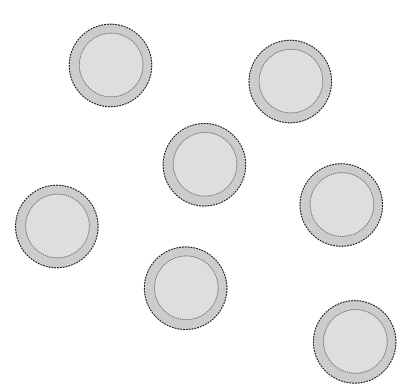
Our computational toolkit contains efficient algorithms to produce packings on surfaces

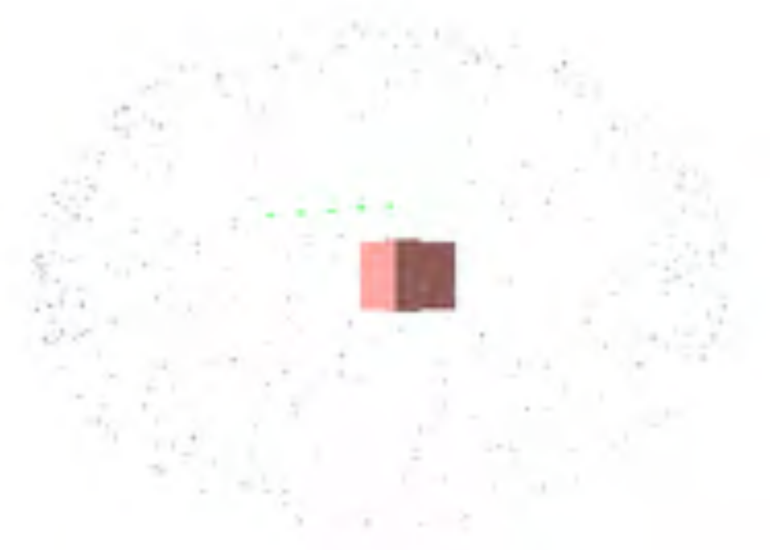
Inflation





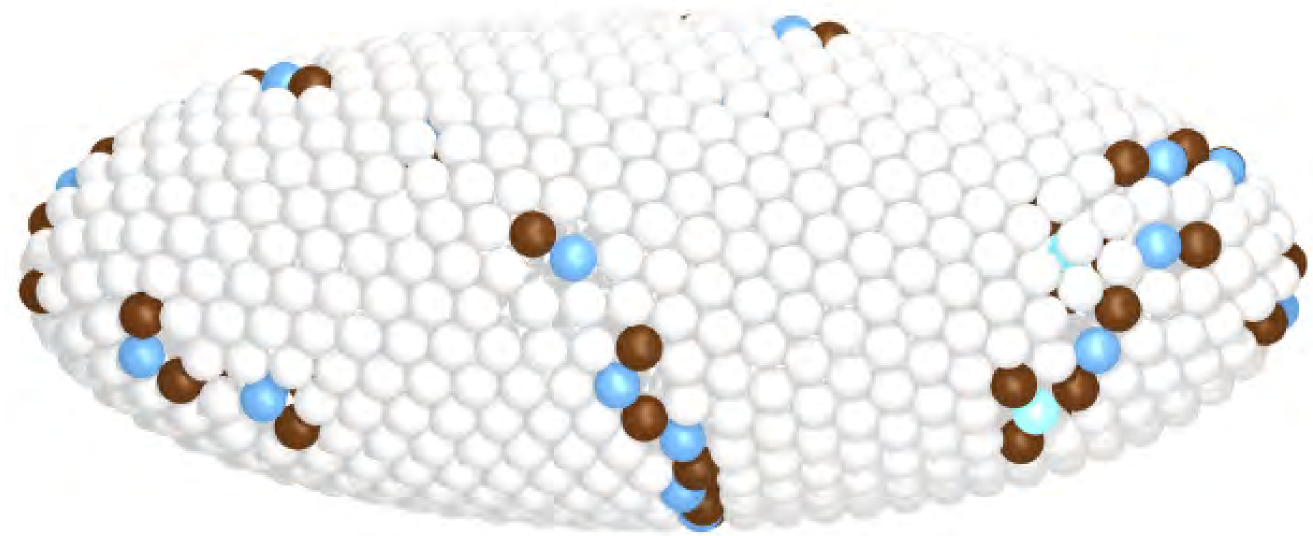
Simulated Annealing

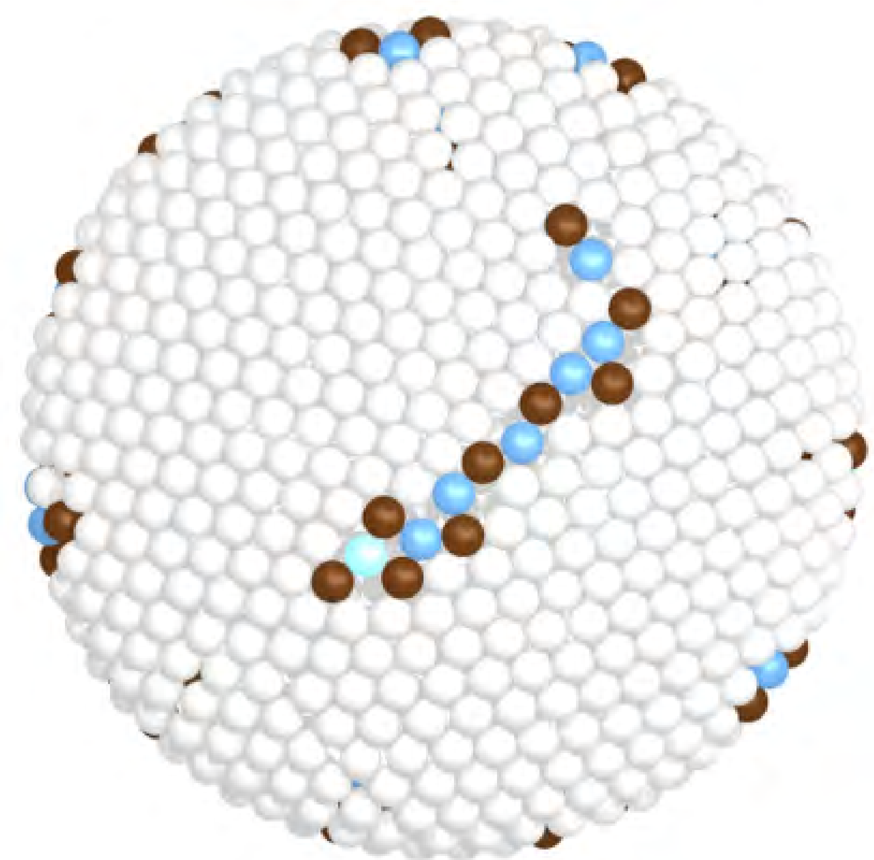




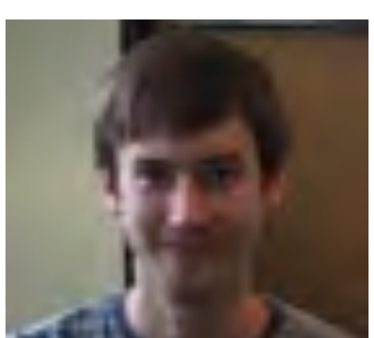
Prolate and oblate ellipsoids have similar defect structures, but they're placed differently

Prolate

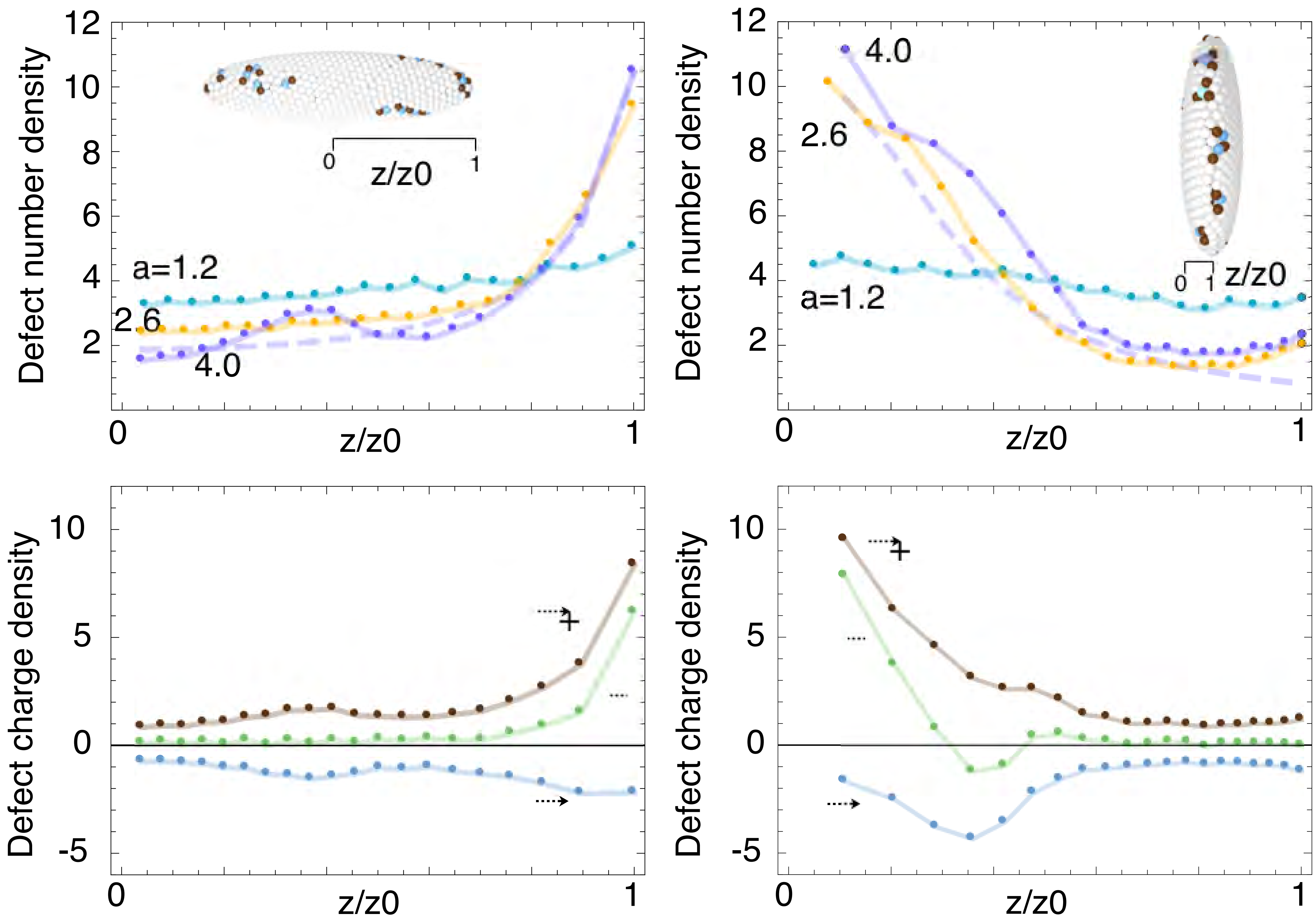




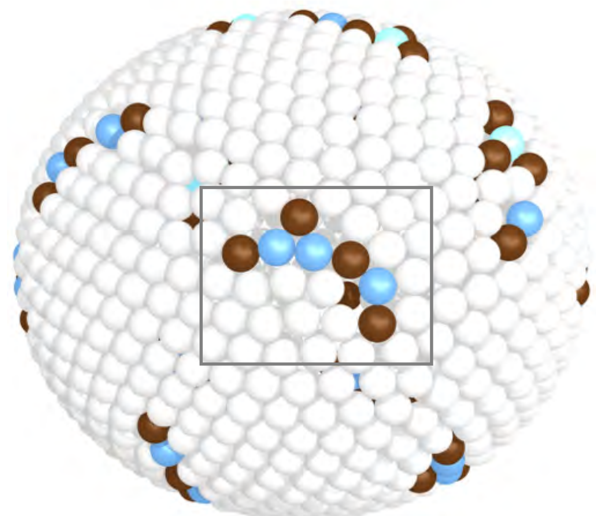
Oblate

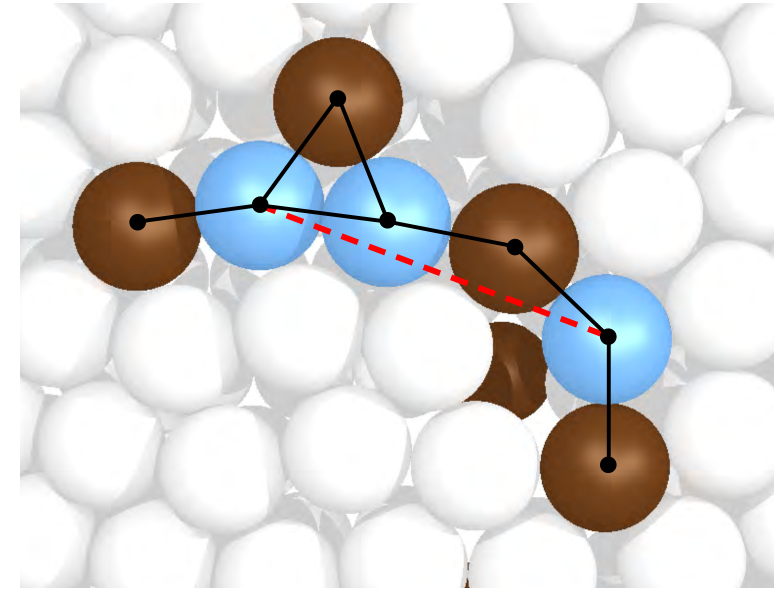


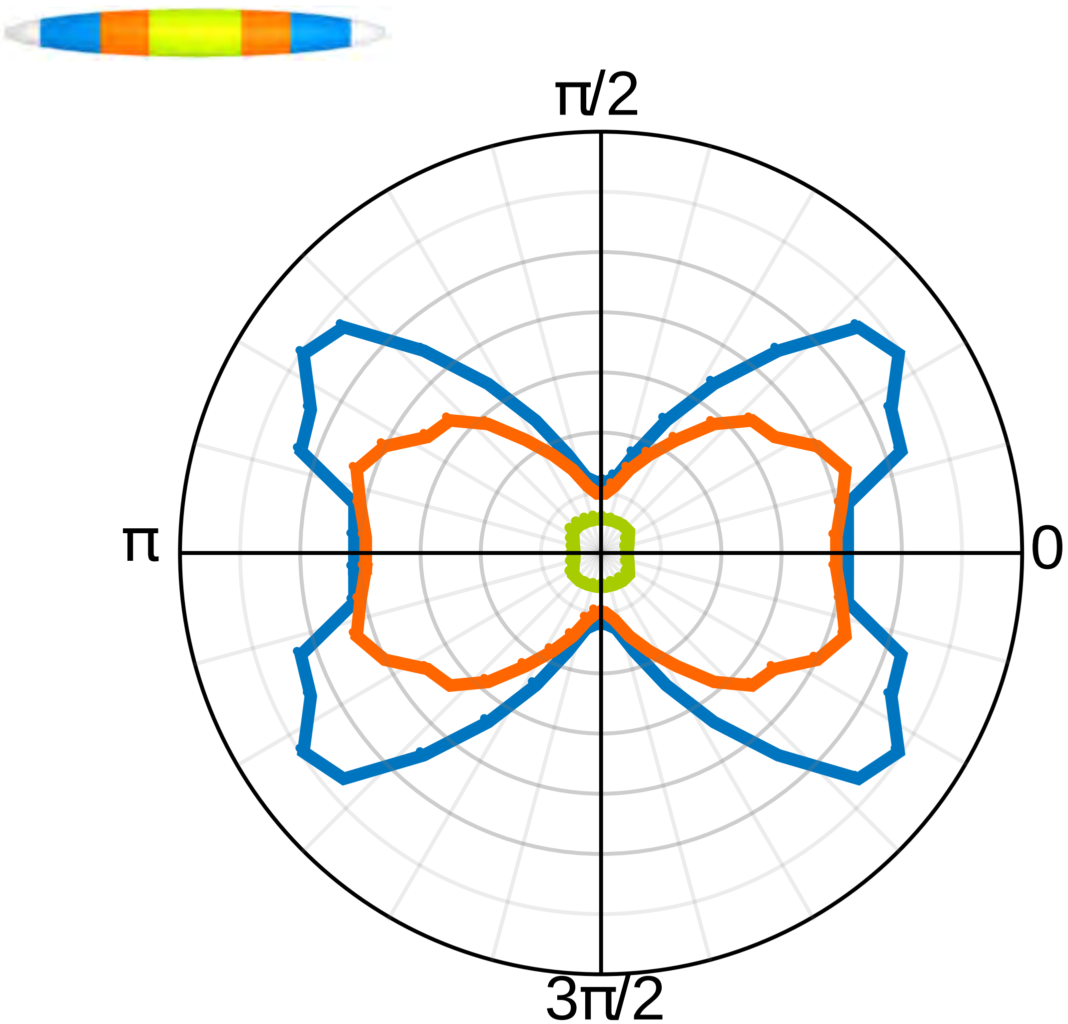
Defects migrate to regions of high curvature

