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Numerical modeling of granular media made of polyhedral particles

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Modélisation numérique discrète des matériaux granulaires

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7 novembre 2010

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Chapitre 1

Numerical modeling of granular media made of polyhedral particles

1.1. Introduction

As soon as we are interested in the simulation of interacting objects raises the issue of the choice of a relevant numerical model and of technical approaches suitable to the solving strategy. It concerns the choice of objects bulk behavior (which reduces to kinematic parametrization if they are considered as rigid), object shape description, contact behavior, contact detection technics and solving strategy (e.g. time evolution, time integration, contact solver, etc.) The principal difficulty comes from the choice of a model and numerical technics and strategies. However models and strategies are usually related. Various models and strategies are already presented in this book (chapters ??, ??, ?? and ??) which explains why this chapter only focuses on specificities and sophistications necessary to the modeling of collection of objects with complex shapes described by polyhedra.

The geometrical description of objects shape is a crucial point concerning the modeling of granular material, particularly when real material are studied. An obvious but too naive choice should be to adopt an “exact” description. It is irrelevant due to the poor gain of taking into account the microscopic complexity of object surface (multi-scale or fractal) with respect to the macroscopic studied phenomenon. On the contrary a too rough geometrical description needs to introduce ad hoc interaction law

able to mimic its phenomenology but difficult to characterize. Considering the modeling of granular material made of non spheric grains, one can find various approaches in the literature :

- some authors, for obvious technical reasons, keep a spherical description of grains and introduce some additional sophistications in the interaction law to fit the macroscopic behavior of the granular material : rolling friction interaction law [ZHO 02, EST 08], modified kinematic of grains through constraining the spin [CAL 03], etc.
- others proposed to use grains made of an assembly of spheres (*cluster* or *clump*), or approximated by super-ellipsoids (also known as super-quadrics) [HOG 98], sphéroïdes [LEE 03], spherolines [POU 05], spheropolyhedra [GAL 10], etc.
- others use polyhedral description.

One can notice that literature concerning the modeling of contact between polyhedral surface is abundant and comes from various community :

- mechanics of materials and structures (usually through finite element technic),
- mechanisms and robots,
- virtual reality, physically based animation, haptic devices,
- granular materials.

Unfortunately all these related works are not obviously exploitable due to some granular material modeling specificities :

- it concerns large and dense collections of objects which means a large set of potential interactions (neighborhood), from 10^3 for small examples to 10^5 for representative ones,
- a large number of interaction are really acting at the same time ;
- dynamics is necessary to compute the rigid body motion of unconstrained objects. A suitable numerical treatment is necessary due to the stiff interaction constraints,
- usually the solution is not unique.

In this chapter, as in the whole book, we only consider rigid bodies. However many ideas can be adapted to deformable objects. One consider a system made of N 3D rigid objects. Each object is defined by a set of generalized coordinates $q(t) \in \mathbb{R}^{n_q}$ defining its current configuration. A body i occupy the domain $P_i(t) \in \mathbb{R}^3$ in the current configuration defined from the initial configuration through $P_i(t) = \varphi(t, q(t))P_i(t_0)$. Without going into details of the various interaction laws used in the modeling of granular material one needs to compute $d(P_i(t), P_j(t))$ the signed distance between objects $P_i(t)$ and $P_j(t)$. In case of separation this distance is strictly positive, in case interpenetration this distance is strictly negative and in case of grazing contact the

distance is equal to zero. Additionally one needs to define a contact frame and various quantities.

This chapter is formally splitted in three parts dedicated to :

- the continuous modeling : rigid body dynamics and parametrization ($q(t)$ choice), geometric description of objects ($\partial P(t)$ choice) and contact detection (computation of $d(q(t))$),
- specificities of taking into account polyhedral particles in numerical implementation,
- applications, and especially results obtained with the software developed by LMGC¹.

1.2. Rigid body dynamics and parametrization

The Newton-Euler formalism is classically used when modeling granular material. The velocity of a rigid body is decomposed in terms of a translational velocity of its center of inertia $v_G = \dot{x}_G$ and the angular velocity Ω expressed in its inertia frame. Denoting R the rotation matrix from the global frame to the inertia frame, one can write :

$$\tilde{\Omega} = R^T \dot{R}$$

where $\tilde{\Omega}x = \Omega \times x$.

Using these notations one can write Newton-Euler equation, in case of nonexistence of contact forces, as :

$$\left\{ \begin{array}{l} M\dot{v}_G = F_{ext} \\ I\dot{\Omega} + \Omega \times I\Omega = M_{ext} \\ \dot{x}_G = v_G \\ \dot{R} = R\tilde{\Omega} \end{array} \right. \quad (1.1)$$

where $M = m\mathbb{I}_{3 \times 3}$ is the mass matrix (diagonal and constant) with m the mass, I the inertia matrix (diagonal and constant).

This rough choice of generalized coordinates $q = [x_G, R]$ and velocities $v = [v_G, \Omega] = T(q)\dot{q}$ can be improved in terms of number of variables or suitability for time integration. In such improvement, the rotation matrix may be related to the angular parametrization of the object orientation, e.g. $R = R(\Theta)$. Various possibilities are available [CRI 97, IBR 97, GER 01, KOZ 10] such as Euler or Cardan angles, quaternions, etc. However, if an explicit or precise parametrization is not required, using the rotation matrix is sufficient.

1. lmgc90 [DUB 03].

Concluding on this topic, one can remark that generally 1.1 is non-linear for any plain objects (not spheres). To avoid this problem it is possible to express the Euler equation in the global frame ($\omega = R\Omega$); an arising drawback is that the inertia matrix won't be any more constant and diagonal.

1.3. Geometrical description of objects

When considering complex-shape objects two geometrical modelization are generally possible :

- Constructive Solid Geometry (CSG). This technic describes a solid object as the combination of basic volumes (cylinder, sphere, cone, tore, etc.) through boolean operations (union, intersection, subtraction, etc.). A cluster of spheres can be seen as a simple CSG model. An object described by this technic has a “perfect” boundary since each basic component is well defined. It allows to compute gap and local frame precisely. However for complex-shape solids this approach is less relevant due to the heaviness of the modelisation.

- Boundary Representation (Brep). This technic consists in modeling the skin of solids sewing geometrical tiles defined by canonical surfaces (generally B-spline, Bézier or NURBS). Each tile is defined through a parametric description. Such Brep model contains two kinds of data : topological and geometrical (surfaces, curves and points). Principal topological data are faces, edges and vertices. A face is a limited part of a surface (restriction). An edge is a limited part of a curve. A vertex lays on a point. A Brep model can be obtained from a CSG model (the contrary is generally impossible). Actually even if this technic is mainly used to build CAD model, it is still few employed for contact modeling due to the necessity of computing in an effective manner the distance between parametrized surfaces [JOH 04].

