Producing dense packings of cubes

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Abstract

In this paper we consider the problem of packing a set of $d$-dimensional congruent cubes into a sphere of smallest radius. We describe and investigate an approach based on a function $\psi$ called the maximal inflation function. In the three-dimensional case, we localize the contact between two inflated cubes and we thus improve the efficiency of calculating $\psi$. This approach and a stochastic algorithm are used to find dense packings of cubes in 3 dimensions up to $n = 20$. For example, we obtain a packing of eight cubes that improves on the cubic lattice packing.

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1. Introduction

A typical packing problem consists in the search for configurations of non-overlapping congruent objects within a fixed compact subset $K$ of $\mathbb{R}^d$, which minimize the wasted volume. Many instances of this problem have produced a large literature, especially when the sets are disks or spheres, see for instance [2,14]. The case of square packings was initiated by Erdős and Graham [3] and has been studied recently by Friedman [4], Stromquist [16], Kearney and Shiu [11]. These authors offer some proofs of optimality of configurations of $n$ squares in a square up to $n = 10$ and for $n = 14, 15, 24, 35$; their proofs rely on the technique of unavoidable points which has been more recently generalized by Nagamochi [15].

The aim of this paper is to explain how to produce dense packings of $d$-cubes in the unit ball $K = B(0, 1)$. The side of the $n$ cubes of an optimal packing in the ball $K \subset \mathbb{R}^d$ will be denoted by $s_n$. Fig. 1 displays on the left the best packing found of eight 3-cubes. All the cubes have side $16/\sqrt{761} > 0.59$. In comparison, the cubic lattice packing displayed on the right is worse since their side equals $1/\sqrt{3} < 0.58$.

We adapt here and generalize the method of [8] to the $d$-dimensional case and we experiment it only for $d = 3$. Roughly, the algorithm consists in generating a random walk:

- Choose randomly $n$ non-overlapping cubes inside $K$.
- Move randomly the $n$ cubes without overlap inside $K$ and inflate them if it is possible. Continue until the packing is jammed.
Notice that the idea of inflating particles to create dense packings of disks in the plane is already there in [12,13]. Their method relies mainly on billiard systems and has inspired subsequent works on disk packings [1,10] and on sphere packings [6].

But how to inflate a configuration \( \mathcal{C} = (q_1, \ldots, q_n) \) of \( n \) cubes in \( K \)? We compute the maximal side \( \omega(\mathcal{C}) \) of the cubes \( q_i \) which prevents from overlapping and keeps confinement in \( K \), then we replace the original side of the cubes of \( \mathcal{C} \) with \( \omega(\mathcal{C}) \). The core of this computation is the evaluation of the maximal inflation \( \psi(q_1, q_2) \) of two \( d \)-cubes: at the side \( \psi(q_1, q_2) \)—the centers and the orientations being fixed—the two cubes contact each to other at their boundaries. Finally, we can rephrase our problem as a maximal separation problem [14]:

To find \( n \) non-overlapping congruent cubes of \( \mathbb{R}^d \) which attain \( s_n = \max_{\mathcal{C}} \omega(\mathcal{C}) \).

Section 2 is devoted to the definition and the computation of \( \psi(q_1, q_2) \), Section 3 deals with \( \omega(\mathcal{C}) \). In Section 4, we focus on the localization of contacts between two congruent \( 3 \)-cubes. In Section 5, we give an account of the algorithm and of the experiments.

**Notation:** Throughout this paper, boldface letters denote either cubes or unit vectors. We denote by:

\[
AB = B - A \text{ the vector joining two points of } \mathbb{R}^d, \\
AB \cdot CD \text{ the dot product of two vectors,} \\
B(M, \varepsilon) \text{ the ball of radius } \varepsilon \text{ and centered at } M, \\
\text{int} X \text{ and } \partial X \text{ the interior and the boundary of a subset } X \text{ of } \mathbb{R}^m, \\
\text{ri} X \text{ the relative interior of a subset } X \text{ of } \mathbb{R}^m, \\
V(q) \text{ (respectively, } E(q)) \text{ the set of vertices (respectively, of edges) of a cube } q.
\]

### 2. The maximal inflation function and its computation

For any cube \( q \) in \( \mathbb{R}^d \), we denote by \( q^k \) the inflated cube of side \( k > 0 \) obtained from an homothety centered at the center \( C(q) \) of \( q \). If \( q_1 \) and \( q_2 \) have distinct centers, we want to find the side \( k > 0 \) for which the inflated cubes \( q_1^k \) and \( q_2^k \) intersect and do not overlap. We now generalize the definition given in [8, p. 99]:

**Definition 1.** The maximal inflation of two cubes \( q_1, q_2 \) in \( \mathbb{R}^d \) with distinct centers is the least positive real number \( k = \psi(q_1, q_2) \) for which \( q_1^k \cap q_2^k \) is not empty.

#### 2.1. Cubes and first steps towards \( \psi \)

Any cube \( q \) of \( \mathbb{R}^d \) is determined by its center \( C = C(q) \), an orthonormal basis \( \mathcal{A} = \{\tilde{a}_1, \ldots, \tilde{a}_d\} \) and its side \( s > 0 \):

\[
q = \left\{ C + \sum_{i=1}^{d} x_i \tilde{a}_i : |x_i| \leq \frac{s}{2} \text{ for all } i \right\}.
\]
We denote by \((C, \mathcal{A}, s)\) the cube (1). For example, the unit cube \([-\frac{1}{2}, \frac{1}{2}]^d\) is \((O, \mathcal{A}_0, 1)\) where \(\mathcal{A}_0\) is the canonical basis. We write \(P = C + \sum_{i=1}^d x_i \tilde{a}_i = (x_1, \ldots, x_d)q\) for each point \(P\) of the cube \(q\).

The various faces of \(q\) are given by

\[
F_{q,i_0}\Delta = \left\{ P = C + \sum_{i=1}^d x_i \tilde{a}_i : x_{i_0} = \omega_0 \frac{s}{2} \text{ and } |x_i| \leq \frac{s}{2} \text{ for all } i \right\},
\]

where \(\omega_0 \in \{1, \ldots, d\}\) and \(\omega_0 \pm 1\). The vector \(\tilde{a}_{i_0}\) is orthogonal to the face \(F_{q,i_0}\Delta\).

Let \(q_1, q_2\) be two congruent cubes with distinct centers \(C_1, C_2\) and orientations defined by the two orthonormal bases \(\mathcal{A} = \{\tilde{a}_1, \ldots, \tilde{a}_d\}\) and \(\mathcal{B} = \{\tilde{b}_1, \ldots, \tilde{b}_d\}\). The vector joining the centers and the vectors of the basis \(\mathcal{B}\) of \(q_2\) decompose in the basis \(\mathcal{A}\) of \(q_1\) as

\[
C_1C_2 = C_2 - C_1 = \sum_{j=1}^d \beta_j \tilde{a}_j \text{ and } \tilde{b}_j = \sum_{j=1}^d \gamma_{ij} \tilde{a}_j.
\]

Lemma 2(a) justifies Definition 1 of \(\psi\) and Proposition 7 shows that \(\psi\) is also the least side \(k\) such that the two boundaries \(\partial q_{i_0}^k\) intersect.

\textbf{Lemma 2.} Let \(q_1 = (C_1, \mathcal{A}_1, s)\) and \(q_2 = (C_2, \mathcal{A}_2, s)\) be two congruent cubes with distinct centers.

(a) The set \(I = \{s > 0 : q_{1,i}^s \cap q_{2,i}^s \neq \emptyset\}\) is an interval of \(\mathbb{R}_+^d\) of the shape \([\psi, +\infty]\).

