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PAPER

Designing architectural materials: from granular form to functional granular material

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Abstract

Designed granular materials are a novel class of architectural material system. Following one of the key paradigms of designed matter, material form and material function are closely interrelated in these systems. In this context, the article aims to contribute a parametric particle design model as an interface for this interrelation. A granular material is understood as an aggregation of large numbers of individual particles between which only short-range repulsive contact forces are acting. Granular materials are highly pertinent material systems for architecture. Due to the fact that they can act both as a solid and a liquid, they can be recycled and reconfigured multiple times and are thus highly sustainable. Designed granular materials have the added potential that the function of the granular material can be calibrated through the definition of the particles' form. Research on the design of granular materials in architecture is nascent. In physics they have been explored mainly with respect to different particle shapes. However, no coherent parametric particle design model of designed particle shapes for granular material systems in architecture has yet been established which considers both fabrication constraints and simulation requirements. The parametric particle design model proposed in this article has been based on a design system which has been developed through feasibility tests and simulations conducted in research and teaching. Based on this design system the parametric particle design model is developed integrating both fabrication constraints for architecture-scale particle systems and the geometric requirements of established simulation methods for granular materials. Initially the design system and related feasibility tests are presented. The parametric particle design model resulting from that is then described in detail. Directions of further research are discussed especially with respect to the integration of the parametric particle design model in 'inverse' design methods.

1. Introduction: designed granular materials in architecture

Designed granular materials are a new class within the overarching research area of architectural material systems [3] (see figure 1). In such a designed granular material, the form and the function of the material are closely interlinked [1, 3–5]. In this context, the article proposes a parametric particle design model as an interface for this form-function interrelation.

Granular materials are defined as very high numbers of individual particles which are larger than

a micrometre. These particles are not chemically or mechanically bonded. Consequently, only short-range repulsive contact forces are acting between them [6-12]. Examples of these materials are sand, gravel or snow [6, 7, 9-12]. In any granular material, the particle form affects the granular material's behaviour which ultimately defines its functionality in the context of an application [4, 8, 11-13].

Based on this observation, in a designed granular material the geometry and the materiality of the particles are developed in order to calibrate the characteristics of the overall granular material

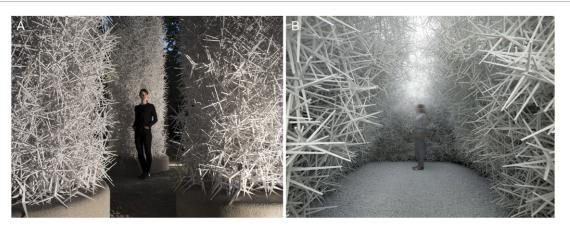


Figure 1. Designed granular materials can be used for architectural construction. (A) If non-convex particles are deployed they can interlock to form vertical structures. Reprinted by permission from Springer Nature Customer Service Centre GmbH: Springer Nature, Granular Matter [1](c) 2016. (B) Spatial enclosures can be created by pouring non-convex particles over a removable formwork of convex particles. The non-convex particles interlock to form a vault or dome once the formwork particles have been removed. Reproduced with permission from [2].

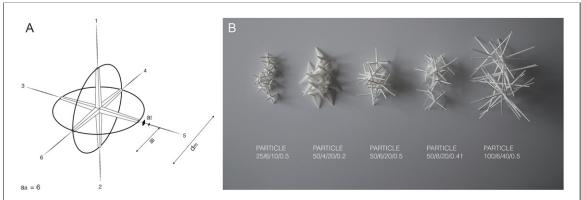


Figure 2. The characteristics of a granular material can be calibrated by adjusting the material and the geometry of its component particles. (A) An initial parametric particle design model was based on the cumulation of platonic solids. It allowed to vary the particles' longest diameter of the convex hull (d_m) , arm amount (a_a) , arm axis length (a_l) and arm taper (a_t) to be varied. Reproduced with permission from [2]. (B) Based on this parametric particle design model different particle types could be developed by varying the input parameters. The particle type index shows the values for these four parameters d_m in millimetres, a_a as a dimensionless value, a_l in millimetres and a_t as a dimensionless value Reproduced with permission from [2].

[1, 3-5]. Hensel and Menges have described architectural material systems as physical structures which can form spatial arrangements and modulate environmental factors, such as sunlight or rain. They have outlined three classes of architectural material systems: (i) 'proliferated component systems', (ii) 'globally modulated systems' and (iii) 'aggregate systems'. In a 'proliferated component system' an architectural structure is composed of units which can be varied according to internal and external functional criteria. In a 'globally modulated system' the architectural structure can be modified by adjusting control-points which affect the overall geometry. In an 'aggregate system' the architectural structure consists of particles which are not bound to each other; structures belonging to this class can be developed through the design of the component particles and the modulation of the boundary conditions [3].

Designed granular materials belong to the third class; that is, 'aggregate systems'. In this context of

architectural materials systems, the design of the particles' form is aimed at achieving architectural functionalities on the level of the overall granular material [3].

Based on this understanding of designed granular materials, the proposed parametric particle design model is an interface for the interrelation between the form of the particles and the function of the granular material for architectural applications. It can be deployed both for so-called 'forward' and 'inverse' methods of design. In a 'forward' design method the process moves from form or cause to function or effect. In an 'inverse' design method it moves in the opposite direction—from function or effect to form or cause [4, 14, 15].

For 'forward' design methods both experiments and simulations could be deployed, yet experiments are the more immediate method especially when treating problems for which no theoretical model exists or predicative models do not offer valid results [14]. These experiments are conducted in the physical realm and require information about the possible geometries for fabrication of the particles. For 'inverse' design methods, simulations are required which have specific underlying geometric models as the basis of their contact-calculations, such as spheres or polyhedra [14, 15]. The proposed parametric particle design model aims to integrate both of these methodological requirements into a coherent model in order to lay the foundation for the quantifiable interrelation of particle form and granular material function.

Within architectural design research, granular materials in general are a highly relevant research field: due to their ability to have both solid and liquid states, they can be recycled and reconfigured numerous times [1, 16–21]. Recycling denotes the reuse of a granular material employed in one structure for deployment in another structure; reconfiguring refers to the rearrangement of parts of a structure during its instalment [2]. Designed granular materials present the specific added possibility of developing material systems with entirely new material characteristics suited for architectural applications which non-designed granular materials do not offer [1, 3–5, 16, 22–24] (see figure 2).

2. Context: designing matter and materials

Research on designed granular materials is situated within the wider context of designing matter and materials. Among the terms used for the field is 'designer matter', as used in areview article by Reis, Jaeger and van Hecke. They define 'designer matter' as a material in which mesoscale structure is the key focus of investigation, as opposed to the material as a continuum at a macroscale or the component elements at the material's microscale [25].