A way to overcome the drawbacks of these geometrical modeling technics consist in describing objects with polyhedra obtained from surfacic or volumic mesh (for technical details see for example [LAU 05, GEU 09]). In the following polyhedra means either simple objects (tetrahedra, cube) or complex ones, even non-convex, described by closed triangulated surface, etc

In order to manage such polyhedral surfaces some data structures are relevant. They allow to find faces or edges adjacent to a vertex, faces adjacent to an edge, edges limiting a face, etc. Various data structures exist [LIN 93, BER 04] ; anyway half-edge structure is efficient [ALU 05].

An other practical advantage of possessing a polyhedral description of an object is to be able to compute some relevant mechanical quantities such as center of inertia (OG), mass (m) and inertia matrix (I) (in a global frame (O, \mathcal{R})). Two approaches are possible :

– if a volumic mesh is available, one computes for each element e of the mesh its center of inertia (OG^e), mass (m^e) and inertia matrix (I^e) in a local frame (G^e, \mathcal{R}) (see [TON 04, SAU 04b] for details) and then uses the classical relations to obtain :

$$m = \sum_e m^e \quad (1.2)$$

$$mOG = \sum_e m^e OG^e \quad (1.3)$$

$$I = \sum_e I^e + md_{\mathcal{R}}(O, G^e)^2 \quad (1.4)$$

where $d_{\mathcal{R}}(O, G^e)$ is a diagonal matrix which terms are the distance between the axes of the frame (O, \mathcal{R}) and (G^e, \mathcal{R}).

– if a surfacic mesh is available same quantities can be computed through surface integrals, see [MIR 96a, EBE 09].

When the mesh loses some topological properties, due to defects in the CAD for example, one speaks of “polygon soup”. This kind of description won’t be considered in this chapter.

In order to increase continuity of polyhedral surfaces spheropolyhedron can be introduced [POU 05, GAL 08]. This surfaces are build sweeping the elements (face, edge, vertex) with sphere; one also speaks of Swept Sphere Volume (SSV). More precisely this object are build using the Minkowski sum of two set of points :

$$A \oplus B = \{x + y : x \in A, y \in B\} \quad (1.5)$$

Recently a more “generic” approach was considered representing objects by a cloud of points [KLE 05]. This approach allow to manage data coming from 3D laser scanning measure.

1.4. Contact detection

1.4.1. Introduction

When performing contact detection various informations are expected depending on the interaction law and on the numerical strategy used to solve the problem.

For example when modeling unilateral contact with a gap-Signorini approach (NSCD chapter ??) one needs to compute precisely the separation distance. With velocity-Moreau approach (NSCD chapter ?? and event driven chapter ??) one needs to know if objects are touching and to evaluate the pre-contact relative velocity. With a deformable contact approach (Molecular dynamics chapter ??) one needs to evaluate the penetration depth and the pre-contact relative velocity.

Practically one needs to know the signed distance (interpenetration/separation) between two objects, contact locus (not necessarily unique), local frame, relative velocities, etc. The literature on contact or collision detection is huge and one can find some reviews in papers [LIN 98, JIM 01, TES 05], PhD thesis [KLE 05, OND 06, ERL 04] and books [BER 04, ERI 05] .

1.4.2. *Hierarchy of contact detection*

Contact detection represents an important part of granular material modeling, in terms of reliability of the solution but also computational effort. In order to reduce this computational effort due to the complexity of algorithms these methods are splitted in various stages :

- broad phase : it consists in building a list of adjacent objects in a given neighborhood (tolerance). This stage used a rough description of the geometry of objects mainly based on bounding volumes ;
- narrow phase : this phase (not mandatory) tries to improve the broad phase detection. For simple objects it can consist in eliminating entries of the list in some straightforward situation. For more complex objects it can consist in specifying which parts of the objects are potentially concerned by contact ;
- contact determination : at this stage one evaluate pairs of objects in contact and contact loci, local frames, distances, etc. Depending on the numerical strategy this stage can be adapted.

1.4.3. *Broad phase*

The aim of this phase is to build quickly a list of adjacent objects. It is mainly based on the proximity of bounding volumes of objects.

Various bounding volumes (BV) exist as illustrated on the figure 1.1 : sphere, Axis Aligned Bounding Box (AABB), Oriented Bounding Box (OBB), k Discrete Orientation Polytope (kDOP), convex hull, etc.

Once evaluating the bounding volume of each objects, it exists mainly three proximity detection approaches :

- space subdivision [MIR 96b]. This approach rely essentially on a bounding sphere approximation of objects. Basically one builds a constant box-mesh where cell size is taken as the diameter of the largest object of the sample. Once computed in which cell (or box) an object is located, rough proximity is computed with objects populating the same cell and the surrounding cells. This is an obvious method which works fine with dense samples made of objects with bounding sphere radius of the same order. In case of loose samples the mesh size can be important but a large amount

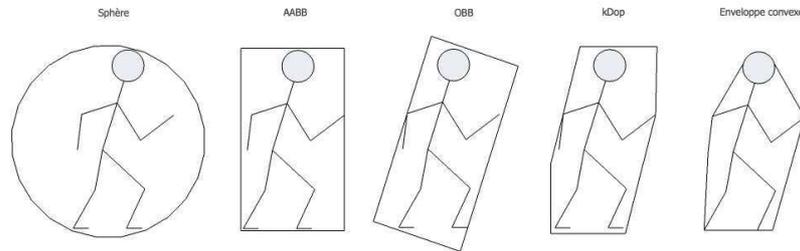


Figure 1.1. *Various bounding volumes*

of cells of the box-mesh are useless. This can be managed using a linked-cell dedicated storage technic as explained in [MUN 04]. In case of highly polydisperse media a hierarchic subdivision approach can be more relevant (see [MIO 07] and [OND 06] for a discussion). Various hierarchic subdivision technic exist : octree, kd-tree, bsp-tree, etc. Due to the computational effort of such technics they are few used.

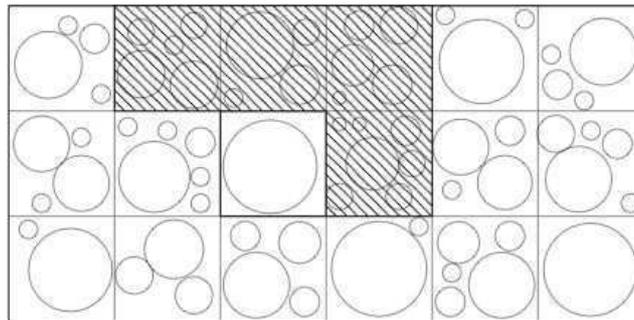


Figure 1.2. *broad detection : space subdivision*

– shadow overlap on an axis (sort and sweep [BAR 90] or sweep and prune [COH 95]). This approach rely essentially on a AABB approximation of objects. In a first step one projects the bounding boxes on axes (figure 1.3). For each axis one sorts the projected intervals in apparition order. Then one sweeps each axis in order to build an active interval list : an interval is added to the list once its beginning is reached and is removed once its end is reached. Each time a new interval is added to the list it means it interacts with intervals in the list, in a such a case the proximity list related to the given axis is increased. The final proximity list is the intersection of the lists build for each axis. Even if this method is not obvious to implement this approach works well. Its main drawback comes from some clustering effects appearing when the sample flatten along one axis. See [ZOM 02] for some optimizations.

