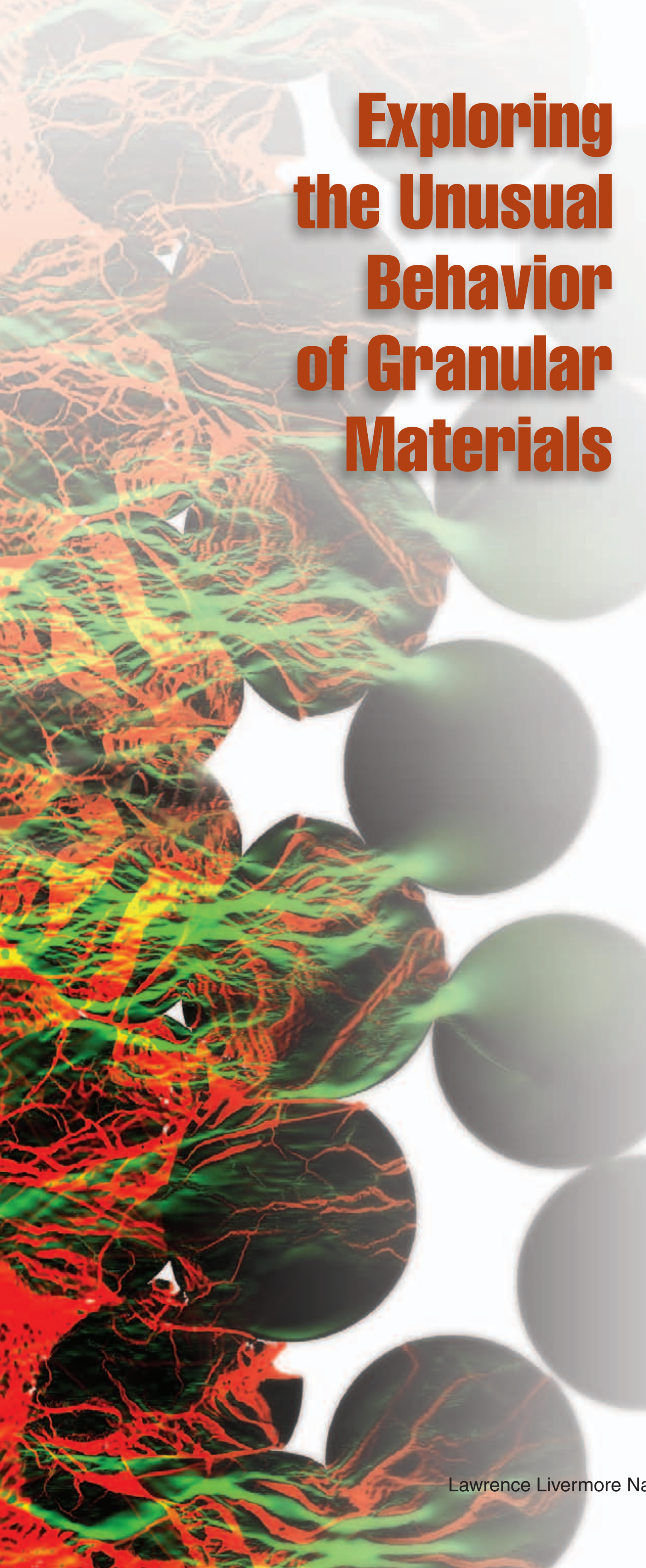
# Exploring the Unusual Behavior of Granular Materials



TRY pushing a pencil through a block of Jell-O, and it penetrates the substance with relative ease. But push that pencil into a bucket of sand, and the farther it goes, the more resistance it encounters. What causes this difference? Friction between the particles strongly affects the behavior of granular materials, such as sand. As a result, these materials respond differently to external forces than liquids, solids, or gases do. This unique attribute—one of many—makes it difficult to predict their flow and mechanical behaviors.