In the present article, the terms 'designing matter', 'designing materials', designed matter' and 'designed materials' are used as close synonyms of 'designer matter', thereby laying the emphasis on the act or past act of design rather than the designers themselves.

Reis, Jaeger and van Hecke understand this notion of 'designer matter' to encompass 'transformative matter, mediated matter[©], smart matter, active matter, metamatter or machine matter' [25].

In order to evaluate each of these related descriptors—'designer matter', designing matter or materials and designed matter or materials—as a suitable overarching term for this emerging field with respect to designed granular materials, some related terms will be briefly reviewed in the following paragraphs. An in-depth review has been conducted in the context of the doctoral thesis by the first author [2].

The notion of 'transformative matter' emphasizes the passing of a substance from one state into another [26]. While granular materials in general have the capacity of a phase change, this aspect is not key to the development of designed granular materials in specific. The term 'transformative matter' appears not to be very widely used.

'Mediated matter' has been introduced by Oxman. The term lays the emphasis on matter or materials which are in interrelation with people and with the surroundings [27–30]. As such this notion can also apply to designed granular materials yet does not address their core aspects.

The concept of 'smart matter' or 'smart material' refers to a substance that reversibly changes properties due to a specific input [31–34]. Only some designed granular materials display this behaviour, so 'smart matter' is not suitable as an overarching term for this entire field.

'Active matter' is considered to be a multi-agent system which uses external energy [35–53]. Even though most such systems are biological, some granular materials are also considered to be 'active matter' systems [54–56]. Yet these applications are fairly specific and 'active matter' is therefore not appropriate as a common term for the wider field of granular materials consisting of designed particles.

The term 'metamatter' or 'metamaterial' refers to elements which are ordered on or in a substrate and which have properties that go beyond what is normally the case in a naturally occurring material [35, 57–69]. Given granular materials are by definition not bound to each other or embedded in a matrix, this term cannot be applied to them.

'Machine matter' is understood to be matter that is developed to act like a machine rather than a mere material [70–75]. This notion is not entirely suitable for designed granular materials, which are always considered as a substance as such rather than as a machine which is acting on a substance.

Other terms related to 'designer matter' which are not listed in the article by Reis, Jaeger and van Hecke might be 'digital materials', 'programmable matter' and 'architectured materials' [76–81].

Within the context of the research on granular materials presented here, the notions of 'designer matter', designing matter or materials as well as designed matter and materials seem to be best suited to describe the overarching research field. The notion of design as interrelating form and function which was prominently put forward by Sullivan in 1896 appears to be especially relevant in this regard: in designing matter or materials one interrelates material form on the mesoscale to material function on the macroscale [4, 14, 82].

3. Current state

An exploration of the current state of research needs to include contributions both from the field of granular physics and of architecture since the research pertains to both fields and ultimately aims to establish an intersection between them. The following sections will thus give a review of both. The projects will be evaluated considering two key questions: (a) has a geometric model been established which uses parameters; that is, placeholders, the values of which can be varied? (b) Does this parametric particle design model integrate geometric principles that respond to fabrication constraints for architecture-scale fabrication of the particles as well as simulation methods for granular materials? To conclude, the novel contributions of the research presented in this article will be highlighted.

3.1. Designed granular materials in architecture

An in-depth review of designed granular materials in architecture has been given in the doctoral thesis [2] on which this section is based.

In architecture several precedent projects have explored the potential of granular materials using designed particles.

One of the first projects was conducted as a Master's thesis by Tsubaki at Cranbrook Academy of Art. He developed particles which were based on two tetrapods at a 30 degree rotation to each other connected by a spine. These were partly poured and partly laid into a scaled dome and arranged into a window-screen [83–85]. The project was pursued further at Tulane University [86]. In this project, a parametric particle design model was not developed. The geometric values were set and kept constant. Only the fabrication and not the simulation of the particles was considered.

Matsuda conducted his Diploma Unit 4 thesis at the Architectural Association School of Architecture (AA). In this project he developed designed particles made from wooden matchsticks. Three matchsticks were joined at their middle to form a six-armed particle. Circa ten thousand of these particles were fabricated and tested. These tests included the investigation of basic system properties, such as the angle of repose of the material, spatial enclosures, such as domes, as well as interaction with possible environmental factors, such as precipitation [5, 20, 21, 87, 88]. A parametric particle design model was developed in this case, yet it was confined to stick-based particles. The integration of simulations was not considered; the model was mainly fabrication-oriented.

In a GPA studio project at Rice University Hawkins and Newell developed designed particles from a sheet material. For one particle two U-shaped pieces were assembled to form either an 'X' or an 'A'. These geometries were developed to allow interlocking of the particles, low particle weight, speed of fabrication and low production cost. Circa three thousand particles of each type were made. Experiments focussed among other things on the construction of larger screens to modulate light transmission

as well as on interaction between people and the material system [20, 21, 23, 89]. Here too a parametric particle design model was developed, but in this case it was confined to sheet-based particles. Fabrication was taken into account; simulations have not been integrated.

In the AA's Emergent Technologies and Design programme, Schertzing and Bayer conducted a studio project in which they up-scaled both the particle geometries and the structural types developed by Matsuda. They fabricated sixarmed particles with diameters of 900, 600 and 300 millimetres. These were poured over a removable formwork into an arch that was able to support live load [20]. This project deployed a scaled version of Matsuda's particles. No specific parametric particle design model was established, yet the principles from the previous project apply. Only fabrication of the particles and no simulation was considered.

At the Swiss Federal Institute of Technology (ETH) Zurich, Gramazio Kohler Research developed the project 'Remote Material Deposition'. In the early stages of the project, designed particles were developed which were made from wooden dowels and velcro. Each dowel was wrapped with two bands of velcro, one with the male and one with the female side in order to allow adhesion between them. These were deposited using a six-axis articulated robot and sensory control [90–94]. In this project only this one particle seems to have been developed and a parametric particle design model may thus not have been established. As in the previous projects, fabrication of the particles was the driving parameter and simulations were again not conducted.

In collaboration with the Self-Assembly Lab at the Massachusetts Institute of Technology (MIT), Gramazio Kohler Research of the ETH Zurich inaugurated the project 'Jammed Architectural Structures'. The key aspect of this project is the reinforcement of granular materials with a string. While the final prototype deploys non-designed particles, several industrially fabricated particles were tested which could also be considered as designed. These were investigated in various combinations with respect to their compressive strength [17, 95-97]. Since ready-made parts were used as particles, a parametric particle design model was not developed. The particles stem mainly from serial production so architecture-scale fabrication of them seems feasible. Simulations were not conducted on these particles but were included in the later stages of the project.

