Detachment Transition in a Model of Convexification of Clusters of Discs

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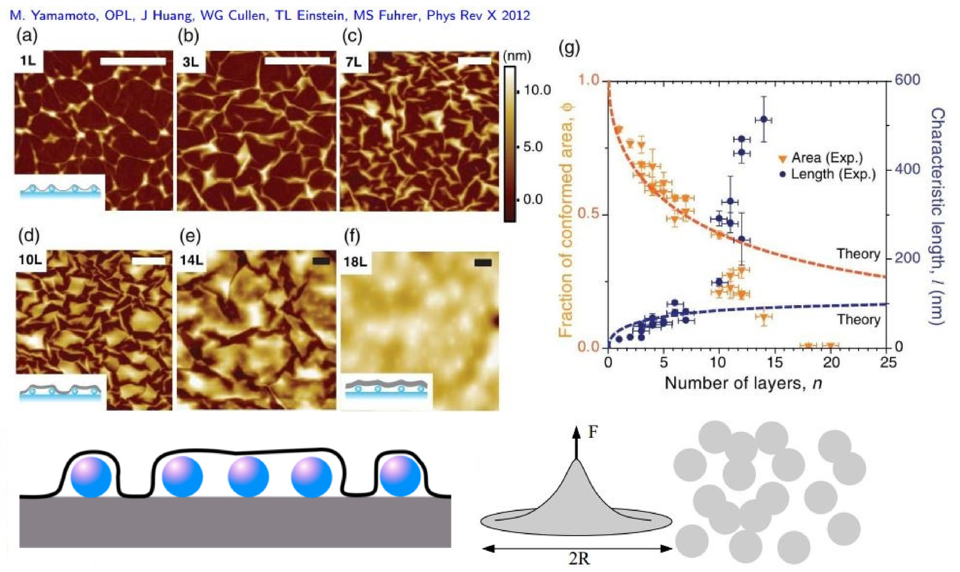
Abstract

Adhesion controlled by the roughness of the surfaces in contact, or by third bodies at the interface, is a recurring problem in contact physics, with applications ranging from geophysics to nanosciences. Inspired by experimental observations [1] of a detachment transition when one increases the density of nanoparticles intercalated between a graphene sheet and a flat substrate, we propose a simple statistical model which displays a similar transition. Experimental observations suggest that the observed transition results from collective effects that expand the detachment zones in the regions where its boundary is concave. Thus, we build a model based on the convexification of percolation clusters associated to individual detachment areas induced by each particle. Numerical simulations reveal that this model exhibit a discontinuous transition, i.e., the transition occurs via a macroscopic avalanche triggered by a microscopic change (here, adding a single particle to the system). Our model therefore shares similarities with explosive percolation and bootstrap percolation models. We also propose a quantitative interpretation of the unbinding transition of graphene with intercalated nanoparticles based on this model.

Inspiration: Experiments



- Unbinding transition observed when increasing the thickness of graphene
- Detachment zones exhibit collective effects

Applications:

- Engineering: Contact mechanics, tribology
- Geology: fragments in faults, fracking
- Graphene: **Strain Engineering**

Other applications of our model:

- Third-bodies problem
- Imbibition in 2D domains with pre-wetted zones
- Linear Separability in 2D classification

Models

Without collective effects: disc percolation

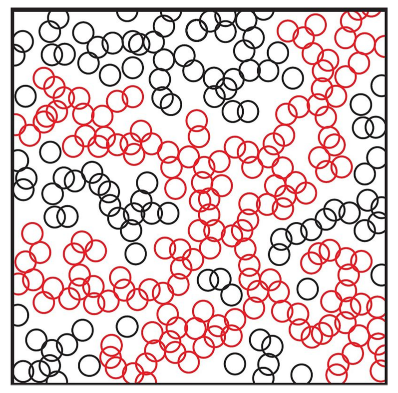
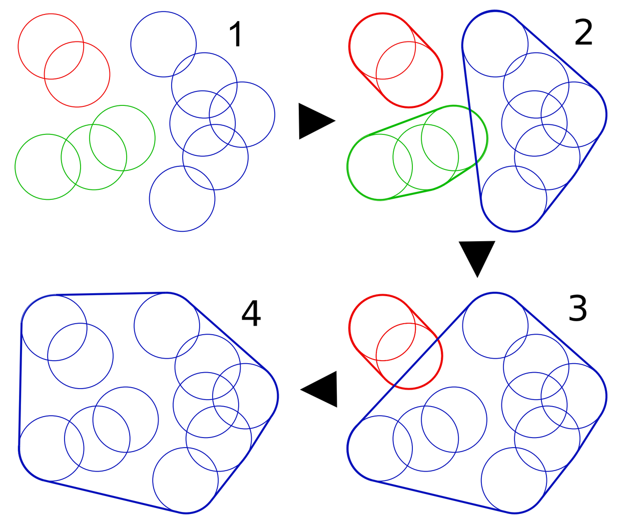


