Characterization of cementitious materials by advanced concurrent algorithm-based computer simulation systems

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Abstract

The traditional discrete element computer simulation system in concrete technology is based on random generators referred to as sequential random (particle) addition (SRA) systems. They generate particles that are not spaced according to situations met in the actual material. This paper indicates the technological relevance of upgrading the concurrent algorithm-based discrete element computer simulation system SPACE discrete element facilities into a new discrete element system, HADES, which can encompass arbitrary particle shapes. The generation of particles is described as is the way particulate structure is formed. The technologically relevant fields are briefly indicated requiring exploration by this concurrent algorithm-based system. Such activities will be undertaken on short terms at Delft University of Technology.
Keywords: arbitrarily shaped particles, concurrent algorithm-based system, cementitious materials, discrete element, and finite element.

1 Introduction

Cementitious materials are of particulate nature on different structural levels. The aggregate is compacted in the fresh concrete into the *jammed state*. It is a strong and hard material, under such conditions roughly taking up three-quarter by volume of the material body, and constituting a load-bearing skeleton that can provide the normal concretes with high compressive strength. The stability of the skeleton is guaranteed by the cementitious “glue”, the cement paste. Moreover, the paste’s quality, which is directly influenced by its fineness and by the water to cement ratio, governs the actual composite’s compressive strength level.

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Additionally, it gives the material its tensile strength. Modern high performance concretes are produced at low water to cement ratio, so the volume content of the cement in the paste may be as high as 60%. The latter is achieved by addition of chemical and fine mineral admixtures, which can also be employed for replacing part of the Portland cement (PC) and can be of pozzolanic or inert nature. All composing parts of the material have influence on engineering characteristics of the composite that will change as a function of time, in the first place as a result of hydration, however also due to complicated interaction processes with the environment. Material optimization would ask for very large numbers of specimens. Certain aspects have been investigated in trial testing and structural research programs, but it would be economically attractive to have reliable computer simulation methods available.

The traditional discrete element computer simulation system in concrete technology is based on random generators to disperse inside the container aggregate particles on meso-level in a cementitious matrix, or cement and eventually other types of mineral admixture particles on micro-level in the watery environment during the fresh state. These systems are referred to as sequential random (particle) addition (SRA) systems. As stipulated elsewhere, they generate particles that are not spaced according to situations met in the actual material on both structural levels [5,7]. As a result, the processes of pore de-percolation, underlying concrete durability, and damage evolution, governing the materials residual strength capacity, will be incorrectly generated; biases declining fortunately during such processes. The latter field was so far the territory of “numerical concrete” [8], which is SRA-generated concrete subjected to finite element analysis. Additionally, SRA systems cannot produce particulate systems with the aforementioned high volume densities. Therefore, we have applied the concurrent algorithm-based discrete element computer simulation system SPACE with success on both structural levels, as witnessed by our two papers [12,13].

A drawback of all these systems is that only spherical particles can be generated. For aggregate of fluvial origin this may be considered not too dramatic. This can also be argued for cement or silica fume, as popular mineral admixture. However, aggregate grains of non-spherical shape are known to lead to lower densities in the jammed state. This has consequences for engineering strength. However, the impact on the nodes in the pore network model [13,14] that can be designed for estimating durability performance could be more dramatic. Realistic packing research on different structural levels with discrete element computer simulation system therefore requires facilities to also generate non-spherical particles. This is pursued by the HADES toolbox. With this package, particles can be of any shape and contacts are force-based rather than impulse-based, as in SPACE system. The surface of objects is no longer described by a mathematical function (such as in case of a sphere), but by a set of interconnected surface elements. In this way any shape can be described. The present paper briefly sketches the actual state of developments and indicates typical fields of application that will be explored in the very near future.

2 Structure generation

2.1 Single particle

To be able generating a particle assembly that corresponds to some actual mixture, one needs to characterize shape first. Once shape has been described by a set of shape parameters, probability curves have to be provided for each parameter so that it becomes possible to predict the probability of a certain shape (*i.e.*, combination of shape parameters) in a mixture. Basically, HADES is designed to handle arbitrary shapes as long as the surface is tessellated by triangular or square surface elements of which the nodes are located on the surface. So far, ellipsoidal shaped and multi-facetted particles have been implemented [18]; more complicated shapes are under development.

