

## Undergraduate Research Projects

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### *Background*

Discrete element modeling (DEM) is becoming an increasingly common tool for investigating the dynamics of particulate systems such as those involving the processing of pharmaceuticals, agricultural and food products, building materials, and chemicals. With DEM, the behavior at the macroscopic scale emerges from specified properties and interactions at the particle level. The method allows one to investigate simultaneously both particle-level and system-level phenomena.

The principles behind DEM are straightforward. The forces acting on individual elements in the system, *e.g.* particles, are calculated using appropriate models. Typical forces include weight, elastic and dissipative contact forces, and cohesive forces. Newton's Laws are then used to determine individual particle accelerations. The resulting accelerations are integrated explicitly in time to generate new particle states. The process is repeated until a specified ending condition is reached.

### *Project 1 Description*

One significant challenge to performing meaningful DEM simulations is applying the algorithm to sufficiently large numbers of particles so that realistic systems may be modeled. Current DEM simulations typically model on the order of  $10^4 - 10^5$  particles, whereas real systems can be comprised of up to  $10^9 - 10^{12}$  particles. Although it remains to be determined what number of simulated particles is sufficient, having the capability to simulate increasingly larger systems is desirable.

In this project, the student will modify an existing serial C++ DEM code to perform contact detection calculations in parallel on either multi-core or cluster-based PCs, depending upon the student's experience. Candidates for the position should have the following background and skills.

1. Strong C/C++ programming skills and familiarity with UNIX.
2. Familiarity with statics and dynamics.
3. Familiarity with parallel programming.

The project may be pursued either for course credit or for pay.

### *Project 2 Description*

In addition to simulating large systems of particles, having the ability to model particle interactions with realistic system geometries is also desired. The movement of material in complex system geometries, such as those encountered in powder mixing and granulation processes, are of considerable practical interest.

In this project, the student will modify existing C++ DEM codes to read a Computer Aided Drafting (CAD) file describing the system geometry in terms of triangular elements, and develop and implement contact detection schemes between spherical particles and the boundary triangle sub-elements (*i.e.* flat surfaces, edges, and corners). Candidates for the position should have the following background and skills.

1. Strong C/C++ programming skills and familiarity with UNIX.
2. Familiarity with statics and dynamics.
3. Familiarity with a CAD package is desirable, but not required.

The project may be pursued either for course credit or for pay.