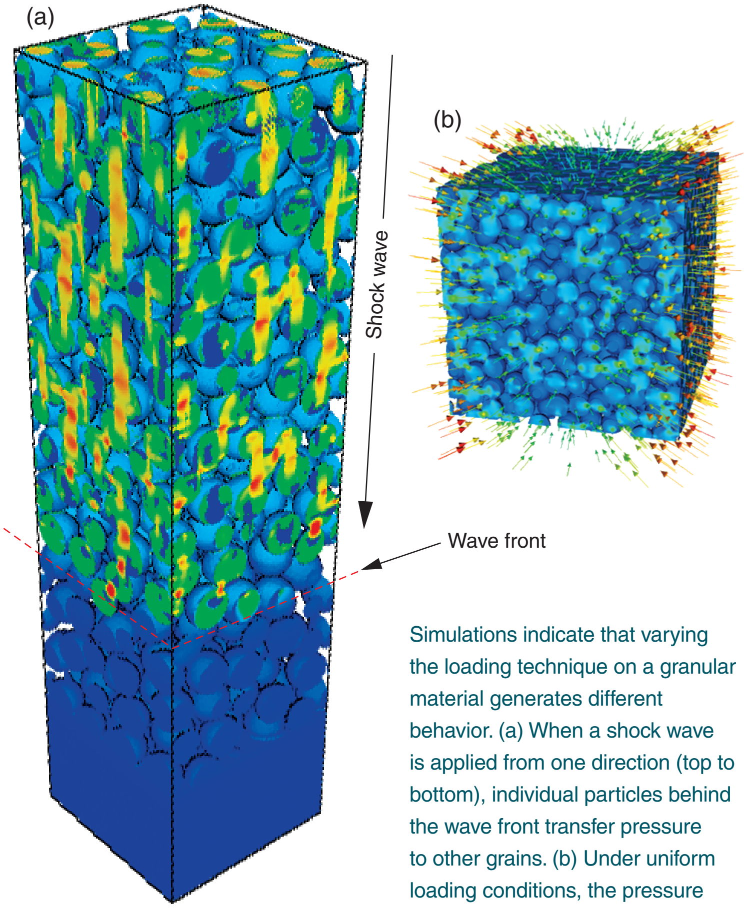
Granular materials stand in a class of their own, separate from other states of matter. Their behavior includes aspects of fluid and solid mechanics and molecular dynamics, but some responses are specific to them. In addition, properties that appear in the bulk material may not be exhibited by individual grains. To better understand these responses, scientists at Lawrence Livermore are developing predictive models to study granular materials under dynamic pressure loads so they can analyze material behavior at multiple scales, from the nanometer scale of grain–grain interactions up to the macroscale flow in a large conglomeration of particles.

"The Laboratory's expertise in experimental science, materials research, and high-performance computing makes us particularly qualified to take on this challenge," says Livermore physicist Tarabay Antoun, who leads the project team. The research effort, which is funded jointly by the Departments of Energy, Defense, and Homeland Security, will provide new modeling capabilities for use in many areas, from pharmaceuticals and agriculture to national security and defense. For example, the Livermore team is applying these models to help develop transparent ceramic armor for military vehicles. The research can also be adapted to study wave propagation in heterogeneous geologic materials and reactive transport processes in porous media such as soils and rocks. Understanding how fluids flow through porous media is vital to various research areas, including carbon sequestration and efforts to protect critical infrastructures from the threat of an earthquake or a terrorist attack.

## Taking a Closer Look

Granular materials vary widely in shape, size, and physical properties. The Livermore research is primarily focused on granular powders, which have the smallest particle sizes. Powders consisting of brittle materials are of particular interest because individual particles can fracture and fragment when compressed, making the material's overall response more difficult to predict. According to Antoun, the Laboratory team is combining experiments and

(left) As a shock wave propagates through a powder, individual grains (black dots) fracture and fragment, producing localized cracks (red lines) in the grains. Colors indicate the progression of damage, with red being the most severe.




Simulations indicate that varying the loading technique on a granular material generates different behavior. (a) When a shock wave is applied from one direction (top to bottom), individual particles behind the wave front transfer pressure to other grains. (b) Under uniform loading conditions, the pressure compacts the grains.

modeling to examine brittle material powders under dynamic loading and determine how changes in stress and strain are related to fracture and fragmentation processes.

Current computer codes used to model granular materials are based on empirical relationships derived from experimental data and do not explicitly account for characteristics such as particle size and morphology. These models consider powder as a continuous medium rather than as a conglomerate of discrete particles. As a result, continuum models cannot capture the grain-scale processes affecting material response, such as how each particle transmits loads to the particles surrounding it.