Ellipsoids are particularly interesting because with only 3 parameters a variety of shapes, ranging from oblate to oblong can be described, as shown in fig. 1. Two extra parameters are introduced that allow a range of differently-shaped particles derived from the ellipsoids fig. 1a-c, namely, maximum size of surface element and maximum angle between the normal vectors to neighbouring surface elements at a node. The latter parameter controls how much the surface mesh follows the actual mathematical shape. Single examples out of ranges of shapes derived from fig. 1a-c are displayed in fig. 1d-f, by changing the maximum size and the maximum angle. In fig. 1d-f for all three cases, the maximum size of surface element and maximum angle are 20 and 60º, which are 2 and 10º for the cases in fig. 1a-c, respectively.

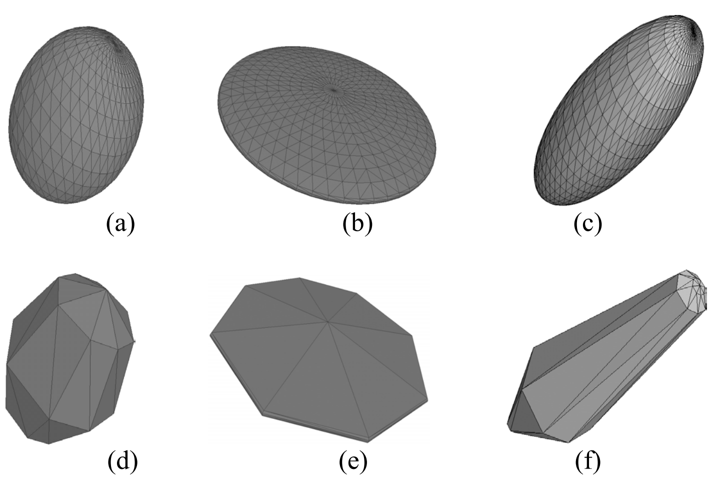

Figure 1: Differently shaped ellipsoids. The lengths of the three semi-axes are 6, 8, 10 in (a), 3, 20, 22 in (b) and 3, 4, 16 in (c), respectively. (d), (e) and (f) are derived from corresponding ellipsoids in (a), (b) and (c).

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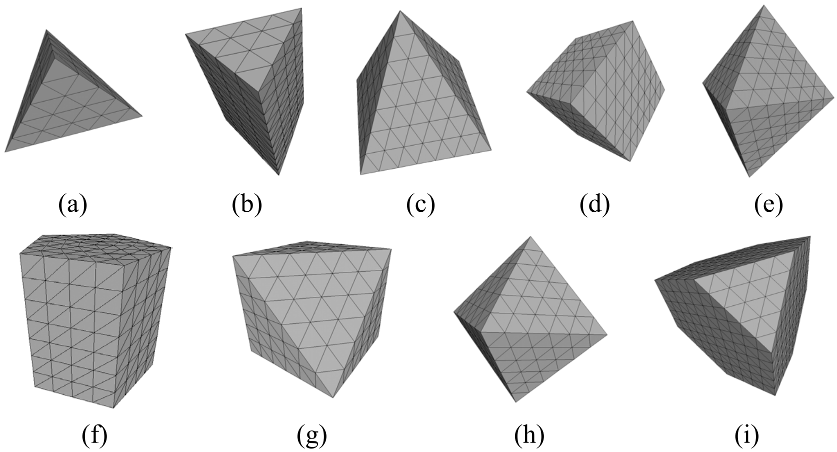

Figure 2: Particles with multi-facetted surfaces. (a) tetrahedron, (b) and (c) pentahedron, (d) and (e) hexahedron, (f) and (g) heptahedron, (h) and (i) octahedron.

A specific group of shapes with 4-8 facetted surfaces are proposed to represent the crushed rock by Guo Wen's [16] based on his investigation. This proposal greatly simplifies the simulation of crushed rock since only two parameters are needed to determine shape and size. One extra parameter of maximum size of surface element is required only by numerical algorithm of interaction between particles and this parameter will not influences the shape of particles with multi-facets. Fig. 2 illustrated the particles with different number of facets.

