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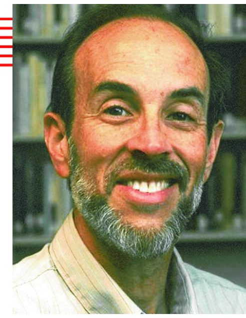

Discrete and Continuum Descriptions of Matter

Jerry Gollub

Physicists often describe nature in two opposing ways, which I characterize as particle and continuum approaches. In the particle approach, we try to understand the properties and dynamics of isolated objects and their interactions. In the continuum approach, on the other hand, we ignore discreteness, use conservation principles to formulate continuum equations, and then solve or simulate those equations to explain complex phenomena.

Here, I illustrate those contrasting methods by describing phenomena that occur in the physics of granular materials and particles immersed in fluids. These phenomena have a host of applications in engineering, geophysics, and astrophysics, and are of considerable intrinsic interest. Although the complementarity of particle and continuum or field approaches also has a long history in our understanding of physics on subatomic scales, it will be interesting to see how that issue plays out in a macroscopic, yet still controversial, context.

In fluid dynamics, a continuum description seems manifestly appropriate because the molecular scale is so much smaller than the scale of typical flows. However, molecular discreteness sometimes plays an important role in fluid dynamics—for example, in describing flow near a solid boundary. Macroscopically, one normally assumes a "no-slip" condition to describe the vanishing of the tangential velocity at the boundary. On the other hand, when fluids are manipulated in microfluidic devices, deviations from the no-slip condition due to molecular discreteness become significant.

Granular physics

In studying the physics of granular materials such as sand, one usually starts from a particle point of view.

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That approach is appropriate and relatively successful when the particles are highly excited, are in random motion, and are undergoing inelastic collisions with one another. This random motion is produced by vibration or shear, either on Earth or in microgravity experiments. A useful paradigm is a granular gas, which is much like an ordinary gas except that collisions between particles are dissipative. Theoretical models often use the concept of a granular temperature, which is proportional to the mean square particle velocity. Modeling the dissipation due to collisions in a granular gas can be subtle; the energy loss depends strongly on the incident energy, a result that is incompatible with the often-used concept of a coefficient of restitution.

Some researchers have used a continuum approximation to obtain a version of hydrodynamics for granular media. The strategy is sometimes useful—for example, in treating energy transport in highly excited granular matter. However, the continuum approach can be problematic. When the degree of excitation is low, gravity often produces persistent contacts between particles, so their interactions are not limited to the isolated collisions that are assumed in justifying a continuum approximation. Also, if you shake a granular medium to excite it, the energy subsequently decays rapidly but unevenly due to huge numbers of inelastic collisions. This collision process leads to inhomogeneities in the local kinetic energy on scales only a few times larger than the particle size. The distribution of internal stresses in both the static and dynamic states is highly nonuniform, and the stresses are transmitted along linear chains of particles, in contrast to the situation in ordinary solids. Researchers have devoted much attention to understanding such effects. Because the inhomogeneities are so prominent, it is difficult to treat the network of forces between interacting particles accurately using continuum methods, although one promising research effort is to determine whether there is some length scale above which spatial averaging makes sense.

Explaining shear flow

An important test of continuum ideas is to predict the response of a granular material to applied shear. The resulting flow is largely confined to thin boundary layers and does not penetrate the entire medium, as would occur in an ordinary fluid. How is this behavior to be understood? A variety of approaches have been proposed. Some scientists use a hydrodynamic picture but allow for complex material properties, such as a viscosity that depends on location and time as a result of variations in the local particle concentration. A simple parameterization of the internal stresses is a simplification, because the local properties are anisotropic and history dependent, and the flow fields vary rapidly in space. Still, continuum theories can often give a decent approximate description and can convey insight.

Other researchers treat sheared granular materials by using particle-based computations instead of hydrodynamics and explain complex phenomena by "molecular" dynamics simulations that model collisions between particles in more or less realistic ways. Particle-based simulations are generally much faster to compute than solving differential equations, and allow one to explore the nature of collisions. Such simulations can successfully describe the development of shocks, which arise when speeds higher than the local "sound" velocity occur. If the material is dilute and highly excited, both particle-based simulations and continuum theory work reasonably well in describing shocks.