Figure 3: Illustration of the model of percolation of discs. In red, the percolating cluster

Iterative convexification



Questions raised:

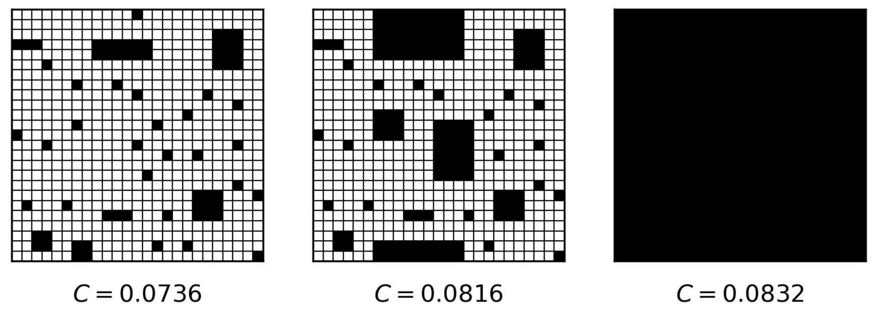
- Order parameter $\Phi(C)$ with $C = \rho_d \pi r_d^2$
- Existence of a transition, threshold value ?
- Continuity of the transition ?

Avalanche of convexifications lead to transition ?

Implementation:

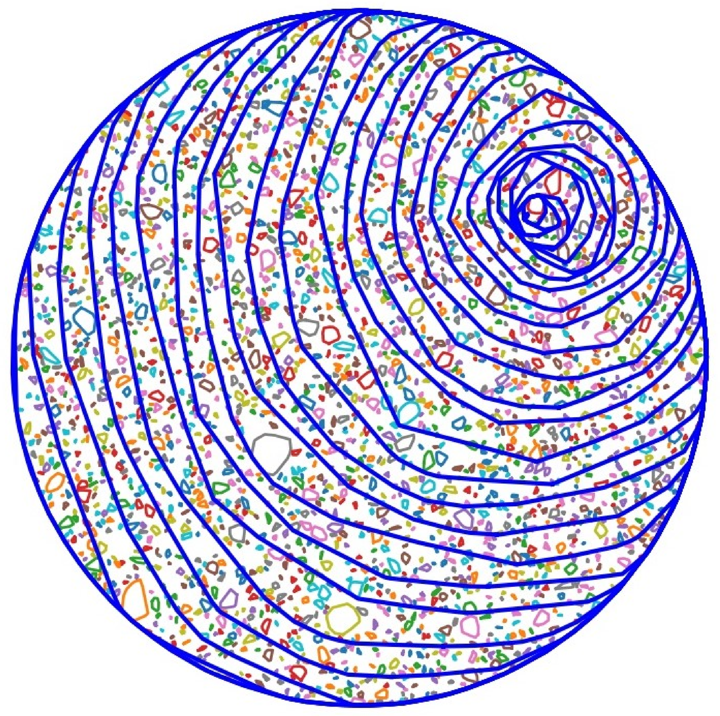
- Discs added one by one (Also some simulations with varying disc radius)
- Free edges or periodic boundary conditions
- Systems containing up to 10^8 discs

