Physicists use a new absorbing-state model to investigate random close packing

August 31 2021, by Ingrid Fadelli

A dense random packing of steel ball bearings, dubbed "Random Close Packing" by Bernal in 1960. Credit: Credit: BERNAL, J., MASON, J. Packing of Spheres: Co-ordination of Randomly Packed Spheres. Nature 188, 910–911 (1960). 10.1038/188910a0

Sphere packing, a mathematical problem in which non-overlapping spheres are arranged within a given space, has been widely investigated in the past. It has been proven that the densest possible packing is a face-centered cubic (FCC) crystal with a space-filling fraction of $\phi_{FCC}=\pi/\sqrt{18}\approx 0.74$.

The densest possible random packing, dubbed random close packing (RCP), on the other hand, is still poorly defined. Past studies and simulations, however, have predicted its volume fraction to be $\phi RCP \approx 0.64$.

Researchers at New York University and Technion- Israel Institute of Technology have recently carried out a study aimed at further investigating the characteristics of RCP, using a new absorbing-state model they developed. Their paper, published in *Physical Review Letters*, confirmed original predictions of the value of RCP, while also representing RCP as a dynamical phase transition.

The work was inspired by a series of experiments carried out by David Pine and Jerry Gollub on the reversibility of particulate suspensions in periodic shear flow. One of the physicists on the team, Paul M. Chaikin, recently invented a model dubbed random organization (RO), which explained the findings gathered by Pine and Gollub in terms of a dynamical phase transition between quiescent and active states.

"Using the RO model and other similar absorbing state models, Dov Levine and Daniel Hexner showed that at the critical point, these models are hyperuniform, a quality that is often associated with vanishing density fluctuations in large scales," Sam Wilken, one of the researchers who carried out the study, told Phys.org. "This was confirmed in my thesis and in a subsequent paper. In my thesis, I extended the RO model to include repulsive interactions and renamed it biased random organization (BRO) to obtain a quantitative fit for my experiments on sheared suspensions."

Absorbing state models are derived from toy models that describe the spread or containment of viruses or diseases. These toy models show that in high-density regions (i.e., highly populated areas), particles (i.e., people) overlap and are considered active (i.e., infected).

Active particles are then given random displacements and spread out within a given space, to reduce their density and activity so that they can eventually become inactive or die out. Alternatively, they could infect neighboring, inactive and absorbing regions with which there were no previous overlaps in activity.

"The competition between infection and dilution determines the fate of a system, which either finds a configuration where no particles overlap (an absorbing state), or continuously evolves forever (an active steady-state)," Wilken explained. "These dynamically disparate states are separated by a critical point (here a critical density) characteristic of a second order phase transition."

RO, the model developed by Chaikin, is one of the first continuous absorbing state models (i.e., reaching on a continuum of space), as opposed to lattice models (i.e., physical models specifically defined on a lattice). The BRO model, introduced by Wilken in his thesis, mixes random and repulsively directed displacements of the active particles and therefore increases the system's critical density.

The BRO model was originally developed with the aim of studying the structures of dilute suspensions. Nonetheless, Wilken and his colleagues felt that it was compelling to investigate the densest possible critical states of the model, as dense packings of particles is a particularly old and fundamental physics problem.

"Surprisingly, our model does not crystallize in the dense critical state limit, where there are small displacements, and instead approaches what has been called random close packing (RCP)," Wilken said. "In this work, we demonstrate that the BRO model belongs to a well-studied class of absorbing state models called the Manna class, sharing universal dynamical exponents like the scaling of the fraction of overlapping particles on the active side of the transition, as well as the power law divergence of the time to arrive at steady state near the critical point."

In their study, Wilken and his colleagues found that critical states at small displacement sizes did not only approach RCP in volume fraction, but also exhibited structural behaviors that had not been previously associated with RCP. These behaviors included the divergence of the nearest neighbor pair correlation function, as well as isostatic coordination (Z = 6, on average each particle has six touching neighbors).

"Additionally, we show that the long-range density fluctuations (in S(q)) of the critical states go to zero in the large size limit as a power law (S(q) ~ q^alpha), where alpha is a universal Manna class exponent," Wilken said. "We believe that the association of RCP with a Manna class dynamical phase transition allows for a clearer path to studying RCP mathematically, especially because previously studied simulation models, like Lubachevsky-Stillinger and soft sphere relaxation, produce structurally identical density correlations."

The researchers found that past simulations and theoretical models converge at RCP, which suggests that this is a special state, as physicist J.D. Bernal had first hypothesized in 1960. Interestingly, in the BRO model used by Wilken and his colleagues, RCP arose as the highest density critical point. Other existing approaches describing RCP enforce constraints such as isostaticity, jamming and hyperuniformity, all of which are emergent properties in the researchers' BRO model.

In the future, the work could inspire further studies focusing on RCP and applications of their model to the sphere-packing problem. So far, the team has primarily explored the structural and dynamical features of the BRO model in 2D bi-disperse and 3D monodisperse systems, yet they would soon also like to use the model to examine other systems.

"In preliminary studies we have found that in 1D and 2D BRO leads to closely packed crystal phases, while in 3D and 4D, it leads to disordered packings," Wilken said. "Introducing shear in 3D BRO simulations leads to crystallization and this points to the interesting role that dimensionality and isotropy play in the geometry and frustration of sphere packings. In the future, we plan to investigate these roles along with the implications on the configurational entropy of the random close packed states."

More information: Random close packing as a dynamical phase transition. *Physical Review Letters*(2021). DOI: 10.1103/PhysRevLett.127.038002.

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