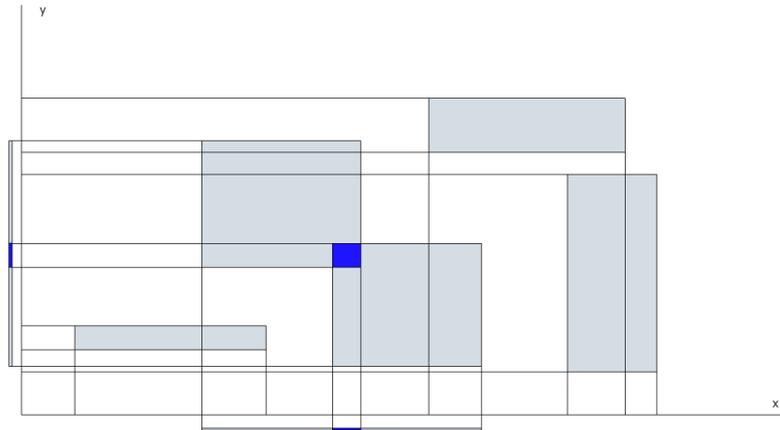


Figure 1.3. *broad detection : sweep and prune*

– triangulation [FER 02]. This approach uses a triangulation of a set of nodes (the center or inertia of objects for example) to determine adjacent objects. This technic is few used and mainly for spheres.

1.4.4. *Narrow phase*

This optional phase uses the adjacent list build during the broad phase in order to remove trivial undesirable cases.

For simple convex objects previous methods can be repeated, e.g. if space partition was used a local shadow overlap on various axes can also be performed.

For more complex objects (large amount of faces or non convex) a boundary volume hierarchy (BVH) can be build in order to compute the bounding volume of sub-parts of an object. The aim is to build progressively a tree where the leafs are basic primitives (triangle) or set of primitives. Each node of the tree contains a set of sub-nodes and their bounding volume (BV). The narrow detection uses these BV-BV detections. Different approaches were used : [HUB 95] for spheres, [BER 97, GOT 96] for AABB, [KLO 98] for k-DOP and finally [BAR 96] for convex hull. Other technics exists using spatial subdivision of objet (shape independent) as octree or bsp-tree. One can also mention technics based on distance field to perform narrow detection [TES 05].

Some of these BVH decomposition are performed in a preprocessing stage which makes them even more efficient.

1.4.5. Contact detection between convex polyhedra

Before diving into the details of contact detection techniques some preliminary ideas need to be introduced.

First its important to remember that different situations may appear (grazing, separated or penetrated contact) and that various numerical methods are available to detect them.

Admitting that ideal grazing contact situation appears, various cases are possible : one contact point (figure 1.4), contact line (figure 1.5) or contact surface (figure 1.6).

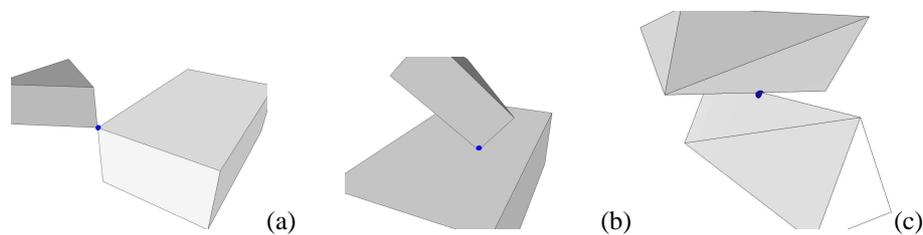


Figure 1.4. One contact point situations

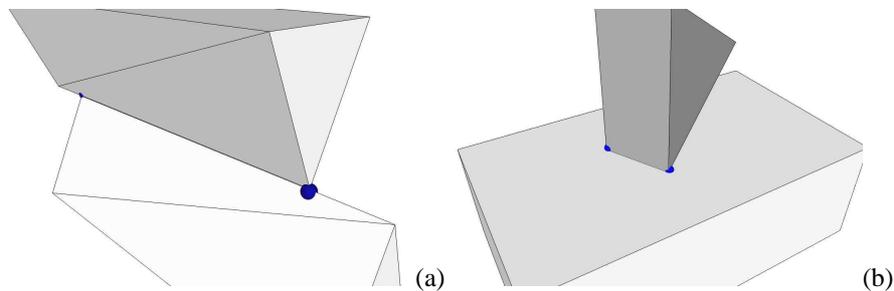


Figure 1.5. contact line situations

Considering these obvious situations raises some issues :

– How to model contact transmitted by a line or a surface ? A classical choice is to assume it can be replaced by a finite number of contact points (see Figures 1.4, 1.5 and 1.6). Some fictitious concavity of line or surface can be assumed as in [MOR 03]. Even if this choice seems interesting it introduces a local non-uniqueness of the contact force distribution. In some obvious situations one can introduce additional relations between nodal contact forces to recover uniqueness [MOR 03, PER 07].

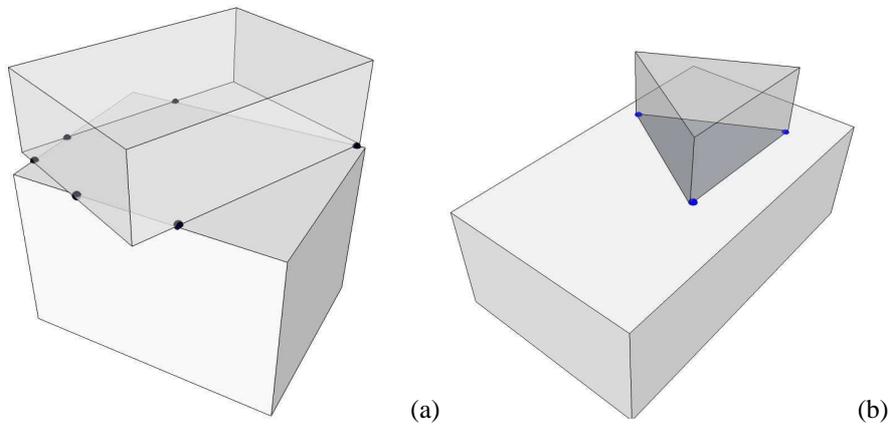


Figure 1.6. *contact surface situations*

– How many contact points are necessary ? Without any modification of the interaction law, a contact line can be represented by two points and a contact surface by three points. Selecting the nodes at the intersection of the edges delimiting the contact surface seems to be a solution. But as illustrated figure 1.6 it is not so easy to select only three points. A lazy solution is to put a large amount of points and let the numerical method select which one is transmitting a contact force. This solution raises collateral problems in terms of management of data : memory size, recovery between two steps, etc.

– How to determine contact node position ? Mechanical stability should be increased if the nodes are positioned on the edges delimiting the contact surface (figure 1.6) but from a practical point of view it is better to position this nodes inside the contact surface.