3.2. Designed granular materials in physics

A detailed review of investigations on designed granular materials in physics which are relevant to architecture has been given in the doctoral thesis [2]. This review was largely based on reviews by Jaeger and collaborators, Franklin and collaborators as well as Behringer and collaborators [4, 13, 16, 98–101].

Philipse of the Van 't Hoff Laboratory for Physical and Colloid Chemistry at Utrecht University investigated granular materials consisting of prolate particles—in other words, rods. He established an interrelation between the particles' aspect ratios and the packing density as well as the fluidity of the granular material that they constituted [102]. A parametric particle design model was not developed as such yet the results were presented as theoretical models which can form the base of a parametric particle design model. Simulations were not conducted, yet the particles are suitable for serial production from rods. Blouwolff and Fraden from the Complex Fluids Group at Brandeis University studied the coordination number of granular cylinders. The coordination number defines the amount of neighbours which one particle has on average. Their results demonstrate that the coordination number increases with increasing aspect ratio. Granular materials consisting of particles with an aspect ratio of 50 formed 'plugs' which were stable enough to be lifted up in one piece [103]. Similar to the previous project a parametric particle design model was not used to design the particles yet the results are presented in a manner which makes them a good basis for a parametric model of particle design. Simulations were not deployed, yet these particles are suitable as well for serial production from rods.

Research on the simulation of particles which are non-convex was conducted in a collaboration between the MoSCoS School of Mathematics and Physics at the University of Queensland, CSIRO Exploration and Mining, the Golder Geomechanics Center at the University of Queensland and the Grupo de Simulación de Sistemas Físicos at the Universidad Nacional de Colombia. The aim was to establish a molecular dynamics (MD) model which allows the characterization of granular materials consisting of such particles. They based the modelling of the particles on 'spheropolytopes'. These were used within the MD simulations to test the clogging behaviour for granular materials consisting of particles with different aspect ratios in a hopper-flow as well as the behaviour of such granular materials under threeaxial compression [104]. The 'spheropolytopes' can be considered a parametric particle design model. Simulations were conducted, yet fabrication of the particles—especially for architecture-scale construction-was not.

A collaboration of LCD, SP2MI and UPMC investigated transport properties of granular materials consisting of so-called 'spiky' particles. Packings of such particles were simulated using a numerical model and then the transport properties of the material, such as permeability, were determined. The results indicated that the porosity of the granular material depends on the so-called 'sphericity' of its component particles [105]. Ellipsoids were added to

a sphere to produce protrusions on that sphere. Overall the particles were regular, and they were mostly isotropic—these geometric operations can be considered a parametric particle design model. The particles were simulated yet fabrication was not considered.

Wouterse, Luding and Philipse investigated granular materials consisting of rods at Van 't Hoff Laboratory for Physical and Colloid Chemistry at Utrecht University and at Multi Scale Mechanics at the Universiteit Twente. They aimed to establish a theoretical model to simulate the relation between 'particle volume fraction' and 'average contact number (C)' and to analyse the average contact number of particles. Among other things, their theoretical results show that the 'average contact number (C)' reaches a maximum of 9 [106]. A model of the rods with different aspect ratios was established which is in principle a parametric particle design model. Simulations were implemented; fabrication was not discussed yet is feasible considering that the particles were in principle rods.

Trepanier and Franklin of the Rochester Institute of Technology conducted research into the disintegration of cylinders consisting of granular rods. The aspect ratios of the rods were set in relation to the heights at which a cylinder is stable [107]. Similar to the previous project, the aspect ratios of the rods were varied, which is a parametric operation. Yet here fabrication of the particles was conducted, which is also suitable for architecture-scale particles. Simulations were not conducted.

A group composed of the School of Physics and the School of Mechanical Engineering at Georgia Institute of Technology and the Department of Physics at Rochester Institute of Technology investigated the characteristics of granular materials consisting of 'u-shaped' particles. The groups studied the formation and the disintegration of columns made from these particles and established both experimental and theoretical models. The particles display a behaviour which the authors call 'entanglement' [101]. A parametric particle design model was developed which varied the length-to-width ratio of the 'u-shaped' particles. The particles were not customfabricated but stemmed from industrial serial production which could be adopted for architecture. Simulations were conducted.

The research on 'u-shaped' particles was continued by Franklin in the School of Physics at the Rochester Institute of Technology. He investigated the granular material consisting thereof under tension. In this state, the material elongates, displaying stickslip behaviour, and eventually breaks. The probability of breakage increases proportionally to the length of the test piece [100]. The same parametric particle design model specifying length-to-width ratio of the 'u-shaped' particles which was developed in the previous project was used again here, yet in this case the ratio was kept constant. The particles were thus

suitable for serial production. Simulations were not deployed.

The Jaeger Lab at the University of Chicago and the Sibley School of Mechanical and Aerospace Engineering at Cornell University conducted an extended investigation of the interrelation between particle shapes and the response of the respective granular materials to confining pressures. Both convex and non-convex particle geometries were tested. The main characteristics of the granular material which were analysed were the packing density, yield stress and Young's modulus. Their results show that under constant confining pressure, the yield stress and Young's modulus can be calibrated by particle shape; yet if confining pressure increases this effect is reduced. With respect to the stiffness of the granular material under confining pressure, two strands of particle shapes could be distinguished based on their 'sphericity': the first group are mainly polyhedral particles which form face-to-face and thus very stable contacts; the second group are particles with arm extensions which form point-like and thus less stable contacts [13]. Several of these particle types have been further analysed with respect to their 'granular plasticity' [108, 109]. A parametric particle design model was not established as such. Defined geometries were used in which values were not varied except for the arm length in a series of hexapods. The architecture-scale fabrication of the particles was not considered. The particles were 3D printed which is quite likely too costly in extremely high numbers. The results were established using experiments not simulations.

Miskin and Jaeger from the Jaeger Lab at the University of Chicago have applied evolutionary algorithms for the 'inverse' modelling of particle geometries. This approach allowed a specific target characteristic to be set, such as the maximum packing stiffness or packing density of a granular material in a given volume, and then particle geometries to be found that best match the target. 'Design rules' for the particles were developed which departed from the fact that spheres are the basis of a discrete element method (DEM) simulation. In order to arrive at a wide range of particle shapes, spheres were iteratively added to an origin-sphere and permanently bonded to each other [15, 110, 111]. The 'design rules' for the particles formed an integral part of the research: they were the basis for the 'inverse' optimization of the granular material and can be considered a parametric particle design model. Simulations were considered from the beginning. 3D printing was used for fabricating the particles, which appears expensive with respect to architecture-scale construction.