"We need to understand compaction behavior in a wide range of particle sizes," says Antoun. "For example, continuum mechanics does not apply to particles at the nanometer scale. Our goal is to develop predictive models that incorporate morphology and material properties so we can explore the physics of material response at levels well below the continuum scale." Using these different methods, the team will be able to simulate material behavior over length and time scales that span several orders of magnitude.

Sophisticated instruments such as atomic force microscopes will measure the strain rate and fracture properties on individual grains of a material. The team will also perform shock compression experiments to characterize materials under dynamic loading. Results from these experiments will then be incorporated in the refined models along with first-principles calculations that are based solely on the fundamental laws of physics. Complex algorithms will calculate properties such as particle size and shape, and adaptive mesh refinement techniques will continually refine individual grid points as the simulation progresses, so that computational resources are used more efficiently.

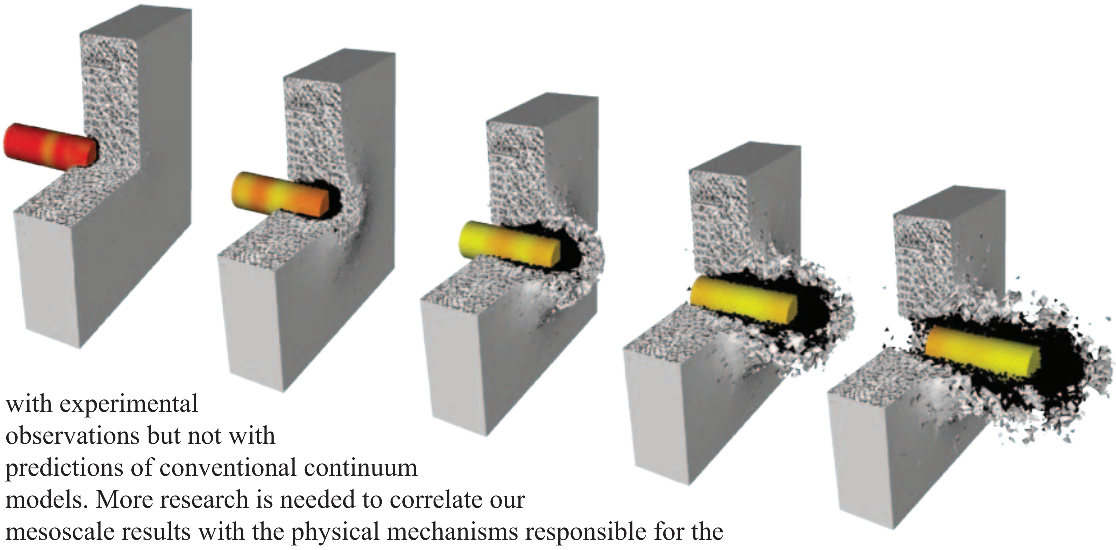
Nano- and microscale simulations will provide information about fracture behavior within individual grains, allowing researchers to visualize processes that they cannot easily observe in experiments. Mesoscale simulations resolve details within 1 millimeter, the same scale achieved in experiments. The team can thus directly compare modeling results with experimental data to validate the codes. Ultimately, the team will develop a macroscale continuum model that incorporates the essential physics of material response at the most basic level. "Our approach to a predictive continuum model is top down," says Antoun. "We'll begin by modeling the material at the macroscale, then progress to the lower scales as needed to gather fundamental information for further refining our macroscale model."

Thus far, the researchers have focused on selecting and characterizing materials and conducting static and dynamic experiments. Their initial simulations are examining powders made of ductile materials, which have a less complicated response than those made of brittle materials. These models will allow the researchers to generate baseline data and test the codes' overall effectiveness. Simulations of brittle materials will begin in the second year of this three-year project.

## Protection at Home and Abroad

Antoun and his colleagues are already working on a variety of applications for the models. With funding from the Department of Homeland Security, they are building detailed models to simulate how rocks and soils will respond to loads generated by seismic events or explosives. "Granular materials are not only pressure sensitive," says Antoun, "but they also behave differently depending on whether they are wet or dry, which influences the effective pressure." Predicting how Earth materials and structures respond to pressure is important to protect vulnerable infrastructure and to develop strategies for mitigating damage from a potential earthquake or terrorist attack.

