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Bespoke particle shapes in granular matter

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Among granular matter, one type of particle has special properties. Upon being assembled in disordered configurations, these particles interlock, hook, almost braid, and – surprisingly, considering their relatively low packing fractions – show exceptional shear strength. Such is the case of non-convex particles. They have been used in the shapes of tetrapods, 'L', 'Z', stars, and many others, to protect coasts or build self-standing structures requiring no binders or external supports. Although these structures are often designed without a comprehensive mechanical characterization, they have already demonstrated great potential as highly resistant construction materials. Nevertheless, it is natural to attempt to find the most appropriate non-convex shapes for any given application. Can a particle shape be tuned to obtain a desired mechanical behavior? Although this question cannot be answered yet, current technological, simulation, and experimental developments strongly suggest that it can be resolved in the next decade. A clear understanding of the relationships between particle shapes, mechanical response, and packing properties will be key to providing insights into the behavior of these materials. Such work should stand on 1) robust and general shape descriptors that encode the complexity of non-convex shapes (i.e., the number of arms, the symmetries and asymmetries of the bodies, the presence of holes, etc.), 2) the analysis of the response of assemblies under different loading conditions, and 3) the disposition and reliability of non-convex shapes to ensure durability. The manufacturing process and an efficient use of resources are additional elements that could further help to optimize particle shape. In the quest of designing bespoke non-convex particles, this paper consolidates the challenges that remain unresolved. It also outlines some routes to explore based on the latest developments in technology and research.

I. Introduction

Have you observed tetrapod-like elements protecting coasts? Or, perhaps, an assembly of rigid stars collectively building a structure? Figure 1 shows complex arrangements of interlocked non-convex particles forming relatively loose structures with remarkable strength and dissipative properties. In many places around the world, concrete non-convex blocks are used for coastal protection due to their easy prefabrication and disposition methods [1–4] (see Fig. 1(a)). These blocks create stable, loose configurations that allow water to enter the cavities and, thus, release the kinetic energy of the waves.

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Figure 1(b) shows a self-standing structure easily reaching a few meters high, requiring no external support or binding materials. These innovative applications expose the great potential non-convex particles possess as construction materials where interlocking, braiding, or stacking elements can dramatically improve mechanical properties [5–11]. In addition, non-convex shapes such as ‘Z’ [11] can also continuously gain shear strength as strains do not necessarily trigger failure, but rather promote particle rearrangement and further interlocking [12–14]. Since the particles used for many of these applications are replicated from a single shape – or a few shapes –, the fabrication processes and disposition of the pieces can be automated for construction in environments of difficult access or that require remote-controlled machinery/robots [15, 16].

It is evident that non-convex particles could vary infinitely in shape. In practice, there are branched, twisted, curved, asymmetric, and even convex shapes with hollowed faces creating truss structures [17–19].

It is natural, then, to inquire into the best shape for a given application. Although intuition may suggest that assemblies of ‘Z’ or ‘L’ shaped particles can develop higher strengths, there are no systematic studies allowing one to determine which non-convex shape performs better than another. So far, studies have used different particle shapes and tested various characterization approaches that produce no comparable results. While the particle shape is central to designing tailored/bespoke granular materials, other aspects such as deposition or assembly methods, particle strength, and constructive processes should also be considered to optimize the particle geometry for a given application.

In the following, we present the challenges that, in our opinion, can be addressed in the near future to make bespoke granular matter the next generation of construction materials.

II. Challenges

i. How is particle geometry described?

Many shape descriptors found in the literature are focused on describing convex shapes (i.e., shapes without cavities) by means of their sphericity, aspect ratio, angularity, flatness, elongation, roundness, and irregularity [22–28]. These parameters often fail to describe the complexity of non-convex shapes or do not allow one to have a straightforward picture of the particle. As an alternative, Fourier descriptors have been used to represent non-convex shapes [29, 30]. However, this method may need a large set of parameters when dealing with asymmetric or highly irregular geometries. In general, there is no consensus on a parameter or a set of parameters to describe the complexity of non-convex bodies.