(b) The intersection \(q_{1,i}^s \cap q_{2,i}^s\) is not empty if, and only if, there exist real numbers \(x_1, \ldots, x_d, y_1, \ldots, y_d\) such that for all \(i\), \(|x_i| \leq s/2\), \(|y_i| \leq s/2\) and

\[
\forall j \in \{1, \ldots, d\}, \quad x_j = \beta_j + \sum_{i=1}^d \gamma_{ij} y_j.
\]

\textbf{Proof.} (a) is straightforward and we omit its proof. (b) Clearly, the intersection \(q_{1,i}^s \cap q_{2,i}^s\) is not empty if, and only if, there exists a point \(P\) with coordinates \((x_1, \ldots, x_d)_{q_1}\) and \((y_1, \ldots, y_d)_{q_2}\) such that

\[
P = C_1 + \sum_{i=1}^d x_i \tilde{a}_i = C_2 + \sum_{i=1}^d y_i \tilde{b}_i \text{ and } |x_i| \leq \frac{s}{2}, \quad |y_i| \leq \frac{s}{2}.
\]

We get

\[
\sum_{j=1}^d x_j \tilde{a}_j = \sum_{j=1}^d \beta_j \tilde{a}_j + \sum_{i=1}^d y_i \sum_{j=1}^d \gamma_{ij} \tilde{a}_j = \sum_{j=1}^d \left( \beta_j + \sum_{i=1}^d \gamma_{ij} y_j \right) \tilde{a}_j,
\]

and the result follows. \(\square\)

We note that \(\psi\) is also the least value of the numbers \(s\) such that there exists a solution \((x_1, \ldots, x_d)_{q_1}, (y_1, \ldots, y_d)_{q_2}\) of Eqs. (4) together with the inequalities \(|x_i| \leq s/2, \quad |y_i| \leq s/2\). The following lemma is reminiscent of Lemma 1 in [8] and gives some easy properties of the function \(\psi\).

\textbf{Lemma 3.} Given two \(d\)-cubes \(q_1, q_2\) with distinct centers, we have:

(a) \(\psi(q_1, q_2) = \psi(q_2, q_1)\).

(b) \(q_1 \cap q_2 = \emptyset\) is equivalent to \(\psi(q_1, q_2) > s\).

(c) \(d(C_1, C_2) / \sqrt{d} \leq \psi(q_1, q_2) \leq d(C_1, C_2)\).

(d) For any \(k \in \mathbb{R}\), we have \(\psi(q_{1,k}^k, q_{2,k}^k) = \psi(q_1, q_2)\).

(e) We have \(\psi(g(q_1), g(q_2)) = \psi(q_1, q_2)\) for any displacement \(g : \mathbb{R}^d \to \mathbb{R}^d\).
2.2. Calculation of $\psi$ in 3-dimension

Here we give a short account on the way of computing $\psi$ in the case of 3-cubes. It is intuitively obvious that two inflating 3-cubes can contact each other either face-to-vertex or edge-to-edge. Thus we have to solve the following linear system of seven equations in seven unknowns $x_1, x_2, x_3, y_1, y_2, y_3, s$:

$$x_j = \beta_j + \sum_{i=1}^{3} a_{ij} y_i \quad \text{for } 1 \leq j \leq 3,$$

$$x_i = \pm \frac{s}{2}, \quad y_j = \pm \frac{s}{2} \quad \text{for } i \in I \text{ and } j \in J,$$

(6)

where the sets $I, J \subset \{1, 2, 3\}$ satisfy $\text{Card } I + \text{Card } J = 4$.

The $2 \times 6 \times 8$ virtual contacts face-to-vertex appear when Card $I$, Card $J \in \{1, 3\}$. The $12 \times 12$ virtual contacts edge-to-edge appear when Card $I = \text{Card } J = 2$. The solutions of the Cramer systems among the 240 previous ones are to be tested on belonging to the cubes, that is $|x_k| \leq s/2$, $|y_k| \leq s/2$ for each $k$. Among all the solutions, we select the one having $s$ positive and minimal; this solution yields a contact and $\psi$.

The complexity of the three-dimensional case is revealed by a moment-thought, for the non-empty intersection $q_1 \cap q_2$ of two non-overlapping cubes with side $s = \psi$ can be equal to

- a vertex common to $q_1$ and $q_2$,
- a vertex of $q_1$ lying in the relative interior of an edge of $q_2$,
- a vertex of $q_1$ lying in the relative interior of a face of $q_2$,
- a point lying in the intersection of two relative interiors of two edges of $q_1$, $q_2$,
- a common edge or a segment included in two edges,
- a segment included in, say an edge of $q_1$ and in a face of $q_2$, this case yielding several subcases,
- a convex polygon $F_1 \cap F_2$—having from 3 to 8 sides—where $F_1$ and $F_2$ are faces of $q_1$ and $q_2$.

Readers interested only by three-dimensional case can skip the following subsection which is devoted to the calculation of $\psi$ in any dimension and to a rigorous proof of this algorithm.

2.3. A general algorithm for computing $\psi$

Let $q$ be a cube of side $s$. Any facet $F$ of $q$ is determined by a subset $I$ of $[1, d]$ and a sequence $(\varepsilon_i)_{i \in I}$ with $\varepsilon_i = \pm 1$ for all $i \in I$, so that

$$F = \left\{ C + \sum_{i=1}^{d} x_i \vec{a}_i : |x_i| < s/2 \text{ for } i \notin I \text{ and } x_i = \varepsilon_i s/2 \text{ for } i \in I \right\}.$$

As a consequence we have $\overrightarrow{F} = \text{span} \{\vec{a}_i : i \notin I\}$ and $\dim F = \dim \overrightarrow{F} = d - \text{Card } I$. For instance, the face $F_{q_{i_0}, \varepsilon_{i_0}}$, see (2), is also the facet defined by $I = \{i_0\}$ and $\varepsilon_{i_0} = \varepsilon_{i_0}$. We recall that the facet of a point $P \in q$ is the facet of $q$ of maximal dimension which contains $P$.

We now show that an extremal point of $q_{1,\psi} \cap q_{2,\psi}$ belongs to at least $d + 1$ faces of the two cubes $q_{1,\psi}$, $q_{2,\psi}$. We obtain so far a generalization of the two-dimensional case: an extremal point of $q_{1,\psi} \cap q_{2,\psi}$ belongs to three edges of the two squares and then is a vertex of one of the two squares.

Proposition 4. Let $P$ be an extremal point of $q_{1,\psi} \cap q_{2,\psi}$. The coordinates of $P$ verify

$$\text{Card}\{i : |x_i| = \psi/2\} + \text{Card}\{j : |y_j| = \psi/2\} \geq d + 1.$$

(7)

In other words the facets $F_1$, $F_2$ of $P$ in $q_{1,\psi}$, $q_{2,\psi}$ verify $\dim F_1 + \dim F_2 \leq d - 1$. 