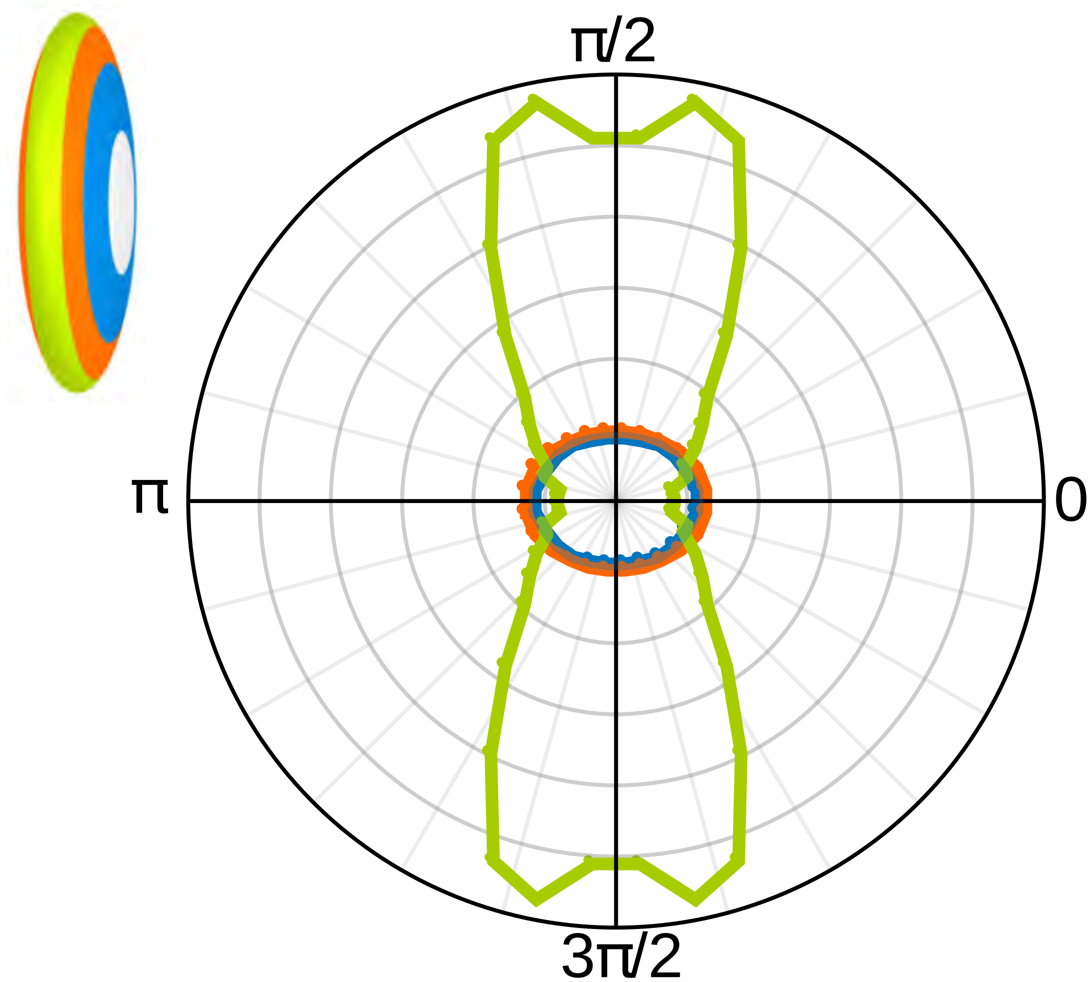


Scars tend to align with lower principal curvature



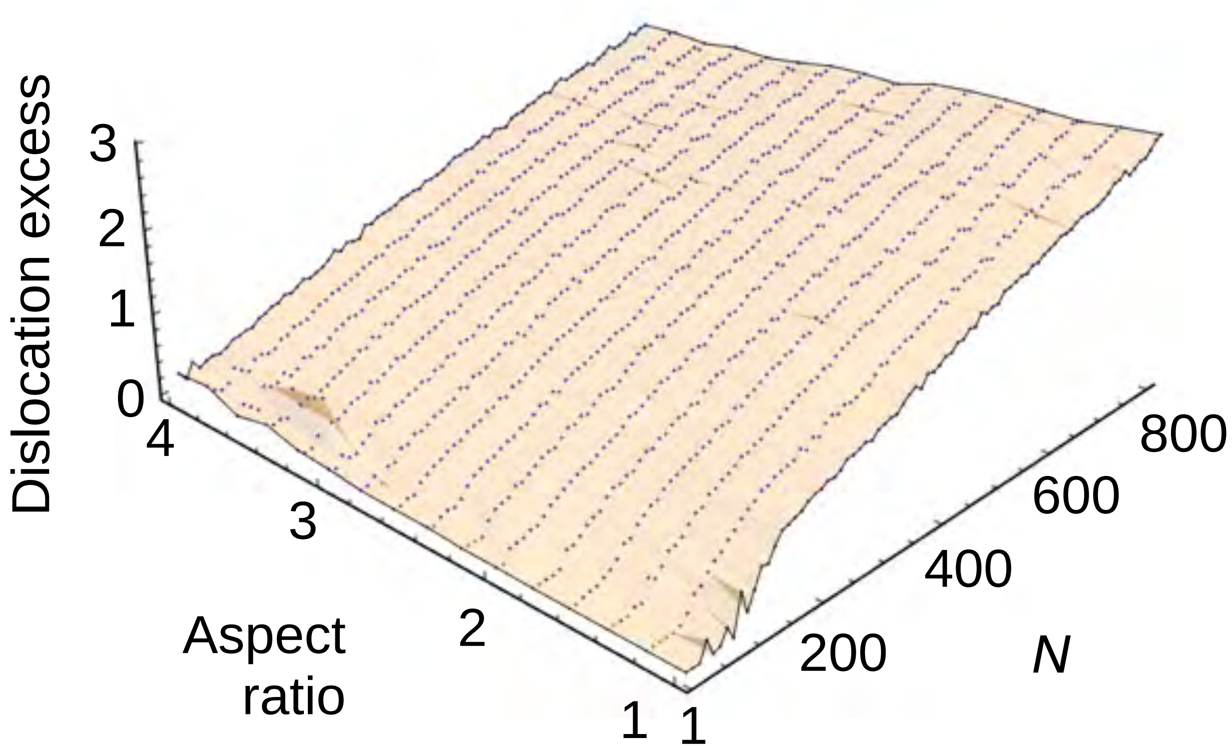




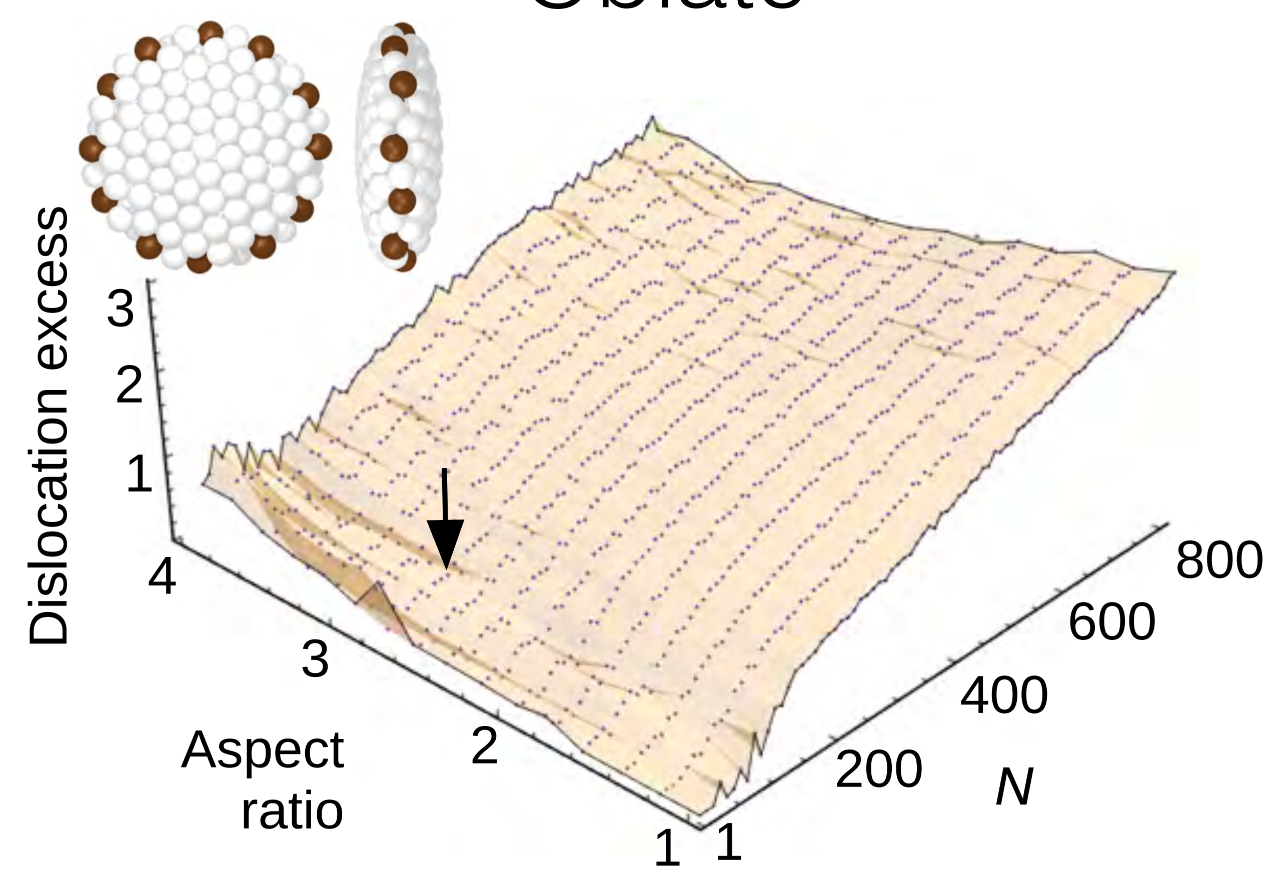


Scar transition is softened

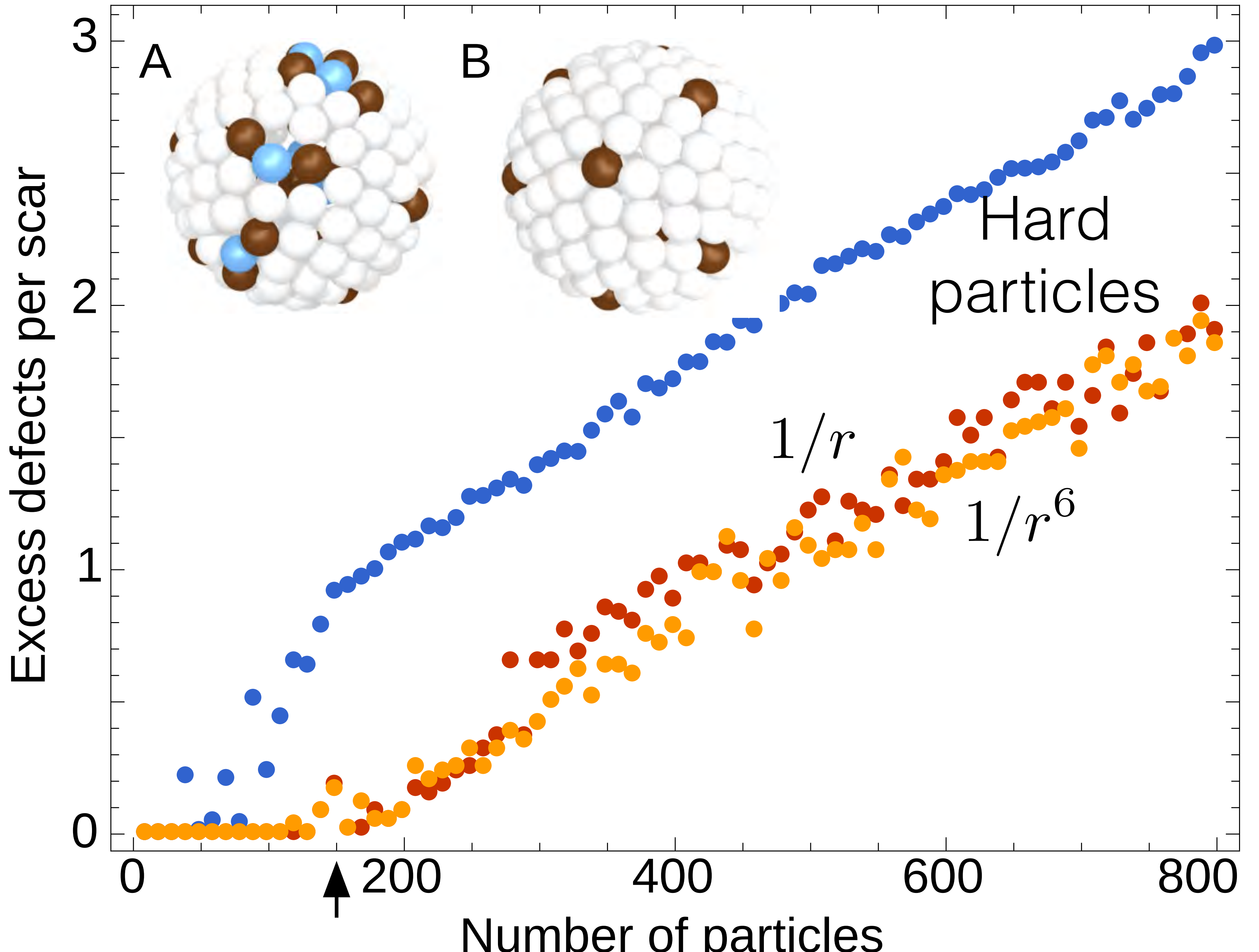
Prolate



Oblate

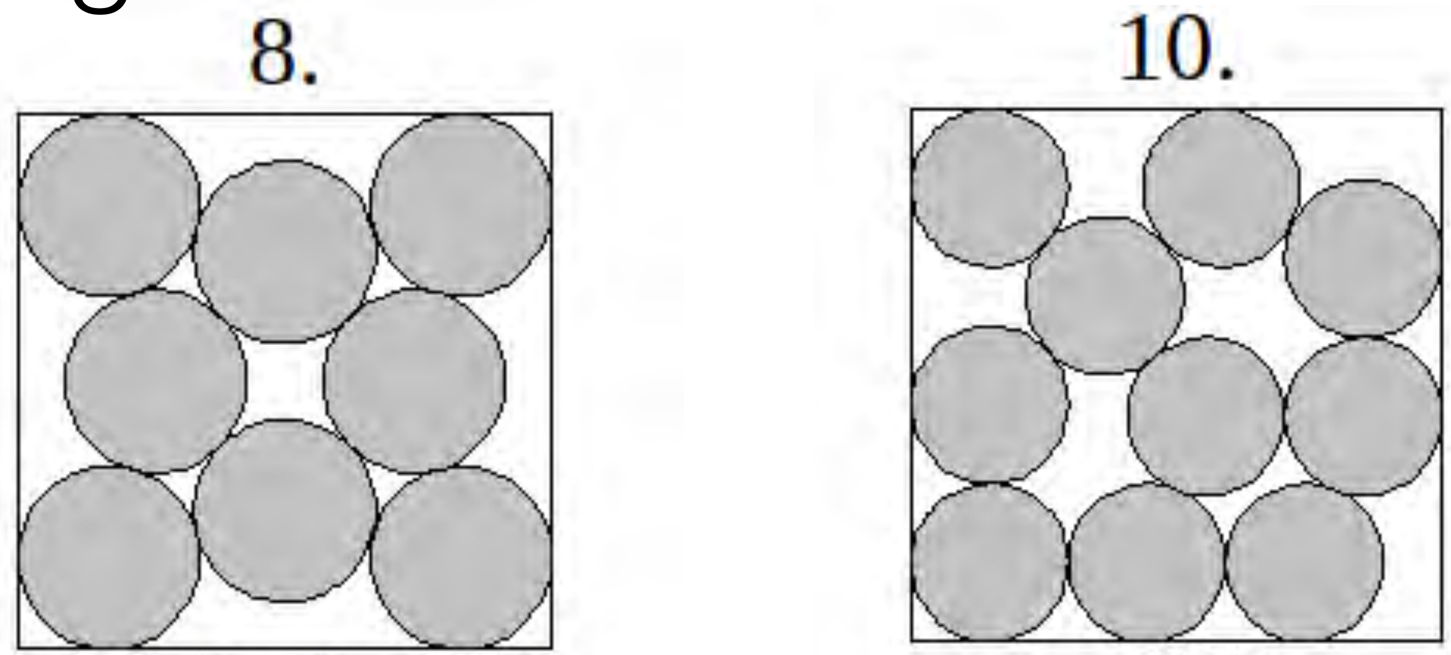


Scar transition is also shifted by inter-particle interactions



Boundary conditions can lead to favorable or unfavorable packing

E.g. Particles in a box



s = 2 + √2 + √6 = 5.863+
Proved by Schaer/Meir in 1964.