Anyway in the following we assume it is relevant to model contact with a reduced number of points. Therefore the various situations (figures. 1.4, 1.5 and 1.6) reduces to look for a limited number of scenario : vertex-vertex, vertex-edge, vertex-face, edge-edge [LIN 93]. Once performed the contact point detection arises the problem of the local frame definition. In some degenerated situations (vertex-vertex, vertex-edge, edge-edge) the uniqueness of the normal is lost and it leads to difficulties in contact force computation.

However the ideal grazing contact situation is too restrictive and few encountered. Practically it is necessary to manage properly the separated contact situation. A first set of methods are based on the fact that if two convex polyhedra are separated (even grazing) it exists a separating plane, e.g. a plane that define two subspaces each one containing an object. The separating plane is not unique in many situations. But when

it exists it can be chosen as a face of one of the two polyhedra or parallel to two edges (one for each polyhedron) and containing one of these edges (the normal of the plane is the cross product of the directions of the two edges) [BAR 90].

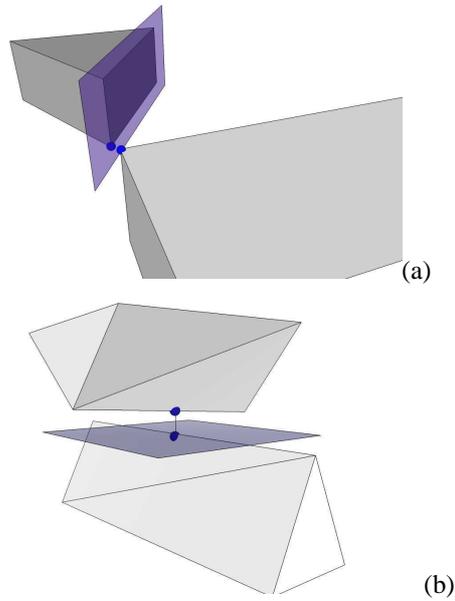


Figure 1.7. *Separating plane*

To summarize, finding a separating plane leads to the fact that the two polyhedra are not interpenetrating. This method is not giving any value of the distance between the two objects. The separating axis method (also named shadow-overlap method by Moreau) is a dual approach. For further details see [EBE 01, SAU 04b].

Cundall has proposed a method suitable for computing the distance between two polyhedra A and B [CUN 88] using the idea of separating plane : the common plane method. One notes G_A (resp G_B) the inertia center of A (resp. B) and X_A (resp. X_B) its set of vertices. Considering a plane P containing the point $M = \frac{G_A + G_B}{2}$ and perpendicular to a normal vector n , one define the signed distances :

$$d^+ = \min\{n \cdot MX : X \in X_A\} \quad (1.6)$$

$$d^- = \max\{n \cdot MX : X \in X_B\} \quad (1.7)$$

The goal of the method is to find n such that $d^+ - d^-$ is maximal. It is an iterative method based on perturbation of the orientation of the normal vector. The process is

initialized using the vector which links the center of the objects or with a previous guess. The main advantage is that it can give a solution even in degenerated situations. The main drawbacks comes from the slow converging iterative process and its poor precision. Using some optimization it can be used for modeling polyhedral granular materials [NEZ 04, PER 07, CHA 08]. This method works even for interpenetrated objects. It was also successfully used to model masonry structures and fractured rock mass [PER 07, RAF 08].

In order to compute more precisely the minimal distance between two objects one can use the Voronoïregion, which allows to do a partition of space around a convex polyhedron based on its elements (vertex, edge, face). Using this unique partition, for a given point outside a polyhedron, it is possible to find the nearest element, as illustrated figure 1.8.

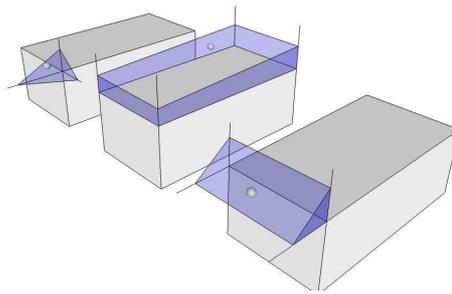


Figure 1.8. *Voronoïregion*

Based on this property iterative algorithms evaluating the minimal distance between the set of elements of polyhedra were developed [LIN 91, LIN 93]. The minimal distance between two convex polyhedron is the minimal distance between the sets of elements. The original method, only able to manage separating or grazing contact, was extended to interpenetrated contact [MIR 98].

This method was used to model polyhedral granular materials in order to find a common plane [NEZ 06]. This rely on the property that the shortest link vector between two convex polyhedra can be taken as the normal of the common plane.

A totally different and original method developed to compute the distance between any convex object can be used [GIL 88]. It relies on the following mathematical notions :

– support function of an object C , which for a vector (v) gives the point C such that :

$$s_C(v) \in C \text{ and } v \cdot s_C(v) = \max\{v \cdot x : x \in C\} \quad (1.8)$$

– convex combination of a set of points X :

$$\text{conv}(X) = \left\{ \sum_{i=1}^n \lambda_i x_i : \sum_{i=1}^n \lambda_i = 1, \lambda_i \geq 0 \right\} \quad (1.9)$$

– proximal point to the origin of the points of a convex set Q :

$$v(Q) \in Q \text{ and } \|v(Q)\| = \min\{\|x\| : x \in Q\} \quad (1.10)$$

In order to compute the minimal distance of a convex set C to the origin one can use the following iterative descent method (see figure 1.9) :

– One initialize the method defining a vector v_0 in the direction of the convex set C , a set of point $W_0 = \emptyset$ and computing $w_0 = s_C(-v_0)$

– For each iteration k one computes $v_k = v(\text{conv}(W_{k-1} \cup w_{k-1}))$ and W_k as being the smallest set X of $W_{k-1} \cup w_{k-1}$ such that $v_k \in \text{conv}(X)$ and $w_k = s_C(-v_k)$

– One stops the process when for example $\|v_k\|$ is no more varying (see [BER 04] for discussions).

In order to use this method one needs to observe that computing the distance between two convex objects A and B is equivalent to compute the distance to the origin of the convex set C which is their Minkowski difference :

$$d(A, B) = \min\{\|x - y\| : x \in A, y \in B\} = v(A \ominus B) \quad (1.11)$$

From a practical point of view it is not necessary to build C , one only needs to be able to compute the support function of the convex set C . Which can be computed using the support function of A and B :

$$s_{A \ominus B}(v) = s_A(v) - s_B(-v) \quad (1.12)$$

For polytopes the support point are the vertices, which leads to easier computation and insure convergence in a finite number of iteration. It was extended to contact with interpenetration [JOU 97, BER 04]. This method was successfully used to model polyhedral granular materials [PET 01].

Concerning contact detection with interpenetration a simple method based on the intersection of soup of triangles can be used [MOL 97, O'R 98, GUI 03]. It was successfully used to model ballast [SAU 04b].

