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Proceedings Paper:

Jia, X, Guadarrama-Lara, R and Fairweather, M (2015) DigiPac/DigiDEM and Applications. In: Erlangen Particle Simulation 2015. Erlangen Particle Simulation 2015, 21-24 Sep 2015, Erlangen, Germany. , pp. 45-46.

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DigiPac/DigiDEM and Applications

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Here we describe a group of particle packing simulation models, all based on a digital representation of the particles, the container and the packing space. They are implemented as software programs called DigiPac and DigiDEM. DigiPac is a collection of four packing models: random-walks (DigiRWP) [1], collision-guided (DigiCGP) [2], random-placement (DigiRPP) and optimal stacking (DigiOSP) [3] packing models respectively. For complex and arbitrary shapes, the use of voxelated objects has the advantages that complex shapes can be handled by simple and efficient computer code for collision and overlap detections and for packing property calculations, and the computing time does not increase with shape complexity. Applications of DigiPac models will be illustrated with examples such as packed columns [2] (Fig.1a), segregation [4] (Fig.1b) and popcorns [5] (Fig.1c). DigiPac packing models are typical Monte Carlo simulations where probabilities are used to control particle movements. It is good at providing packing predictions for trend analysis and is generally much faster than DigiDEM. DigiDEM, on the other hand, tends to provide more quantitatively accurate results and can simulate dynamic processes as well as the packing structures, but at a high computational cost. This is because DigiDEM is a lattice implementation of the Discrete Element Method where which way and how much each particle moves are determined by calculating physical interaction forces and solving Newton's equations of motion in very small time steps. Potential applications of DigiDEM are illustrated through sieving by vibrating screen (Fig.1d) and stirring of packed bed, etc. In addition to packing, the software suite also contains modules to calculate some properties of common interest, such as permeability (using Lattice Boltzmann Method) [6] (Fig.1e), effective thermal or electrical conductivity (using Finite Difference Method) (Fig.1f), dissolution [7] (Fig.1g) or chemical reaction in porous media, sintering, and light scattering etc. In all these calculations, the aim is to link particle characteristics to microstructure of packing then to their properties. Difference between the different models will be explained and illustrated. Challenges, bottlenecks and possible solutions will be described, and finally future development will be highlighted [8-9].

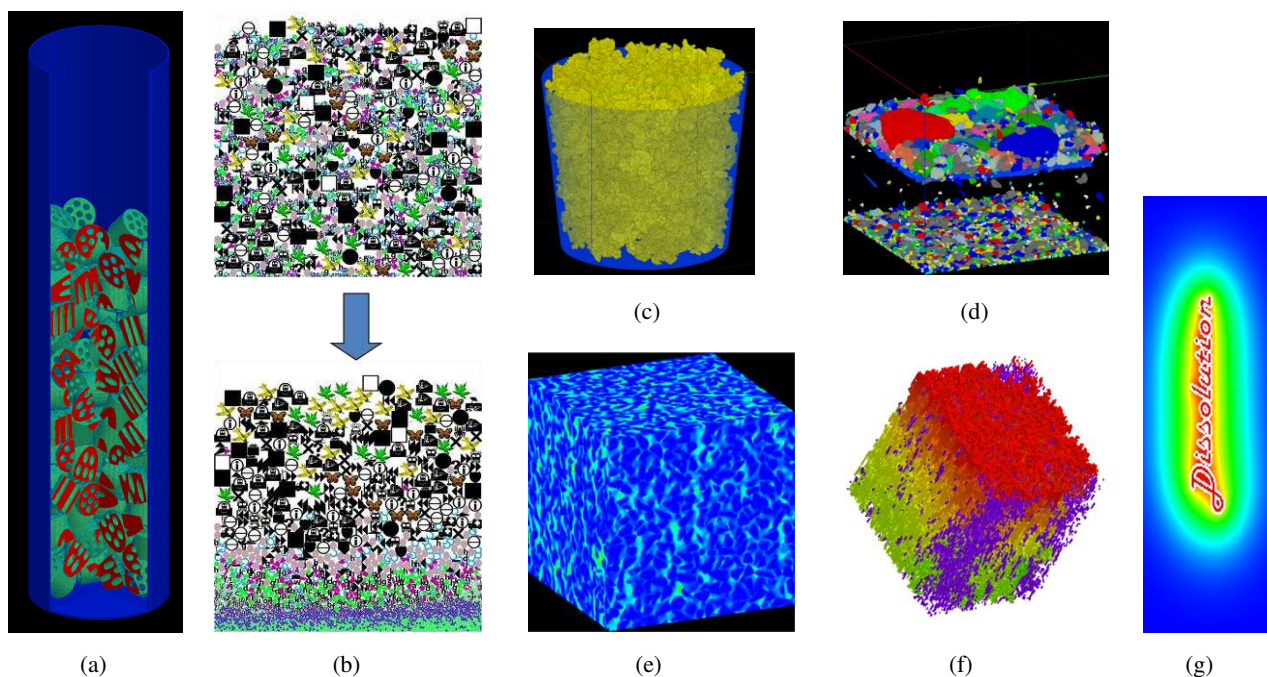


FIG. 1. (a) Packed column. (b) Segregation. (c) Popcorns. (d) Vibrating screen. (e) LBM simulated flow in porous medium. (f) Temperature distribution through a porous material. (g) Concentration distribution of dissolving solids.

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