Packing of bubbles and soft spheres in cylindrical confinement

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The model: Confined soft spheres

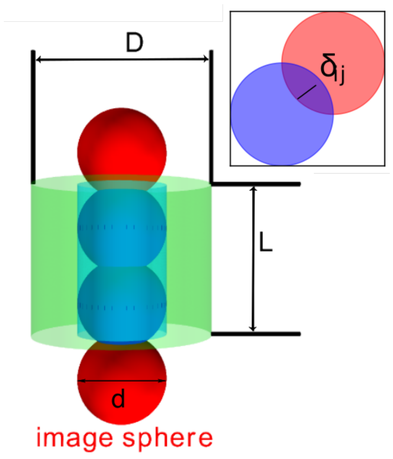


Figure 1: Definition of overlap and lengths.

- Soft interaction dependent on overlap:
$$U_{\text{soft}}(\delta_{ij}) = \varepsilon\delta_{ij}^2$$
- Soft confinement dependent on wall overlap:
$$U_{\text{conf}}(\rho_i) = \varepsilon\rho_i^2$$
- Periodic boundaries at top and bottom: image spheres twisted by angle α
- pressure term $pV = p\pi\left(\frac{D}{2}\right)^2 L$
- Energy:
$$E(\{\vec{r}_i\}, L) = \sum_{ij}^{N} U_{\text{soft}}(\delta_{ij}) + \sum_{i}^{N} U_{\text{conf}}(\rho_i) + pV$$

The Algorithm: Energy minimisation

- Start from random initial configuration
- Find energy minimum for given pressure p
- The Basin-Hopping algorithm
  - Monte-Carlo type algorithm
  - Global min. method in combination with direct min. (BFGS)
  - Directed random walk in parameter space $(3N + 2)$
  - `niter` steps with `stepsize` at temperature T

In the limit of hard spheres (no overlap)

hard spheres = no overlap

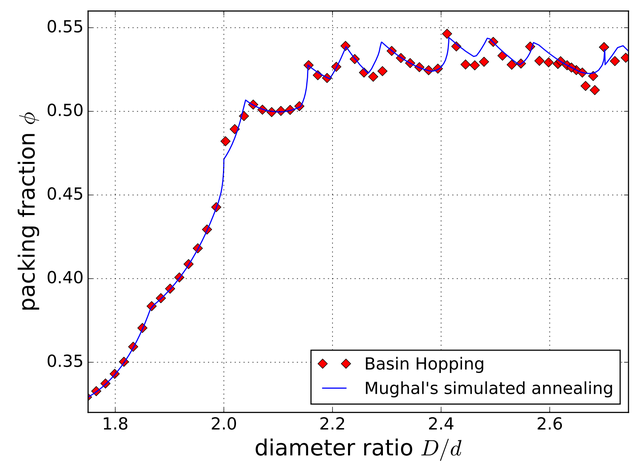


Figure 2: Comparison with present hard sphere methods [5, 3]

For each diameter ratio D/d:

1. decrease packing fraction $\phi = {}^{NV_{\text{sphere}}}/_{V}$
2. minimise energy
3. if overlap: continue with 1.
4. else: hard sphere packing found

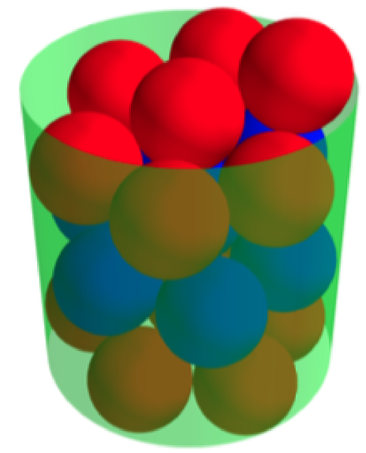


Figure 3: Hard sphere packing.