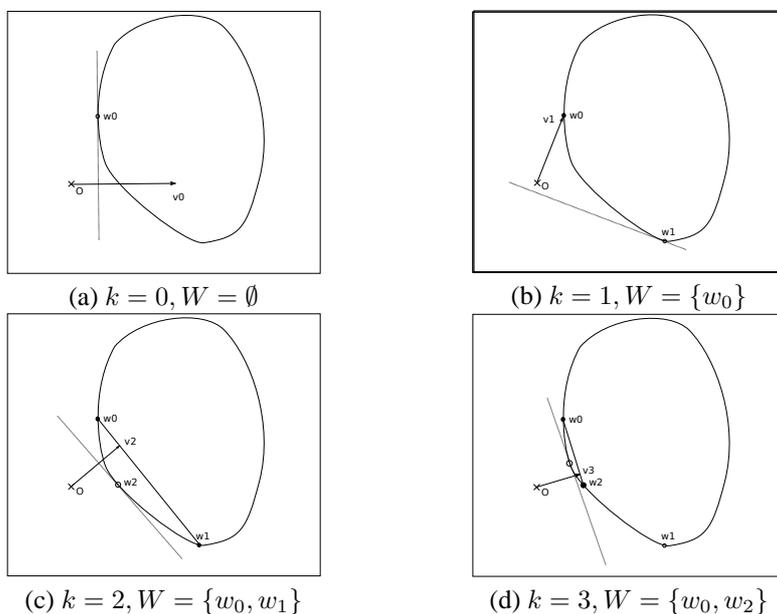


Figure 1.9. iterations of the GJK method

Finally it can be mentioned that contact detection methods developed by the finite element community are also available [LAU 02].

All the available methods are now presented. More or less they were all extended to contact with interpenetration in order to give the interpenetration depth, e.g. the smallest translation needed to obtain a grazing contact. Obviously one can consider the orientation of this vector as the normal vector at the contact point. Unfortunately this choice is not relevant in some degenerated situations (figure 1.10a).

A pseudo energy minimization was proposed to solve this problem [FEN 04]. Anyway it seems that a natural solution consist in using the causality of interpenetration, which uses the consistency of the path followed by objects. Roughly, knowing a separated configuration and a velocity it is possible to build a normal vector (figure 1.10b).

In order to control interpenetration between objects one can adapt the time step [ACA 08] or interpolate the trajectory in order to evaluate the position of objects to grazing contact [BAR 89, BAR 90]. Depending on the solving strategy one adopts the suitable solution.

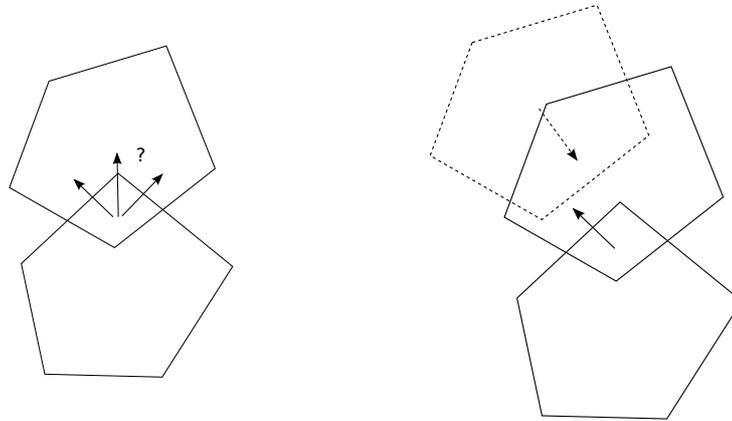


Figure 1.10. *Spatial consistency to insure suitable normal definition*

Once computed the distance and the normal between objects, one needs to define the contact locus (e.g. where the contact forces will act). Only contact occurring along a line or surface raise issues. The following approach allow to build this points :

- build a common plane (as meant by cundall) between A and B objects.
- do a projection on this plane of a subset X_A^ϵ (resp. X_B^ϵ) of the vertices of A (resp. B) nearer to the plane than a given tolerance ϵ (figure 1.11a)
- build the convex hull of the projected nodes X_A^ϵ and X_B^ϵ (figure 1.11b)
- compute the intersection of these convex hulls (figure 1.11c)
- choose contact points in this domain and rebuild distance, normal, etc. (figure 1.11d)

To conclude one can mention the elegant method proposed by [MER 07] to perform contact detection between polygonal surfaces using sphero-polygons which allows to obtain unicity and continuity of normal along the surface. Sphero-polygons were already used to model granular materials [PET 01, GAL 08].

1.4.6. Contact detection between non convex polyhedra

Contact detection between non convex polyhedra is a difficult task. Most of the methods split the problem using one of the following two approaches :

- a bounding box hierarchy as explained in section 1.4.4. Once two bounding boxes are crossing contact detection technics between the polygonal surfaces embedded may be performed as explained in section 1.4.5.

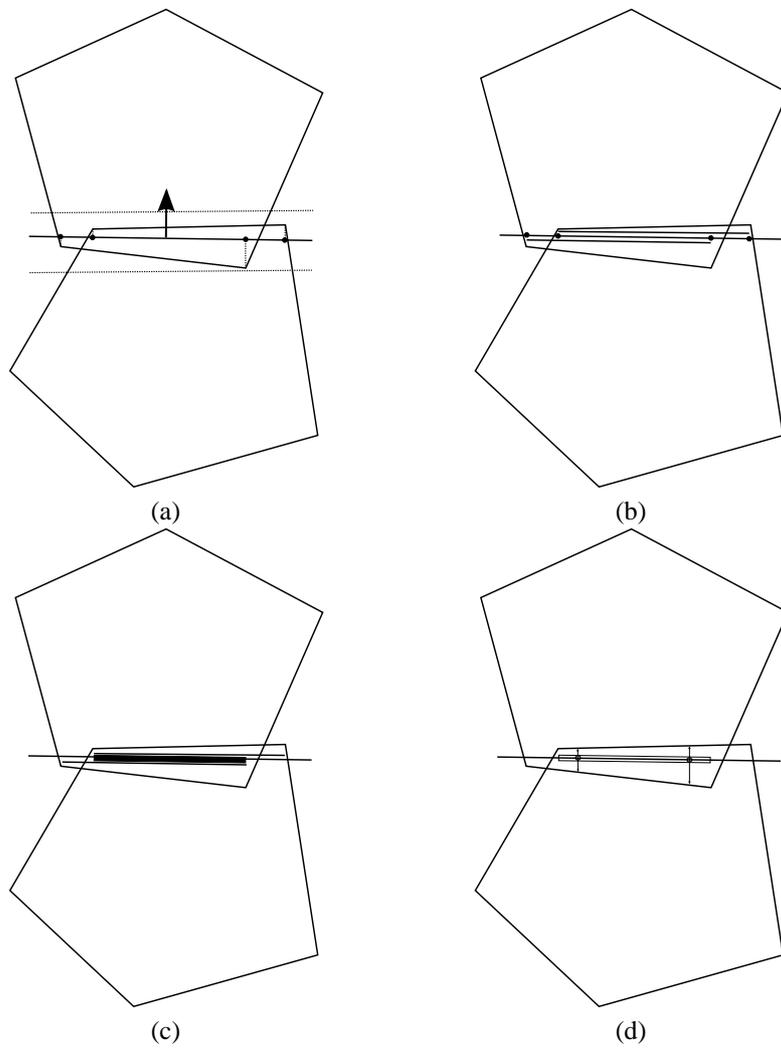


Figure 1.11. Steps to compute contact points

– a decomposition of non convex object in a set of convex objects (*cluster*). Such decomposition may be performed by hand or automatically [LIE 08, RAT 09].