Again at the Jaeger Lab at the University of Chicago, Murphy conducted research on granular materials for architectural structures. More specifically he was aiming for granular materials suitable for the construction of arches and columns with high

aspect ratios. The key functional criteria for the granular material were pourability of the material during construction and self-confinement under external loads once the material has been poured into place. A group of shapes was identified and called 'Z', 'U' and 'Z₉₀' depending on the orientation of two arm extensions in a backbone. 'Z' particles can be poured most easily and show the highest strain-stiffening; 'U' particles form strings which are the hardest to disentangle; 'Z₉₀' display the highest rigidity [98, 112, 113]. The particle model is parametric since it allows the orientation of the arms on the backbone to be set as variables. Architecture-scale fabrication of the particles was considered, as was the simulation of the particles using bonded spheres.

A research team of the Department of Mechanics Engineering at the South China University of Technology and of the Department of Mechanics and Aerospace Engineering at Peking University published research on 'maximally dense random packing (MDRP)' of so-called 'intersecting spherocylinders'. The team deployed a 'geometrically based relaxation algorithm' which showed good correspondence with earlier simulations and experimental results. These simulations were used to interrelate the aspect ratio of the arms of the spherocylinders and the 'MDRP' of the overall granular material. Among others the results show that the 'MDRP' is higher in '2D intersecting spherocylinders' than in '3D intersecting spherocylinders' and packing density decreases with increasing aspect ratio of the particles' arms [114, 115]. The team of South China University of Technology in cooperation with Electric Power Research Institute of Guangdong Power Grid Cooperation further expanded the group of particle shapes to those that can be produced by the deformation or assembly of rods [116]. The particles have clearly defined geometric variables which in essence is a parametric particle design model. As in most of the previous cases from granular physics, simulations were conducted, yet in this case also a specific fabrication method—rods—was considered.

A group composed of the Laboratory of Energy Science and Engineering, the Department of Mechanical and Process Engineering and the Institute of Energy and Process Engineering at the ETH Zurich as well as the Swiss Federal Laboratories for Materials Science and Technology (Empa) presented research on the interrelation between the morphology of 2D and 3D packings of highly non-convex particles and the contact forces occurring in these packings. According to the authors these types of particles show the capacity to bear both compressive and tensile loads even though there is no cohesion between them. The team deployed a newly developed DEM model as a means of investigation. The 'sphericity' of the particles was used as a variable parameter. Their results show—among other things—that the distribution of contact forces of 3D packings in the normal direction

of compression becomes increasingly heterogeneous if particle 'sphericity' is decreased; whereas in 2D packings this distribution is not affected by the particle 'sphericity' [117]. This project clearly establishes a particle model with variable parameters for the particles' 'sphericity' and simulations are deployed. Yet suitable fabrication methods are not included in the development of the particle model.

3.3. Contributions to the current state

In architecture several initial parametric design models for particles have been established yet they have been closely connected to specific fabrication methods and are thus in principle projectspecific. These parametric particle design models do not integrate those geometries which are required for simulation, yet fabrication of the particles for architecture-scale construction is considered or at least possible in all projects. In granular physics parametric particle design models are established in most projects as a basis for quantitative analysis, yet in every project these are confined to quite a small group of project-specific particle shapes except in the case of the work by Miskin and Jaeger at the University of Chicago [15, 110, 111]. The projects consider either fabrication or simulation; only three of them integrate both [98, 101, 112, 113, 116].

In this context, this article contributes on two levels. First, it presents the crucial aspects of a design system which mainly defines the key principles that need to be considered when designing particles for granular materials. This design system is complemented by feasibility tests conducted in research and teaching. It has been developed in a doctoral thesis and related teaching modules [2]. Second, a parametric particle design model is introduced which is a specification of this more generic design system. The parametric particle design model integrates three aspects. First, it allows particles to be designed with consideration of their geometric type and materiality to produce a wider group of particle shapes than the previously established models have allowed. This wide scope of possible geometric types and materials also makes them an advancement from the most integrated parametric particle design models which have been presented in the research by Gravish and collaborators, Murphy and collaborators as well as Meng and collaborators [98, 101, 112, 113, 116] which consider a confined group of particle geometries and related serial fabrication methods only. Second, it considers the geometric requirements for the fabrication of particles which are suited for architecture-scale construction. And third, it integrates those geometries which are suitable for the simulation of these granular materials using DEM. This parametric particle design model is intended to be an interfacing tool for architectural design and granular physics as well as a starting point for the 'inverse' design of granular materials.

4. Methods

The parametric particle design model has been developed on the basis of a design system. This design system has been presented in the doctoral dissertation by the first author [2]. On the one hand the design system is a classification for particle systems as well as construction systems suitable for granular materials [2]. The category of particle systems—which is the main category relevant in the context of this article—is further distinguished by geometric and material characteristics of the particles as well as particle mixes [2]. On the other hand the design system proposes key parameters for each of its categories which can be used as an interface for collaborations between architecture and granular physics [2]. The design system is based on the investigation of preceding projects in architecture and granular physics as well as on feasibility tests in research and teaching conducted in the context of architecture [1, 99, 118–120] (see figure 3).

The parametric particle design model refines the key categories of this design system. It details the generic parameters given for each category into definite geometries which integrate three core aspects: (i) selection of fabrication processes of the particles which may be suitable for architectural applications, mainly through considering the particle's dimensions and the estimated production cost; (ii) geometric possibilities and constraints of these fabrication processes; (iii) translation of the analogue geometry into a digital geometry with respect to the models used for DEM simulations. The parametric particle design model has been developed using a visual programming language which is embedded in a 3D computer-aided design software application. As a reference for the simulation software a commercially available DEM software package has been used [121].

5. Results

Initially the design system categories and related feasibility tests will be introduced here as they are developed in the doctoral thesis [2]. Then the parametric particle design model will be presented in terms of these design system categories.

5.1. Design system and feasibility tests

The entire design system encompasses categories for particle systems and related construction systems [2]. Here, only those categories are introduced which are relevant to the design of the individual particles themselves, namely the dimension, geometric types and geometric variability.

The testing and thus the validation of the behaviour of the designed granular materials occurs through both experiments and simulations (see figure 4). These can—for example—give an indication whether a granular material consisting of

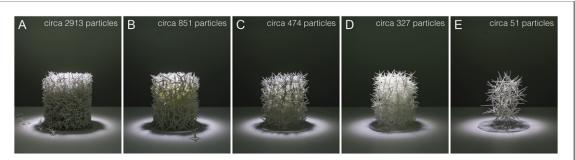


Figure 3. The particle types presented in figure 2(B) were tested with respect to their packing density. Experiments were repeated 20 times and the mean packing density for a fixed volume was calculated. The figures show one probe and the average particle count of (A) particle type 25/6/10/0.5. Reprinted by permission from Springer Nature Customer Service Centre GmbH: Springer Nature, Granular Matter [1] (c) 2016. (B) particle type 50/4/20/0.2 [24] John Wiley & Sons. (C) particle type 50/6/20/0.5. Reprinted by permission from Springer Nature Customer Service Centre GmbH: Springer Nature, Granular Matter [1](c) 2016. (D) particle type 50/8/20/0.41. Reproduced with permission from [2] and (E) particle type 100/6/40/0.5. Reprinted by permission from Springer Nature Customer Service Centre GmbH: Springer Nature, Granular Matter [1](c) 2016.