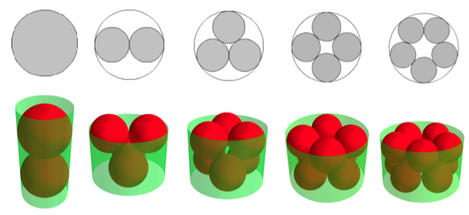
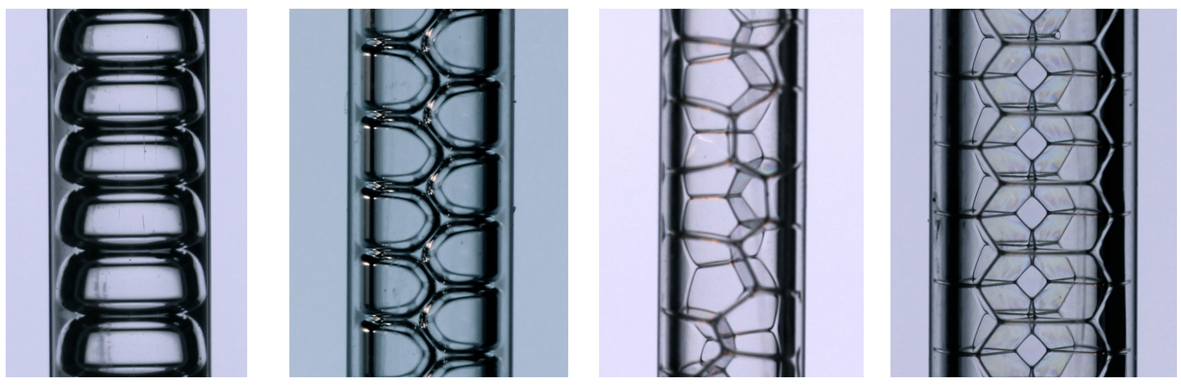


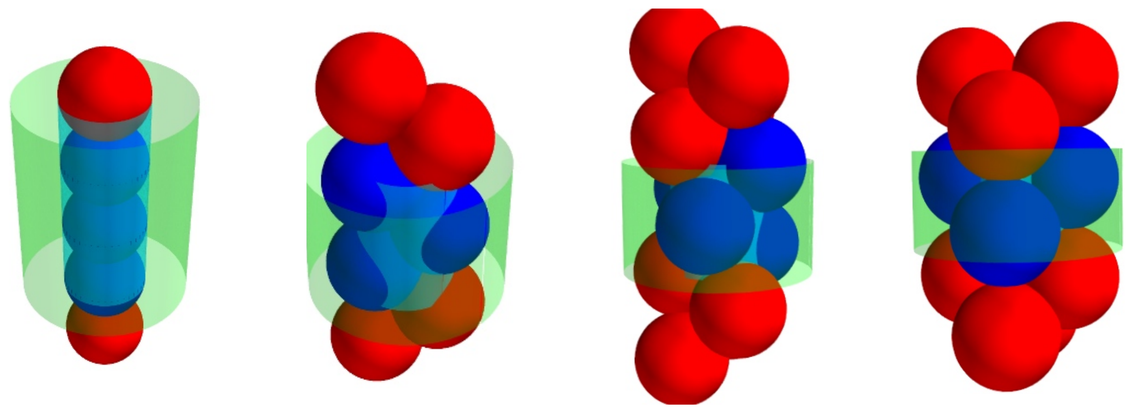
Figure 4: Columnar crystals.

Experimental structures



Bamboo **(2, 1, 1)** **(3, 2, 1)** **(4, 2, 2)**

Simulation structures



Coexistence of two structures

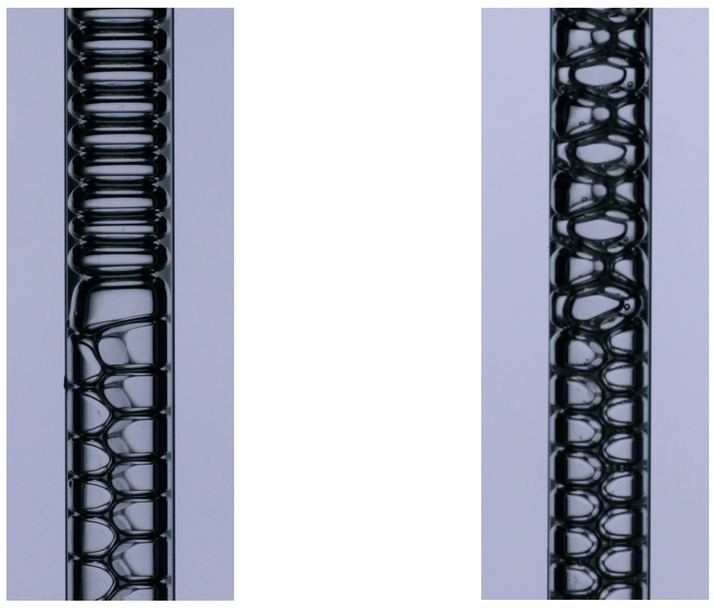


Figure 5: Bamboo and stair case (2, 1, 1).