1.5. Numerical implementation

1.5.1. Introduction

Taking into account polyhedral particles in a modeling software of granular material is not an impossible task. The main difficulty comes from contact detection. In the following (1.5.2) we give a list of existing libraries based on the methods presented before. However it remains necessary to adapt the contact report to the numerical strategy used to model the problem (see section 1.5.3). To conclude we will detail some choices made in the software we develop (section 1.5.4).

1.5.2. Libraries dedicated to contact detection

Various *open source* libraries, using the algorithms described before, are available on the WEB :

- I-collide [COH 95] : this tool rely on the Lin-Canny algorithm which uses the Voroniregion [LIN 91, LIN 93]. It can take into account large collection of convex or poly-convex objects, sorting potential couples of contacting objects with a *sweep and prune* method. It can use temporal coherence to improve detection.

http://www.cs.unc.edu/~geom/I_COLLIDE.html

- RAPID [GOT 96] : this tool compute contact considering polyhedral surface as a *polygon soup*. It uses a bounding box hierarchy (OBB tree) of objects. It is particularly suitable for objects made of a large number of triangles.

<http://www.cs.unc.edu/~geom/OBB/OBBT.html>

- V-collide [HUD 97] : this tool uses the narrow detection of I-collide and the fine detection of RAPID.

http://www.cs.unc.edu/~geom/V_COLLIDE.html

- V-clip [MIR 98] : this tool rely on an extension of the Lin-Canny algorithm due to Mirtich, which can cope with interpenetrating objects. It detects contact only between two objects.

<http://www.cs.sunysb.edu/~algorithm/implement/V-CLIP/distrib/>

- SOLID [BER 04] : this tool uses a GJK method and a bounding box hierarchy (AABB). It allows to perform contact detection between rigid or deformable objects.

<http://www.win.tue.nl/cs/~gino/solid/>

- PQP [LAR 00] : this tool consider objects as a polygon soup and uses swept sphere volumes to search contacts.

<http://www.cs.unc.edu/~geom/SSV>

- CollDet proposes a large set of tools in a framework able to perform contact detection.

<http://cg.in.tu-clausthal.de/research/collidet/index.shtml>

Additional informations are available on the following web site :
<http://gamma.cs.unc.edu/research/collision/packages.html>

1.5.3. *Problems related to numerical strategy*

Various paradigm of numerical strategy exist and are presented in this book. Without coming into the details of such methods some, remarks related to their use with polyhedral particles can be made :

- static or quasi-static methods (chapter ??). Considering polyhedral particles seems straightforward once contact detection (taking into account several contact points) is performed.

- explicit contact methods (chapter ??). These methods assume contact force is proportional to some overlap between particles. Therefore the results of such methods are deeply depending on the interpenetration distance and normal vector computation. Introducing several contact points to model linear or surface contact may be tricky with respect to there number, location and to the value of the rigidity [ZAV 09]. Using too small rigidity vanishes the interest of using polyhedral shapes because it won't respect the geometrical constraints. Using too stiff rigidity may introduce some numerical troubleshooting as oscillations. Furthermore it seems difficult to give a physical meaning to contact rigidity.

- event-capturing methods (chapter ??). As previously this method depends on the precision of contact detection, especially the normal vector. When considering interaction law written in terms of relative velocity only grazing or interpenetrated potential contact are treated, which rely essentially on the knowledge of the normal vector at contact point. However it implies that the impenetrability constraint is only controlled by the choice of the time step. Considering interaction law written in terms of distance allows to achieve impenetrability constraint for any reasonable time step. However the contact frame is implicit (it depends on the unknowns). It is relevant to use an explicit configuration but its choice is not unique. One can consider the configuration known at the beginning of the time step or at some intermediate time. A *leapfrog* approach was proposed by Moreau [MOR 03].

- event-driven methods (chapter ??). In this method the only difficulty is to evaluate precisely impact time in order to sort contact events and drive the simulation.

Furthermore one needs to notice that when considering polyhedral particles the non linear term appearing in the Euler equation (1.1) no more vanishes. In a confined and dense granular material, where the spin velocity is small, it can be relevant to integrate it explicitly or to make it vanishing.

A technical problem arise when considering interaction laws with internal variables (damage, cumulated path, etc) as cohesive model for example. In this situation it is necessary to find a relevant way to store contact history (using a Verlet mapping

for example) which may be tricky when considering several contact points between two objects.

1.5.4. Choices made in LMGC software

Modeling of polyhedral granular media was initiated at LMGC during the PhD of Saussine [DUB 03, SAU 04b]. Many improvements are still performed, for example see the work of Pérales et al [PER 07]. Here we will summarize some choices we did in our software ².

As presented in section 1.2, object orientation may be given by the rotation matrix R independently of any parametrization. However one needs to integrate the spin velocity Ω to update the rotation matrix at each time step. Two methods are available :

– if the spin rotation is very small a kind of linearization may be performed. Each vector of the inertia frame e_i^t is modified due to an increment of rotation $\Delta t \Omega$ using the following relation :

$$e_i^{t+\Delta t} = e_i^t + \Delta t \Omega \times e_i^t \quad (1.13)$$

This obvious technic needs some re-orthogonalization of inertia frame to keep numerical precision.

– to overcome the previous method drawback we use the algorithm proposed by Hughes *et al.* [HUG 80] which preserves orthogonality and metric of the principal inertia frame.

Concerning contact detection the following steps are performed :

– space subdivision broad phase. Big particles are not considered when computing the size of the boxes.

– narrow phase : obvious non contact situation are removed using a separating axis technic (*shadow-overlap*). The axis are taken in the set of the normal vectors to the triangular faces of the polyhedra.

– contact detection : two methods are used.

- triangle intersections [SAU 04b] which can only be used with contact law written in term of relative velocity,

- common plane (as meant by Cundall) [PER 07] which can be used with any interaction law. The normal to the plane can be determined using various technics.

The code was modularly designed in order to mix various mechanical models (rigid, deformable, etc), to perform contact detection between various shapes and to use various simulation strategies.

2. available at <http://www.lmgc.univ-montp2.fr/~dubois/LMGC90>

1.6. Examples

1.6.1. *Ordered media*

Masonry structures can be considered as an ordered discrete media made of polyhedral objects.