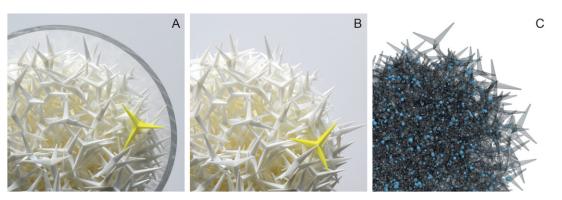


Figure 4. Experiments and simulations are used to explore the properties of a newly developed granular material and its suitability in the context of architectural construction. (A) In an experiment tetrapodal particles are contained inside a cylinder. They have been designed varying the particle dimension, arm amount, axis length and arm taper. The particles used in this experiment have the values 50/4/20/0.2 [2]. (B) The particles remain stable to form a column after the outer cylinder has been removed [2]. (C) A DEM simulation allows to analyse contacts in the designed granular material consisting of the tetrapodal particles. The amount of contacts in a granular material can be one indicator of its stability. Reproduced with permission from [2].

designed particles remains stable or if it is unstable and thus not suitable for the formation of space-forming architectural structures. However, also instability can be desirable behaviour in architectural design, for example when considering a formwork which needs to flow out of a mould. Evaluating the suitability of a specific designed granular material and its behaviour thus requires a clear identification of its exact evaluation criteria relevant for architectural construction and design.

5.1.1. Dimension

The longest diameter of a particle's convex hull defines the dimension of a particle (see figure 5). The convex hull is the smallest possible convex polygon or polyhedron that encompasses all points of a given set of points. In the case of a particle this set of points are those vertices that define the particle's geometry. The dimension of a particle is relevant for, among other things, the establishment of-dimensional ratios between the individual particle and the overall structure as well as for the determination of size grading in particle mixes [2].

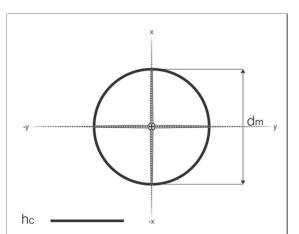


Figure 5. The longest diameter of the convex hull (hc) of a particle defines the particle's dimension ($d_{\rm m}$). Reproduced with permission from [2].

A feasibility test—or rather a suitable application scenario—of the dimension of particles was conducted as part of an initial parametric particle model for symmetrical non-convex particles. This parametric particle model allowed particle geometries to be

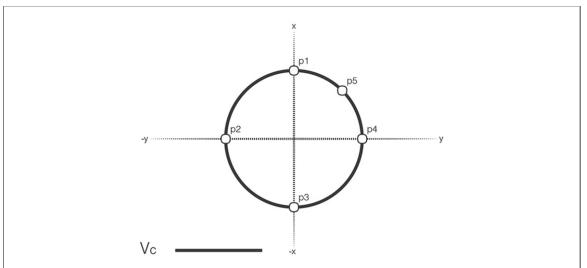


Figure 6. In a convex particle the convex volume (V_c) which is here shown as two-dimensional section encloses all lines connecting all points pertaining to the particle's geometry. Reproduced with permission from [2].

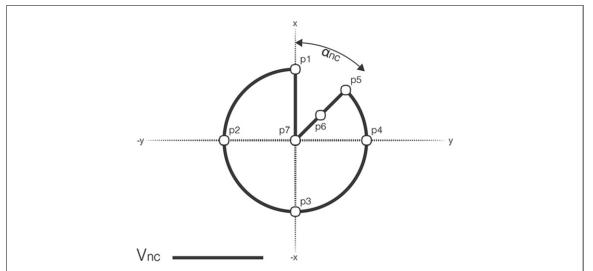


Figure 7. In a non-convex particle the non-convex volume $(V_{\rm nc})$ which is here shown as a two-dimensional section does not enclose all lines connecting all points pertaining to the particle's geometry. The degree of non-convexity can be defined by the angle $\alpha_{\rm nc}$. Reproduced with permission from [2].

designed with the exact same dimension yet different arm amounts. This way it could be used to investigate the effect of arm amount only on the packing density of granular materials consisting of these particles [2].

5.1.2. Geometric types

A geometric type is understood to be the set of features which bring forth a characteristic and distinct group of behaviours in a granular material consisting of these particles. Three main categories of geometric types have been established: (a) convex, (b) non-convex and (c) double non-convex. This characterization is based on the observed behaviour—or functionality—of the granular material consisting of these geometric types through feasibility tests [2].

(a) Convex: a particle is called convex if its enveloping surface contains all lines connecting all points pertaining to its geometry (see figure 6). The enveloping surface is the surface that describes

the actual geometry of the particle and it is therefore not always equivalent to its convex hull. Examples of the group of convex particles are spheres or ellipsoids. Very generally the particles pertaining to this category have the ability to flow. Considering this behaviour, one extreme of the geometries pertaining to the convex category would be spheres, the other rods with high aspect ratios: whereas granular materials consisting of spheres can be poured in any orientation, those consisting of rods can only be poured in longitudinal orientation to the rods. The capacity of a granular material to flow is extremely relevant for the material to be easily poured into place during the construction phase of an architectural structure [2].

A comparative feasibility test of examples of the three geometric types shows that spherical particles

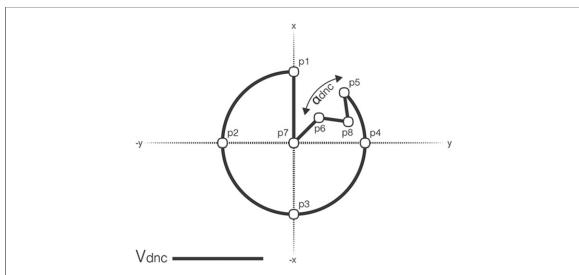


Figure 8. In a double non-convex particle the double non-convex volume $(V_{\rm dnc})$ which is here shown as a two-dimensional section does not enclose all lines connecting all points pertaining to the particle's geometry on two geometric scales. The degree of double non-convexity can be defined by the angle $\alpha_{\rm dnc}$. Reproduced with permission from [2].