2.2 Multiple particles

Next, a set of particles (ellipsoids or polyhedron) is generated by using size and shape distribution curves that approximate the composition of an actual mixture. The individual particles are than positioned in a non-overlapping, but rather dilute way in some region or container. This region can be defined by periodic boundaries, rigid boundaries or partly periodic and partly rigid boundaries. Each particle is given a random initial linear and angular velocity. The particles are than, iteratively displaced to a position that is obtained by integrating the velocity over some (very small) time period. Similarly, the velocity of a particle at the next iteration, or time, is calculated by integrating the force (linear) or torque (angular) that acts on each particle. Currently gravitational forces, paste friction and contact forces between particles mutually or between particles and other objects in the simulation have been implemented.

Moreover, the boundaries, periodic or not, can be dynamically moved according to the user-defined function. In this way, a number of experiments can be simulated. For example, by providing some sinusoidal motion of the container, shaking can be simulated, and along with it, size segregation of the

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particles (under the influence of gravitational force), as show in fig.3. Dense packing can be obtained in this way, but it is also possible to move the periodic or rigid walls of the container towards each other thereby increasing the volume density of the mixture. By measuring the force or stress that is exerted by the particles on these container walls one can decide when the 'jammed state' is reached.

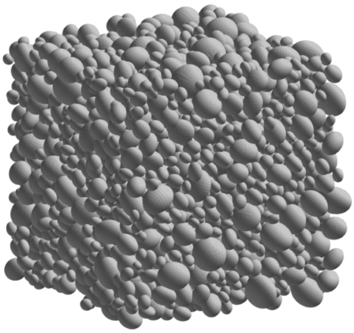

Figure 3: Highly compacted system of ellipsoidal particles of type (a) generated by HADES in container with periodic boundaries.

3 Possible applications

3.1 Optimum mix design

How do we do that, making concrete in virtual ‘reality’? What characteristics of the complex, particulate material should be incorporated in this so-called *compucrete*? Such questions must have been at the minds of those coming up with the first systems in the 70s of the previous century, such as that of Roelfstra [3], which formed the starting point of the “numerical concrete” concept of Zaitsev and Wittmann [15]. Basically, these and later developed systems in concrete technology rely on random RSA algorithms [1,2,9]. In RSA systems, particles are placed proceeding from large to small on preconceived positions of a Poisson field. Violation of physical conditions by overlap leads to *rejection and re-generation*. So, part of the Poisson field positions cannot be exploited, since spacing with other points is insufficient. The consequences are that, firstly, new positions should be randomly assigned to remaining particles until overlap is avoided. This is a time-consuming process, whereby the number of re-generations dramatically increases when the volume fraction is approaching a level of only 35%. In Williams and Philipse [7] an upper limit of 38.5% for spherical particles is mentioned, which is in qualitative agreement with Ballani [10] where in most cases the production of compucrete with 40% spherical aggregate failed. So, *practical* arguments plea for application to low density grain mixtures only. Secondly, instead of having series of particles close together in compucrete, in conformity with Poisson point processes, on average a more uniform dispersion is obtained.

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Clustering, a *natural phenomenon in particulate matter* [4], is therefore very poorly represented by RSA systems. On the contrary, the concurrent algorithm-based computer simulation systems SPACE and HADES imitate the production conditions of concretes and have been demonstrated realistically incorporating the clustering phenomenon in compucrete.

The SPACE and HADES systems realize compaction by a dynamic algorithm, which is also supposed to imitate the production stage of the material, as stipulated earlier. The forces added to the particles can be manipulated, so that "sticky" particle contacts (or particle repulsion) during the production of the model material can be simulated. Also gravity effects can simply be included. River gravel and broken rock aggregates compact to different densities in the jammed state at equal grading (obtained by sieving), so HADES generation of compucrete will be required for simulation of crushed aggregate. SPACE application for this purpose in case of river gravel aggregate has resulted in good agreement with experimental observations [12].

3.2 Dynamic effects on particle mixtures

The study on the effect of *compaction energy* (in the construction industry as well as in laboratory testing) on possible size segregation can be pursued by HADES system. Although the concurrent algorithm in SPACE is based on a dynamic Newtonian stage, but it is impulse-based, this does not automatically allow studying effects of vibration characteristics (frequency, amplitude) on particle packing. The latter phenomenon is widely denoted as "Brazil nut effect" (BNE) in the international literature, and recognized as a relevant phenomenon in many branches of industry where they deal with transport or vibration/shaking of particles. The situation is shown quite complicated, and received intense attention in many articles issued during the present century in leading journals. Apart from the normal BNE, the reversed BNE is reported (Nature 429, May, 2004, 352-353), and even the horizontal BNE (Physics News Update, nr 653 #3, Sept. 2003). Relative densities and frequency details play a role, but the phenomenon is far from established, and some of the mechanisms are still of speculative nature.