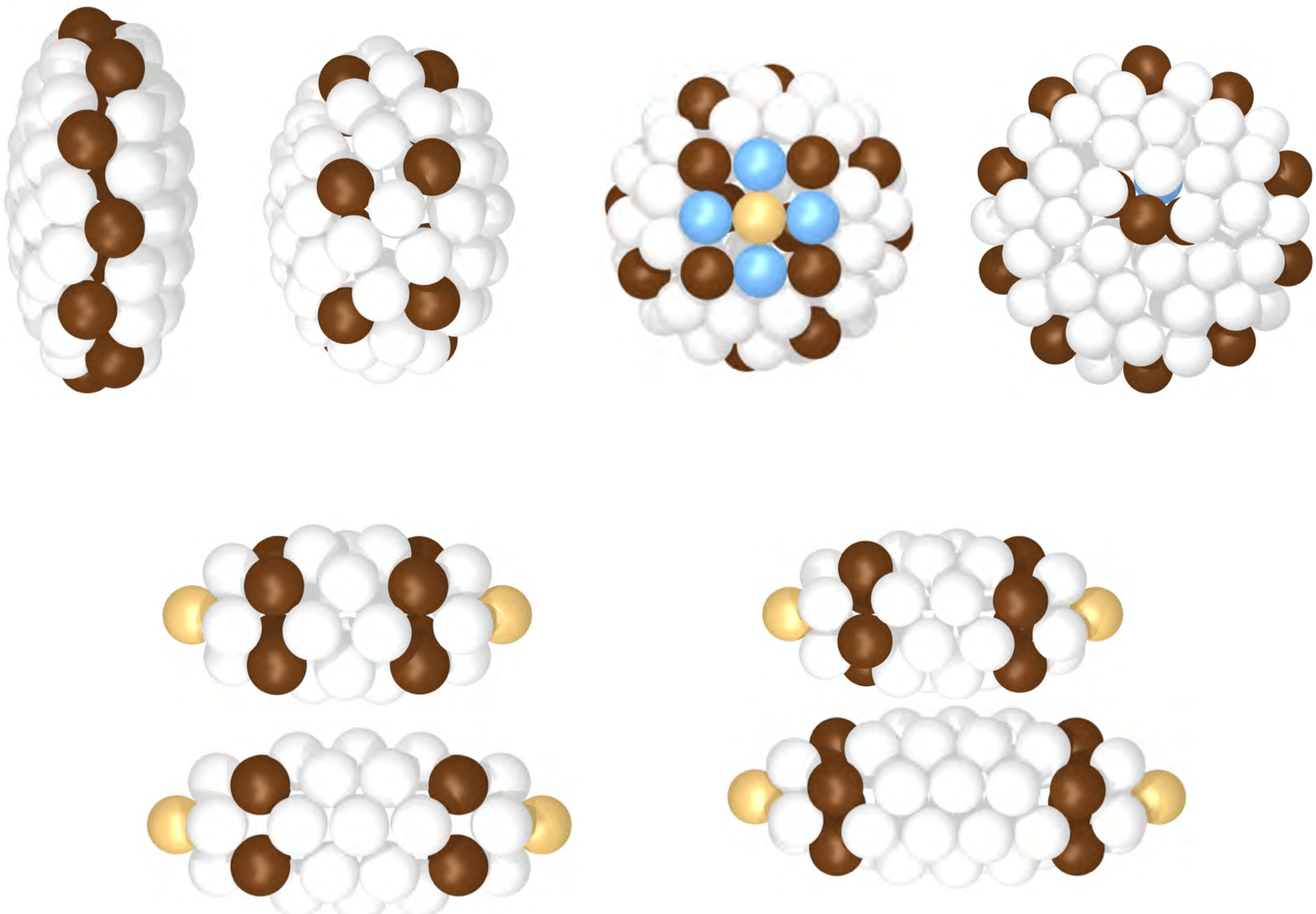
s = 6.747+
Proved by De Groot in 1990.

Particle packings break ellipsoidal symmetry.

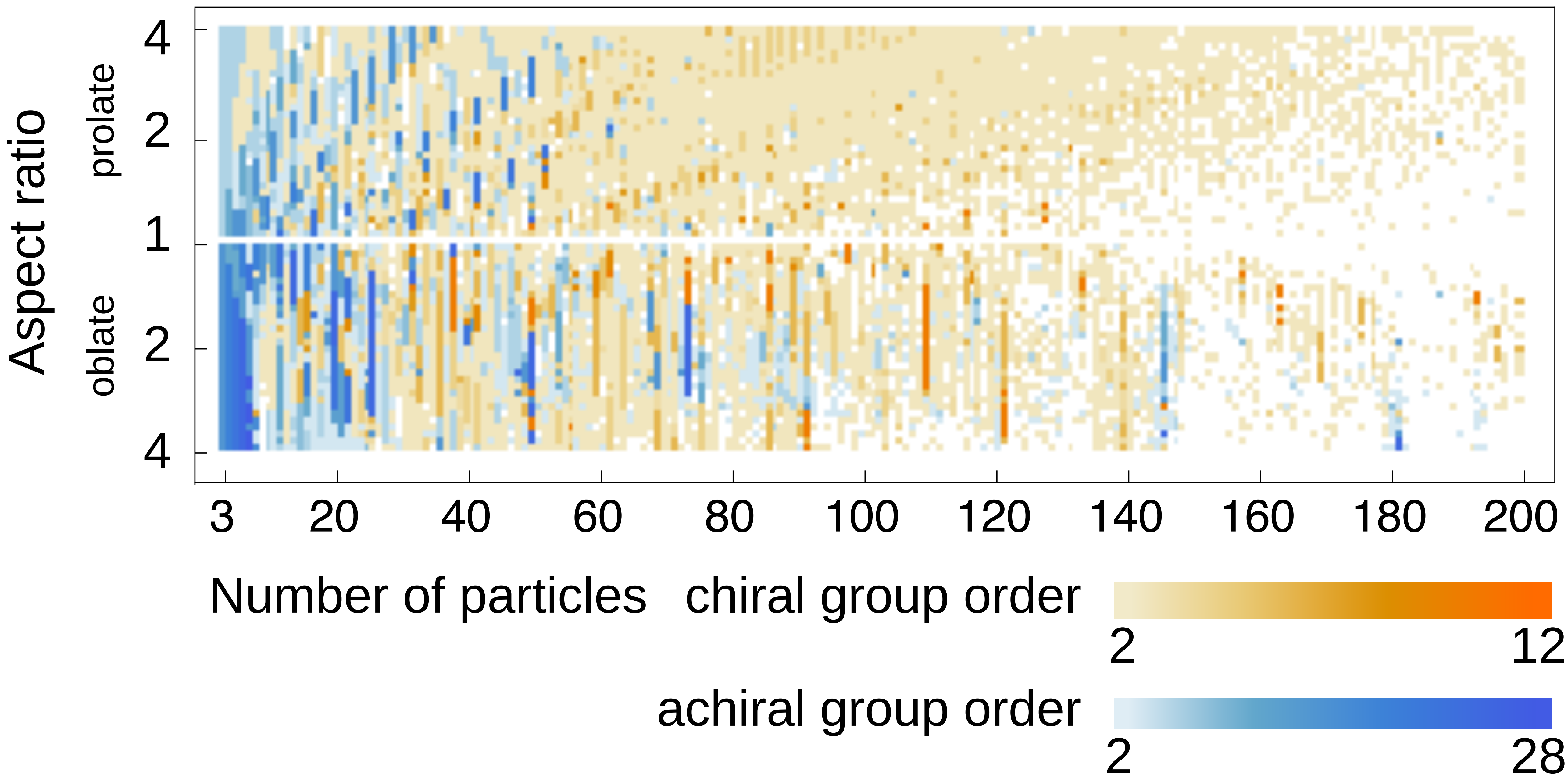
Packings must fall into a subgroup of ellipsoidal symmetry group $D_{\infty h}$

…but which?

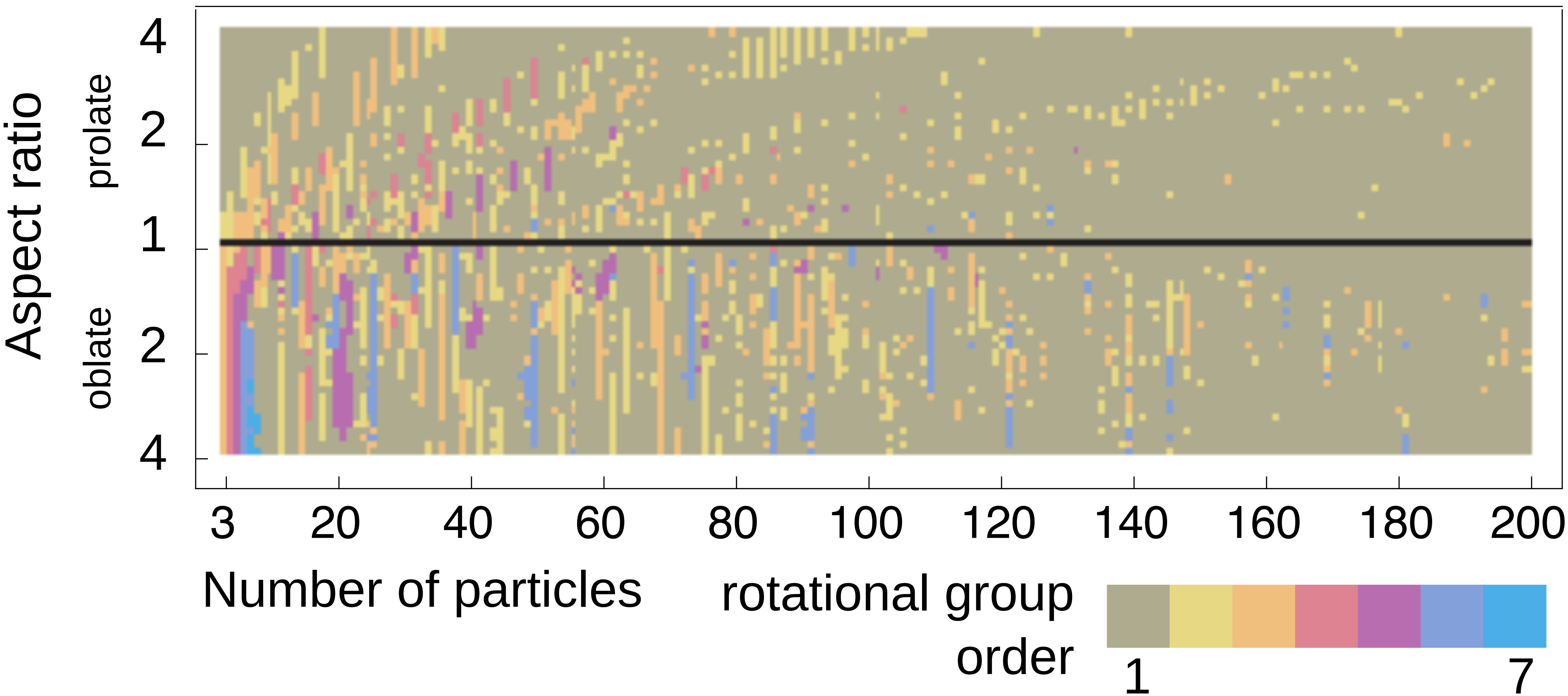
Commensurate packings



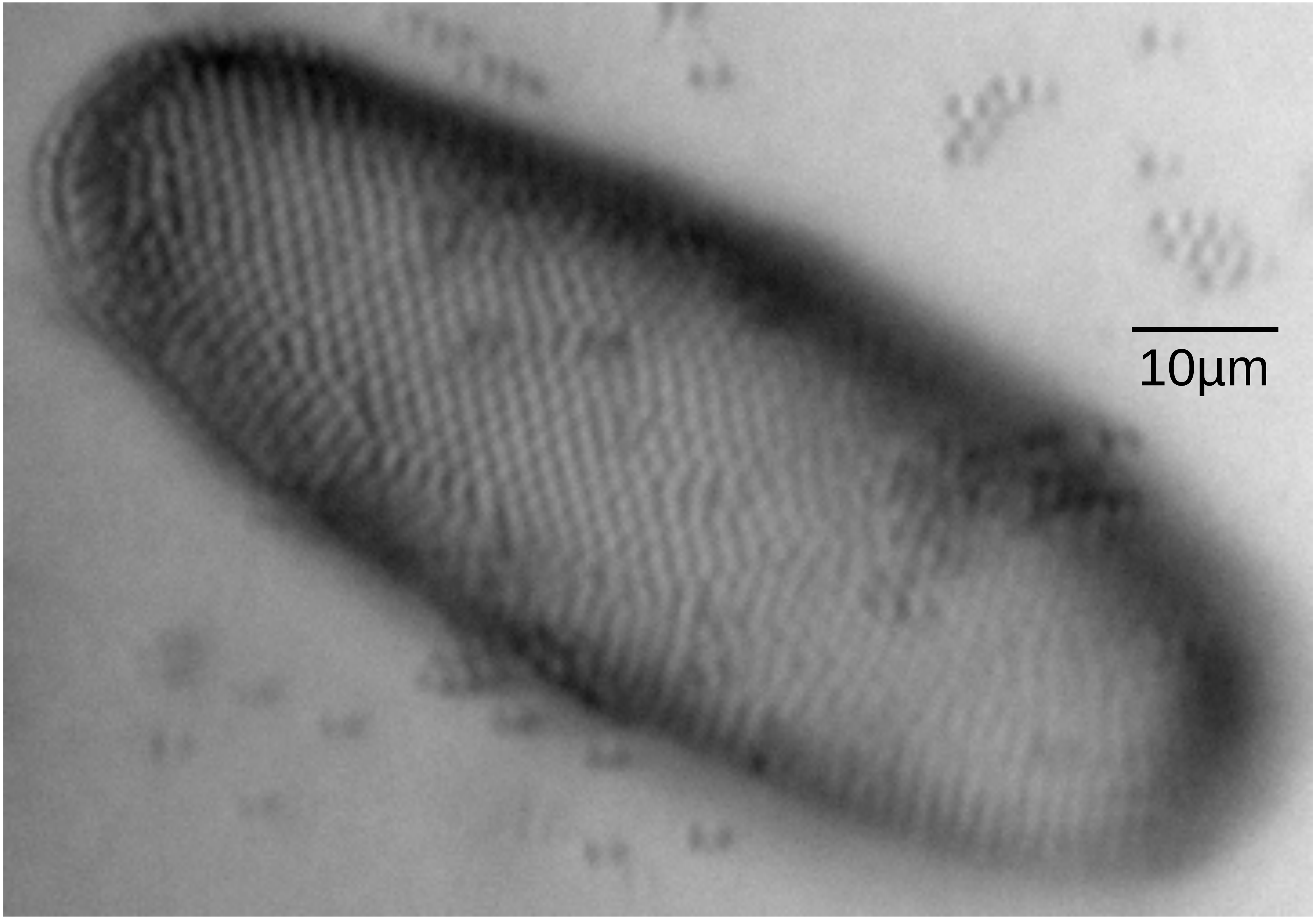
Commensurate packings



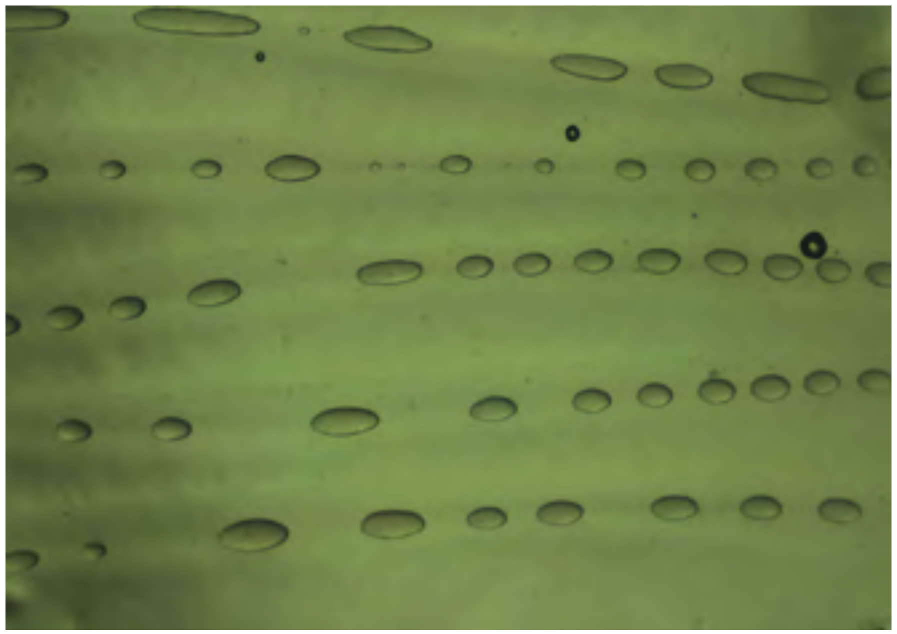
Commensurate packings

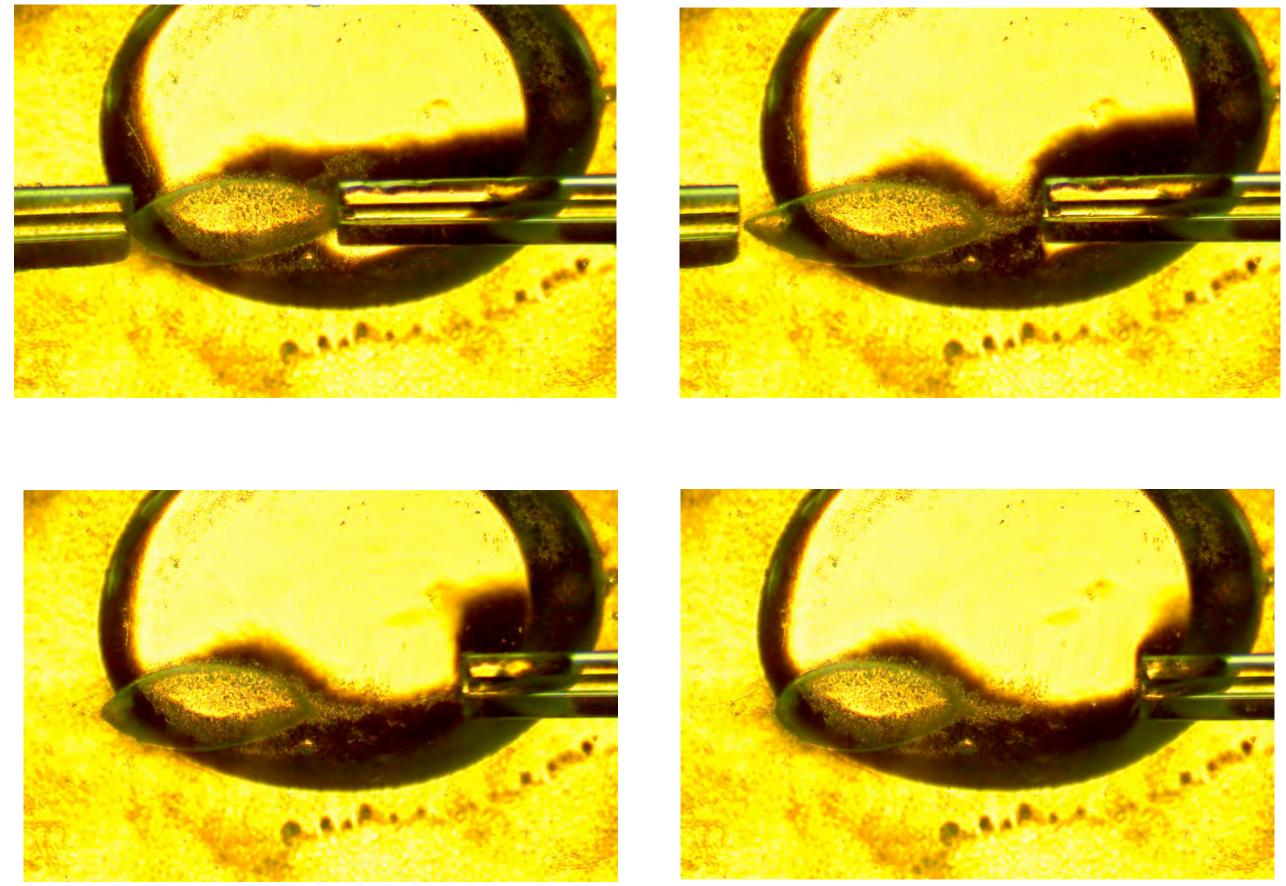


Having predicted these shapes, we've now seen them:

