CHAOTICALLY INTERACTING HARD PARTICLES CREATE ORDER OUT OF CHAOS

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Examples of application of an algorithm which imitates dynamics of an ensemble of interacting hard spherical particles in a constrained geometrical shape are discussed.
In the first example we are trying to achieve the highest density packing of a given number N of equal disks in a given geometric shape. The packing is generated by first placing randomly zero-diameter disks inside the container and then letting them expand uniformly without overlaps. Standard laws of elastic collisions are applied to bounce off the disks when they are attempting to overlap.
This chaotic procedure generates many interesting new patterns and symmetrical structures, including hexagonally packed fragments, "grains," with each grain having generally different orientation. Irregularity concentrates along the grain boundaries, as do the "rattlers," the disks that are not rigidly fixed in their positions but trapped in the cages formed by their fixed rigid neighbors or boundary walls if any.
The size of the grains increases as the expansion rate decreases.
For a sufficiently slow expansion a single hexagonal "crystal" emerges.
The crystal usually contains interesting structural deviations and insertions caused by the fact that the enclosing volume does not fit exactly a perfect hexagonal arrangement of the a priori chosen number of disks *N*.
For the cases of packings in a circle, a square, and an equilateral triangle, an interesting phenomenon of pattern repetition was observed. It appears that as number of disks N takes on an increasing sequence of values,
$N= N(1)$, N(2) .... N(k),...,
the packings follow a well-defined pattern.
Several such patterns and for each pattern its corresponding sequence of N's have been found.
The sequence may extend to infinity, for a shape that agrees with the perfect hexagonal order, like an equilateral triangle. Or it may cease to exist above some threshold value N* when the enclosing shape does not agree with the hexagonal order, like the shapes of a circle or square.
In the second example we study crystalline-amorphous interface in 3D structures The size of spherical particles is fixed but the container is shrinking so that the particle assembly becomes packed. Some particles are selected to represent the crystallic "seed." They are placed in prespecified ordered positions and can not move during the compression. The other particles are free to follow the mechanics of elastic collisions. It appears that the interface structure and parameters depend very much on the geometry of the "seed."
In the third example, after the expanding particle configuration (in 3D) achieves a certain density, the expansion stops and the particles continue their chaotic motion. If the stopping point is chosen appropriately, then after a while one sees a rapid spontaneous ordering (crystallization) of the previously disordered (amorphous) ensemble.