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ParticlePack: Packing a Peck of Pickled Peppers
by Gary Friedman

A newly released version of LLNL's ParticlePack shape-packing code includes features that have significantly enhanced the simulation of high explosives, propellants, and additive manufacturing for DOE, DoD, NASA, and their contractors.

ParticlePack is a preprocessing geometrical shape-packing code that generates objects for ALE3D, LLNL's multiphysics, massively parallel, arbitrary Lagrangian–Eulerian simulation tool. ParticlePack is part of the ALE3D package that is distributed to Government facilities and their contractors, and the code development is supported in-part by DOE Advanced Simulation and Computing (ASC) Program.

ParticlePack was created to help define packs of similar objects (e.g., grains, ball bearings, fuel pellets, manufacturing powders) for use in the ALE3D simulations. Today, the new version of the code is reducing problem setup time and improving the input accuracy for ALE3D.

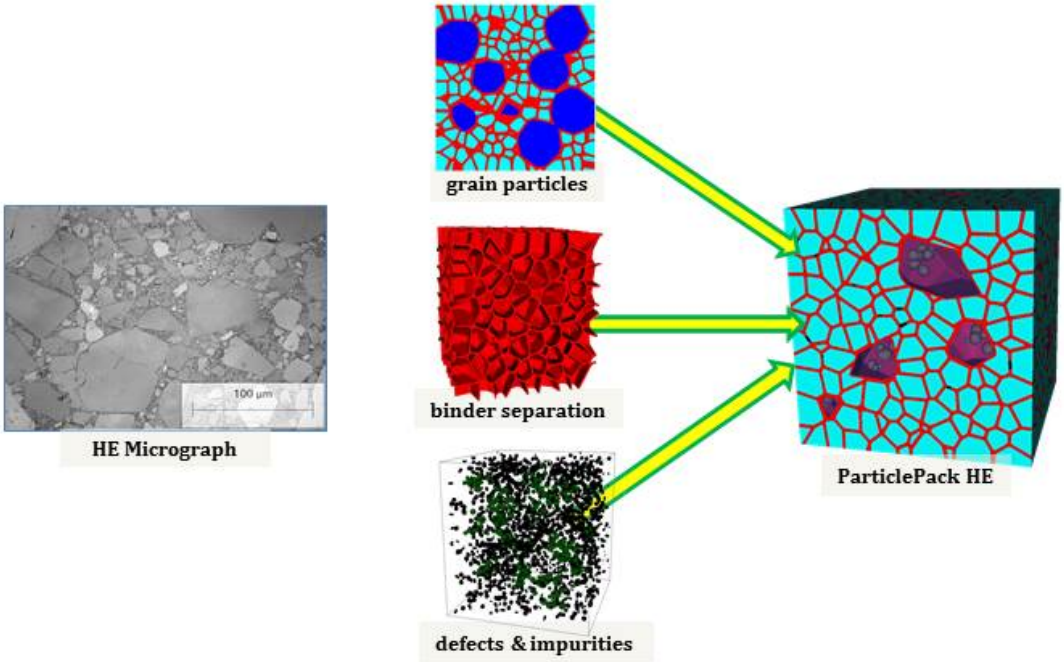
"As scientists continue meshing very detailed, mesoscale objects, there are times they need to 'inject' material shapes into an existing background mesh," explained Gary Friedman, developer of ParticlePack. "In ALE3D terminology, this is referred to as 'shaping.' This is where ParticlePack comes into play."

ALE3D already has a full set of basic shaping capabilities, but ParticlePack adds the ability to define a set of particles that are tightly packed into a space and shaped into an ALE3D model. Although ParticlePack's primary function is to shape objects into a background mesh, the code also provides an option to generate the particles as conformal mesh objects.

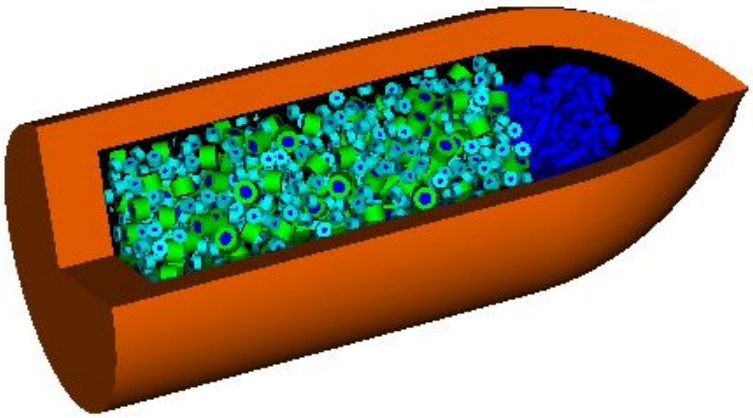
In addition, the code allows users to choose multifaceted grains, spheres, cylinders, or slabs for the particles and pack them into spherical, cylindrical, or rectangular enclosures. Users can define their particle size distribution using discrete size sets, Gaussian size distributions, or bimodal size distributions. Options are available to the user to set separations between particles. This is useful for modeling binder between high explosive grains. Users can also specify material types based on particle volumes, particles with a coating layer, and particle defects. Particles can be randomly positioned in the pack or packed in a lattice pattern.

The new version of ParticlePack incorporates algorithms to generate shape files that take advantage of the massively parallel shape generation capabilities in ALE3D. "We now have the capability to generate and shape millions of particles in a couple of hours," Friedman said.

Currently, ParticlePack is in the final stretch through a five-year plan to add enhancements that will be used in a wide range of high performance computing applications, benefitting DOE, DoD, and NASA. As part of the ALE3D modeling and simulation code, ParticlePack is helping scientists and engineers investigate the safety and performance of munitions and rocket motors, and pushing the limits of new manufacturing methods, like 3D printing.



Modeling HE Grain Structure



Fuel Pellets in Projectile

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