Effects of shape have been reported relevant for aggregate grains and binder particles. The shape effect was extended to fibres in Physical Review papers; so that fibre reinforcement in compacted concrete will basically be subjected to this effect, too. A wide variety of fibres (in size, aspect ratio and material) are used, as well as types of aggregate (with a wide range in volumetric densities). Also workability is low for precast elements and can be quite high for on-site placement of concrete. The assessment of safe ranges for compaction conditions should therefore be established for a variety of compositions. This would be of high economic relevance, since segregation may negatively affect performance.

It will add to our studies of other size segregation phenomena inflicted by rigid surfaces during compaction (mould for aggregates, and aggregate grains for cement particles). This size segregation phenomenon finally leads after hydration to the location of percolated porosity in a thin zone immediately neighbouring all the aggregate's surfaces, and thus to a spatial interconnected network structure that governs durability issues [13]. On the somewhat longer run, it will be scientifically highly interesting and technologically extremely relevant to see whether BNE will interfere and how with such size segregation phenomena. Fig. 4 demonstrates the simulation of typical dynamic granular effects such as size segregation by vibration (the so called BNE) as generated by HADES system in 2D.

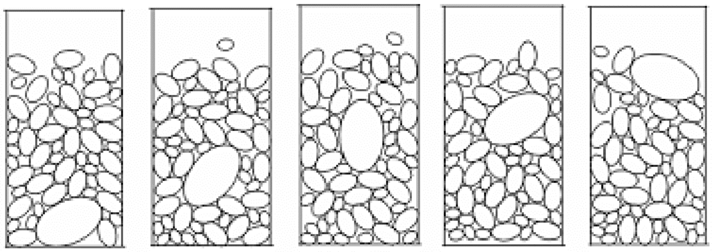


Figure 4: Brazil Nut Effect simulated by HADES in 2D.

3.3 Workability

The methods for workability and compactability testing are numerous and highly uncorrelated. The methodology can be characterized by a large degree of pragmatism, and a minor scientific basis. Specific solutions have been developed for sub-sectors of the concrete technology field, whereby simplicity under given conditions (either on-site or for laboratory testing) prevail. Some methods with overlapping fields of usage have been compared as to ease of use, simplicity of equipment, and stability or reproducibility of outcomes. The "Summary of concrete workability test methods" [17] offers a good survey.

Computer simulation would allow for an economic approach to such problems and could unify (at least partly) the methodology on fundamental issues. Compucrete is employed for the purpose, whereby the effect of the existing equipment on the compucrete can be simulated. Cementitious materials contain high amounts of aggregate, so particle interference will be a major mechanism governing workability of the mixture. Conventional RSA-based systems cannot (or, cannot economically) simulate particulate materials in this high-density range. This application of HADES will require *adaptations of the computer simulation methodology*.

A selection of most promising methods will be simulated and outcomes mutually compared. Only a small number of the methods in vogue employ vibration, thereby better resembling workability during compaction. Vibration is necessary for workability testing of SFRC (because of thixotropy). This situation will certainly be covered.

The common used slump test is simulated for fresh concrete with different fluidities as shown in Fig. 5. The calibration work will be done in near future.

3.4 Strength and damage estimation

SPACE and HADES have been extended with the possibility to generate unstructured finite element meshes in which the material structure is explicitly modelled. Within these meshes, three components can be distinguished: aggregates, the cement matrix and the interfacial transition zones (the thin cement layer around each particle of which mechanical properties are different from those in bulk cement). Fig.6 shows all three components. These meshes can be constructed because SPACE and HADES provides a full description of the material structure. Consequently, it is possible to provide the mesh generator with a function that defines the element size as a function of the distance to the nearest aggregate surfaces, for example. In this way, the interfacial transition zone (ITZ)—important for many mechanical properties in concrete—can be modelled with relative small elements while the elements within aggregates can be taken much larger.