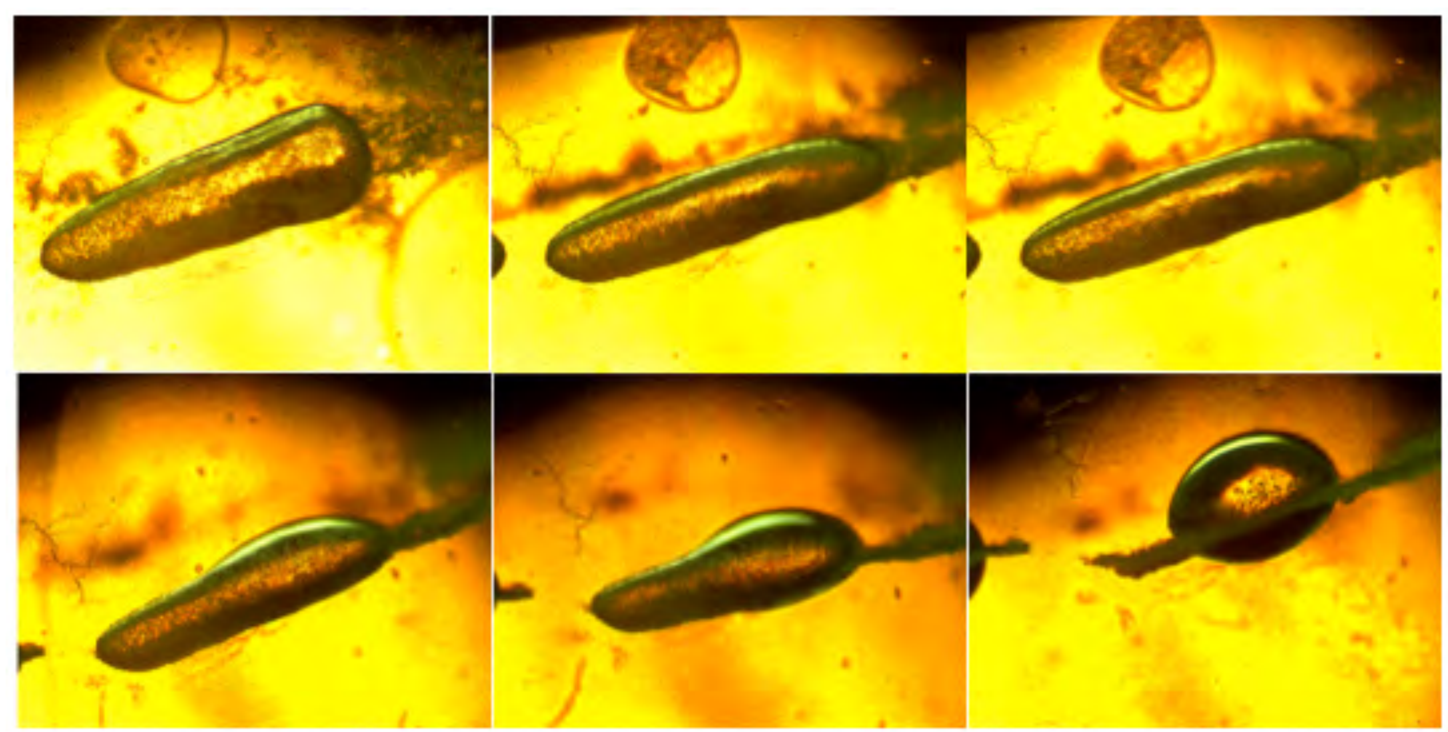


And we now have multiple ways of making them…

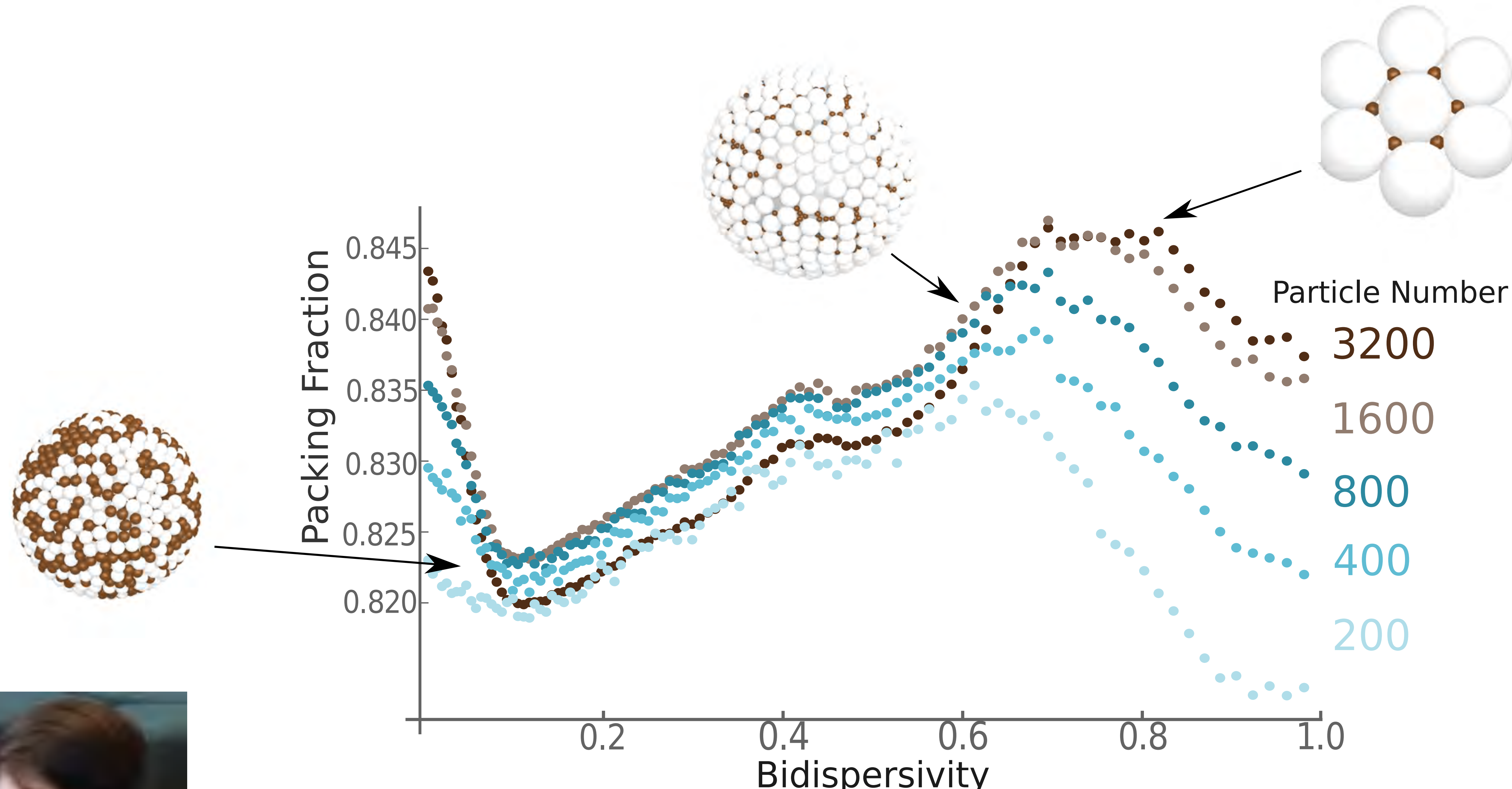




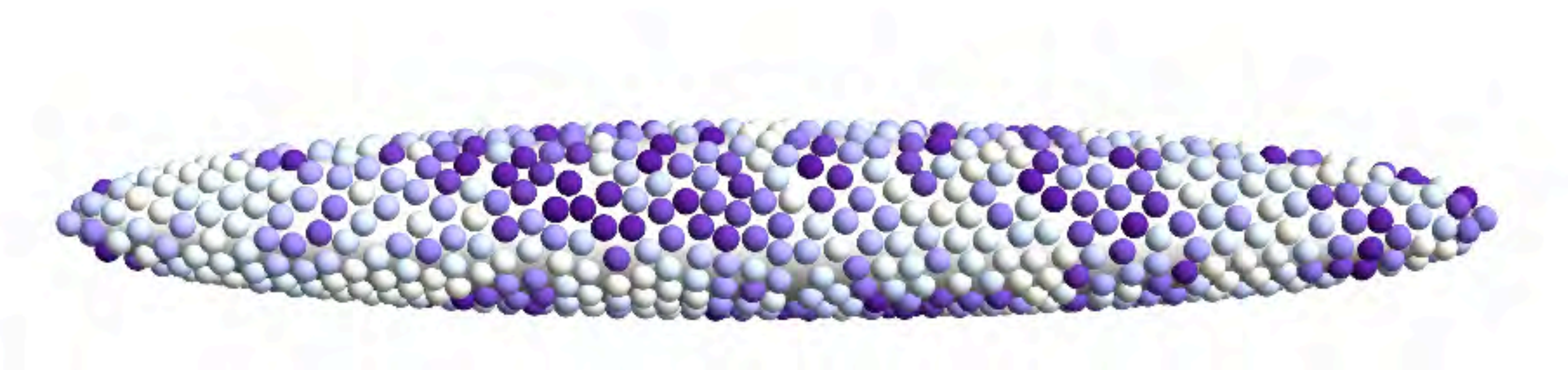
…and controlling stability by changing the chemical environment.

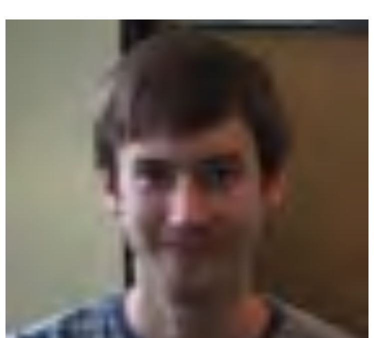


Bidispersity disprupts crystallinity

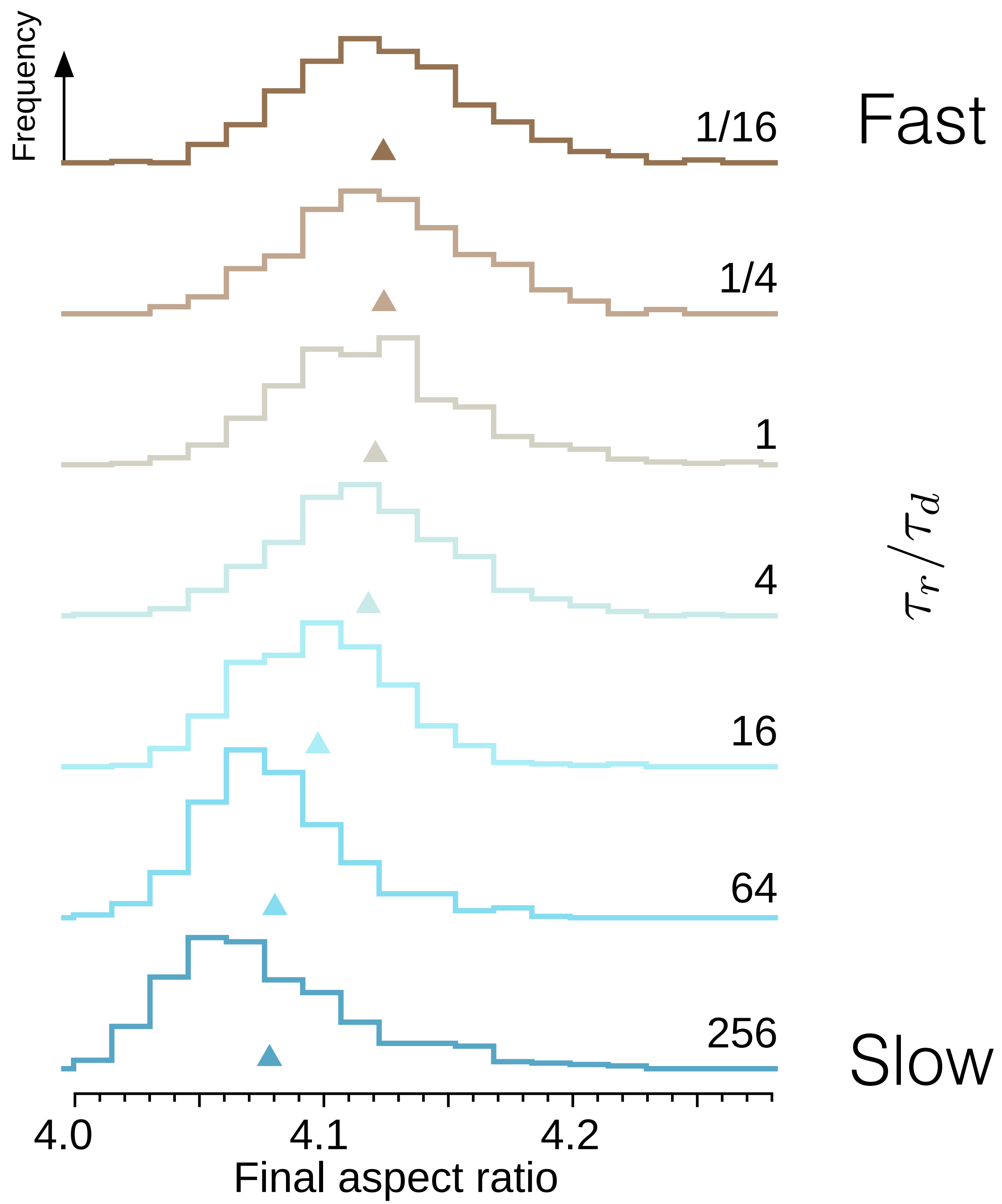


What is the effect of dynamics?