The first challenge is the development of simple and robust geometrical descriptors, allowing one to compare different families of particle shapes. This descriptor - or set of descriptors - should be able to encode as much information as possible regarding the characteristics of non-convex shapes, such as the number of arms, symmetry or asymmetry of the body, the presence of holes, recurrent patterns, among others. Furthermore, any descriptor should be sufficiently clearsuch that its definition maps directly into basic or elemental parameters.

Once the descriptors are set, efforts should be focused on systematically linking them to the mechanical behavior (compaction, shear strength, rheology of quasi-static and inertial flows) and packing properties of particle assemblies. For this, experiments and simulations are valuable tools that should be developed to work in synergy and mutually enrich each other’s observations.

ii. Physical experiments

In experiments, for example, the technology of 3D printing has allowed one to precisely control the shape of particles to be later assembled in structures [31]. Although some studies have performed qualitative characterization of the resistance of non-convex particle assemblies [5, 9, 10, 32], only a few have quantitatively assessed their mechanical response and packing properties [11, 33–36]. The current technological capabilities suggest that hundreds - or even thousands - of particles can be built and tested in standard devices (triaxial, shear cells, rheometers, etc.). However, to the best of our knowledge, this has not been done. Besides, it is unclear how to scale up the obtained properties from the laboratory scale to large size applications such as coastal barriers.

The second challenge is related to the fabrication

(a) (b)

Figure 1: Examples of structures built using non-convex particles: a) coastal barrier (public image by Pok Rie [20]) and b) aggregate wall (with permission of Karola Dierichts [21]).

of non-convex shapes and the mechanical characterization of assemblies either in standard equipment or non-conventional devices (e.g., large-scale shear boxes [37, 38]).

Up to now, the physical characterization we have mentioned refers to macroscopic mechanical or packing properties. However, it is well known that such responses are related to the mechanics at the scale of the particles and their contacts [39–41]. Recently, several efforts have been put into characterizing the mechanics at such small scales. For instance, novel fast digital image analysis allows one to track a particle's positions when loaded [42–45]. Among them, it is worth mentioning the use of photo-elastic particles, which can not only display the contact network, but also permits us to estimate the force and stress intensities within the particles [46–49].

Despite the advances in these experimental approaches, their use is seldom seen when it comes to non-convex particle assemblies.

The third challenge corresponds to exploring the microstructure and force transmission mechanisms within assemblies of non-convex bodies. This requires the development of robust and efficient digital image analyses capable of dealing with complex entangled particles that are often ambiguous, difficult to identify one from another.

iii. Numerical simulations

An alternative means to probe the packing properties and load distribution within a granular sample is numerical simulations. To simulate discrete matter, some of the most popular approaches are the discrete-element method (DEM) [50–52], and the material point method (MPM) [53–55]. In particular, DEM strategies have proven to be quite advantageous since they provide a detailed description of the micromechanics of granular materials (e.g., particle connectivity, fabric anisotropy, contact force network, etc.) while being capable of dealing with collections of rigid [56, 57] and deformable bodies [58–60] of varied sizes and shapes [61, 62], under a large variety of boundary conditions.

Even though the simulation of non-convex granular assemblies is in rapid development today [17, 63–70], these works also expose some of the limitations of the current modeling approaches. First, the shape of the bodies is sometimes represented using clumped spheres [71], sphero-polyhedra [72, 73] or superquadrics [74]. Although these strategies allow one to use well-known methods for convex bodies, the discretization of the shapes may add artificial textures on the surfaces, or they can be rapidly limited when pointy geometries or sharp edges need to be considered. Other strategies that discretize bodies using multiple vertices and faces to represent the particles often require excessive storage space and expensive I/O operations that penalize the number of particles that can be considered. Secondly, contact detection strategies require further optimization and are computationally prohibitive when dealing, for instance, with elongated or long-armed bodies. Since contact detection is often based on the overlapping of spheres enveloping the bodies, such approaches can largely overestimate potential contacts in the case of non-convex particles, which can dramatically slow down the time stepping evolution of a simulation. Finally, it remains difficult to draw clear comparisons between studies given the broad spectrum of particle shapes considered and the lack of a consensus, once again, in the parameters to describe non-convex geometries.

