Sandia National Laboratories

Discrete Element Modeling

Need

Any physical process that involves the disaggregation and movement of material is best modeled with discrete element methods (DEM) rather than continuum methods such as finite elements. Discrete element methods have been under development since the early 1970's. Until recently, most of the capabilities available allowed treatment of certain particle shapes such as spheres or ellipses. Modeling real physical processes with this limitation of particle sizes requires significant simplification.

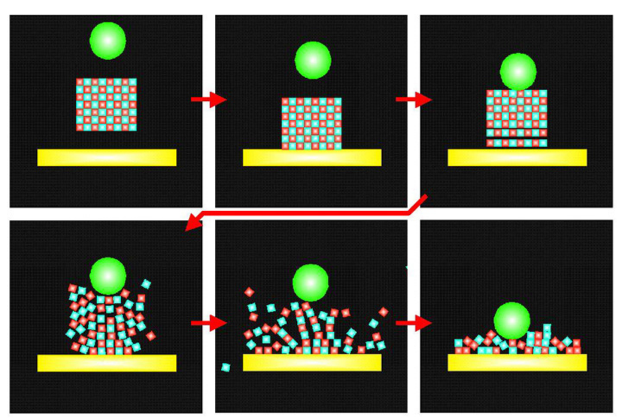
Coupled processes present significant challenges to engineers today. One of those challenges is treatment of the coupling between solid particles and fluid flow. Processes of this type include sand production in oil wells and manufacturing processes where particles are carried by fluids to their final destination.

Description

Treatment of a Variety of Particle Shapes

A relatively new capability being developed by Sandia National Laboratories and the Massachusettes Institute of Technology Civil Engineering and Environmental Engineering Department allows treatment a large variety of particle shapes in the same calculation. This research has produced a 2-D discrete element computer code called MIMES that creates an interactive environment where the user can define discrete element simulations using a variety of particle shapes and physical characteristics. MIMES is suitable for modeling any physical process where the material is not a continuum. It is especially adept at modeling granular materials such as gravel, sand, rock and ceramics that are subjected to fluid induced forces. An example MIMES simulation is shown below.

This simple discrete element simulation shows a block of squares and a sphere falling under the influence of gravity. The block of squares rebounds from a fixed block and then interacts with the sphere and the fixed block. This type of simulation is very easy to set up and simulate with MIMES.



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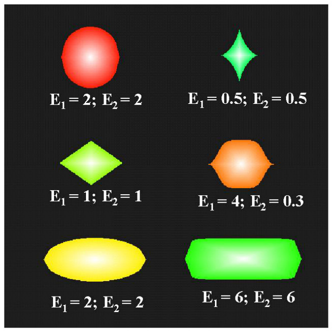
A new type of discrete element has been developed which is based on the concept of superquadrics. These are obtained by changing the exponents in the elliptical equation as shown to the left. The ability of MIMES to treat different particle shapes is not limited to spheres, ellipses, rectangles and superquadrics. MIMES can also treat particles with arbitrary shapes that are defined as n-sided polygons as shown to the below on the right.

Superquadric Discrete Elements

Elliptical Equation

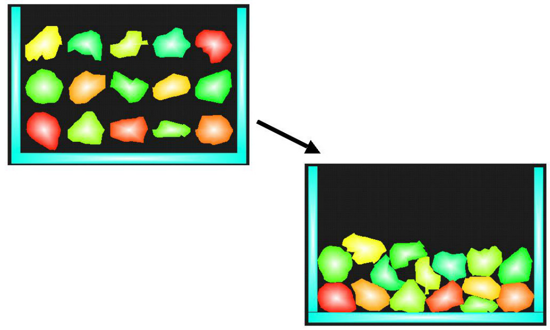
$$\frac{X^{E_1}}{a} + \frac{Y^{E_2}}{b} = 1$$

Where:
E_1 = X exponent
E_2 = Y "
a = X axis length
b = Y " "



A wide variety of particle shapes can be obtained by varying the exponents in the equation of an ellipse. The axis length can also be varied to change the aspect ratio of the particles.