Figure 6: stair case and (2, 2, 0).

Results for the soft sphere simulation

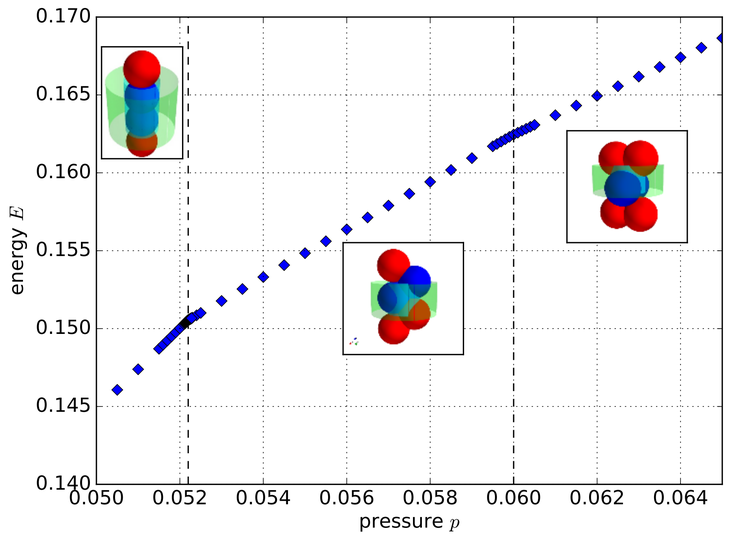


Figure 7: Energy per particle E for different pressures p.

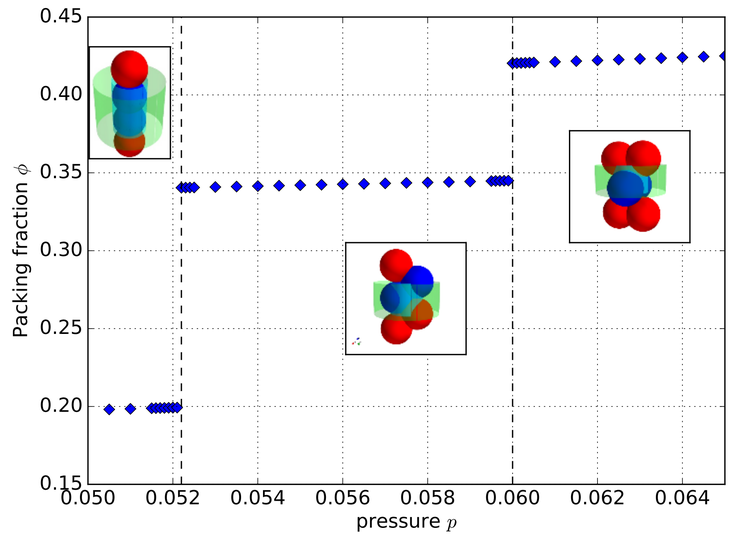


Figure 8: Packing fraction ϕ for different pressures p.

References

[1] K. A. Brakke. *The Surface Evolver.* In: *Experimental Mathematics* 1 (1992), pp. 141–165. [2] D. J. Durian. *Bubble-scale model of foam mechanics: Melting, nonlinear behavior, and avalanches.* In: *Phys. Rev. E* 55 (1997), pp. 1739–1751. [3] L. Fu et al. *Hard sphere packings within cylinders.* In: *Soft Matter* (2016), pp. 2505–2514. [4] S. Hutzler, D. Weaire, and R. Crawford. *Moving boundaries in ordered cylindrical foam structures.* In: *Philos. Mag. Part B* 75 (1997), pp. 845–857. [5] A. Mughal et al. *Dense packings of spheres in cylinders: Simulations.* In: *Phys. Rev. E* 85 (2012), p. 051305. [6] T. E. Oliphant. *Python for Scientific Computing.* In: *Comput. Sci. Eng.* 9 (2007), pp. 10–20. [7] S. Tobin et al. *Ordered polyhedral foams in tubes with circular, triangular and square cross-section.* In: *Colloids Surf. Physicochem. Eng. Asp.* 382 (2011), pp. 24–31.

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