Figure 9. The different characteristics of designed granular materials consisting of convex, non-convex and double non-convex particles can be observed when pouring them into a cylinder and subsequently removing it by pulling it upwards. (A) Convex particles flow out of the cylinder, (B) non-convex particles form a stable column, (C) double non-convex particles entangle so that they can be pulled up as a cluster.

flow out when a cylinder is removed within circa 1 second: no interlocking occurs (see figure 9(A)). This characteristic has been deployed for instance in the context of a removable formwork for arches, vaults or domes: here, convex particles—spheres—flow out of an arch or vault consisting of non-convex particles—hexapods. This combination of properties of two different designed granular materials was the basic formative principle of the architectural structure shown in figure 1(B) [2].

(b) Non-convex: a particle is called non-convex if its enveloping surface does not contain all lines connecting all points pertaining to its geometry (see figure 7).

Consequently these particle types have at least one internal angle larger than 180 degrees. Subtypes pertaining to this group are those particles with arm extensions—like tetrapods—yet in general any geometry with an indentation can fall into this cate-

gory. Particles belonging to this category have in principle the capacity to interlock. An interdependence between the geometric features defining the geometry as non-convex, such as the amount of arm extensions or the internal angle, can be established for each use case. This capacity to interlock is crucial in the context of architecture where a state of stability is required of the granular material when a structure is inhabited

In the comparative feasibility test hexapods form a stable column when a cylinder is removed from the top (see figure 9(B)). The architectural structure shown in figure 1(A) makes use of this property [2].

(c) Double non-convex: a double non-convex particle displays non-convexity on two geometric scales (see figure 8). Through this geometric operation hooks are formed. Particles do not flow at all if subject to gravitation since they strongly interlock or, rather, entangle. Dissolution of such

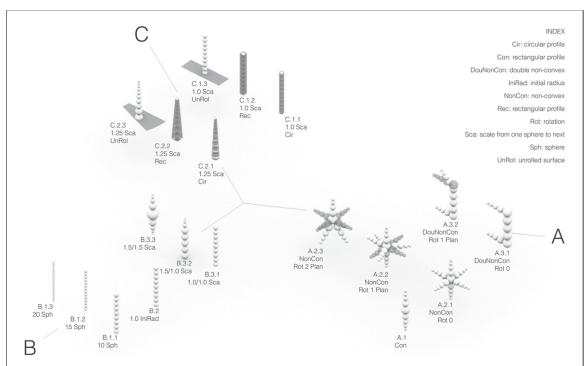


Figure 10. The parametric particle design model integrates requirements for the geometric types of the particles, for the particles' fabrication at architectural scale and for the simulation of the granular material consisting of these particles. Parameters can be varied with respect to the geometric type (A), the definition of the individual arm of a particle (B) and the choice of fabrication method (C).

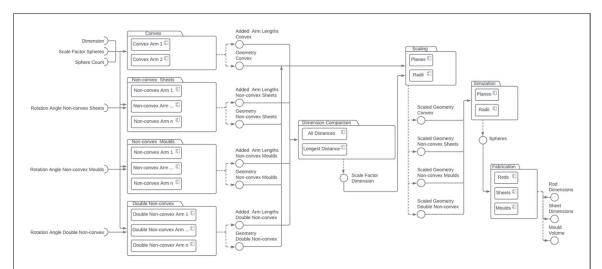


Figure 11. The unified modeling language diagram of the main components of the parametric particle design model shows the entire data stream from the inputs to the simulation and fabrication outputs. In principle five stages can be distinguished: the generation of the geometry through user inputs, the dimension comparison, the scaling of the geometry, the simulation output and the fabrication output.

a granular material can occur through the induction of vibrations. Of the three main geometric types, these have the least ability to flow and are thus highly pertinent as a construction material when considering permanent structures, yet handling in the process of pouring the granular material into place can be intricate [2].

In the comparative feasibility test S-shaped particles can be picked up as a whole (see figure 9(C)). Several loose particles flow out yet the structure settles into a drop-like form. A scaled prototype con-

ducted by Alexander Kretzschmar in the framework of a Bachelor's seminar investigated the dissolving of an entangled granular material consisting of double non-convex particles, its subsequent re-entanglement in a spatial formation as well as the final disentanglement of the granular material [2]. A prototype at architectural scale using this principle has not yet been conducted.

5.2. Parametric particle design model

The parametric particle design model is a specification of the design system presented in the previous section. It encompasses three key aspects: the geometric categories presented in section 5.1, suitable fabrication methods and those geometries which are required for the numerical simulation of granular materials (see figures 10 and 11). In the following sections it will be presented in terms of its variable and non-variable inputs as well as its non-variable outputs.

5.2.1. Inputs and outputs of the parametric particle design model

Geometry: the parametric particle design model integrates the aspects of the design system which have been presented in section 5.1: (a) dimension of the particles and (b) the three geometric types.

- (a) Dimension: as a parameter this is both a variable input and an output of the parametric particle design model. The variable input defines the desired dimensional ranges which for example can be used within the search space of an optimization process. The output is a fixed number value.
- (b) Geometric types: the geometric types are embedded as variable inputs in the parametric particle design model as potential axes of extension from a point of origin. In the convex mode this extension can happen only in one axis, which is set as the z-axis in the model. The variable inputs for the convex geometric type are the arm amount, the sphere count and the scale factor from one sphere to the next. The radius of the initial sphere can also be varied, yet this effect is cancelled out by the dimensioning operation outlined in (a). In the non-convex mode the extension occurs in at least two directions from the point of origin. The variable inputs for the non-convex type are the arm amount, the sphere count, the scale factor from one sphere to the next and the angle of rotation of the arms. The non-variable input is the radius of the initial sphere which is given by the convex core geometry of the particle. In the double non-convex mode the endpoint of a given axis of extension can form the point of origin for a new extension at an angle to the original one. As for the non-convex geometric type the variable inputs for the double non-convex geometric one are the arm amount, the sphere count, the scale factor from one sphere to the next and the angle of rotation of the arms. The non-variable input is again the radius of the initial sphere which is given by the radius of the last sphere of the convex core geometry. The non-variable outputs for all three geometric types are the base planes and radii of the spheres described in the paragraph 'simulation'.

Fabrication: the input parameters which allow fabrication methods to be chosen consider those fabrication processes that deploy (a) rods, (b) sheets or (c)

moulds. The three fabrication methods are modelled with surfaces that envelope the spheres which the particles are composed of for simulation as outlined in the paragraph 'simulation'. This category of the parametric particle design model is mainly relevant as an output for the preparation of fabrication data for the particles.

