COUNTING ALL REGULAR OCTAHEDRONS IN \( \{0, 1, \ldots, n\}^3 \)

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Abstract. In this paper we describe a procedure for calculating the number of regular octahedrons that have vertices with coordinates in the set \( \{0, 1, \ldots, n\} \). As a result, we introduce a new sequence in The Online Encyclopedia of Integer Sequences (A178797) and list the first one hundred terms of it. We adapt the method appeared in [11] which was used to find the number of regular tetrahedra with coordinates of their vertices in \( \{0, 1, \ldots, n\} \). The idea of this calculation is based on the theoretical results obtained in [14]. A new fact proved here helps increasing the speed of all the programs used before. The procedure is put together in a series of commands written for Maple.

1. INTRODUCTION

In this note we complete the work begun in the sequence of papers [2], [9]-[14] about equilateral triangles, regular tetrahedra, cubes, and regular octahedrons all with vertices having integer coordinates. Very often we will refer to this property by saying that the various objects are in \( \mathbb{Z}^3 \). Strictly speaking these geometric objects are defined as being more than the set of their vertices that determines them, but for us here, these are just the vertices. So, for instance, an equilateral triangle is going to be a set of three points in \( \mathbb{Z}^3 \) for which the Euclidean distances between every two of these points are the same. The main purpose of the paper is to take a close look at the regular octahedrons in \( \mathbb{Z}^3 \). The simplest example of a regular octahedron with integer coordinates for its vertices is

\[
OC_1 := \{[0, 1, 1], [1, 0, 1], [1, 1, 0], [1, 1, 2], [1, 2, 1], [2, 1, 1]\},
\]

which can be obtained from the usual unit cube in \( \mathbb{R}^3 \), multiplying the vertices by a factor of two and then taking the coordinates of the centers of the new faces. It turns out that this procedure gives all such octahedrons as shown in [14]:

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**Theorem 1.1.** Every regular octahedron in $\mathbb{Z}^3$ is the dual of a cube that can be obtained (up to a translation with a vector with integer coordinates) by doubling a cube in $\mathbb{Z}^3$.

Referring to Figure 1 (b), we showed that if the regular octahedron $IJKLMN$ is in $\mathbb{Z}^3$, then so is the cube $BB_1C_1IH_1LOM$ and vice versa. This defines a one-to-one correspondence between the classes of cubes (invariant under integer translations) and the classes of regular octahedra (invariant under integer translations) in $\mathbb{Z}^3$. In [12] we determined a sequence of irreducible cubes, one from each of the classes of cubes invariant under integer translations and cube symmetries. For each one of these cubes we can construct as before a regular octahedron, obtaining this way a sequence of irreducible regular octahedrons.

2. Some new ingredients and other theoretical facts

In [12], we improved and adapted the earlier code for counting all cubes with vertices in $\{0, 1, ..., n\}^3$ and extended the sequence A098928. In this paper, the usual techniques and ideas are going to be the same except some counting procedure that is very efficient in comparison to what we had before. We are going to treat this in the general case so, let us suppose that these objects can be either equilateral triangles, regular tetrahedrons, cubes or regular octahedrons with vertices in $\mathbb{Z}^3$. For such an object, say $O$, we can translate it, within $\mathbb{Z}^3$, to $O'$ that is in the positive octant and in such way each plane of coordinates contains at least one vertex of $O'$. Let us denote by $\alpha_0$ the number of objects in $C_m$ obtained by applying to $O'$ all 48 possible symmetries of the cube $C_m$. These symmetries are generated in the following way: first we have symmetries with respect to the middle planes and compositions, for example

$$(x, y, z) \rightarrow (m - x, y, z), \quad (x, y, z) \rightarrow (m - x, m - y, z), \quad (x, y, z) \rightarrow (m - x, m - y, m - z),$$

in a total of eight including the identity, then each one of these is coupled with one of the six permutations of the variables ($S_6$). These transformations form a group isomorphic with the group
COUNTING ALL REGULAR OCTAHEDRONS IN \( \{0, 1, \ldots, n\}^3 \)

of all \( 3 \times 3 \) orthogonal matrices having entries \( \pm 1 \) and it is also known as the group of symmetries of a cube or of a regular octahedron. It is isomorphic to \( S_4 \times \mathbb{Z}_2 \). We are going to denote this group by \( S_{\text{cube}} \) although it is usually known under the name of (extended) octahedral group and denoted simply by \( O_h \).