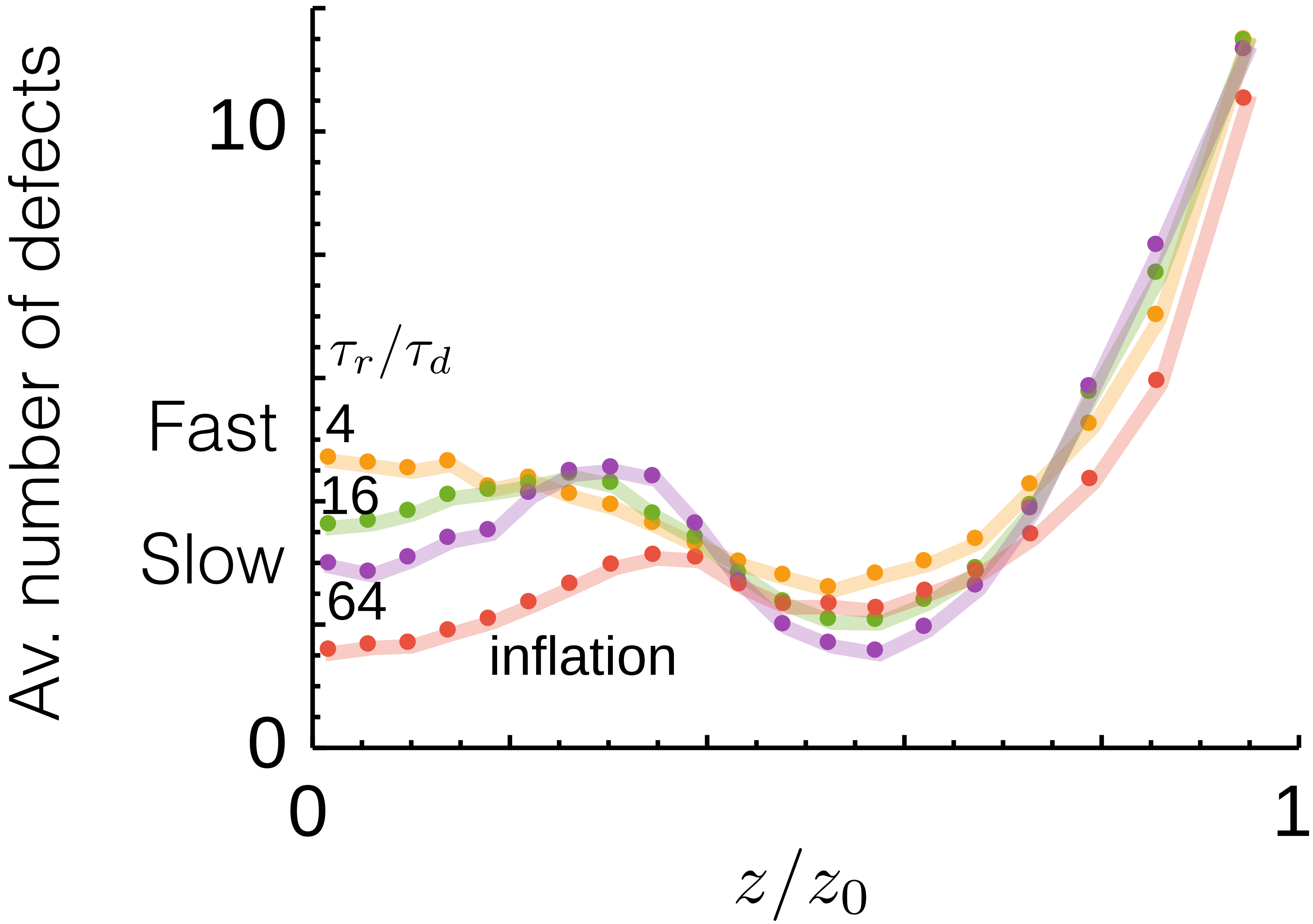




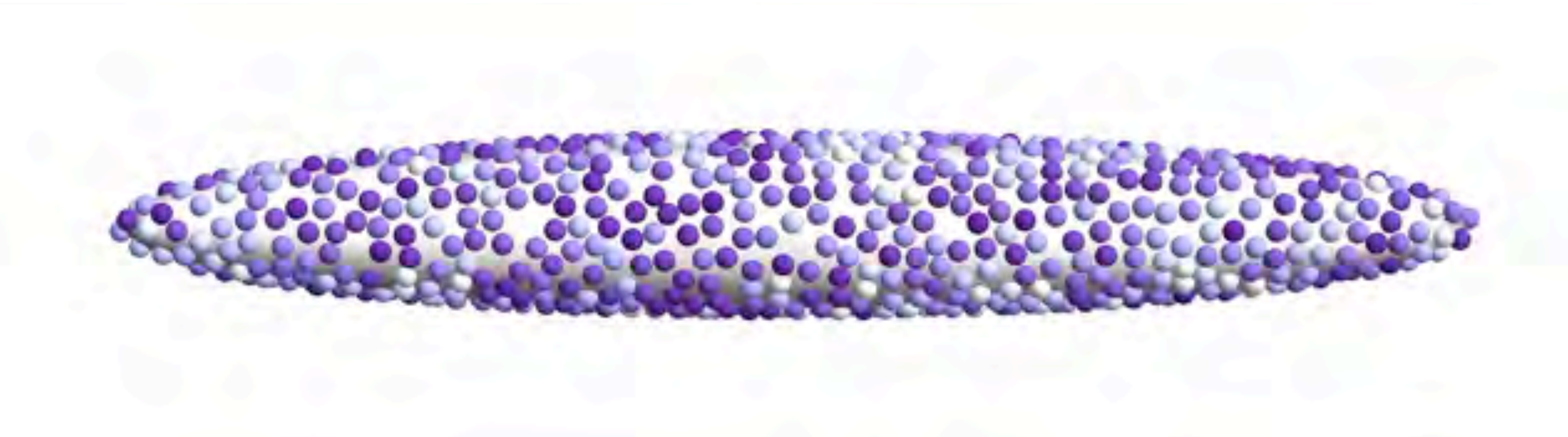
Slower relaxation leads to later arrest



Faster relaxation relocates defects to the center

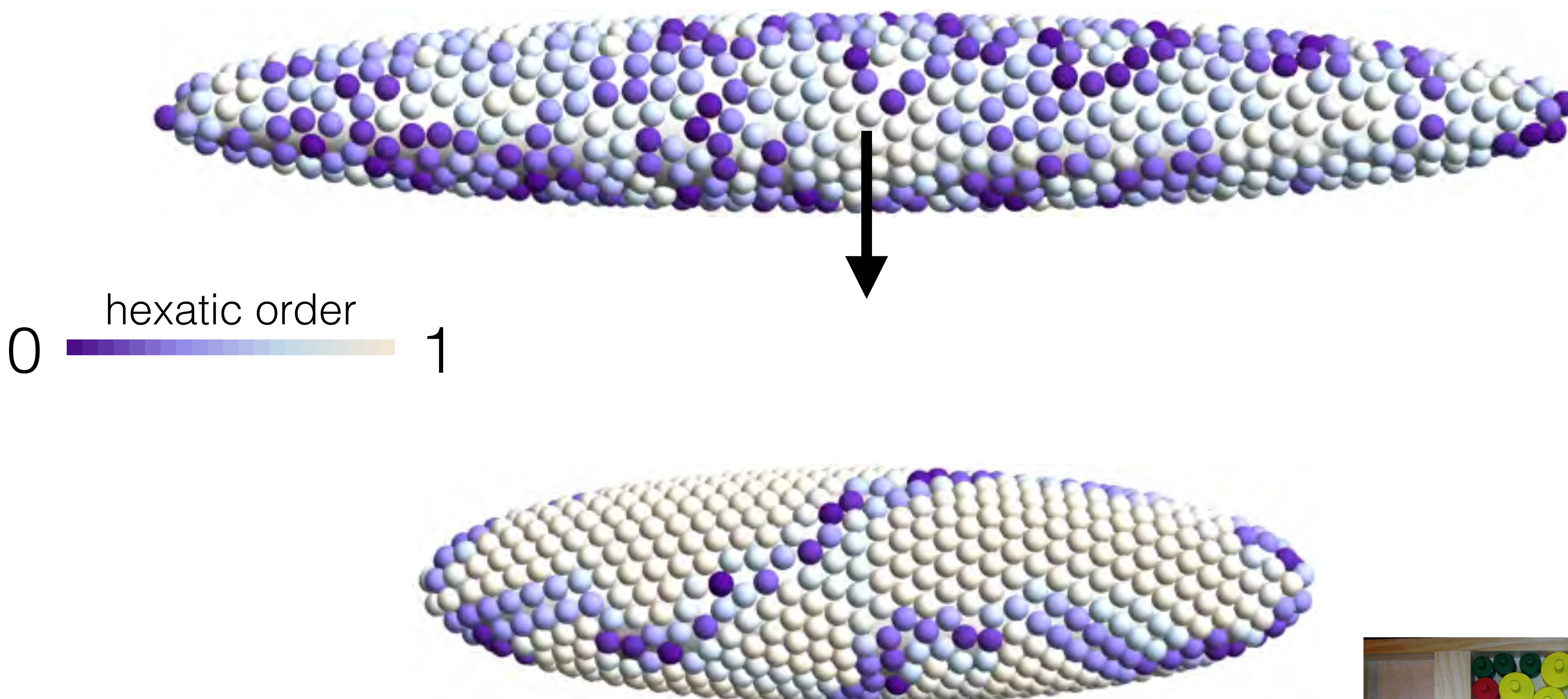


We are currently investigating the effect of inter-particle interactions



Weak short-range attractive interaction

Are the final states jammed?



Packings can be categorized by the types of motion available to particles

Locally jammed—each particle is trapped by its neighbors.

Collectively jammed—collective motions cannot unjam the system

Strictly jammed—collective motions + boundary deformations cannot unjam the system

New category:
Metric jamming—collective motions + surface evolution cannot unjam the system

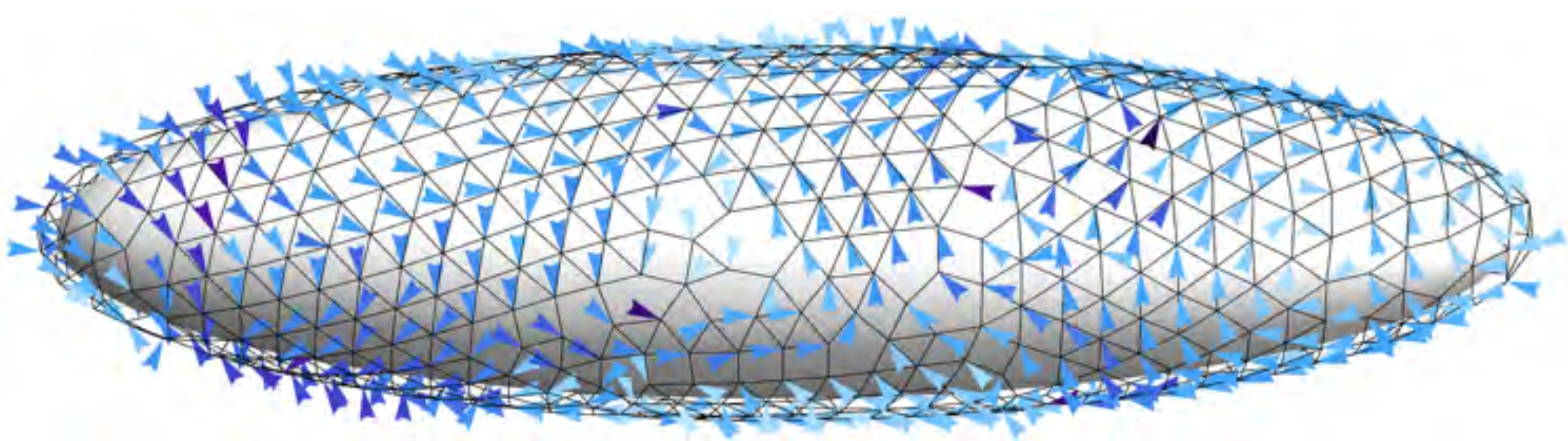
A linear program uncovers feasible motions that may unjam the system

$$\max_{\Delta\mathbf{R}} \mathbf{F}^{\mathrm{T}}\Delta\mathbf{R} \quad \text{subject to} \quad \mathbf{A}^{\mathrm{T}}\Delta\mathbf{R} \leq \Delta\mathbf{l} \quad \text{(impenetrability)}$$

$$|\Delta\mathbf{R}| \leq \Delta R_{\max} \quad \text{(boundedness)}$$

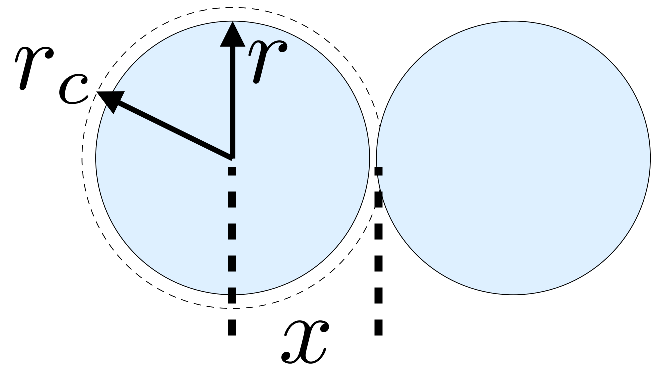
new constraint: $\Delta\mathbf{R}^{\mathrm{T}}\mathbf{N} = 0$ (surface constraint)

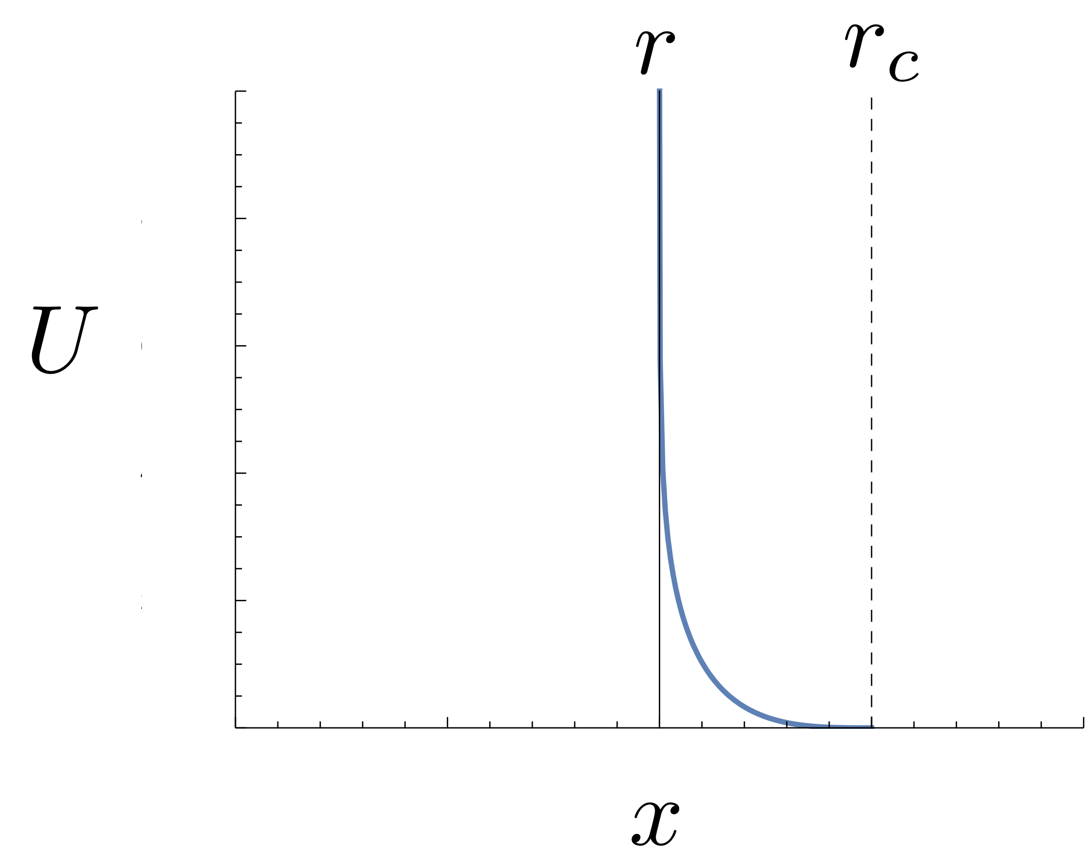
Resulting unjamming motion:



(adapted from A. Donev's work)

We also use minimization of an auxiliary energy functional to condition the packings





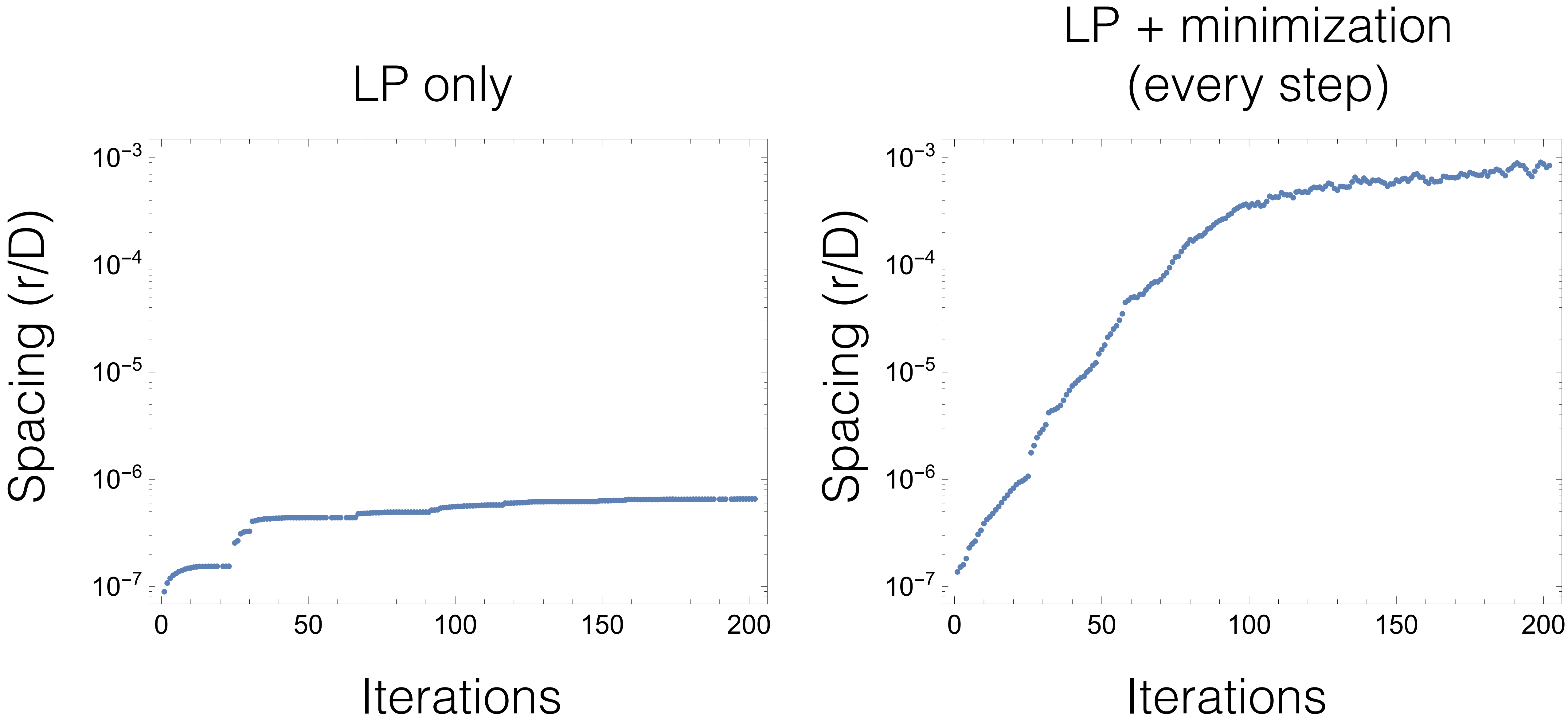
$$U = -(x-r)^2 \log(x-r)$$

smooth at cutoff

hard core w/ soft repulsion

Minimize by gradient descent

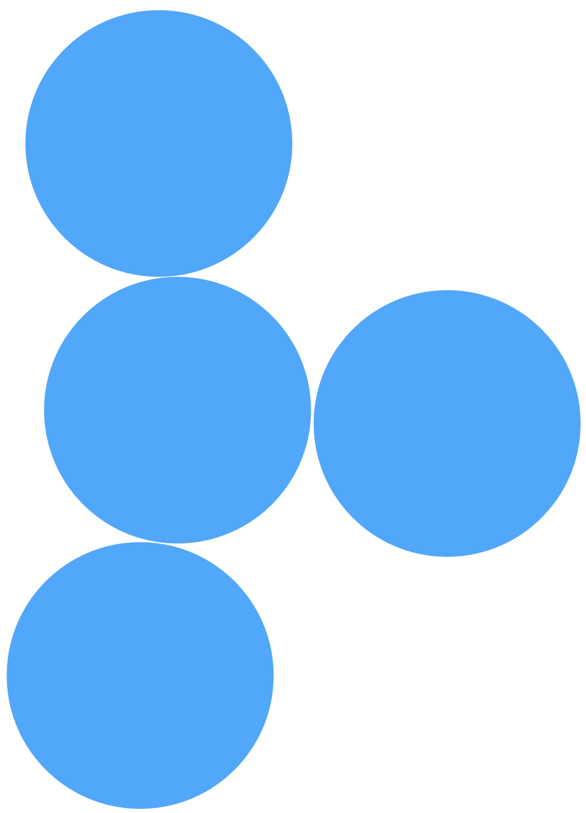
Combining linear program with energy minimization quickly finds unjamming motions.