- (a) Rods: the input for rods allows an element of choice between a circular or a rectangular profile which is extruded along the axis of a particle arm using the isocurves of its component spheres. The profile can be scaled using the scale factor input described in the paragraph 'geometry' in order to model tapering towards the ends of the particle. The output is a surface model for fabrication as well as a cut-length if prefabricated rods are deployed.
- (b) Sheets: the non-variable input for this fabrication method is a rectangular profile that is wrapped around the circular isocurves of the component spheres of an arm extension. Again the profile can be scaled to model tapering towards the ends of the particle with the scale factor input described in the paragraph 'geometry'. The planes of arm extensions are variable inputs. Here, the choice is between arm extensions that occur in one plane only and arm extensions that occur in perpendicular planes. Another option is the use of a developable surface—for example with metals. This last option is modelled by a cylinder that can be unfolded. The output is a surface model for fabrication.
- (c) Moulds: here, the non-variable input considers two-piece moulds, which implies that undercuts in either side of the mould need to be avoided. Again, profiles can be either circular or rectangular, and tapering towards the end of an extension can be modelled using the scale factor input of the arms outlined in the paragraph 'geometry'. The output is the mould volume for computer numerically controlled (CNC) fabrication.

Simulation: a DEM software package has been assumed as the simulation environment with which the parametric particle design model is interfacing. The package uses circles in two-dimensional models and spheres in three-dimensional ones to compute the forces and torques of the particles. If particle geometries are non-spherical these spheres are bonded in order to form so-called clumps [121–123]. An early benchmark comparing this software package to one that uses polygonal blocks has shown that these clumps are faster to compute than polyhedral models if particle numbers exceed one thousand [124].

In order to ensure that the particle geometries can be simulated in the DEM software package, the parametric particle design model uses spheres as a nonvariable input. These are generated using the output base planes and radii of the three geometric types as described in the paragraph 'geometry' above. A tapering arm extension is modelled by spheres that decrease in size. The non-variable outputs are the sphere surfaces, centre points and radii which can be exported to the DEM software package.

5.2.2. Applications of the parametric particle design model

There are three main areas of application for the parametric particle design model: (a) simulations for 'inverse' modelling, (b) digital fabrication and (c) experiments for comparative characterization of the particles. The model can be used following exactly this sequence of steps from (a) to (c) which would be considered a conventional route of optimizing the particle design. Yet it can also be deployed in any other order that a specific working process requires.

- (a) Simulations: in numerical simulations the parametric particle design model can be used as a direct input. Here, this input is based on the modelling of bonded spheres presented in section 5.2.1. Through variation of one specific parameter or a combination of parameters the particle design can be calibrated for specific functions of the resultant granular material by 'inverse' modelling.
- (b) Fabrication: based on the surface representation presented in section 5.2.1 the parametric particle design model allows files to be exported that are immediately suitable for fabrication.
- (c) Comparative experiments: experiment series comparing different variables of the particles can be set up so that the exact geometric values are compared to the experimental results. For this purpose particles can be digitally fabricated in sufficiently high numbers based on the parametric particle design model. The exact geometric values are then known and can be directly matched with the experimental results.

5.2.3. Architectural evaluation parameters for the parametric particle design model

The parametric particle design model has been developed as a proposed interface between architectural design and construction and granular physics, with one very promising area of future application being the inverse optimization of the particle shape using DEM simulations.

For any such optimization, metric evaluation parameters which describe functional criteria for architecture need to be defined. These evaluation parameters need to address the following aspects of architectural construction: (a) fabrication speed and cost, (b) behaviour of the granular material during construction, (c) load-bearing behaviour of the structure and (d) environmental modulating of the structure.

- (a) Fabrication speed and cost: these are typically evaluated in particles per hour and cost per particle. The evaluation can be conducted in close collaboration with an industrial partner for fabrication of the particles.
- (b) Behaviour of the granular material during construction: here, the pourability of the granular material is the key characteristic. Metrics used in the rheology of granular materials can be deployed, such as the viscosity (η) . These can be obtained using DEM simulations.
- (c) Load-bearing behaviour of the structure: architectural structures are exposed to compressive, tensile and shear forces. Compression and tension are usually measured in newtons (N), whereas shear is measured in pascals (Pa). DEM simulations can be deployed to evaluate these parameters.
- (d) Environmental modulating of the structure: apart from being load-bearing, architectural structures have the role of modulating environmental influences, such as light, sound, heat or humidity, in order to create inhabitable spaces. Light modulation can be measured in illuminance, with the unit being the lux (lx); sound modulation in sound absorption with the dimensionless absorption coefficient; heat modulation can be explored by heat capacity (C_{th}) of the granular material, with its unit being joules per kelvin ($J K^{-1}$); and humidity modulation in the difference between external and internal relative humidity; which is typically given as a percentage. All of these require either experimental testing or specific environmental testing software packages into which the DEM model can be imported for evaluation.

5.2.4. Case study: particle shape-optimization for fabrication

As a case study for the parametric particle design model a particle shape optimization for mould fabrication has been conducted. The case study refers back to the particle production process used for the first two full-scale architectural demonstrators (see figure 1). The particles have been developed based on the cumulation of Platonic solids [2]. Yet, the development of the particles was conducted using 'forward' methods of design that were mainly based on geometric operations. The case study thus investigates what could be done differently—and possibly better—using the parametric particle design model as part of the design process. The previously developed particle had six arms—a hexapod. It had a diameter of 300 millimetres and was produced using injection moulding (see figure 12). These features are taken on for the case study which will be presented in the following paragraphs.

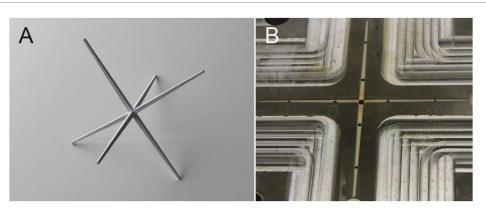


Figure 12. The particles which were mainly used for the construction of the architectural demonstrators shown in figure 1 have been produced using injection moulding. (A) The particle was based on the cumulation of a cube resulting in a six-armed particle, a hexapod, with the values 300/6/40/0.5. (B) The mould for injection moulding was produced using CNC fabrication. Reproduced with permission from [2].

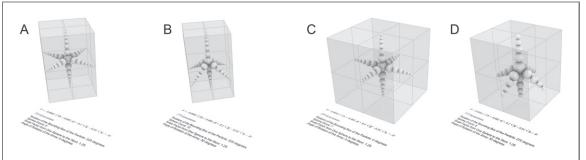


Figure 13. The evolutionary solver was run for each of the four fitness functions: (A) fitness function 1 minimizing volume of the bounding box of the particle (V_b) and the angle of rotation of the arms lying in the xy-plane (A_r) , (B) fitness function 2 minimizing V_b and maximizing A_r , (C) fitness function 3 maximizing V_b and minimizing A_r and (D) fitness function 4 minimizing V_b and maximizing V_b

As a non-variable input parameter the dimension is set to 300 millimetres. The arm amount is six and the rotation of the four arms lying in the world xyplane is enabled. Variable input parameters for the optimization algorithm are the rotation of the bounding box volume of the particle, the sphere count, the scale factor from one sphere to the next as well as the rotation angles of the arms lying in the world xyplane. The rotation of the bounding box volume of the particle occurs in the world xy-plane, the sphere count is set between 2 and 10, the scale factor from one sphere to the next between 1 and 1.25 and the angle of rotation of the arms between 0 and 30 degrees. All arms are treated equally in this case study yet a non-equal setting of the input parameters is also possible.