A first example (more details in [SAU 04b]) is based on an experimental work due to C. Fort (Marseille). It consists in submitting a wall made of wood bricks to a ground translation. The wall is made of 105 bricks putted on 10 layers. Two dimensions of bricks are used, large ones (95) which measure $H = 4.9\text{cm}$, $L = 12.4\text{cm}$ and $l = 6.2\text{cm}$, and small ones (10) with L divided by 2. The numerical results were obtained considering a friction coefficient between 0.6 and 0.7. Figure 1.12 shows the relevance of the numerical solution compared to the experimental results

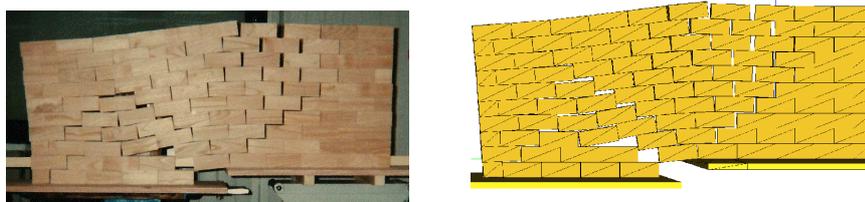


Figure 1.12. *Experimental and numerical displacement pattern of a wall submitted to foundation differential motion*

A second example concerns the computation of the equilibrium state under gravity of the “Pont du Gard” (South of France) [CHE 04]. The bridge is made of 35000 blocks (figures 1.13 a and b) which dimension were obtained by measures. The pillars settle on rigid foundations. Friction coefficient is taken as $\mu = 0.3$. Figure 1.13c shows the distribution of contact pressure supported by blocks and figure 1.13d shows the contact network at blocks interfaces.

This example illustrated the capability of the method to model large systems.

1.6.2. *Disordered media*

Concerning shape of objects, size distribution, compacity, etc granular materials are more disordered than masonry structures. However modeling tools are the same.

In the following are presented some results of studies performed at LMGC in collaboration with SNCF on the modeling of ballast [SAU 04b, SAU 04a, AZÉ 07a]. For

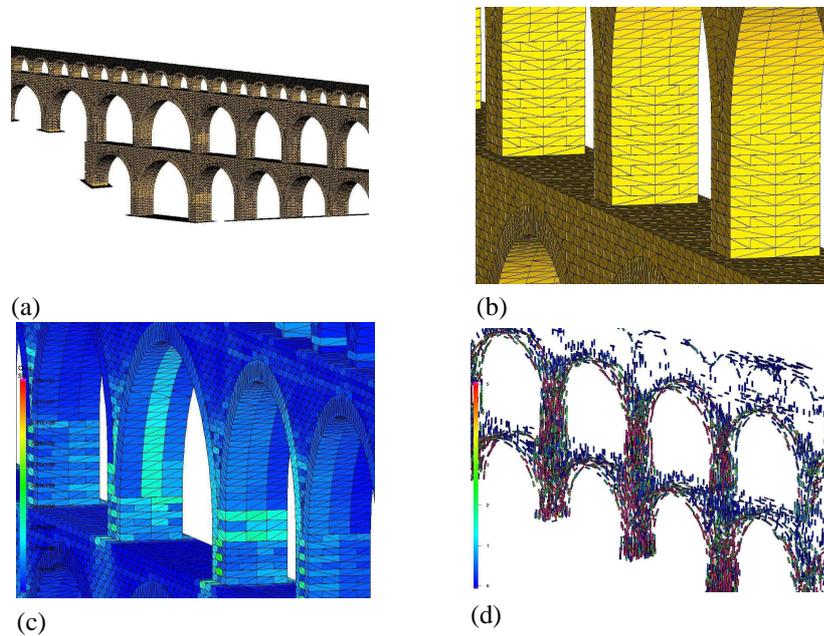


Figure 1.13. *Pont du Gard modeling. (a) and (b) geometry, (c) pressure on blocks, (d) contact forces*

all examples particle shapes come from digitalized grains. Each particle belongs between 8 vertices and 12 faces to 27 vertices and 70 faces (see for example figure 1.14). For such granular material one can study the influence of particle shapes on its macroscopic behavior (force transmission, texture, etc.).

We can start considering a tri-axial test with quasi-static load [AZÉ 07b, AZÉ 09].

The sample is made of 36933 polyhedra (figure 1.15) : 50% with a diameter $d_{min} = 2,5cm$, 34% with a diameter $3,75cm$ and 16% with a diameter $d_{max} = 5cm$. This size distribution is a relevant approximation of ballast material. Such sample contains $7.1 \cdot 10^5$ vertices and more than 10^6 faces.

The friction coefficient between grains is equal to 0.5 and between grains and box walls to 0. Normal and tangential restitution are taken equal to 0. The sample is submitted to a vertical rate of deformation (by the vertical wall) while applying a constant horizontal stress. In [AZÉ 09] a detailed analysis of the material rheology is given. It can be related to the contact force distribution. Figure 1.16 gives the probability density function of punctual, linear and surface contact forces, as well as the contact network.

One can also consider the dynamical behavior of such material [AZÉ 06, AZÉ 08]. As an illustration we consider a sample made of 1200 particles with the same property

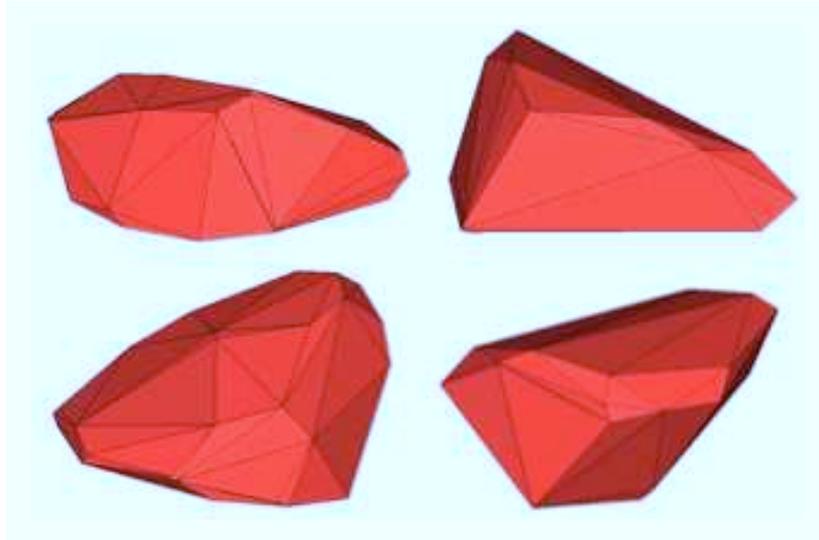


Figure 1.14. *Sample of digitalized ballast grains (courtesy of SNCF)*

than before. The sample fill a cubic box (figure1.17) and is submitted to a cyclic horizontal force $f(t)$:

$$f(t) = \frac{(f_{max} + f_{min})}{2} - \frac{(f_{max} - f_{min})}{2} \sin(\omega t),$$

where f_{max} and f_{min} are the maximum and the minimum of the compression force.