Bootstrap Percolation

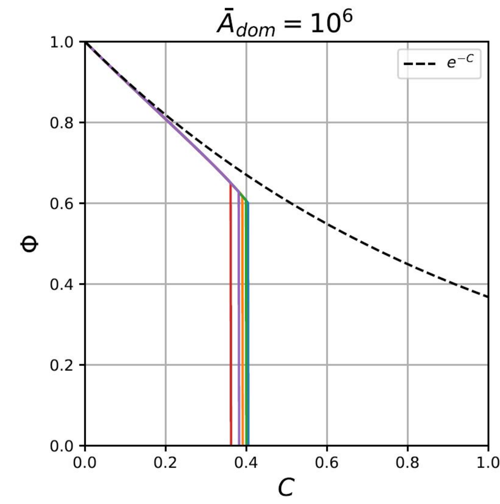


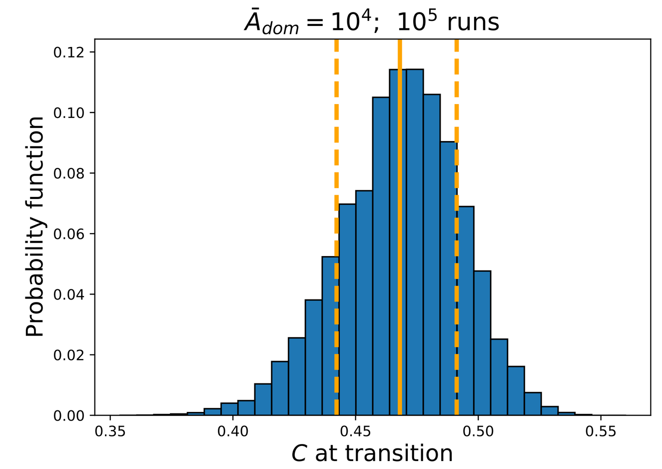
Is our convexification model a continuous, isotropic generalization of bootstrap percolation ?

Results: Macroscopic Avalanches



43121 → 43122 discs





- Mechanism of transition: an avalanche of convexifications when a critical disc is added
- Discontinuity over one realization
- Distributed transition

Results: Finite Size Effects

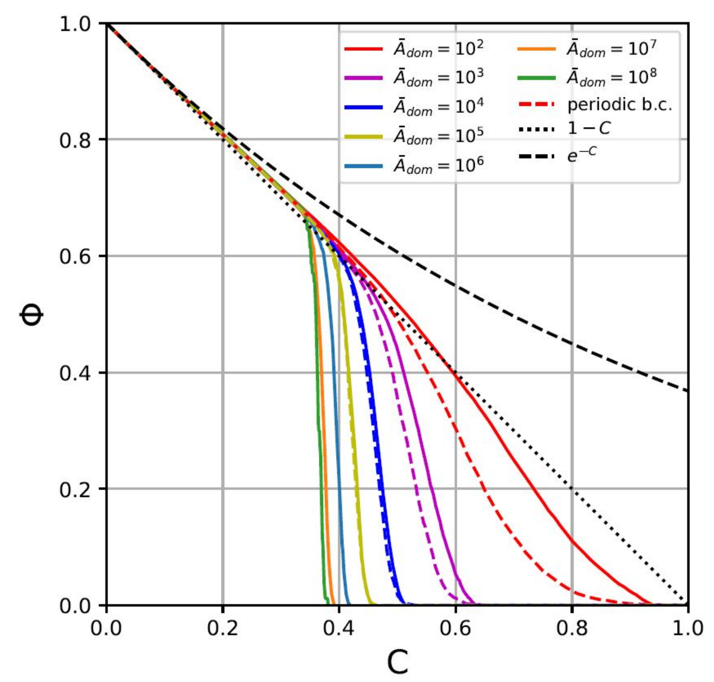
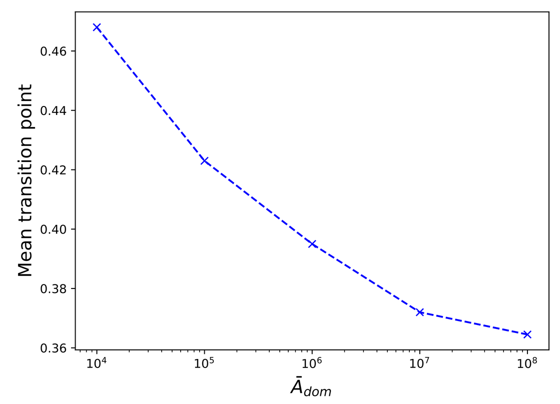
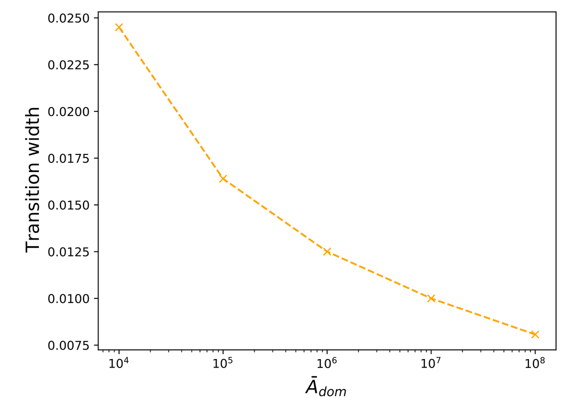