The optimization is conducted with the in-built evolutionary solver of the modelling environment which has been used for the development of the parametric particle design model. For this case study the default settings of the evolutionary solver have been applied. A runtime limit of 1.5 hours has been implemented. The initial state is set with a 0 degree rotation of the bounding box volume, a sphere count of 10, a scale factor from one sphere to the next of 1 and an angle of rotation of the arms to be at 0 degrees to the world *xy*-plane.

The evaluation parameters for the evolutionary solver are the volume of the bounding box volume of the particle (V_b) , the arm length (A_l) , the scale factor from one sphere to the next (S_f) , the sphere count (S_c) and the sum of angle of rotation of the arms which are lying in the world xy-plane (A_r) . The bounding box volume of the particle and the scale factor of one sphere to the next are key aspects for fabrication, since the size of the bounding box defines the amount of material required for the making of the mould and the scale factor from one sphere to the next defines the arm taper. As a consequence, the bounding box volume should be minimized in order to save material and the arm taper should be maximized since an arm taper enables the finished particle to be removed more easily from the mould. The sphere count is relevant for future simulations. It should be kept low in order to save computational time. Arm length and arm rotations are key parameters for the functionality of the particles. In this case study the arm length was optimized to be as high as possible as this enables interlocking of the particles. The angle of rotation of the arms was minimized as well as maximized, where minimization denotes that the arms are lying in the world xy-plane and maximization that they are rotated downwards. These two different sets of results can serve as an input for future simulations or experiments which evaluate the effect of the angle of rotation of the arms on the characteristics of the overall granular material. These evaluation parameters were embedded in the following fitness function (F) for the minimization of the angle of rotation of the arms:

(a)
$$F = -0.0001\sqrt{V_b} + 0.001A_1 + 0.1\sqrt{S_f} - 0.01$$

 $\sqrt{S_c} + A_r$

The fitness function (*F*) for the maximization of the angle of rotation of the arms is:

(b)
$$F = -0.0001\sqrt{V_b} + 0.001A_1 + 0.1\sqrt{S_f} - 0.01\sqrt{S_c} - A_r$$

In order to show the effect of the bounding box volume of the particle on the solution, V_b is allowed to be maximized, and the fitness function is written as:

(c)
$$F = 0.0001 \sqrt{V_b} + 0.001 A_l + 0.1 \sqrt{S_f} - 0.01 \sqrt{S_c} + A_r$$

As a comparison the fitness function for the maximization of the bounding box volume of the particle is tested also with the maximization of the angle of rotation of the arms and written as:

(d)
$$F = 0.0001 \sqrt{V_b} + 0.001 A_l + 0.1 \sqrt{S_f} - 0.01 \sqrt{S_c - A_r}$$

For each of the fitness functions an optimization was run. Function 1 ran over 214 generations before it self-terminated (see figure 13(A)). The optimal solution had a rotation of the bounding box of the particle of 225 degrees a sphere count of 9 spheres per arm, a scale factor from one sphere to the next of 1.25 and an angle of rotation of the arms lying in the *xy*-plane of 0 degrees.

Function 2 was completed after 275 generations (see figure 13(B)). The optimal solution had a rotation of the bounding box of the particle of 225 degrees, a sphere count of 10 spheres per arm, a scale factor from one sphere to the next of 1.25 and an angle of rotation of the arms lying in the world *xy*-plane of 30 degrees.

Function 3 was terminated after 139 generations (see figure 13(C)). The optimal solution had a rotation of the bounding box of the particle of 0 degrees, a sphere count of 7 spheres per arm, a scale factor from one sphere to the next of 1.25 and an angle of rotation of the arms lying in the world xy-plane 0 degrees.

Function 4 took 172 generations to complete (see figure 13(D)). The optimal solution had a rotation of the bounding box of the particle of 270 degrees, a sphere count of 5 spheres per arm, a scale factor from one sphere to the next of 1.25 and an angle of rotation of the arms lying in the world *xy*-plane of 30 degrees.

Varying the fitness function thus allows to calibrate the weighting of the input parameters in response to fabrication criteria: if mould-material is expensive, one would choose functions 1 and 2 for optimization, if material cost does not play a role, functions 3 and 4 can also be considered; if simulation

is one of the key aspects of the overall project, those functions that show a minimum in sphere count can be favoured.

All of the solutions have a range of top 10, 25 and 50 per cent of genomes. These can also be considered if a wider spread of results should be included in a future development stage of the project.

6. Discussion

A review of projects from both architecture and granular physics that investigate designed granular materials has shown that design models for particles rarely address the requirements for both realms of research, namely the possibility of a wide spectrum of geometric types, the consideration of architecture-scale production of the particles and the use of those geometries required for a numerical simulation. Yet in the context of designed granular materials in architecture there is a need for such a design model for particles: it is required in order to establish a loop between optimization via simulation, digital fabrication and investigation through experiments. These digital loops are standard practice in a range of other fields in architectural design research. The proposed parametric particle design model is an approach to establishing such an interface. Ultimately, this will allow granular materials to be designed that respond to a range of specifically architectural evaluation parameters, as outlined in section 5.2.3.

The proposed case study indicates the use of the parametric particle design model for the optimization of particles in the fabrication phase. It shows how a set of input variables can be optimized based on a set of evaluation parameters which are relevant for fabrication as well as for future simulations and experiments.

7. Further research

In future applications of the parametric particle design model, preference can be given to digital chains or digital loops from simulation to fabrication to experimentation. Thus particle designs can be numerically simulated in an 'inverse' manner, which means that first the desired characteristics of a granular material are defined and from that the shape of the particles is found through optimization of their geometric features [4, 14, 15, 110, 111]. Digital fabrication can then be conducted directly from this numerical optimization. Experiments then serve to verify or falsify the simulation results or to discover new relevant features of the granular materials which can again be used as an input for another set of simulations.

Parameters to be optimized could include the geometry of the particle including the symmetry and

non-symmetry of the particles for example by weighting input and evaluation parameters differently for different arms, the size-grading of a specific particle geometry through using different dimensions of it or the mixing ratio of different geometric types.

In this manner designed granular materials for architecture can increasingly be optimized for a set of parameters from simulation, fabrication and experimentation—especially with respect to actual architectural evaluation criteria.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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