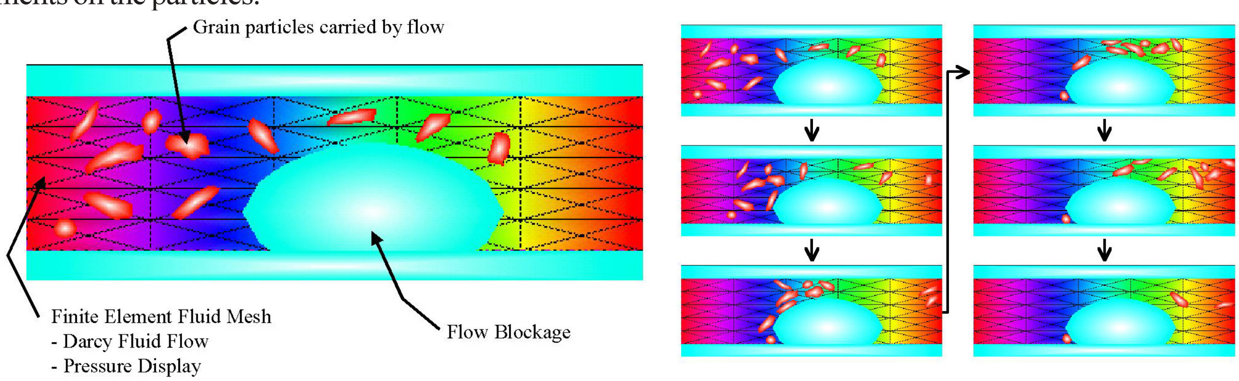
Sand Grain Simulation



The particles in this simulation were digitized from a sandstone photo-micrograph. The particles are allowed to settle under the influence of gravity. Sandstone discrete element models can be generated by randomly picking a shape from this library of particle shapes and scaling the particles to match a specific size distribution.

Coupled Fluid-Flow/Particle Motion

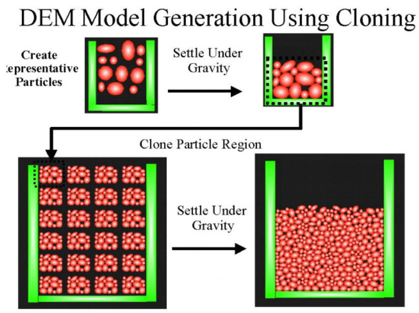
Another advance made in the past few years in the Sandia/MIT research has been in the area of coupled fluid-flow and particle motion. Coupling is accomplished by performing the fluid flow calculation using Darcy computational techniques and integrating the fluid pressures around each discrete element to obtain the fluid-induced forces and moments on the particles.

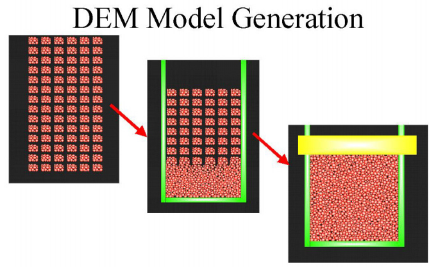


The fluid flow grid in this simulation is shown in the background with color representing the pressure in the fluid. Sand grain shaped particles are being carried by the fluid flow around an obstruction in the channel.

Discrete Element Model Generation

A significant challenge in discrete element modeling is creation of the model itself. This is especially true if the model is to contain particles of different sizes and shapes. A new method has been developed as part of this research which makes it possible to quickly and efficiently generate discrete element models with large numbers of particles which have accurate particle shapes and size distribution.