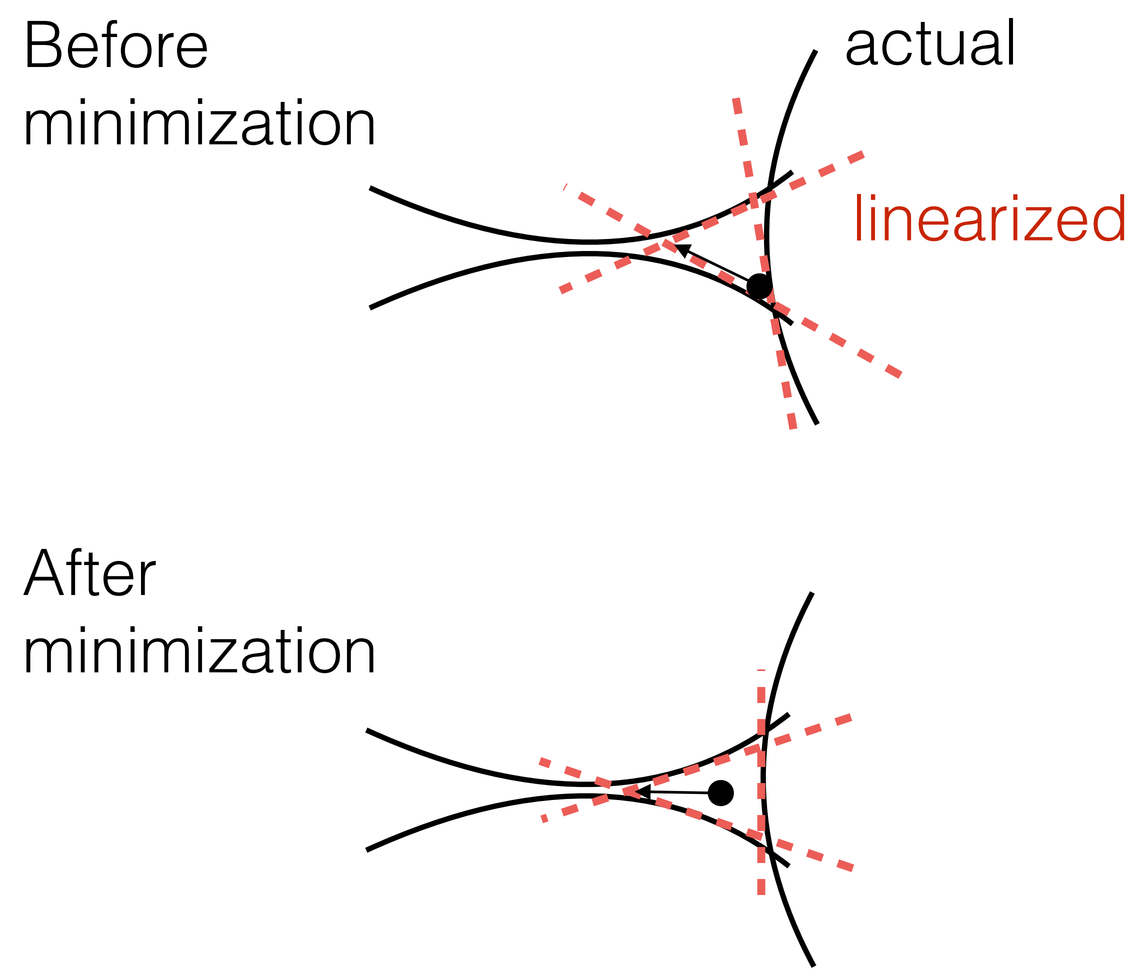
~6 min

Minimization better conditions the problem by shifting particles to the center of the jamming polytope

Particle configuration

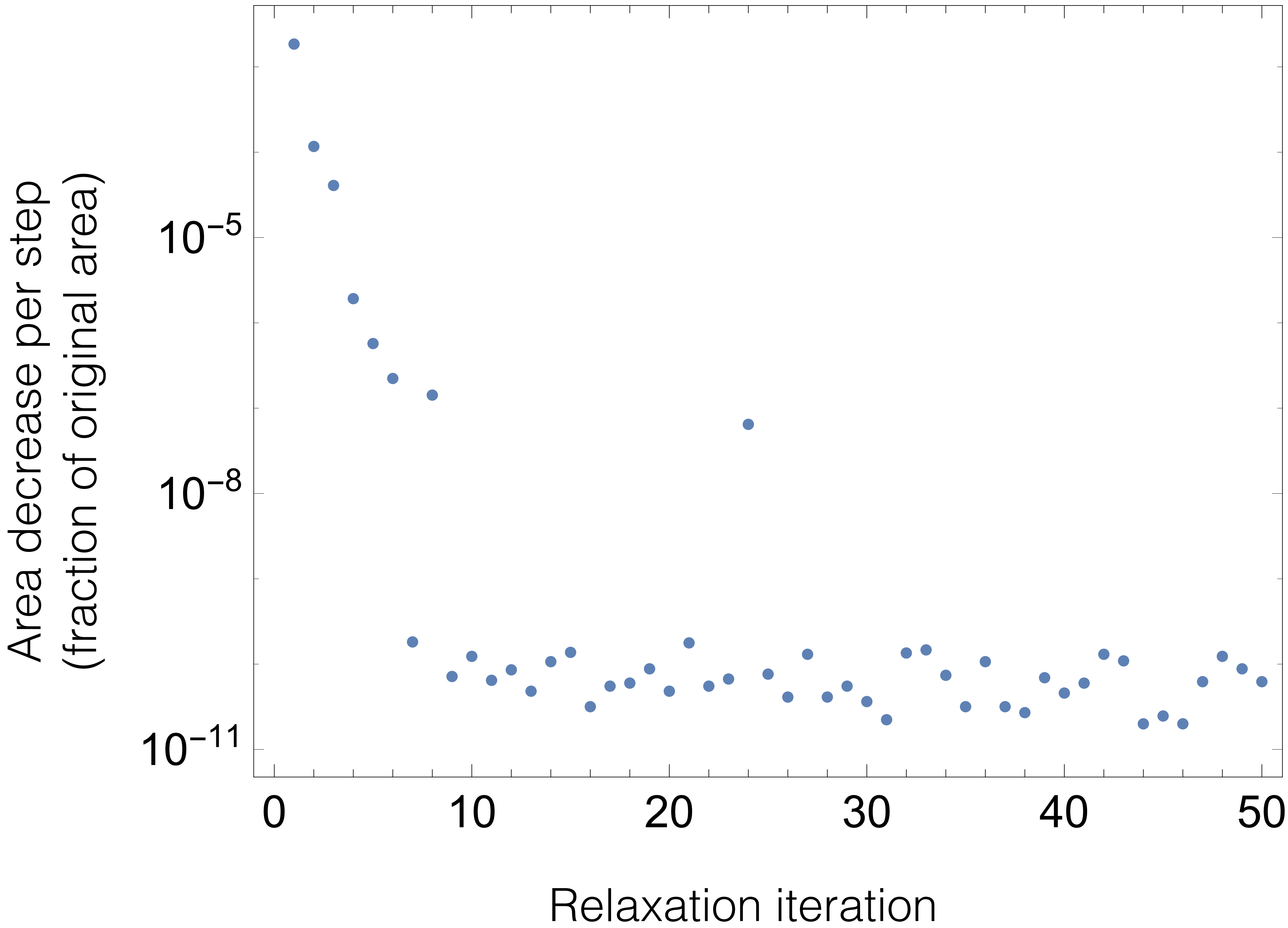


Jamming polytope

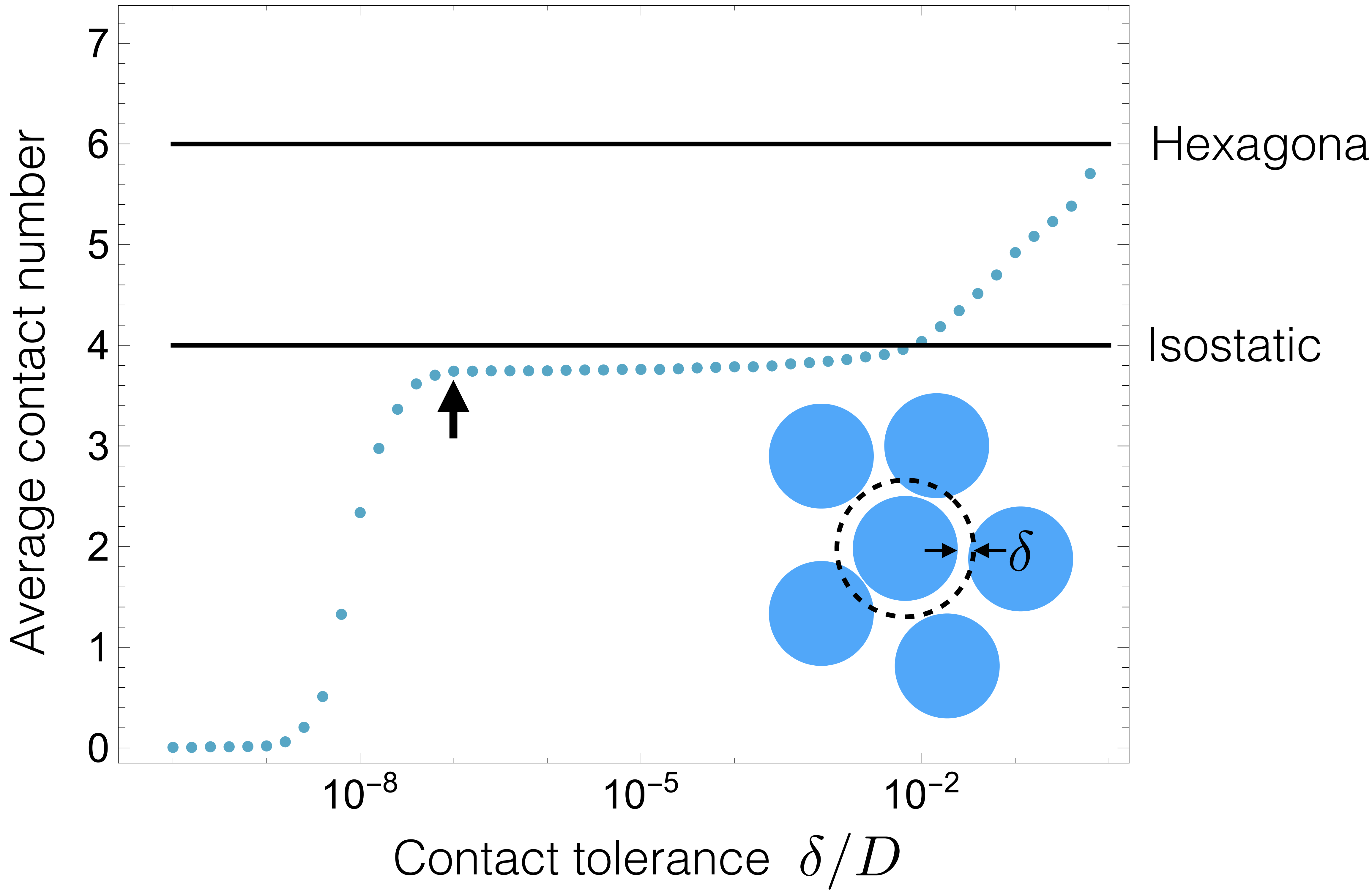


Better motions can be found from center of polytope

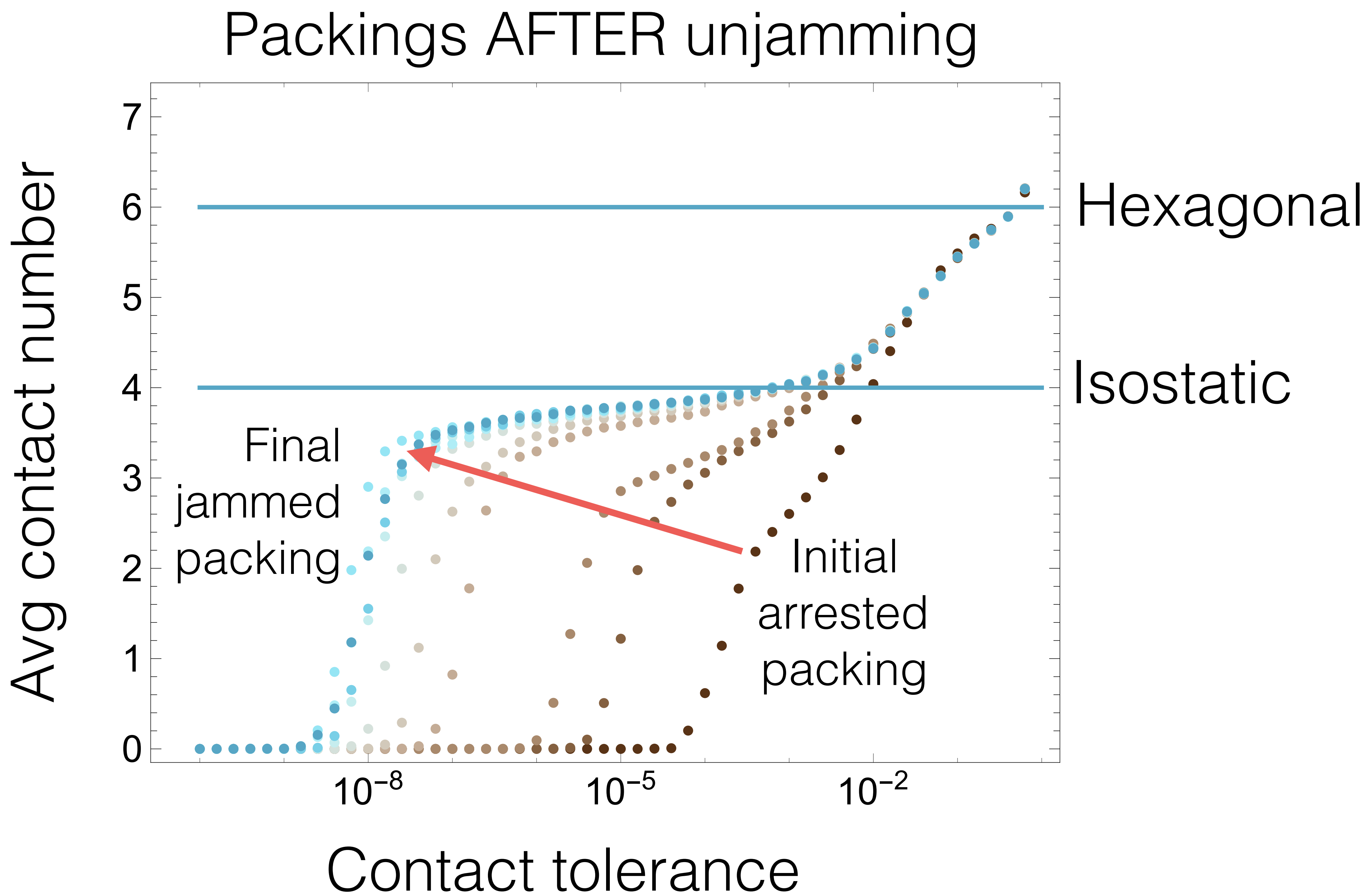
Repeated unjamming and relaxation creates better packings



