PackingSim

PoreSim RESEARCH CONSORTIUM

Overview

PackingSim is a flexible tool for generating computer-simulated packed beds and particulate materials. It is unique because of the much wider range of physical constraints that can be imposed by the user, as compared with other packing algorithms.

Algorithm

A simulated annealing algorithm is used to minimize the difference between the packing structure and a user-defined target. The annealing process occurs via a series of Monte-Carlo perturbations that can include movement, rotation, addition/removal, change in size, and/or exchange of particles.

The advantage of this approach is the flexibility in imposing constraints on the packing structure. The main disadvantage is that simulated annealing can be slow. Tests suggest that speed is a problem mainly if long-range spatial correlations are used.

Examples

The figures shown below illustrate the power and flexibility the PackingSim algorithm. Figure 1 is a sphere packing with a strong spatial correlation in particle size. Figure 2 is a packing of non-spherical particles; mixtures of different shapes are also being simulated. Figures 3 and 4 show packings that conform to more complex, non-periodic boundaries (a reactor tube and a fractured rock respectively). Figure 5 is an image of a one-million sphere random packing.

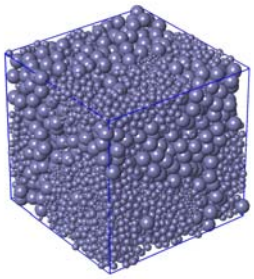

Figure 1

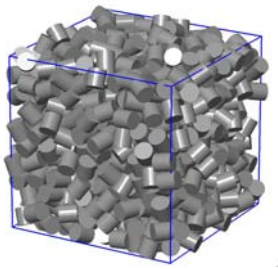

Figure 2

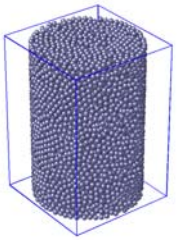

Figure 3

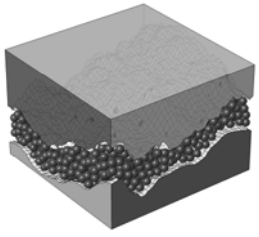

Figure 4

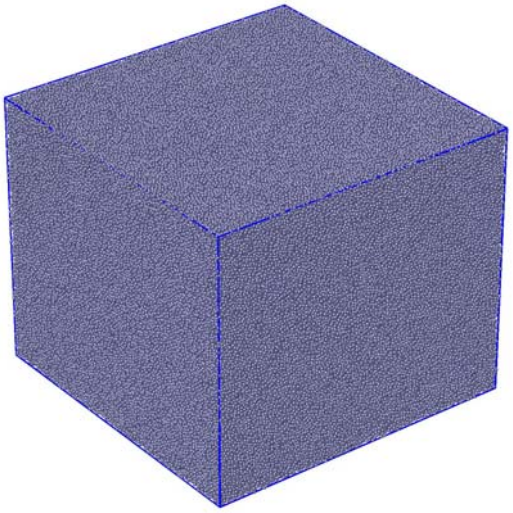

Figure 5