Understanding the compaction behavior of the material (figure1.18) needs once more to analyze local behavior as the contact force distribution and evolution (figure 1.19).

1.6.3. Conclusion

There are no insurmountable conceptual or technical issues taking into account polyhedral particles in a discrete media simulation as soon as objects kinematics and contact detection are managed. However specific difficulties coming from the chosen simulation strategies may arise.

Building a simulation tool remains only the first step in the analysis. Due to the deep influence of particle geometry on sample macroscopic behavior specific post-processing tools need to be developed and are not a straightforward adaption of existing one.

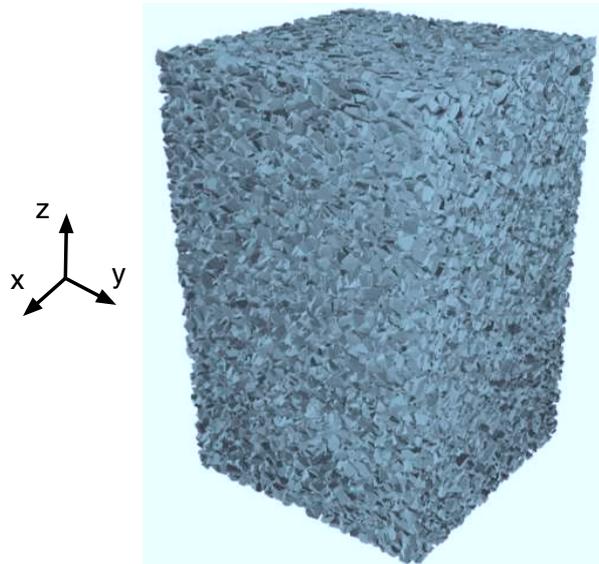


Figure 1.15. *Triaxial test : sample geometry*

To conclude one have to notice that a fine study of the influence of the modeling choices on the macroscopic behavior is not available.

I want to thanks people who contribute to the development of the modeling tool (Gilles Saussine, Robert Pérales) and the analysis methodology (Farhang Radjai, Emilien Azéma, Ali Rafiee, Marc Vinches).

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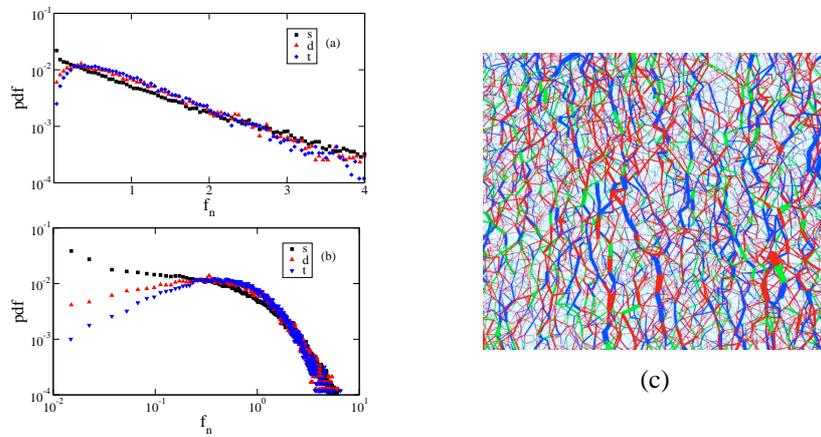


Figure 1.16. Probability distribution functions of radial forces at simple (s), double (d) and triple (t) contacts on log-linear (a) and log-log (b) scales.
 (c) Map of contact forces projected along branch vectors at $\varepsilon_q = 0.4$. Line thickness is proportional to the force. The simple, double and triple contacts are in red (dark gray), in green (light gray) and in blue (black).

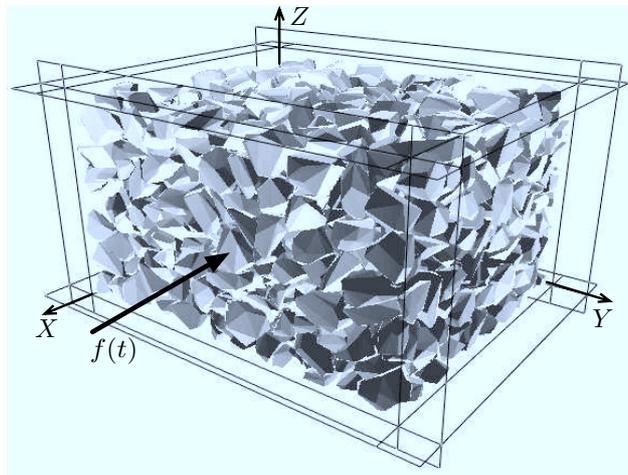


Figure 1.17. A snapshot of the packing inside a box with a free wall over which the driving force $f(t)$ is applied along the x direction.

[AZÉ 07b] AZÉMA E., RADJAI F., PEYROUX R., SAUSSINE G., « Force transmission in a packing of pentagonal particles », *Physical Review E*, vol. 76, p. 1-16, 2007.

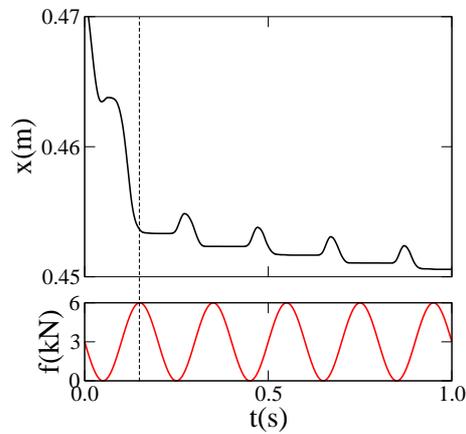


Figure 1.18. The evolution of the x displacement of the free wall (up) in response to harmonic loading (down).

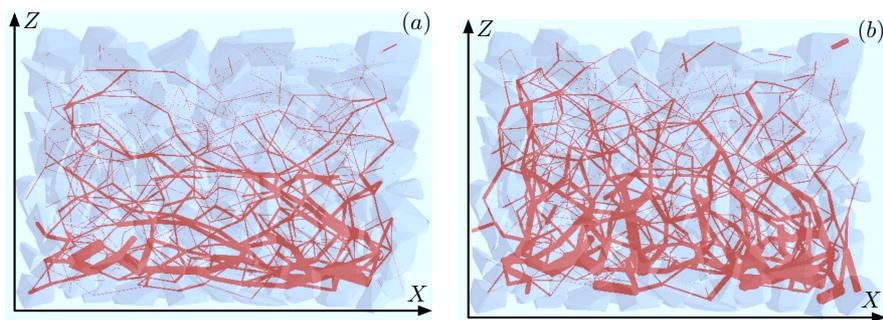


Figure 1.19. Normal forces in the passive (a) and active (b) states in a section of the packing parallel to the xz plane. The segments connect particle centers with a thickness proportional to the normal force.

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