Table 1
Calculation of the maximal inflation of two d-cubes

- Set \( \psi := d(C_1, C_2) \)
- For \( u \) from 0 to \( d - 1 \) do
  - For \( v \) from 0 to \( d - 1 - u \) do
    - For each subsets \( U, V \) of \([1, d]\) with \( Card \ U = u \) and \( Card \ V = v \) do
      - Choose signs \( \epsilon' \) for \( i \not\in U \) and \( \epsilon'' \) for \( j \not\in V \)
      - Write the linear system \( AZ = b \) given by Eqs. (9)
      - If \( ker(A) = 0 \) and \( b \in Im \ A \) then
        - Find the unique solution \( Z = (s, (x_i), (y_j)) \) of \( AZ = b \).
      - If \( |x_i| \leq s/2, |y_j| \leq s/2 \) for all \( i, j \in U \times V \) and \( \psi \geq s \) then \( \psi := s \).
- Result: \( \psi = \psi(q_1, q_2) \)

Proof. Let \( s > 0 \) such that \( q_1^s \cap q_2^s \neq \emptyset \) and \( P \) be a point of \( q_1^s \cap q_2^s \) with coordinates \((x_1, \ldots, x_d)_{q_1}, (y_1, \ldots, y_d)_{q_2}\). The real numbers \( s, x_1, \ldots, x_d, y_1, \ldots, y_d \) are solutions of the \( d \) equations (4) given in Lemma 2, together with the \( 4d \) constraints \( |x_i| \leq s/2, |y_j| \leq s/2 \). We define

\[
U = \{i : |x_i| < s/2\}, \quad V = \{j : |y_j| < s/2\}, \quad u = Card \ U, \quad v = Card \ V
\]  

(8)

to be the sets of indices of inactive coordinates and their cardinals. So, the point \( P \) verifies \( 2d - (u + v) \) active constraints \( x_j = \delta_j s/2 \) for all \( i \not\in U \) and \( y_j = \delta_j s/2 \) for all \( j \not\in V \). Denoting by \( I_U \) the indicatrix of a subset \( U \), the system becomes

\[
x_j I_U(j) - \sum_{i=1}^d a_{ij} y_i I_V(i) + \frac{s}{2} \left( \delta_j (1 - I_U(j)) - \sum_{i=1}^d a_{ij} \delta_j s (1 - I_V(i)) \right) = \beta_j
\]  

(9)

for all \( j = 1, \ldots, d \). This linear system can be written \( AZ = b \) where \( Z = (z_0, z_1, \ldots, z_{u+v}) \) is the vector containing the \( u + v + 1 \) unknowns \( s, (x_i)_{i \in U}, (y_j)_{j \in V} \) (in that order) and where \( A \) is a matrix with \( d \) rows and \( u + v + 1 \) columns. In turn, we denote by \( Z_P \in \mathbb{R}^{1+u+v} \) the vector \((s, (x_i)_{i \in U}, (y_j)_{j \in V})\) relative to the point \( P \in \mathbb{R}^d \), the active coordinates being removed. Conversely, a solution \( Z = (z_i)_{0 \leq i \leq u+v} \in \mathbb{R}^{1+u+v} \) of Eqs. (9) gives rise to a point \( P = (x_i)_{q_1} \in \mathbb{R}^d \), the inactive coordinates of which are \( z_1, \ldots, z_u \) and with active coordinates the numbers \( (z_0/2) \delta_j \). This point \( P \) belongs to \( q_1^s \cap q_2^s \) provided that \( s = z_0 > 0 \) and \( |x_i| \leq s/2, |y_j| \leq s/2 \).

We now suppose that \( P \in q_1^s \cap q_2^s \) and the number of active constraints is strictly less than \( d + 1 \), and we are going to show that either \( s \neq \psi \) or \( P \) is not extremal. We have \( u + v \geq d \), and then the kernel of the matrix \( A \in L(\mathbb{R}^{1+u+v}, \mathbb{R}^d) \) is not trivial: there exists a non-zero vector \( z^* \in \mathbb{R}^{1+u+v} \) such that \( Az^* = 0 \). Then the vector \( Z' = Z_P + z z^* \) is a solution of \( AZ = b \) and, if \( z \) is small enough, satisfies the constraints \( |x_i'| < s/2, |y_j'| < s/2 \) for \( i \in U, \quad j \in V \). This vector \( Z' \) gives rise, as before, to a point \( P' = P + z P^* \) with coordinates \((x_1', \ldots, x_d')_{q_1}, (y_1', \ldots, y_d')_{q_2}\). The inactive coordinates of \( P' \) are components of the vector \( Z' \), while the active coordinates of \( P' \) are equal to \( \delta_j' (s + x z_0)/2 \) for all \( j \not\in U \), and \( \delta_j' (s + x z_0)/2 \) for all \( j \not\in V \). If \( z \) is small enough, the point \( P' \) belongs to \( q_1^{s'} \cap q_2^{s'} \) with \( s' = s + x z_0 \).

First, we suppose that \( z_0^* \neq 0 \). We choose \( z \) small enough and having the opposite sign of \( z_0^* \), then set \( q_1^{s'} \cap q_2^{s'} \) is not empty with \( 0 < s' < s \) and we get \( s \neq \psi \) by Lemma 3(a). Second, we suppose that \( z_0^* = 0 \); for all \( z \) small enough, the points \( P \pm z P^* \) belong to \( q_1^{s'} \cap q_2^{s'} \). We obtain a segment \( [P - z P^*, P + z P^*] \) included in \( q_1^{s'} \cap q_2^{s'} \) and then the point \( P \) is not extremal.

The inequality for the facets is an easy consequence of (7) since we have \( dim \ F_1 = u \), \( dim \ F_2 = v \). \( \square \)

The preceding proposition and its proof yield an algorithm for computing \( \psi \). Indeed, by the Krein–Milman theorem the set \( q_1^{\psi} \cap q_2^{\psi} \) has extremal points, and by (7), all of them have at least \( d + 1 \) active coordinates in the two frames. The inactive coordinates of these extremal points and \( \psi \) are solutions of the system of \( d \) equations (9) with \( u + v + 1 \) unknowns, see (8). So, it suffices to solve all those systems with \( u + v \leq d - 1 \) and to store the various values of \( s \) when the constraints \( |x_i| \leq s/2, |y_j| \leq s/2 \) are verified. Finally, \( \psi \) is obtained as the minimum between the remaining values of \( s \). This algorithm is displayed in Table 1, there again \( A \) is the matrix of system (9).

**Corollary 5.** The algorithm described in Table 1 is valid.
Proof. We keep notation and framework of Proposition 4. Let us explained why in Table 1, the systems $AZ = b$—given by (9)—which are not Cramer have been removed. We show that their solutions cannot return either $s = \psi$ or an extremal point $P$ of $q_1^\psi \cap q_2^\psi$. First, the case $b \notin \text{Im } A$ does not matter. Second, let us consider the case $\ker A \neq 0$ and $b \in \text{Im } A$. Let $Z = (z_i)$ be some solution of $AZ = b$, then the general solution is $Z' = Z + az^*$ with $z^* \in \ker A$. It gives rise to points $P' = P + xP^*$ of $\mathbb{R}^d$. If the first coordinate $z_0^*$ of $z^*$ equals 0, then for $x$ small enough the point $P'$ is in $q_1^\psi \cap q_2^\psi$ with $s = z_0^*$. As before, we deduce that $P$ is not extremal. If $z_0^* \neq 0$, the point $P'$ lies in $q_1^\psi \cap q_2^\psi$ where $s' = s + az_0^*$ for $a$ small enough. For $s$ such that $az_0^* < 0$, we get an admissible solution with $s' < s$ and then $s \neq \psi$. □

In practice, the procedure writes and solves first of all the square systems with $u + v = d - 1$. If all those systems verify $\ker A = 0$, then the procedure stops and we have found $\psi$. Indeed, if an extremal point verifies $u + v < d - 1$, it is also a solution of a square system obtained by forgetting some active coordinates. The number of those square systems can be evaluated with Vandermonde’s convolution formula:

$$
\sum_{u+v=d-1} 2^{d-u}2^{d-v} \binom{d}{u} \binom{d}{v} = 2^{d+1} \sum_{k=0}^{d-1} \binom{d}{k} \binom{d}{d-1-k} = 2^{d+1} \binom{2d}{d-1}.
$$

For instance in dimensions 2–5, we would have to handle 32, 240, 1792, 13,440 square systems. The whole procedure of Table 1 involves 48, 496, 4864, 46,464 “rectangular” linear systems for the same dimensions.