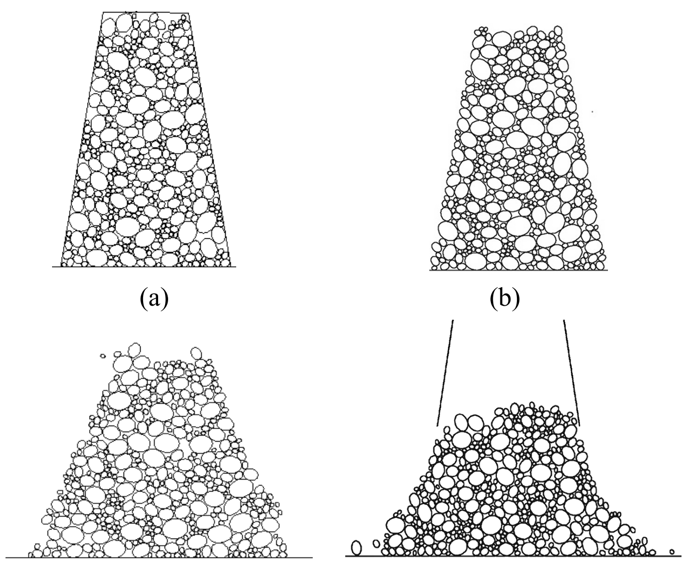
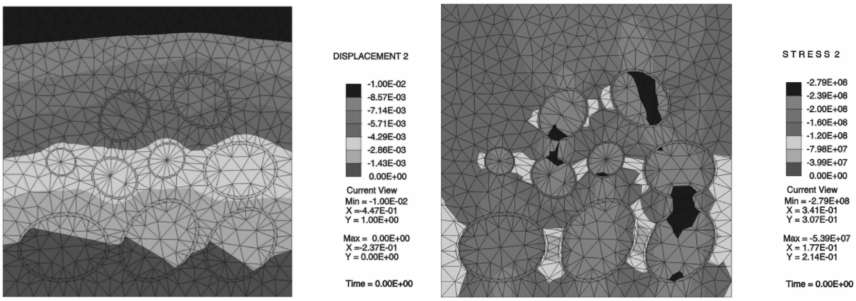


Figure 5: Slump simulation tests. (a) fresh concrete before test; (b) slump tests of concrete with low fluidity; (c) slump test of concrete with medium fluidity; (d) slump test of concrete with high fluidity.

Figure 6 presents a simple example of mechanical analysis. A specimen consisting of 9 particles and matrix is generated by HADES. The data are sent to mesh generator Gmsh [19], whereupon the displacement distribution (Fig.6a) and stress distribution (Fig.6b) under simple tension loading are analyzed by finite element analysis program FEAP [20]. Further studies on strength and damage estimation are foreseen for the near future.



(a) (b)

Figure 6: Displacement (a) and stress field (b) in HADES generated particulate system.

3.5 Durability estimation

Production of computer-simulated *compucrete* can reduce time and efforts bestowed on assessment of geometrical properties of material structure. Results are reliable in so far compucrete's geometric properties that are under investigation are realistic. Aggregate in concrete takes up about three-quarters of the material's volume. This high density cannot be realized by conventional SRA systems. Moreover, particle dispersion (configuration) at lower produced densities is far from realistic. Both deficiencies can be overcome with concurrent algorithm-based SPACE and HADES systems, as is experimentally demonstrated in our paper [12].

A complete and operational system for structure analysis particularly focusing on pore characteristics is elaborated in our paper [13]. The developed methodology will be applied to concrete for pore structure analysis by means of the pore network model for concrete durability. Different technical parameters and production conditions can be incorporated into this physics model.

4 Discussion

SPACE allows investigating hard core particle packing problems up till the jammed state inside and outside concrete technology whereby particles can be considered spherical. Internal forces that govern the packing process can be emphasized. Hydrated states in concrete technology are covered as well, allowing for studies such as self-healing capacity [11] and pore de-percolation [5]. Particle systems that change their packing due to external static or dynamic forces (resulting in flow), and the inclusion of arbitrary shape that has shown to have impact on the density of aggregate at the jammed state enforced the development of HADES. Its 3D version is gradually becoming operational, and will be used for exploration of the territories indicated herein.

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5 Conclusions

This paper demonstrates that the concurrent algorithm-based discrete element computer simulation systems SPACE and HADES are capable of exploration of fields of major technological and economic relevance, the mechanical and durability properties of concrete. They allow for tackling material optimization problems whereby particle packing is especially a major issue; the new version incorporates arbitrary particle shape, and allows the simulation of effects of external forces on the particulate material.

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