Surprises

Some phenomena in the physics of granular materials are surprising and problematic to model. A granular mixture that partially fills a horizontal tube rotating about its axis tends to unmix, with different particles forming separated bands on long time scales. Particle-based theories are cumbersome for describing band formation, which occurs gradually over times corresponding to millions of collisions. Continuum models based on variations of the dynamic angle of repose (the angle made by a flowing material with respect to the local horizontal plane) can account for many features of the observations, but still falls short of fully describing the phenomenon.

An important problem that may benefit from a continuum approach is the occurrence of large geological landslides that sometimes bury towns. These avalanches can travel long distances, apparently behaving as a fluid even though they are composed of coarse material that may include trees and boulders the size of houses. The photograph at right of Devils Postpile National Monument shows a macroscopically linear slope that, despite being composed of large rodlike boulders, resembles what one finds on much smaller scales for sand. Several interesting continuum approaches to understanding avalanches have been proposed. In one approach, the material is considered to be a mixture of solid and liquid phases that can interconvert in response to perturbations.

Rod-shaped boulders at Devils Postpile National Monument near Mammoth Lakes, California, form a well-defined mean angle of repose despite their large size and complex shapes. Continuum models can describe some properties of granular systems on large scales. (Photo by Charles Webber, © California Academy of Sciences.)

Particles in fluids

How does one deal with the extremely common situation of suspensions, that is, fluids containing particles? Examples include the transport of sand in the oceans, sand-forming dunes in air, the motions of colloidal particles in fluids, and the suspended particles that are used in catalytic reactors. Particles moving in a fluid react to the background, but they also interact with each other in complex ways. For these problems, it seems that neither the particulate nor the hydrodynamic (continuum) approach adequately describes all observed phenomena. It may be beneficial to combine the two approaches in creative ways.

In some cases, relatively simple phenomena can be isolated and understood. For example, closely spaced particles suspended in a liquid shear flow experience a kind of chaotic motion due to their interactions; their motion accurately mimics the thermal diffusion of molecules in a liquid, although the cause is quite different. Fluids that contain suspended particles also manifest pattern-forming instabilities, and those patterns can sometimes be treated using hydrodynamic models in which the particles affect the fluid's rheology. If particles move relative to the fluid—for example, as a result of imposed vibration—the particles experience hydrodynamically generated attractive forces that can lead to ordered arrangements. Similar interactions between particles also affect sedimentation in fluids. Analysis of continuum equations can potentially lead to insights into the dependence of instabilities on parameters, information that is hard to obtain in other ways.

When even a small amount of liquid is added to a dry granular material, the material's cohesion increases dramatically, as anyone who has made sandcastles knows. The increased cohesion is caused by the surface tension of liquid trapped in the narrow gaps between the particles. Those forces aren't simple to simulate, but are of great significance. For example in soil mechanics, the prediction of the stability of soil on slopes is a critical problem.

Experimental challenges

The difficulties in constructing robust particle-based models of granular-flow phenomena are compounded by difficulties in measuring the properties of individual particles. The typical time interval between collisions can be extremely short in dense granular materials, so measurements of instantaneous velocities are impractical. The effective viscosity of a granular medium (with or without an interstitial fluid) diverges as a critical particle density is approached. Therefore, measuring small fluctuations in the actual density (or filling fraction) is both important and difficult. The surface properties of particles also affect frictional interactions. Thus, problems in measuring individual particle properties may lead one to favor continuum modeling. Other methodological issues arise in numerical simulations. Especially when a liquid is present, a full two-phase simulation of the particles and fluid is a demanding challenge.

The complementary strengths of particle-based and continuum approaches are needed to explain many phenomena involving granular and fluid dynamics. Experiments conducted in my own laboratory and in many others show both approaches to be useful, and eliminating either one leads to trouble. We can best make progress by using the two views appropriately, sometimes in combination. Similarly, discrete and continuum modeling have contributed to other areas of physics, such as the gravitational interactions of stars and galaxies, and the dynamics of large nuclei. I invite you to imagine phenomena in your own field in which a single modeling approach does not tell the whole story.

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