Let $q_1, q_2$ be two congruent cubes having distinct centers. For conciseness, we omit the proofs of Proposition 7(a) and (b). The statement (c) is a first step towards the localization of contacts between cubes.

Corollary 6. The sets $I = \{s : q_1^s \cap q_2^s \neq \emptyset\}$ and $I' = \{s : \partial q_1^s \cap \partial q_2^s \neq \emptyset\}$ are equal.

Proof. Obviously, we have $I' \subset I$. Conversely, if $s \in I$, by Krein–Milman theorem, the non-empty convex compact set $q_1^s \cap q_2^s$ has extremal points. Such an extremal point $P$ has at least $d + 1$ active coordinates by (7). Hence $P$ has at least one active coordinate in each cube and we conclude that $P \in \partial q_1^s \cap \partial q_2^s$, that is, $s \in I'$. □

Proposition 7. (a) The number $\psi$ is the only positive real number for which $\text{int } q_1^\psi \cap \text{int } q_2^\psi$ is empty and $\partial q_1^\psi \cap \partial q_2^\psi$ is not empty.

(b) We have $q_1^\psi \cap q_2^\psi = \partial q_1^\psi \cap \partial q_2^\psi = \partial (q_1^\psi \cap q_2^\psi)$.

(c) There exist a face of $q_1^\psi$ and a face of $q_2^\psi$ which both contain the whole set $q_1^\psi \cap q_2^\psi$.

Proof of (c). By (b), $q_1^\psi \cap q_2^\psi$ is included in $\partial q_1^\psi$ which is nothing but the union of all the faces of $q_1^\psi$. We remark that if $M, M'$ belong to $q_1^\psi \cap q_2^\psi$, they cannot verify $M \in F \setminus F'$ and $M' \in F' \setminus F$ where $F, F'$ are two distinct faces of the cube $q_1^\psi$. Indeed, a convexity argument together with inspection of coordinates show that in that case the relative interior $\text{int } M, M'$ is contained in the interior of $q_1^\psi$. We have also $[M, M'] \subset q_1^\psi \cap q_2^\psi \subset \partial q_1^\psi$ yielding a contradiction. We have shown that at least one face of $q_1^\psi$ contains $q_1^\psi \cap q_2^\psi$. The same holds for $q_2^\psi$. □

3. Confinement and inflation of a configuration of $n$ cubes of $\mathbb{R}^d$

3.1. Confinement

In this subsection, we compute the largest real number $k > 0$ such that the homothetic cube $q^k$ is included in some compact and convex subset $K$ of $\mathbb{R}^d$. If $C(q)$ belongs to the interior of $K$, we define $\varphi(q) = \max \{k > 0 : q^k \subset K\}$. We give two formulas for $\varphi(q)$ when $K$ is a cube or a ball. First, we easily get:

Lemma 8. Let $K$ be a convex compact subset of $\mathbb{R}^d$ and $q$ be a cube of $\mathbb{R}^d$ such that $C(q) \in \text{int } K$. For each vertex $S \in V(q)$, there exists only one strictly positive number $\mu_S$ such that $C + \mu_S CS \in \partial K$. Then

$$
\varphi(q) = s \min_{S \in V(q)} \mu_S.
$$
Let $K$ be the cube $[-L, L]^d$. We denote by $(c_1, \ldots, c_d)$ the coordinates of the center $C$ and by $(x_{1,S}, \ldots, x_{d,S})$ the coordinates of any vertex $S \in V(q)$. Then

$$\varphi(q) = s \cdot \min_{S \in V(q)} \{ \mu_{1,S}, \mu_{2,S} \},$$

where

$$\mu_{1,S} = \min_{i=1,\ldots,d} \left\{ \frac{L - c_i}{x_{i,S} - c_i} : x_{i,S} > c_i \right\} \quad \text{and} \quad \mu_{2,S} = \min_{i=1,\ldots,d} \left\{ \frac{L + c_i}{c_i - x_{i,S}} : x_{i,S} < c_i \right\}.$$

Proof. Due to Lemma 8, we have to compute all values $\mu_S$. The number $(L - c_i)/(x_{i,S} - c_i)$ is the ratio of the homothety centered at $C$ which maps the vertex $S$ onto the face $x_i = L$ of the cube $[-L, L]^d$. Similarly, the number $(L + c_i)/(c_i - x_{i,S})$ is the ratio of the homothety centered at $C$ mapping $S$ onto the opposite face $x_i = -L$. We discard all negative values among all the previous ratios of homothety, and we get $\mu_S = \min\{\mu_{1,S}, \mu_{2,S}\}$. □

Lemma 10. If $K$ is the ball $B(O, 1)$ of $\mathbb{R}^d$, we have

$$\varphi(q) = s \min_{S \in V(q)} \left\{ \frac{-OC \cdot CS + \sqrt{(OC \cdot CS)^2 - (OC^2 - 1)CS^2}}{CS^2} \right\}.$$

Proof. Indeed, in order to compute the numbers $\mu_S$ given in Lemma 8, we have to solve the equation $||OC + \mu CS||^2 = (CS)^2 \mu^2 + 2(OC \cdot CS)\mu + (OC)^2 = 1$. This yields the above value for $\mu_S$ since the other root is negative. The formula for $\varphi(q) = s\min_{S \in V(q)} \mu_S$ follows. □

3.2. Maximal inflation of a configuration

Let $Q_{n,d,s}$ be the manifold of configurations $\mathcal{C} = \{q_i\}_{i=1}^n$ of $n$ congruent cubes with distinct centers in $K$ and side $s$. In the report [9], we prove that the mapping $\psi(q_1, q_2)$ is continuous on the manifold of configurations of two cubes of $\mathbb{R}^d$ — we use in this proof the Hausdorff metric.

Definition 11. For any $\mathcal{C} = (q_1, \ldots, q_n) \in Q_{n,d,s}$, there exists an unique packing $(q_{1,\omega(\mathcal{C})}, \ldots, q_{n,\omega(\mathcal{C})})$ having the same centers and the same bases as the cubes of $\mathcal{C}$ and of maximal side. The value of $\omega(\mathcal{C})$ is given by

$$\omega(\mathcal{C}) = \min \left\{ \min_{1 \leq i \leq n} \varphi(q_i), \min_{1 \leq i < j \leq n} \psi(q_i, q_j) \right\}.$$ 

The mapping $\omega : Q_{n,d,s} \rightarrow \mathbb{R}_+$ is continuous.

If $K$ is compact, the packing problem amounts to maximize the continuous and non-differentiable function $\omega$ on the compact space $Q_{n,d,s}$.

4. Localization of the contact between two cubes of $\mathbb{R}^3$

We address here the problem of determining the faces of the cubes $q_1^\psi$ and $q_2^\psi$ on which the contacts hold and we give an answer in Proposition 12. Indeed, effective computations of dense configurations imply a huge amount of evaluations of $\psi$ and localization of contacts decreases the intricacy underlying each evaluation.

Until the end of this paper, we suppose $d = 3$.

4.1. Localization

For any cube $q = (C, \mathcal{A}, s)$ and for $k = 1, 2, 3$ and $\varepsilon = \pm 1$, we define the sextant $\mathcal{S}(q, k, \varepsilon)$ as the cone centered at $C$ and generated from the face $F_{q,k,\varepsilon}$, see (1). A point $M = C + \sum_{i=1}^3 x_i \vec{a}_i$ belongs to $\mathcal{S}(q, k, \varepsilon)$ if and only if $|x_k| = \varepsilon x_k \geq \max |x_i|$. A cube has six sextants, all independent of the side $s$. Sextants generalize the quadrants defined
in [7]. If a point $M$ belongs to the interior of $\mathcal{S}(q, k, s)$, we note $\mathcal{S}(q, M) = \mathcal{S}(q, k, s)$. If the point $M$, distinct from the center of the cube, lies on the boundaries of two or three sextants, we choose indifferently $\mathcal{S}(q, M)$ as one of those.

