11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

CONCRETE MESOSTRUCTURE GEOMETRY MODELLING WITH GROWING AND COLLIDING HARD SPHERES

Thomas Titscher[1], **Jörg F. Unger**

[1] Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany, thomas.titscher@bam.de

Key words: *concrete, mesoscale, geometry modelling, molecular dynamics.*

The geometry of concrete on the mesoscale is relevant for a realistic numerical simulation. On the mesoscale, concrete is multiphase material consisting of a cement paste and particles (aggregates). There are two entirely different approaches to obtain the particle geometry, either by visual analysis (e.g.: X-ray) of real specimens or by a numerical geometry model. The latter one, used in this work, is far more flexible and allows a fast creation of a virtual specimen geometry. The grading curve and the particle volume fraction are the input parameters of the geometry model.
For dynamic simulations, e.g. wave propagation, the maximum time step depends on the element length (CFL-condition), which is directly related to the minimum distance between particles. Thus, the overall numerical cost and accuracy is significantly influenced by the particle distance.

There are several algorithms for the geometry creation. In the first step, the number of particles and the volume of each particle is determined based on the input parameters. The particle placement is the next step. It is required that particles do not overlap. A common approach is to randomly place each particle successively into the specimen. If it overlaps with existing particles, either a new random position is picked (*take-and-place* algorithm [2]) or the particle is slightly moved (*stochastic-heuristic* algorithm [1]). These algorithms do not allow movement of already placed particles. This results in loosely packed geometries with a relatively small maximum volume packing.
In order to guarantee a minimal particle distance, the algorithms are slightly modified. During the placement process, the size of each particle is temporarily increased. After the placement of all particles, the additional volume is removed and now available for meshing. This modification leads to a (temporary) increased particle density and requires very densely packed particles.

The Lubachevsky-Stillinger algorithm [3] simulates molecular dynamic processes using hard particle collisions. By applying it to growing spheres in a box with periodic boundaries, a very high sphere density (random closed packed) can be obtained [4].

In the present paper, this idea is adapted to concrete particles. Infinitesimal spherical particles with random initial velocities are randomly placed into the specimen. As time progresses, they freely move in space and their diameters grow. Collisions with other particles or boundaries are fully elastic. When the particle size distribution matches the desired grading curve, the particles can be further increased temporarily to maximize the particle distance.
For an efficient and precise collision handling, collision events are predicted and scheduled by using an event list. Each time step is adapted to the next collision event. After each collision, the event list is updated for all events involving the collided spheres.
Different particle placing algorithms are compared to the present one. The achievable maximum particle distance, the randomness of the particle positions and the performance are investigated. The influence of the grading curve and the volume fraction on these results is further discussed.

REFERENCES

[1] J. P. B. Leite, V. Slowik and J. Apel. Computational model of mesoscopic structure of concrete for simulation of fracture processes. *7th International Conference on Computational Structures Technology/4th International Conference on Engineering Computational Technology, Lisbon, Portugal*, 2004.

[2] E. Schlangel and J. VanMier. Simple Lattice Model for Numerical Simulation of Fracture of Concrete Materials And Structures. *Materials and Structures*, Vol. **25**(153), 534–542, 1992.

[3] B. Lubachevsky and F. Stillinger. Geometric Properties of Random Disk Packings. *Journal of Statistical Physics*, Vol. **60**(5-6), 561–583, 1990.

[4] A. Donev; S. Torquato and F. Stillinger. Neighbor list collision-driven molecular dynamics simulation for nonspherical hard particles. *Journal of Computional Physics*, Vol. **202**(2),737–764, 2005.