Contact number must be assessed as a function of contact tolerance

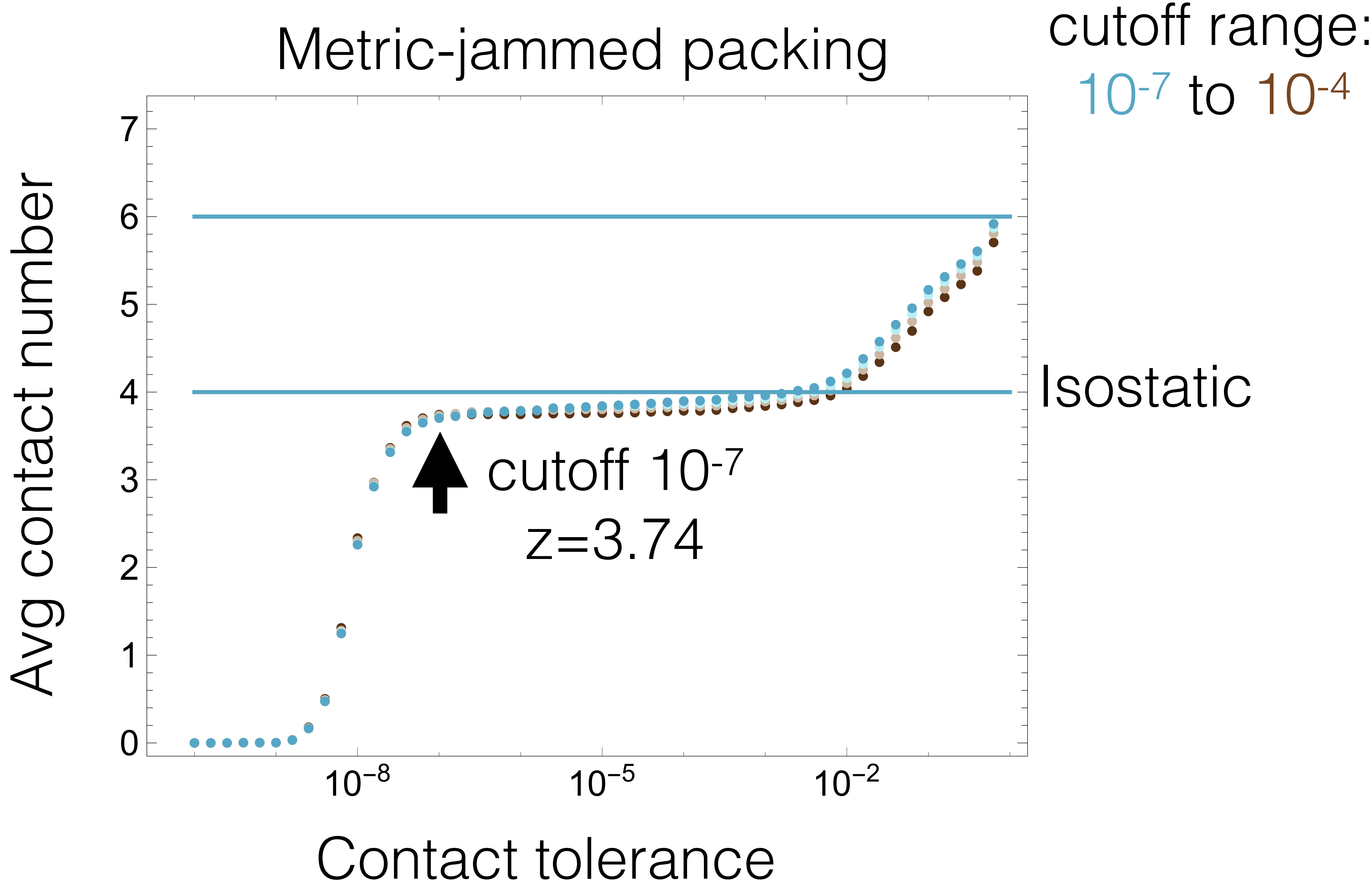


Packing approaches isostaticity as contact tolerance is increased.



Rattlers

Contact number plot is insensitive to the cutoff for removing rattlers



Mechanical stability requires four contacts per particle.

of degrees of freedom = # of constraints

n particles in 2D → 2n degrees of freedom

Z contacts per particle → nZ/2 contacts (each contact is shared between two particles)

→ $Z=4$ for spheres in 2D

This need not be the case on curved surfaces due to the nonlinearity of the surface constraint

6 particles on a sphere

6*2 = 12 degrees of freedom

6*4/2 = 12 contacts

OK!

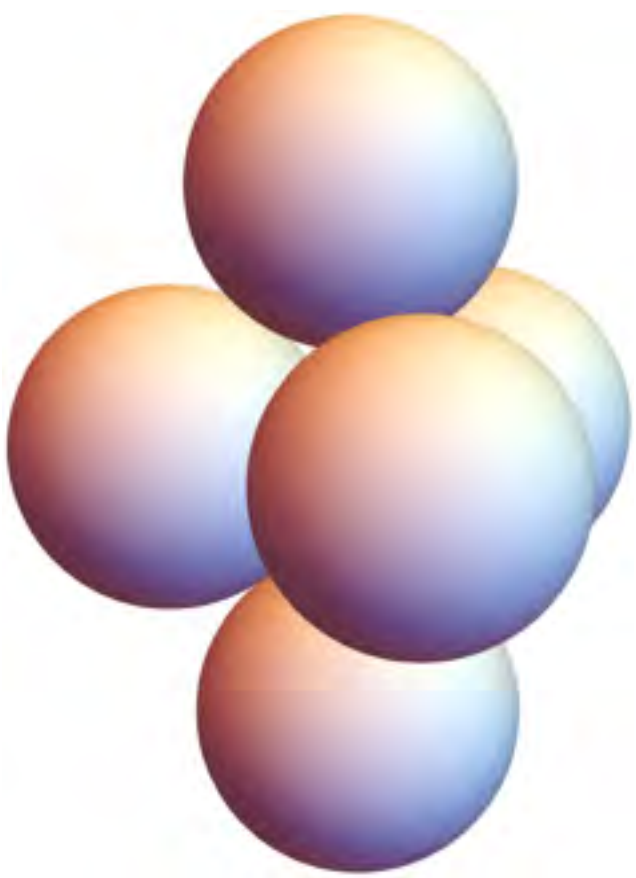
5 particles on a commensurate ellipsoid

5*2 = 10 degrees of freedom

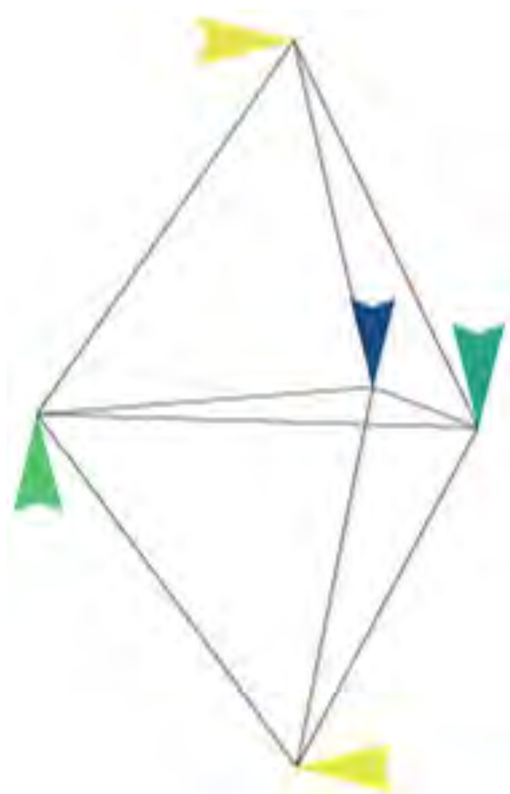
(3*4+2*3)/2 = 9 contacts

Apparently unstable?

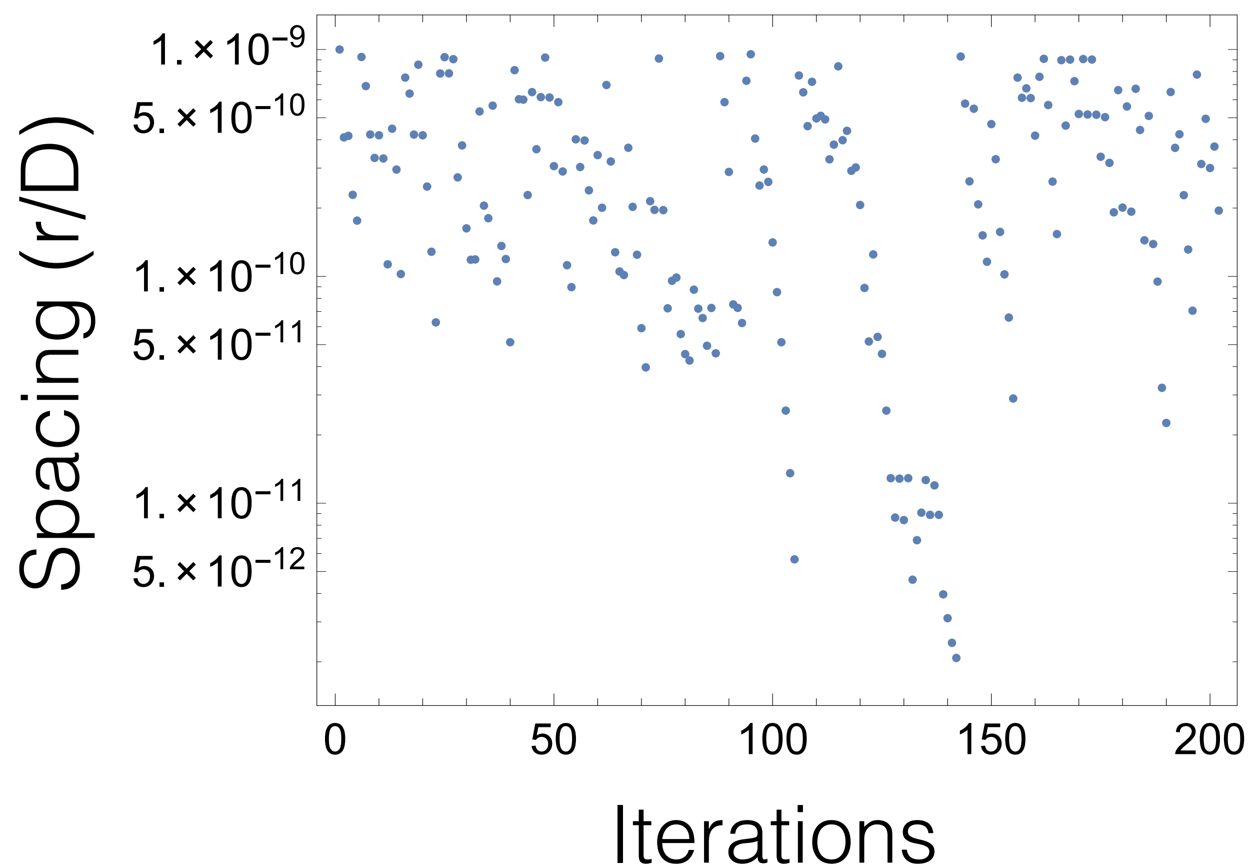
Our counterexample is unstable with respect to linearized constraints, but not with respect to the full problem



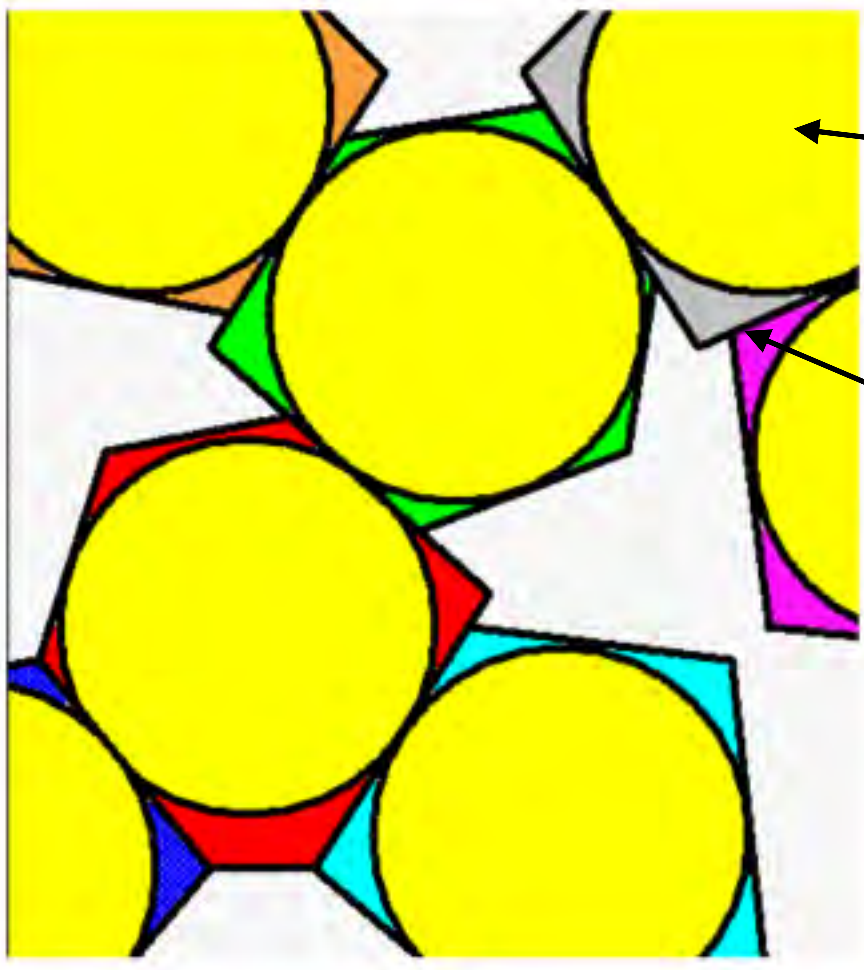
Linear program finds an "allowed" motion



But applying it doesn't unjam the packing



Nonspherical packings can also be under constrained



2D nonspherical particles require Z=4

Spheres can rotate
(but we don't care)

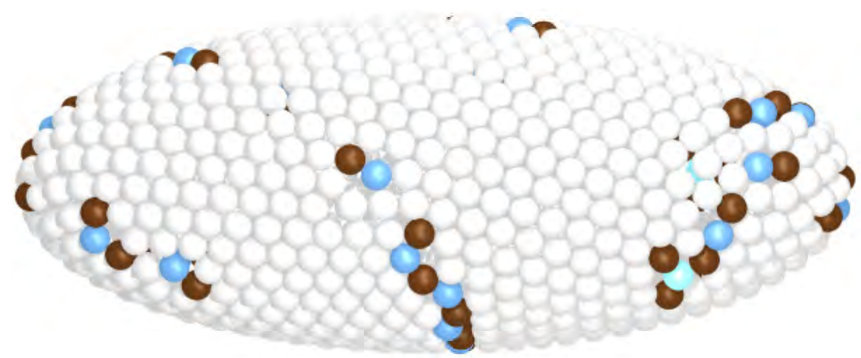
Add faces:
Break rotational symmetry,
but still stable without adding contacts

Appears underconstrained, but low curvature faces add constraints at higher order

