The Summer Undergraduate Research Fellowship (SURF) Symposium
6 August 2015
Purdue University, West Lafayette, Indiana, USA

Optimization in the Simulation of Jammed Polyhedral Particles

Joseph W. Mynhier
School of Electrical and Computer Engineering, Purdue University
Ishan Srivastava and Timothy S. Fisher
Birck Nanotechnology Center and School of Mechanical Engineering, Purdue University

ABSTRACT

Energy loss due to poor transport properties in electrically and thermally conducting materials, such as battery electrodes and thermoelectric composites, contributes to the energy inefficiency of electronic devices. For conductive materials composed of granular materials, particle-particle contact topology strongly governs the efficiency of energy transfer. Although there is a large body of existing work on the arrangements made by granular materials comprised of spherical particles, less is known about the mechanically stable arrangements of granular materials made of convex polyhedra. This project seeks to create a computer simulation of the solidification of convex polyhedra from a diffuse state into a jammed state under varying external states-of-stress. In order to optimize the runtime performance, the most time consuming regions within the code were identified. Four areas for improvement were identified and algorithms and libraries were evaluated for speedup in each case. Trials of polyhedral intersection detection were made with spatial gridding and sweep and prune. Intersection calculation implemented with CGAL was evaluated. Triangulation and tetrahedralization, were implemented and evaluated with TetGen and Triangle++ respectively. Parallelization was implemented with OpenMP. Initial results indicate that a significant speedup has been achieved as compared to the existing program. Now this program can allow researchers to simulate the jamming and stress/strain-response of a significantly large number of polyhedral particles in less time, including possibly via online naoHUB simulation tools, which will increase the pace at which new research can be conducted.

KEYWORDS

Jamming, non-spherical packing, granular materials, optimization