In [7], if $d = 2$ we have proved that

$$q_1^\psi \cap q_2^\psi \subset \mathcal{S}(q_1, C_1) \cap \mathcal{S}(q_2, C_1).$$

This result is no longer true for $d = 3$: Fig. 2 exhibits $q_2$ touching $q_1$ at $P$ on the “upper” face of $q_1$, and the sextant $\mathcal{S}(q_1, P)$. The center $C_2$ is outside $\mathcal{S}(q_1, P)$ and thus $P$ does not belong to $\mathcal{S}(q_1, C_2)$. In this example we get that $q_1^\psi \cap q_2^\psi$ is not included in $\mathcal{S}(q_1, C_2)$.

Let $q_1$ and $q_2$ be two congruent cubes. Recall that $C_1C_2 = \sum_{j=1}^3 \beta_j \vec{a}_j$, see (3). It is always possible to change the basis $(\vec{a}_1, \vec{a}_2, \vec{a}_3)$ of $q_1$ to $(\vec{v}_1 \vec{a}_1, \vec{v}_2 \vec{a}_2, \vec{v}_3 \vec{a}_3)$ with $\vec{v}_i = \pm 1$, in such a way that we obtain $\beta_3 \geq \beta_2 \geq \beta_1 \geq 0$.

**Proposition 12.** Let $q_1$ and $q_2$ be two congruent non-overlapping cubes. W.l.o.g., we assume that the coordinates of the center of $q_2$ in the basis of $q_1$ satisfy $\beta_3 \geq \beta_2 \geq \beta_1 \geq 0$. If $\beta_3 \neq \beta_1$, then we have

$$q_1^\psi \cap q_2^\psi \subset F_{q_1^\psi, 3, 1} \subset \mathcal{S}(q_1, 3, 1) = \{ (x, y, z) \in \mathbb{R}^3 : z \geq \max(|x|, |y|) \}$$

or

$$q_1^\psi \cap q_2^\psi \subset F_{q_2^\psi, 2, 1} \subset \mathcal{S}(q_1, 2, 1) = \{ (x, y, z) \in \mathbb{R}^3 : y \geq \max(|x|, |z|) \}.$$

This result although elementary is somewhat involved and we defer its proof to the next subsection. The aim of the following easy result is to reduce the complexity arising in explicit calculations of $\psi$. More precisely, it allows to break the calculations when $C_2 \in \mathcal{S}(q_1, 3, 1)$ and when $q_1^\psi \cap q_2^\psi$ contains a vertex $P' \in q_2^\psi$ which belongs also to $F_{q_1^\psi, 3, 1}$. Indeed, in that case $P'$ comes from the “lowest” vertex $P$ of $q_2$, which amounts to saying that its third coordinate $x_3 = C_1P \cdot \vec{a}_3$ in the basis of $q_1$ is minimal. But the converse also holds, under a mild hypothesis:

**Proposition 13.** Let $q_1$, $q_2$ be two non-overlapping congruent cubes of $\mathbb{R}^3$ of side $s$. We suppose that $C_2 \in \mathcal{S}(q_1, 3, 1)$. Let us choose among the eight vertices of $q_2$ a vertex $P$ minimizing the third coordinates $x_3 = C_1P \cdot \vec{a}_3$ in the basis of $q_1$. We have

$$\psi = \psi(q_1, q_2) = \left( \frac{1}{2} - \frac{1}{s} C_2P \cdot \vec{a}_3 \right)^{-1} (C_1C_2 \cdot \vec{a}_3),$$

provided the homothetic vertex $P' = C_2 + (\psi/s) \cdot C_2P \in q_2^\psi$ belongs also to the face $F_{q_1^\psi, 3, 1}$ of $q_1^\psi$. 

Fig. 2.
Proof. For each $s' > 0$, the point $P' = C_2 + s'/s \cdot C_2 P$ is a vertex of $q_1^{s'}$. If $P'$ belongs to the upper face $F_{q_1^{s'},3,1}$, then the common side $s'$ is a solution of the equation $\mathbf{a}_3 \cdot C_1 P' = s'/2$. Solving $\mathbf{a}_3 \cdot (C_1 C_2 + s'/s \cdot C_2 P) = s'/2$ with respect to $s'$ yields (11). Our assumption is $P' \in F_{q_1^{s'},3,1}$ where $s'$ is given by (11). Since $P' \in q_1^{s'} \cap q_2^{s''}$ we get $s \leq s' \leq s''$ by Lemma 3(a). Now, each point $(x_1, x_2, x_3)_{q_1}$ of $\text{int } q_1^{s'}$ obviously satisfies $x_3 < s'/2$. Due to the choice of $P$ among the vertices of $q_1$ and by convexity, each point $(t_1, t_2, t_3)_{q_1}$ of $\text{int } q_2^{s''}$ satisfy $t_3 > s'/2$. We conclude that $\text{int } q_1^{s'} \cap \text{int } q_2^{s''} = \emptyset$ so that $s' \leq s'', \text{ and } s'' = s'$. □

4.2. A faster computation of $\psi$

When computing $\psi$, the number of systems (6) is decreased with Propositions 12 and 13. Recall that without localization, the algorithm requires writing, solving and testing the solutions of 240 systems of three linear equations with three unknowns. We apply instead the following steps:

- Reorder the coordinates of $C_2$ in the basis of $q_1$, that is, choose $(i_1, e_1), (i_2, e_2), (i_3, e_3)$ with $e_i = \pm 1$, such that $e_3\beta_{13} \geq e_2\beta_{12} \geq e_1\beta_{11} \geq 0$. Change the basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ of $q_1$ to $(e_1\mathbf{a}_i, e_2\mathbf{a}_i, e_3\mathbf{a}_i)$. Now, we have $C_2 \in \mathcal{S}(q_1, 3, 1)$.
- Do the same for the center of $C_1$ in the basis of $q_2$.
- Apply Proposition 13 to detect a percussion of $q_2$ on the “upper” face $F_{q_1,3,1}$ of $q_1$. The success of this stage gives $\psi$ and stops the computations. If not, permute the cubes and do the same.
- Proposition 12 shows that it is possible that $q_2$ strikes $q_1$ at a vertex of $P \in q_2$ on one of the faces $F_{q_1,2,1}$ and $F_{q_1,3,1}$. The case $P \in F_{q_1,3,1}$ was treated in the previous step. We get eight systems corresponding to possible percussion on $F_{q_1,2,1}$. When permuting the two cubes, we have eight other systems.
- Proposition 12 gives $49 = 7 \times 7$ systems corresponding to possible contacts between edges of $q_1$ and $q_2$. Indeed, the two faces $F_{q_1,2,1}$ and $F_{q_1,3,1}$ are bounded by seven edges and similarly for $q_2$. However, it is easy to show that the edge $F_{q_1,3,1} \cap F_{q_1,2,1}$ of $q_1$ cannot match $q_1 \cap q_2$ and the number 49 can be replaced with $36 = 6 \times 6$.

4.3. Proof of Proposition 12

This subsection is devoted to the proof of Proposition 12. When $q_1^\psi \cap q_2^\psi$ contains a vertex $P$ of $q_2^\psi$, we say that the square $q_2$ strikes the square $q_1$ at the vertex $P$.