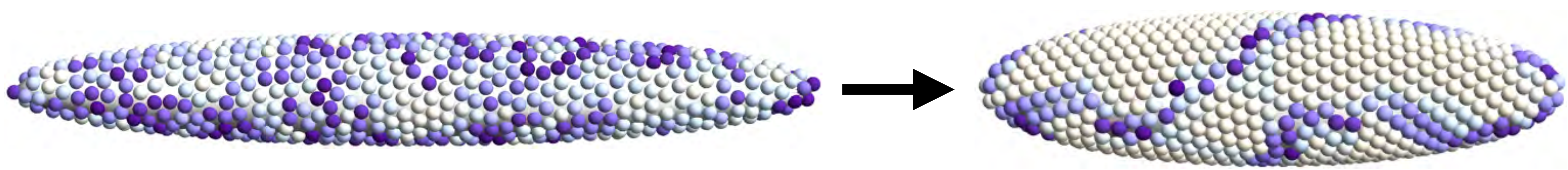
Donev et.al., PRE 2007

Summary

Geometry largely controls placement and type of defects

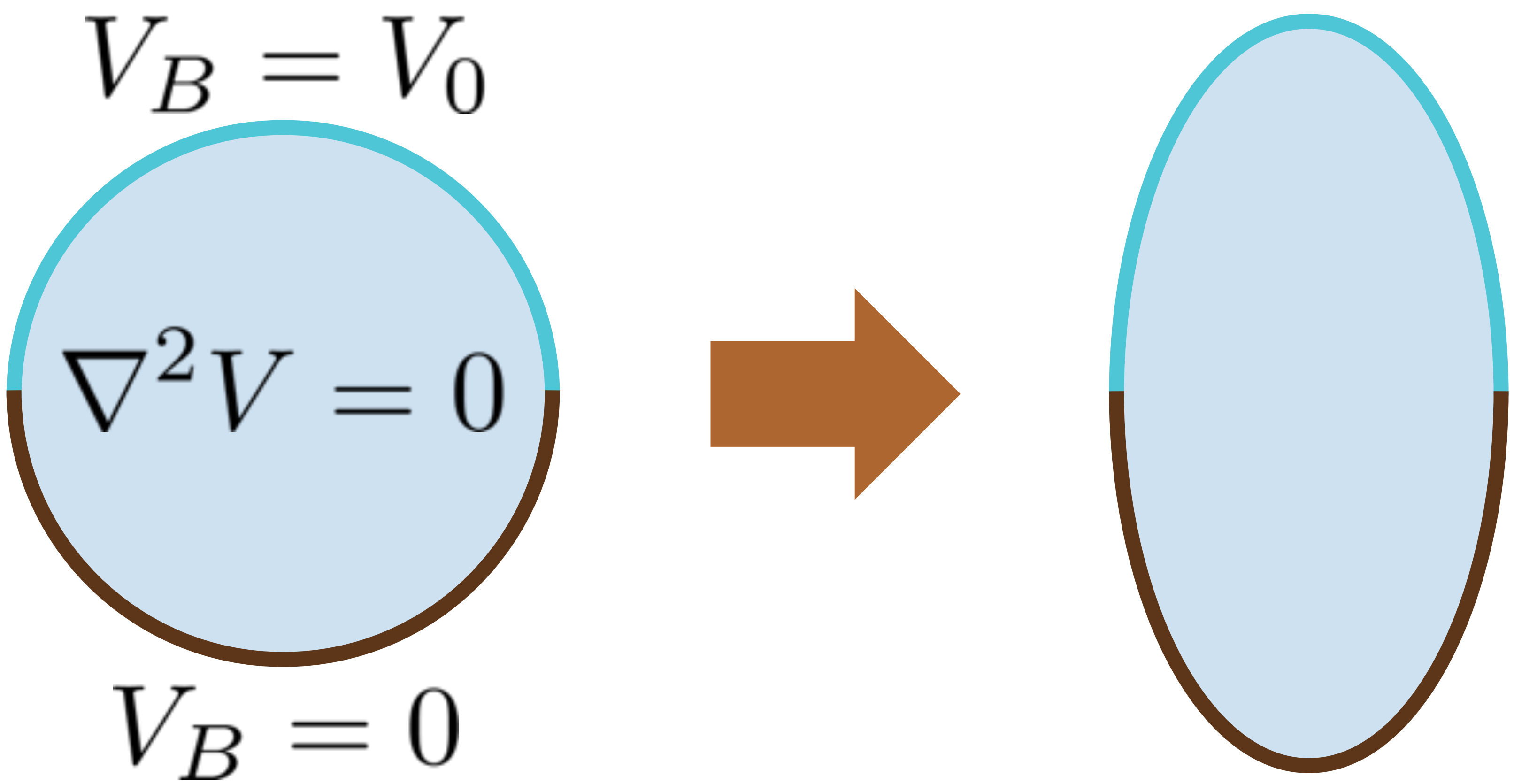


Dynamics alters the preferred position and affects the point of arrest



The initially arrested state then evolves towards a new **metric jammed** state through glassy dynamics

We're now looking at problems where order and shape co-evolve



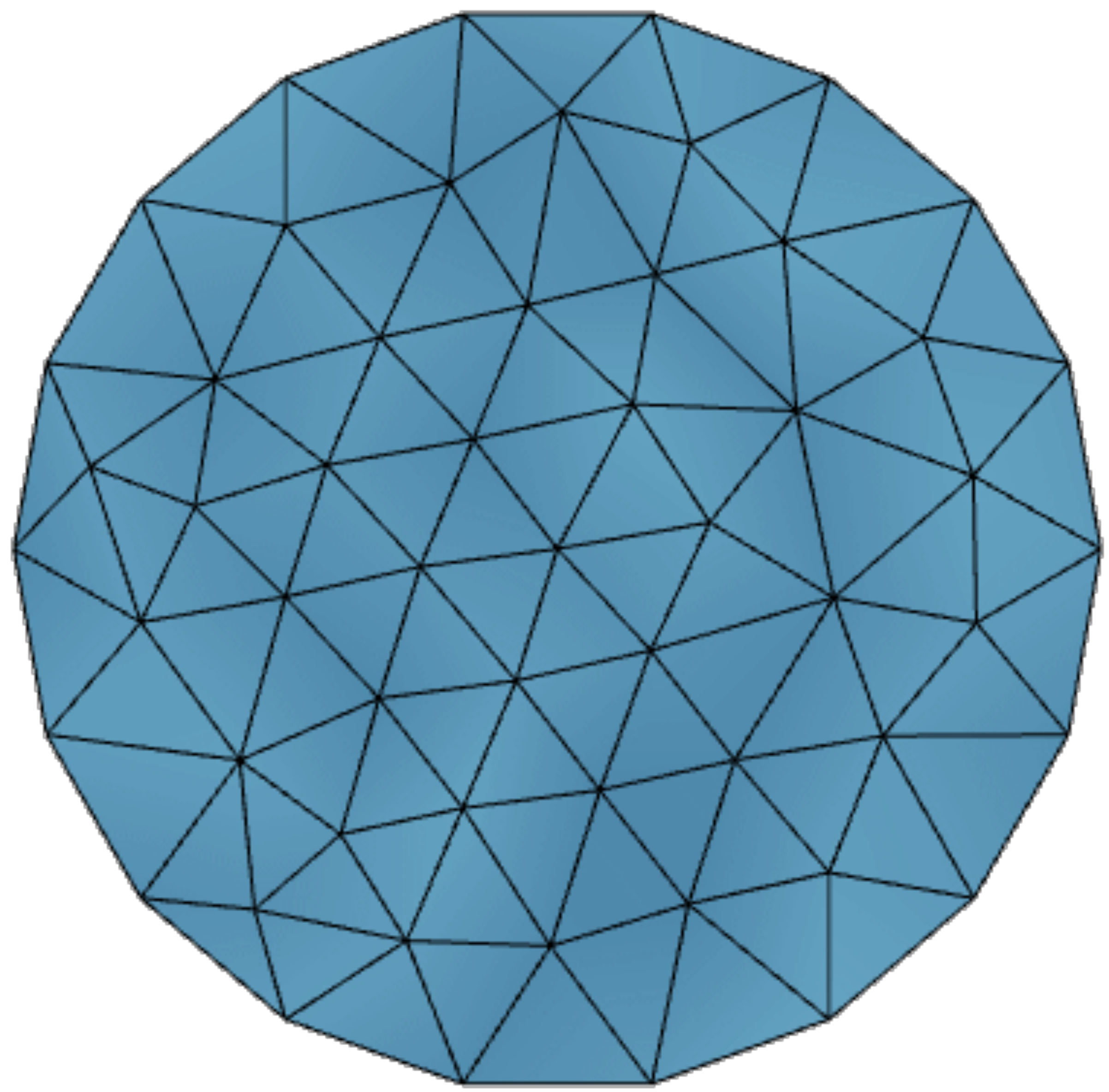
Minimize: $$E = \sigma \int_{\partial C} dl + \epsilon_0 \int_C (\nabla V)^2 dA + W \int_{\partial C} (V - V_B)^2 dl$$

Line tension — Electrostatic — Boundary Condition

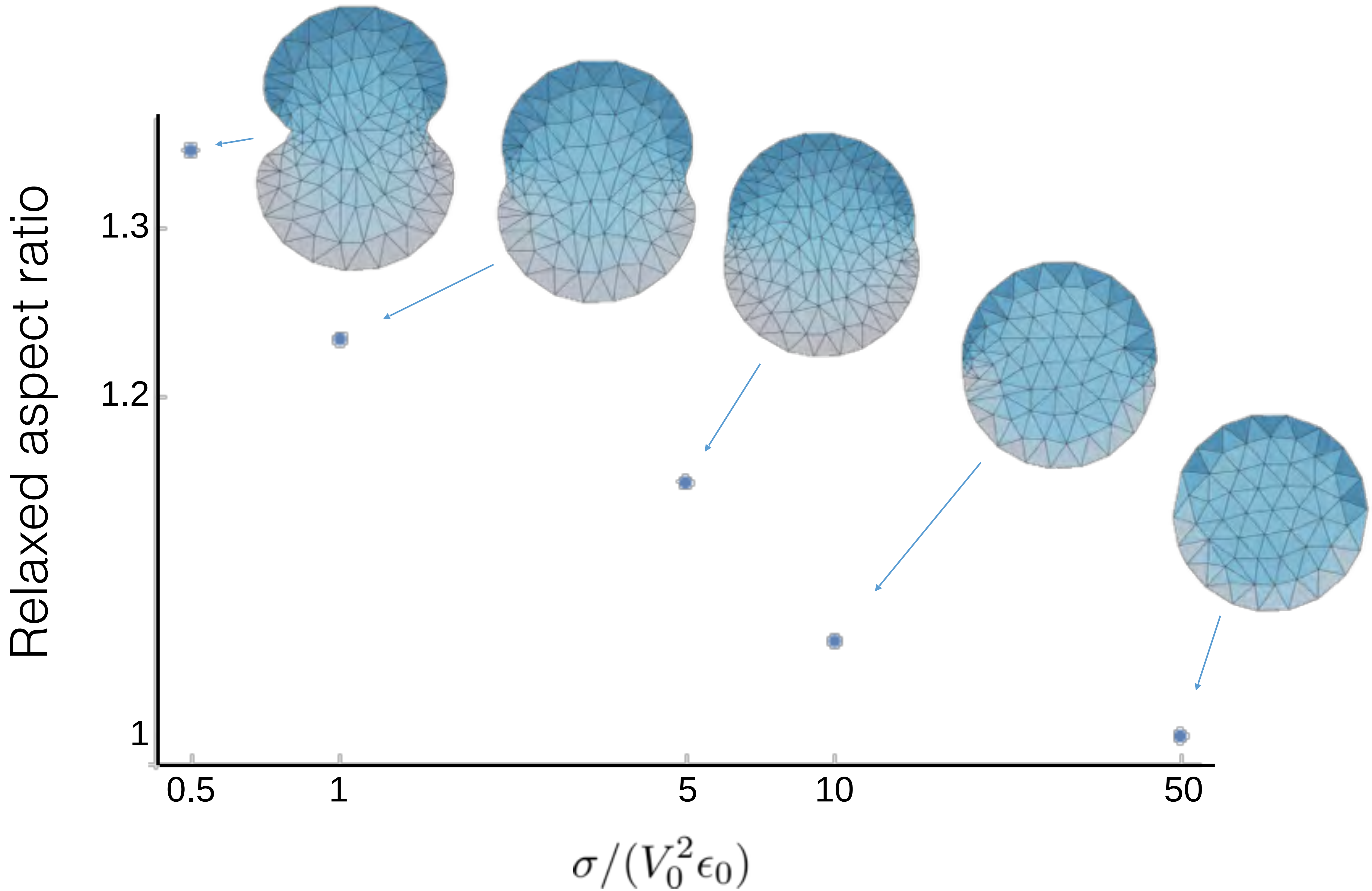
Subject to: $$\int_C dA = A_0$$

Area constraint

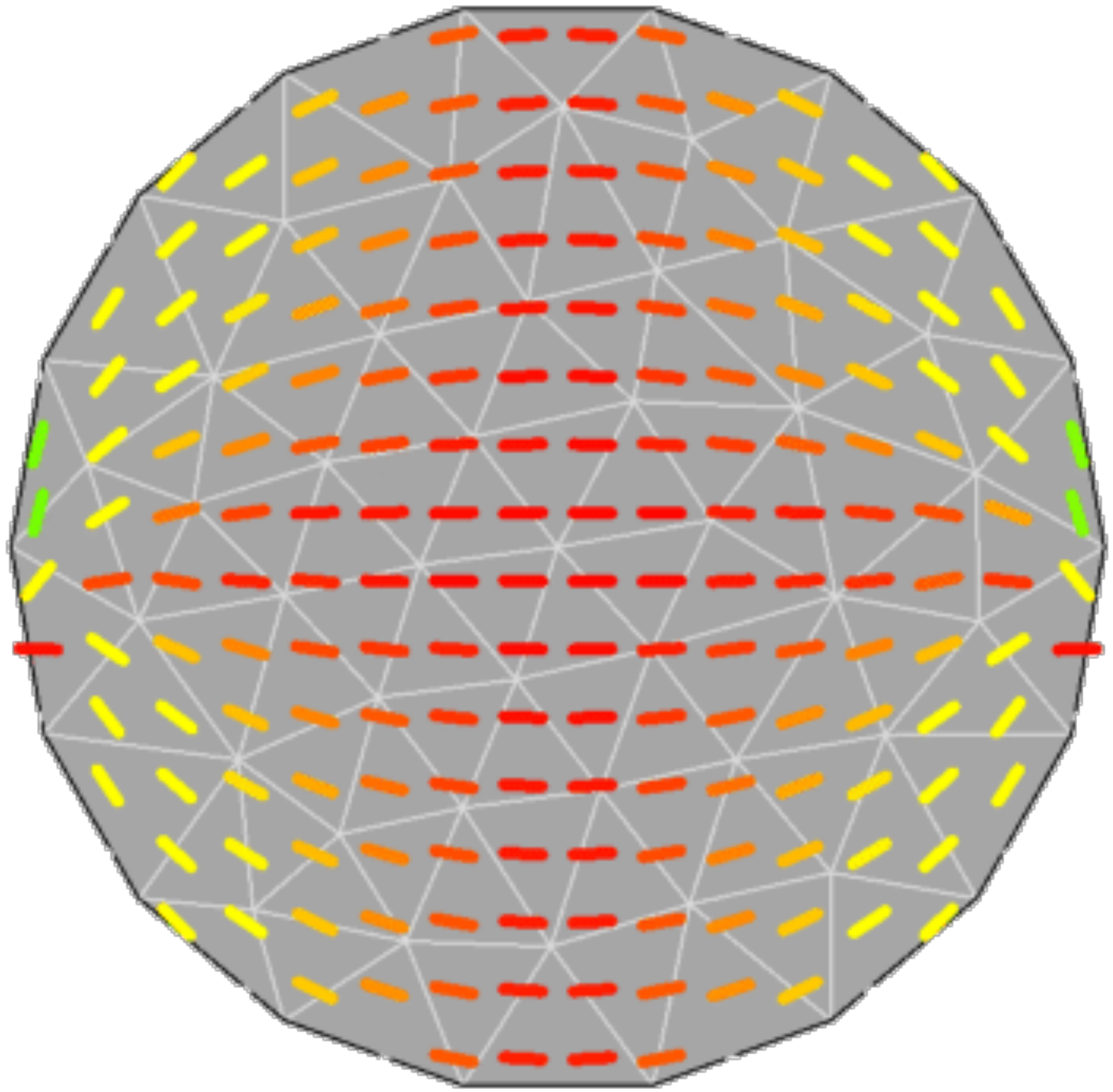
Finite element simulation with *Morpho*.



Relative strengths of line tension and voltage difference control aspect ratio

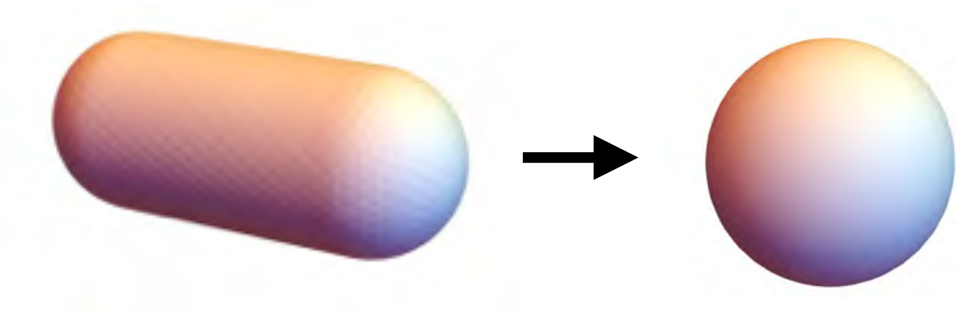


A LC in a flexible geometry requires simultaneous minimization of shape and order

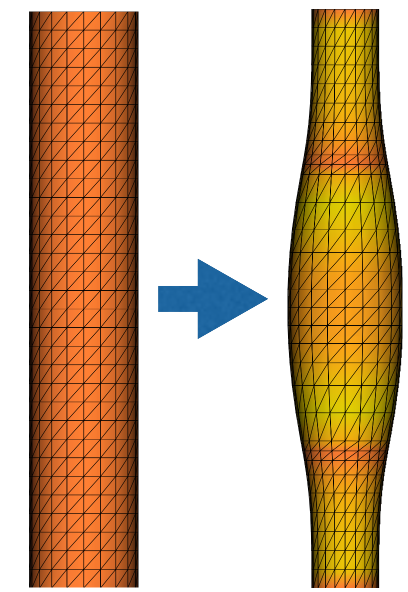


morpho *a language for shape*

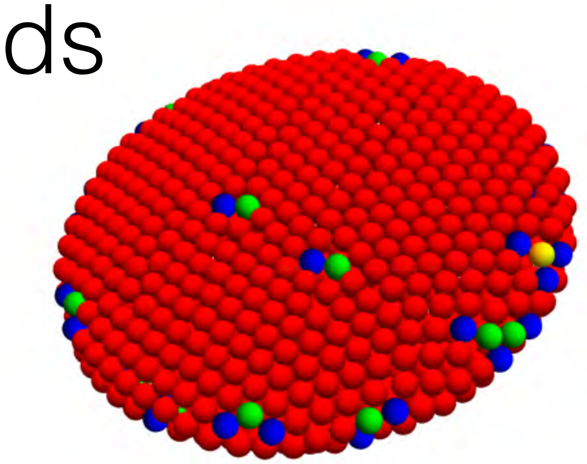
Surface minimization



Multicomponent systems



Particles and interacting manifolds



Minimize **arbitrary** functionals defined on a manifold C

$$\int_C f(q, \nabla q) d^n x + \int_{\partial C} g(q, \nabla q) d^{n-1} x$$

with respect to a set of field quantities q defined on it

and the shape of the manifold.

I'd like to thank…

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softmattertheory