The fourth challenge is to develop new algorithms that provide an accurate representation of non-convex shapes while facilitating or optimizing contact detection. These developments should be conceived and developed as scalable, highly parallel algorithms that could be used in cluster computing (e.g., HPC and GPU computing). Equally important will be validating the well-known micromechanical analyses of granular materials to any particle shape by means of simulation campaigns over a broad range of parameters.

The advances on the experimental and simulation axes will naturally lead to the validation of the numerical models that, then, can be extended to more complex particle shapes and boundary conditions. Extensive systematic simulation studies, in which one can clearly control the physical and numerical parameters, can thus provide further insights into the mechanical behavior of granular matter composed of non-convex bodies.

III. Tuning particle shape for applications

While theoretical, experimental, and numerical approaches are valuable tools to explore the mechanics of granular media, the applications or industrial stakes may determine pertinent features that particles and assemblies should exhibit. As mentioned before, coastal protection structures have consisted of various shapes, including tetrapods, tripods, cubes, dolossa, etc. Even though all of them dissipate energy and contribute to erosion prevention, it is not clear which features led engineers to prefer one shape over others.

The fifth challenge is to develop methodologies to tune particle shape for a specific application, based on the thorough geometrical and mechanical characterization of non-convex shapes.

Although the mechanical response of the granular assemblies can often be the key parameter to choose a specific particle shape, other elements accounting for the durability and reliability of the structures should also be considered. For instance, additional analyses may include the breakage strength of the particles, the settlements over time due to particle rearrangement, the capabilities for particle manufacturing, and the initial conditions of the arrangements (e.g., deposition, preloading, etc.).

More recently, the scarcity of materials due to supply chain unreliability and the need for reducing ecological footprints are issues that call for the reusability of the individual bodies, or for their being manufactured from local materials. This last challenge is indeed broader and may involve the science of new composite materials from renewable sources. Nevertheless, the task may largely benefit from advances in the mechanics of granular media of varied shaped bodies.

IV. Summary and perspectives

Arrangements of non-convex particles often present outstanding properties regarding their shear strength, mainly due to their capacity to hook, interlock, and entangle. These materials also present low packing fractions which favor efficient energy dissipation, as in the case of coastal barriers. Despite the multiple advantages non-convex particle assemblies can display, their mechanical behavior is still poorly understood. Indeed, there are no methodologies to determine what shapes provide more strength than others, and it is not clear how to optimize particle shape for a given application.

To correctly match non-convex particle shapes to applications, a series of challenges need to be overcome. They include 1) the development of robust - yet simple - geometrical descriptors, allowing one to compare different shapes; 2) the generation of particle assemblies for systematic studies on their mechanical properties with experiments and numerical simulations. The synergy between experiments and numerical modeling will be key to rapidly gathering insights on the mechanical behavior of these materials; 3) the micro-mechanical analyses to understand the particularities of these materials that lead to their exceptional macroscopical properties; and finally, 4) the identification of additional elements that limit the range of possibilities for particle shape or allow one to optimize the mechanical properties for a given application.

State-of-the-art experiments and simulations suggest that these challenges can be successfully addressed in the near future. In terms of experiments, X-ray tomography, 3D printing, and digital image analyses are promising tools and strategies largely used for convex grains, awaiting generalization to any particle shape. Regarding numerical modeling, discrete-element approaches seem to present a privileged framework for exploring the macro and microscopic responses of assemblies of complex shaped bodies. However, this task requires several improvements in the algorithms' efficiency and their scalability to work on highly parallelized environments. Although artificial intelligence (AI) is just debuting in the field of granular materials [75, 76], it is going to be an essential tool for the optimization of particle shapes under a set of constraints. These AI tools will benefit from the experimental and numerical axes of research and can shed light into more fundamental aspects concerning a unified geometrical descriptor for non-convex grains and the physics of granular media.

Optimizing particle shapes in granular matter will also benefit from multidisciplinary contributions including mathematics, statistics, computer science, chemistry, among others. Although we focused our exposition on civil structures, this is a topic spanning different fields of material technology, engineering, architecture, bio-inspired materials, etc. Undoubtedly, materials composed of non-convex particles may be the next generation of building materials for optimized structures based on the idea of tailored granular matter or bespoke particle shapes.

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