We consider the set $\mathcal{C}(q_1, k, \varepsilon)$, the elements of which are the points $C$ such that there exists a congruent cube $q_2$ centered at $C$, which strikes $q_1$ at a point of the interior of the face $F_{q_1,k,\varepsilon}$, see Fig. 3. Formally,

$$\mathcal{C}(q_1, k, \varepsilon) = \left\{ C \in \mathbb{R}^3 : \exists q_2, \text{ side } (q_2) = \text{side } (q_1), C(q_2) = C, \text{ int } q_1 \cap \text{int } q_2 = \emptyset \text{ and } \exists P \in V(q_2), P \in \text{int } F_{q_1,k,\varepsilon} \right\}.$$  

We give a description of $\mathcal{C}(q_1, 3, 1)$ in the frame $(C_1, \mathcal{A}_1)$ of $q_1$ and for clarity we choose $k = 3, \varepsilon = +1$ and $s = 2$.

The bounded set $\mathcal{C}(q_1, 3, 1)$ is not compact and is the union of:

- the parallelepiped $-1 < x, y < 1, 2 \leq z \leq 1 + \sqrt{3}$,
- the intersection of the half-space $z \geq 2$ with the four balls defined by the inequalities: $(x-e_1)^2 + (y-e_2)^2 + (z-1)^2 < 3$ with $e_1 = \pm 1$ and $e_2 = \pm 1$,
- the intersection of the half-space $z \geq 2$ with the four cylinders defined as $|y| \leq 1, (x-e)^2 + (z-1)^2 < 3$ for $e = \pm 1$, and $|x| \leq 1, (y-e')^2 + (z-1)^2 < 3$ for $e' = \pm 1$.

The boundary $\partial \mathcal{C}(q_1, 3, 1)$ is the union of:

- an upper square which is obtained for the centers of cubes $q_2$ which strikes $q_1$ at $P \in \text{int } F_{q_1,3,1}$ and such that the diagonal $PC_2$ be orthogonal to the face $F_{q_1,3,1}$,
- four spherical surfaces which correspond to centers $C$ of cubes $q_2$ in the half-space $z \geq 2$ and such that $q_2$ strikes $q_1$ at a common vertex $P \in V(q_1) \cap V(q_2)$ among the four vertices of the face $F_{q_1,3,1}$,
four cylindrical surfaces which correspond to centers $C_2$ in the half-space $z \geq 2$ and such that $q_2$ strikes $q_1$ into the relative interior of an edge of $F_{q_1,3,1}$.

- a lower soft square which is the intersection of the plane $z = 2$ with the nine volumes alluded to in the preceding description of $\mathcal{C}(q_1, 3, 1)$. This is the union of the three subsets with defining inequalities:

\[
\begin{align*}
|x| &\leq 1, \quad |y| \leq 1 + \sqrt{2}, \quad z = 2, \\
|x| &\leq 1 + \sqrt{2}, \quad |y| \leq 1, \quad z = 2, \\
(x - e_1)^2 + (y - e_2)^2 &< 2,
\end{align*}
\]

for some $e_1 = \pm 1, e_2 = \pm 1$. This soft square arises when the cube $q_2$ strikes $q_1$ and is parallel to $q_1$, more precisely when $\tilde{a}_3 = \pm \tilde{b}_i$ for some $i$.

Coming back to the proof of Proposition 12, we note that $C_2 \notin q_1$ and then $\beta_3 = \max \beta_i > 1$. We suppose w.l.o.g. that $q_1 = [-1, 1]^3$ and $\psi = s = 2$, thus $q^\psi = q_1$. Since the three sets $q_1 \cap q_2, \mathcal{S}(q_1, 3, 1), \mathcal{S}(q_1, 2, 1)$ are convex, we are left to show that all extremal points of $q_1 \cap q_2$ either belong to the sextant $\mathcal{S}(q_1, 3, 1)$ or to the sextant $\mathcal{S}(q_1, 2, 1)$. We assume that $P$ is an extremal point of $q_1 \cap q_2$. One of the three following cases occurs.

**Case I:** The point $P$ is a vertex of $q_2$ and lies in the relative interior of a face of $q_1$. We need to prove that if $P \notin F_{q_1,i,1}$, then $P \in F_{q_1,i,1}$. We now show that $P$ cannot belong to any of the four other faces. If the point $P$ belongs to the relative interior of $F_{q_1,i,1}$, then $C_2$ belongs to $\mathcal{C}(q_1, 1, 1)$ and we show that its coordinates $\beta_i$ cannot verify $\beta_3 \geq \beta_2 \geq \beta_1 \geq 0$ and $\beta_3 \neq \beta_1$. Indeed, using the above description, we see that the set $\mathcal{C}(q_1, 1, 1)$ is the union of the sets defined by the inequalities

\[
\begin{align*}
-1 < y, \ z < 1, &\ 2 \leq x \leq 1 + \sqrt{3}, \\
x &\geq 2, (x - 1)^2 + (y - e_2)^2 + (z - e_3)^2 < 3 \text{ with } e_2 = \pm 1 \text{ and } e_3 = \pm 1, \\
x &\geq 2, |y| \leq 1, (x - 1)^2 + (z - e)^2 < 3 \text{ for } e = \pm 1, \\
x &\geq 2, |z| \leq 1, (x - 1)^2 + (y - e')^2 < 3 \text{ for } e' = \pm 1.
\end{align*}
\]

If we have $\beta_3 \geq \beta_2 \geq \beta_1 \geq 0$, an obvious verification shows that the triple $(\beta_1, \beta_2, \beta_3)$ cannot satisfy any of the preceding four sets of inequalities except for the case $\beta_3 = \beta_2 = \beta_1 = 2$—which verify the second bullet—and this case has been rejected. As a consequence, it is impossible that $P$ belongs to the relative interior of $F_{q_1,i,1}$. Similar computations show that a point of $\mathcal{C}(q_1, 1, -1), \mathcal{C}(q_1, 2, -1)$ or $\mathcal{C}(q_1, 3, -1)$ cannot verify $\beta_3 \geq \beta_2 \geq \beta_1 \geq 0$. Hence, the percussion point $P$ either belongs to $F_{q_1,3,1} \subset \mathcal{S}(q_1, 3, 1)$ or to $F_{q_1,2,1} \subset \mathcal{S}(q_1, 2, 1)$. 

Fig. 3. A cube $q_1$ and a set $\mathcal{C}(q_1, k, \varepsilon)$. 

- $\mathcal{C}(q_1, k, \varepsilon)$ is an extremal point of $q_1, F_{q_1,3,1}$.
Case II: The point $P$ is a vertex of $q_1$. We have $d(C_2, P) \leq \sqrt{3}$. If $P \in F_{q_1, 3, 1}$, then the intersection of the ball $B(P, \sqrt{3})$ with the sextant $\mathcal{S}(q_1, 3, 1)$ is contained in $q_1$. Indeed, the inequalities $0 \leq x, y \leq z$ and $(e_1 - x)^2 + (e_2 - y)^2 + (z + 1)^2 \leq 3$ imply $0 \leq x, y \leq z \leq \sqrt{3} - 1$. Hence $C_2 \in \mathcal{S}(q_1, 3, 1) \cap B(P, \sqrt{3}) \subset q_1$ which is impossible by definition of $\psi$. We conclude—$P$ being a vertex—that $P \in F_{q_1, 3, 1}$, so that $P \in \mathcal{S}(q_1, 3, 1)$.

Case III: The point $P$ belongs to the intersection $e_1 \cap e_2$ of two edges $e_1$ of $q_1$ and $e_2$ of $q_2$. We first exclude the subcase where $P$ belongs to an edge of the lower face $F_{q_1, 3, 1}$. Otherwise, we would have $P = (x, y, -1)_{q_1} \in e_1 \cap e_2$ with $e_1 \in E(q_1)$ and $|x| = 1$ or $|y| = 1$. Since the distance $PC_2$ must verify $||PC_2|| \leq \sqrt{3}$ and since $\beta_3 \geq 1$ we get $4 \leq ||PC_2||^2 = (\beta_1 - x)^2 + (\beta_2 - y)^2 + (\beta_3 + 1)^2 \leq 3$, contradiction.