In a project funded by the Department of Defense, the team is working with researchers at Purdue University to examine how objects penetrate sand under dry and saturated conditions. "Our mesoscale model indicates that wet sand is easier to penetrate than dry sand," says Antoun. "This result is intriguing because it agrees



Snapshots from a simulation show a projectile hitting a plate of transparent ceramic armor. As the object moves through the armor, the material turns into a granular powder (black) around the impact zone.

with experimental observations but not with predictions of conventional continuum models. More research is needed to correlate our mesoscale results with the physical mechanisms responsible for the observed behavior."

Modeling granular materials could also help protect military vehicles. Transparent ceramic armor—a heavy, see-though material mounted as a protective windshield on tanks and other vehicles—behaves like a granular material when hit by a projectile such as a bullet, radiating pressure away from the damaged area. "With computational models, we can see in exquisite detail how a bullet affects the armor," says Antoun.

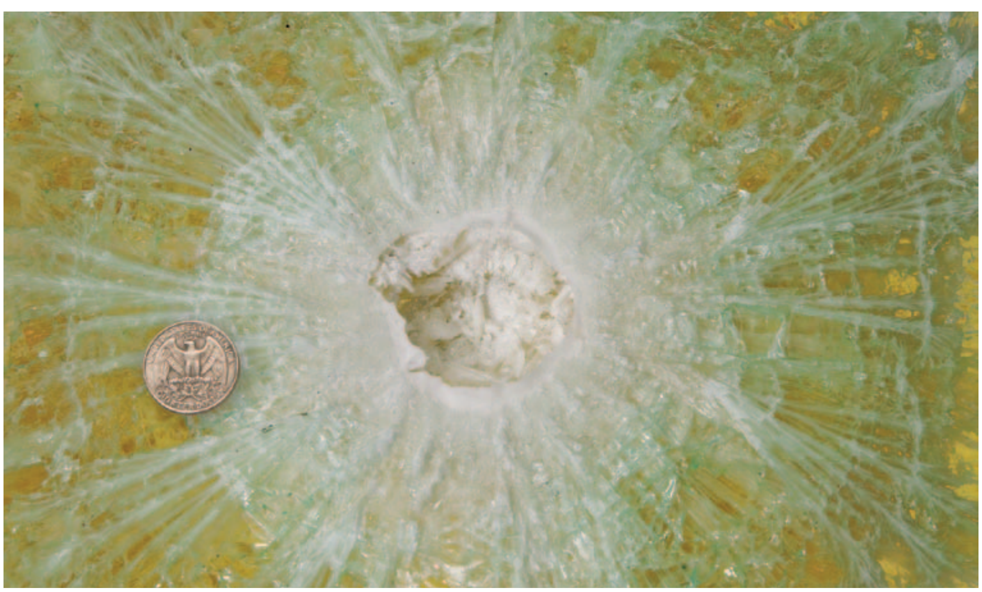
Transparent ceramic armor is built to conform to many specifications. It must withstand extreme temperature variations, transmit infrared light for night-vision equipment, and withstand gunfire, making it notoriously difficult to develop. By advancing predictive capabilities for granular materials, Antoun hopes to significantly reduce the time and cost required to produce the next generation of transparent ceramics.

## The Power of Supercomputers

"Granular materials have never been studied with the kind of detail we are working to achieve," says Antoun. Until the last decade, computing technology was not advanced enough to simulate materials in three dimensions, especially at the small scales of interest to the Livermore team. Extremely powerful computers, such as those at Lawrence Livermore, are needed to perform calculations at such detailed resolutions.

"Through the Laboratory's Computing Grand Challenge Program, we received 500,000 hours of computing time a week on BlueGene/L for our research," says Antoun. With this resource, the team will be able to peer into the fundamental physics of granular material response and examine the intricate interactions between individual grains—paving the way for exciting advances in materials science.

*—Caryn Meissner*



When a projectile penetrates transparent ceramic armor, damage radiates from the entry point outward, creating an intricate web of cracks within the material.

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