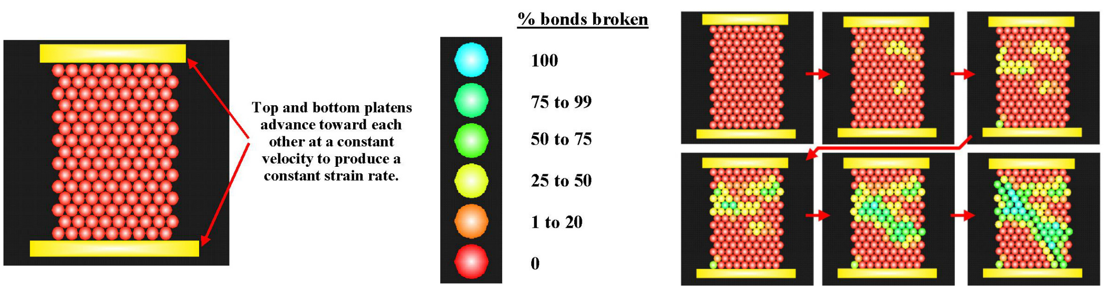




A few particles that capture the shape and size distribution required for the model are created and allowed to settle under the influence of gravity to remove void space. Groups of particles can then be copied and cloned to create larger models. Void space is removed from the particle assemblages through gravity settling as well as weights on the top surface. This method of generating discrete element models is new and unique. It allows creation of models for simulating the behavior of rocks, such as sandstones, as well as assemblages of granular materials and ceramics particles.

Computational Geomechanics

Discrete element methods have been developed to model the behavior of rock which is basically a discontinous bonded material. Sandstone behavior is especially amenable to modeling with bonded discrete elements. Bonding between discrete elements treats the cement between grains in a sandstone. When sandstones are placed in unconfined compression, as in a laboratory test, they usually develop failure planes where all the deformation is localized. It is important for bonded discrete element models to capture this behavior in order for there to be confidence in modeling the response of the sandstone to more sophisticated loading conditions.

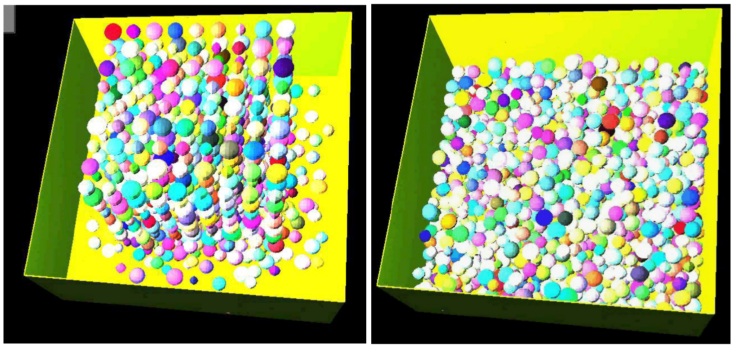


(a) (b) (c)

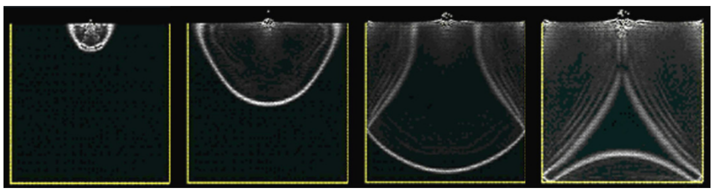
a) A computer simulation of an unconfined compression test where the end plattens move toward each other at a fixed velocity. b) Particle bonds break under loading based on exceeding the cement strength in tension, compression or shear. These bonds simulate the effect of cement in a sandstone, concrete or other geomaterial. As bonds are broken the color of the particles are changed to indicate the percent of bonds broken. c) MIMES simulation of an unconfined compression test where the bond breakage eventually localizes on a plane through the model and all of the deformation of the specimen occurs as slip on the created fracture plane.

3-D Discrete Element Modeling

Significant advances have also been made by Sandia and MIT on the computational efficiency of Three-Dimensional discrete element modeling. Much of this improvement is accomplished through increased efficiency of the contact detection algorithms that are used to track particle contact. Having detected particle contact the appropriate contact physics is applied to simulate the collision and rebound of the particles. Transient stress wave propagation through granular materials does not follow traditional wave theory. An example illustrating this phenomenon is shown on the next page.



A block of 3-D spherical discrete element particles is dropped into a box. The unique and unseen portion of this simulation is speed at which the calculation can be done due to improvements in the efficiency of the contact detection algorithms.



Transient stress wave propagation through an assemblage of bonded 3-D discrete elements due to the impact of a single particle in top center of the model. The wave is also interacting with the rigid sides of the container. The reflected waves also interact with each other.

References

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