Second, we discard the case where $P$ belongs to one of the two edges of the face $F_{q_1, 2, -1}$ which are not included in the faces $F_{q_1, 3, \pm 1}$. Otherwise, let $P = (x, -1, z)_{q_1}$ with $|x| = 1$ and $|z| < 1$. We have $||PC_2||^2 = (\beta_1 - x)^2 + (\beta_2 + 1)^2 + (\beta_3 - z)^2 \leq 3$, and this implies $(\beta_2 + 1)^2 \leq 3$ whence $0 \leq \beta_1 < \beta_2 \leq \sqrt{3} - 1 < 1$. Now, the point $N = P + uPC_2$ has coordinates

$$X = u(\beta_1 - x) + x, \quad Y = u(\beta_2 + 1) - 1, \quad Z = u(\beta_3 - z) + z$$

with $x = \pm 1$ and $|z| < 1$. For small $u \in [0, 1]$ we obtain $|X| < 1$, $|Y| < 1$ and $|Z| < 1$ and so $N \in \text{int } q_1$. Obviously, $N = P + uPC_2 \in \text{int } q_2$ for $u$ small enough, this is not possible since the two cubes do not overlap. We conclude that $P$ belongs either to an edge of $F_{q_1, 3, 1}$ or to an edge of $F_{q_1, 2, 1}$.

Finally, by Proposition 7(c) there exists one face $F$ of $q_1$ which contains the whole intersection $q_1 \cap q_2$. The preceding three cases and Krein–Milman theorem show that this face $F$ is $F_{q_1, 3, 1}$ or $F_{q_1, 2, 1}$. By transitivity, $q_1 \cap q_2$ is included in $\mathcal{S}(q_1, 3, 1)$ or $\mathcal{S}(q_2, 2, 1)$. $\square$

Remark. The two cases described in Proposition 12 occur. The more frequent case $q_1^{\psi} \cap q_2^{\psi} \subset \mathcal{S}(q_1, 3, 1)$ appears for instance when $C_2 \in \mathcal{C}(q_3, 3, 1)$. The less frequent case $q_1^{\psi} \cap q_2^{\psi} \subset \mathcal{S}(q_1, 2, 1)$ holds if we choose $C_2 \in \mathcal{C}(q_1, 2, 1) \cap \text{int } \mathcal{S}(q_1, 3, 1)$ which is not empty (for instance, if $s = 2$ the center $C_2 = (0, 2, 2, 2)_{q_1}$ is convenient). Without proof, we add: $\mathcal{C}(q, k, s) \cap \mathcal{C}(q, k', s') \neq \emptyset$ and $\mathcal{C}(q, k, s) \cap \text{int } \mathcal{S}(q, k', s') \neq \emptyset$, if $k \neq k'$.

5. Computation of dense configurations of $n$ cubes of $\mathbb{R}^3$

5.1. The algorithm

We give here a short account of effective calculations of dense configurations. The whole code has been written in the language C and executed on a computer with a CPU at 2 GHz. First of all we heavily use Euler angles $\theta_1, \theta_2, \theta_3$ for storing the coordinates of the vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ which give the orientation of a cube $q$. In other words, a cube without specified side becomes $q = (C, \theta_1, \theta_2, \theta_3)$ and its basis can be read from the columns of the Euler matrix $E(\theta_1, \theta_2, \theta_3)$:

$$\begin{pmatrix}
\sin \theta_3 \sin \theta_1 + \cos \theta_1 \cos \theta_3 \cos \theta_2, & \cos \theta_1 \sin \theta_3 - \sin \theta_1 \cos \theta_3 \cos \theta_2, & \cos \theta_3 \sin \theta_2 \\
\cos \theta_3 \sin \theta_1 - \cos \theta_1 \cos \theta_3 \sin \theta_3, & \cos \theta_1 \cos \theta_3 + \cos \theta_2 \sin \theta_1 \sin \theta_3, & -\sin \theta_3 \sin \theta_2 \\
-\cos \theta_1 \sin \theta_2 & \sin \theta_2 \sin \theta_1 & \cos \theta_2
\end{pmatrix}.$$  

It is well-known that every matrix $M$ of $SO(3, \mathbb{R})$ is equal to some Euler matrix $E(\theta_1, \theta_2, \theta_3)$.

The whole program that we summarize in Table 2 is a simple adaptation from the one appearing in [8, Section 6] and we record it for the sake of completeness. We have denoted by $\mathcal{H}_X$ the uniform law of probability in a compact subset $X$ of $\mathbb{R}^m$. In Procedure 1, the non-overlapping cubes of a configuration $\mathcal{C}$ move randomly inside $K$ and we expect that the cubes spread out. The integer $N_\alpha$ stands for a number of attempts to move the cubes and the real number $\eta$ controls the amplitude of these moves. Procedure 2 iterates the preceding, the amplitude $\eta$ follows dynamically the improvement or not of $\omega(\mathcal{C})$. The procedure BilliardOfCubes can be run with parameters such as $\eta_1 = 0.01, \eta_2 = 10^{-12}$, $N_\alpha = 600, s = \omega(\mathcal{C})$, where $\mathcal{C}$ is a random configuration created at the very beginning of the run. Many thousands executions of Procedure 2 allow to find good configurations $\mathcal{C}_0$ which become inputs of Procedure 4. Indeed, a jammed configuration $\mathcal{C}_0$ need to be slightly perturbated with Procedure 3 and we get a configuration $\mathcal{C}_1$. We expect then that BilliardOfCubes($\mathcal{C}_0', s, \eta, \eta/\text{factor}, N_\alpha$) improves $\omega(\mathcal{C}_0)$ and in this case we get $\mathcal{C}_1$, and so on.
Table 2
Billiard algorithm for 3-cubes packings in \( K \)

**Procedure 1:** RandomWalking(\( \mathcal{E}, s, N_s, \eta \))

- For \( k \) from 1 to \( N_s \) do:
  - Choose randomly a cube \( \mathbf{q}_k = (C, \theta_1, \theta_2, \theta_3) \) in \( \mathcal{E} \)
  - Choose \( C' \) following \( \mathcal{U}_{B(C,0)\cap K} \) and \( \theta'_j \) following \( \mathcal{U}_{B(\theta_j,0)} \)
  - Set \( z := (C', \theta'_1, \theta'_2, \theta'_3) \)
  - If \( \min_{j \neq i} |\phi(z, \mathbf{q}_j)| \geq s \) and \( |\phi(z) - s| \) then \( \mathbf{q}_i := z \)

**Procedure 2:** BilliardOfCubes(\( \mathcal{E}, s, \eta_1, \eta_2, N_s \))

- \( \eta = \eta_1 \)
- While \( \eta > \eta_2 \) do:
  - RandomWalking(\( \mathcal{E}, s, N_s, \eta \))
  - If \( \omega(\mathcal{E}) > s \) then \( s := \omega(\mathcal{E}) \) and \( \eta := 2 \star \eta \) else \( \eta := \eta/2 \)

**Procedure 3:** Perturbation(\( \mathcal{E}, s, \eta \))

- For \( i \) from 1 to \( n \) do:
  - Let \( C \) be the center of \( \mathbf{q}_i \)
  - Let \( \theta_1, \theta_2, \theta_3 \) be the Euler angles of \( \mathbf{q}_i \)
  - Choose \( C' \) following \( \mathcal{U}_{B(C,0)\cap K} \) and \( \theta'_j \) following \( \mathcal{U}_{B(\theta_j,0)} \)
  - Set \( \mathbf{q}_i := (C', \theta'_1, \theta'_2, \theta'_3) \)
  - Let \( s := \omega(\mathcal{E}) \)