Figure 1: $\Phi(C)$ averaged over realizations. Various system sizes and both boundary conditions





- Asymptotic transition at finite C or zero C ?
- Very slow convergence

Comparison with Experiments

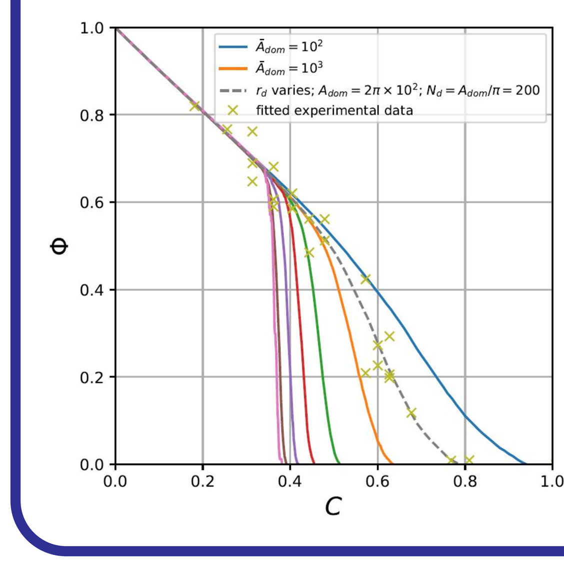
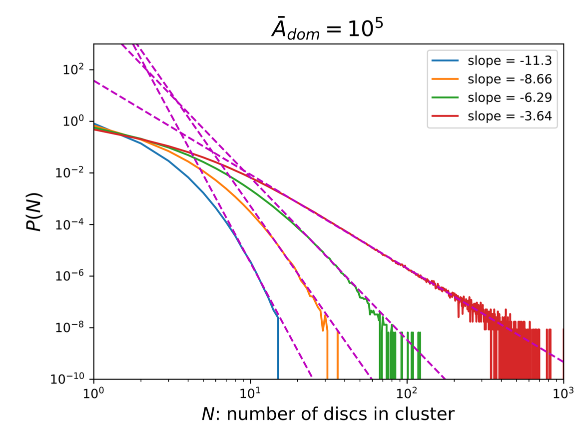
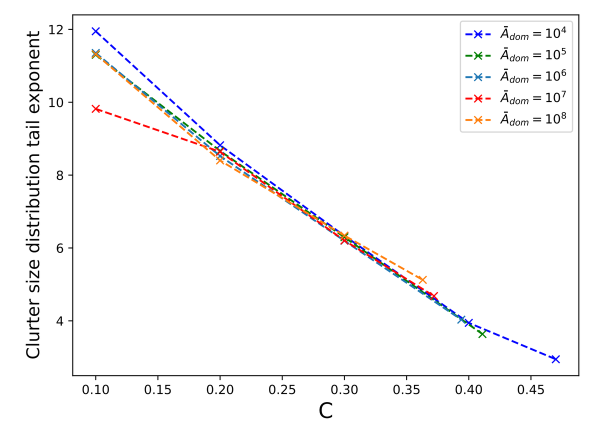


Figure 2: Crosses : fitted experimental data, compared with simulation results

Comparison with our system size gives a characteristic lenght $l \simeq 1\ \mu m$

Cluster Size Distribution





- Power laws tails at finite C
- Exponents depend on C, not on system size
- Exponents depend linearly on C

References

[1] Mahito Yamamoto, Olivier Pierre-Louis, Jia Huang, Michael S. Fuhrer, Theodore L. Einstein, and William G. Cullen. The princess and the pea at the nanoscale: Wrinkling and delamination of graphene on nanoparticles. *Physical Review X*, 2(4), 2012.

[2] Raissa M. D'Souza and Jan Nagler. Anomalous critical and supercritical phenomena in explosive percolation. *Nature Physics*, 11(7):531–538, 2015.

[3] E. T. Gawlinski and H. E. Stanley. Continuum percolation in two dimensions: Monte Carlo tests of scaling and universality for non-interacting discs. *Journal of Physics A: Mathematical and General*, 14(8), 1981.

[4] Alexander E. Holroyd. Sharp metastability threshold for two-dimensional bootstrap percolation. *Probability Theory and Related Fields*, 125(2):195–224, 2003.