**Procedure 4:** WithPerturbations(\( \mathcal{E}, \eta_1, \eta_2, \text{factor}, N_s \))

- \( s := \omega(\mathcal{E}) \)
- \( \mathcal{E}_0 := \mathcal{E} \)
- \( s_0 := s \)
- \( \eta := \eta_1 \)
- While \( \eta > \eta_2 \) do:
  - Perturbation(\( \mathcal{E}, s, \eta \))
  - BilliardOfCubes(\( \mathcal{E}, s, \eta, \eta/\text{factor}, N_s \))
  - If \( s > s_0 \) then \( s_0 := s, \mathcal{E}_0 := \mathcal{E} \) and \( \eta := 2 \star \eta \) else \( \mathcal{E} := \mathcal{E}_0 \) and \( \eta := \eta/2 \)

This method of calculation readily generalizes to any dimension and any confining compact set \( K \) provided we dispose of a formula or a procedure for computing \( \phi(\mathbf{q}) \). Nevertheless, we suppose that the lack of localization for percussion together with the increasing complexity w.r.t increasing \( d \) will considerably slow down the calculations.

### 5.2. Dense packings of cubes in a sphere

In this subsection, we give some comments on the densest packings found of \( n \) cubes in the unit sphere up to \( n = 20 \). Instead of dealing with \( s_n \), we agree to give the value of \( \delta_n = 2/s_n \) which is the diameter of the smallest sphere into which it is possible to pack \( n \) unit cubes. The configurations were found with computer and some of them are displayed hereafter, see [9] for the others. For \( n = 1, \ldots, 13 \) except for the values \( n = 6, 10 \), we succeeded in giving an algebraic construction of the complete packing, that is, a few parameters model giving all the coordinates of the vertices of the configuration. A virtue of these models is that they ascertain the contacts between cubes at prescribed points and also that distinct cubes do not overlap, that is, to say the packings exist. These models have confirmed the computed values of \( \delta_n = 2/s_n \) with a high level of accuracy. As our computer has several times given these configurations, we are confident in the optimality of the algebrized packings and we lay them out as conjectures.

- \( n = 1 \): The smallest sphere which contains a cube of side \( s = 1 \) has diameter \( \delta_1 = \sqrt{3} \).
- \( n = 2 \): The two unit cubes can share a common face and lie in a sphere of diameter \( \delta_2 = \sqrt{3 \times 2} = 2.4495 \).
- \( n = 3 \), Fig. 4: Here, at least two cubes \( \mathbf{q}_1, \mathbf{q}_2 \) have the same basis and a common face. The lower cube \( \mathbf{q}_3 \) can freely rotate with respect to the axis \( (C_3, O) \) through the center of the sphere. We get \( \delta_3 = \sqrt{3 \times 163}/2^3 = 2.7642 \).
- \( n = 4 \), Fig. 4: At least three cubes of the best packing found have the same basis, the fourth cube having a degree of freedom. Eight vertices are on the unit sphere, they appear as bullets. Among them, in an appropriate frame, the three
Fig. 4. Best packings found for $n = 3$ and 4.

Fig. 5. Best packings found for $n = 5$ and 6.

vertices $(s/2, s/2, z), (s/2, \beta, z + 2s), (s, \beta - 2s, z + 2s)$ lead to an algebraic equation for $s = 2/\delta_4$ from which we obtain $\delta_4 = \sqrt{3 \times 756.443}/2 = 2.9422$.

- $n = 5$, Fig. 5: Up to a rotation, all five cubes have the same basis, the four lower are glued along a common edge, this edge containing the center of the sphere. The fifth cube can rotate freely with respect to the diameter containing this edge. In an appropriate frame, two vertices $(s/2, s/2, z + 2s)$ and $(s, s, z)$ are on the sphere, this leads to a quartic equation for $s = 2/\delta_5$ from which we obtain $\delta_5 = 3\sqrt{17}/4 = 3.0924$.

- $n = 6$, Fig. 5: The high level of complexity of the best packing found is astonishing w.r.t. the smallness of $n = 6$. The four upper cubes have a common basis. The two remaining are tilted with an angle 49.93°. Eight vertices belong to the unit sphere. An algebraic construction of the packing leads to a polynomial system with nine unknowns and nine equations of which six are nothing but the belongness of six vertices to the unit sphere. Newton’s method has confirmed our experiments and given $\delta_6 = 3.2542$.

- $n = 7$, Fig. 6: The best packing found is a crux composed of a central cube together with six adjacent and parallel cubes. Some degree of freedom appear because rotations of external cubes are allowed. In the frame of the central cube, one vertex has coordinates $(s/2, 3s/2, z/3)$ and lies on the sphere, this gives $\delta_7 = \sqrt{11}$.

- $n = 8$, Fig. 1: The cubic lattice packing of eight unit cubes in a sphere of diameter $2\sqrt{3} = 3.4641$ is not optimal. Indeed, we found a dense packing composed of two hats of four cubes which realizes $\delta_8 = \sqrt{761}/8 = 3.4483$. We obtained this value by considering the two vertices $(s/2, 3s/2, z + 2s)$ and $(s/2, s, z)$ which are on the unit sphere.
Fig. 6. Best packings found for $n = 7$ and $9$.

Fig. 7. Best packings found for $n = 10$ and $13$.

Fig. 8. Best packings found for $n = 14$ and $20$.

- $n = 9$, Fig. 6: This packing can be disassembled in three equal stairs of three cubes of side $s$, each stair being orthogonal to the other two. The first step has height $s$ and depth $h$, the second step has equal height and depth $s$, the third has height $h$ and depth $s$. The whole configuration can be modeled with four parameters, two of which being
Table 3
Conjectured values of $\delta_n$

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Fig. 9. Two distinct views of the best packing found of 11 cubes in a cube.

$h$ and $s$. We obtain easily that $s$ is solution of $2729x^4 - 920x^2 + 16 = 0$, so that $\delta_9 = 2/s = \sqrt{2729/(115 + 16\sqrt{41})} = 3.5426$ and $s = 0.5645$. Similarly, $h$ is solution of $2729x^4 - 2332x^2 + 64 = 0$ so that $h = 4\sqrt{2/(583 + 85\sqrt{41})} = 0.1685$.

- $n = 10$, Fig. 7: The best packing found of 10 cubes reveals many tilted cubes. We needed a week of calculation to obtain the sixth first digits of $\delta_{10}$.
- $n = 11$ to 13, Fig. 7: The best packing found of 13 cubes is composed of one central cube and six pairs appending to it. All cubes have the same basis and it is easy to find that $\delta_{13} = \sqrt{14} = 3.7417$. The best configurations found of 11 and 12 cubes lead us to conjecture that $\delta_{11} = \delta_{12} = \delta_{13}$ and they are obtained by deleting one or two cubes of the previous packing of 13 cubes. In this process some cubes do not remain jammed.

- $14 \leq n \leq 20$, Fig. 8: Those configurations are too much complicated to provide workable algebraic constructions. Moreover, computations become heavy and really intensive. Some of them have been obtained only once and might not be optimal.

In Table 3, we have summarized the diameters of the smallest spheres containing a packing of $n$ unit cubes. Algebraic and experimental values are rounded up and displayed with eight digits.
The previous methods and algorithms apply equally well to the search of dense packings of cubes in a cube. Friedman [5] provides such packings. For \( n = 11 \), we improve his bound \( \delta_{11} \leq 2 + 2\sqrt{2}/5 + \sqrt{3}/5 = 2.9121 \) with the packing of 11 unit cubes displayed in Fig. 9. The new bound becomes \( \delta_{11} \leq 2.89443924 \).

Acknowledgments

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References