If we think of \( \alpha_0 \) as the cardinality of

\[
\text{Orbit}(O') := \{ s(O') | s \in S_{\text{cube}} \},
\]

which is, by the first theorem of isomorphism of groups, the same as the cardinality of the group factor \( S_{\text{cube}}/G \), where \( G \) is the subgroup of \( S_{\text{cube}} \) of those symmetries that leave \( O' \) invariant. The structure of subgroups of \( S_{\text{cube}} \) is known and for each divisor of 48 there is a subgroup of that order. Hence, we expect \( \alpha_0 \) to be in the set \( \{1, 2, 3, 4, 6, 8, 12, 16, 24, 48\} \) and most of the time to be 48 since an arbitrary object \( O' \) in \( C_m \) is unlikely to be invariant under any of the symmetries of \( S_{\text{cube}} \).

Then, we denote by \( \alpha \), the cardinality of the set of all the objects counted in \( \alpha_0 \) and their (all possible) integer translations that leave the resulting objects in \( C_m \). Also, we denote by \( \beta \) the objects counted in \( \alpha \) which are in \( \{0, 1, \ldots, m\}^2 \times \{0, 1, \ldots, m-1\} \). Finally, let us denote by \( \gamma \) the number of objects counted in \( \beta \) which are in \( \{0, 1, \ldots, m\} \times \{0, 1, \ldots, m-1\}^2 \). Then, we found a formula that gives the number of objects obtained from \( O \), under all symmetries and translation that leaves the resulting object in \( \{0, 1, \ldots, k\}^3, k \geq m \).

This fact has been essentially proved in Theorem 2.2 in [10]. The formula that gives this number is

\[
N(O, k) = (k - m + 1)^3\alpha - 3(k - m)(k - m + 1)^2\beta + 3(k - m + 1)(k - m)^2\gamma. \tag{1}
\]

Let us suppose that the object \( O \) can be squeezed within a box of dimensions \( m \times n \times p \) (\( m \geq n \geq p \)), i.e. up to symmetries and translations, \( O \) can be transformed to \( O' \) fitting snugly into

\[
B_{m,n,p} := \{0, 1, \ldots, m\} \times \{0, 1, \ldots, n\} \times \{0, 1, \ldots, p\}.
\]

We can similarly consider all eight reflections compatible with the box \( B_{m,n,p} \) of the form

\[
(x, y, z) \rightarrow (m - x, y, z), \quad (x, y, z) \rightarrow (m - x, n - y, z), \quad (x, y, z) \rightarrow (m - x, n - y, p - z), \text{ etc.}
\]

Let us denote the group of these transformations by \( S_b \). We notice that each one of these transformation leaves the object \( O' \) inside the box \( B_{m,n,p} \). From case to case, depending of what the values \( m, n \) and \( p \) are, we may have the result of some or all of the permutation transformations applied to \( O' \) still in \( B_{m,n,p} \). Hence, we will denote by \( \omega(O) \) the cardinality of the set
BoxOrbit(\mathcal{O}’) := \{ [s_1 \circ s_2](\mathcal{O}’) | s_1, s_2 \in \mathcal{S}_0 \}.

Let us look at an example. Suppose \mathcal{O} (equal with \mathcal{O}’) is the equilateral triangle given by its vertices:

\{[0,2,2],[5,7,0],[7,0,1]\}.

We observe that \mathcal{O} \in B_{7,7,2}. Then one can check that BoxOrbit(\mathcal{O}) is the collection of eight triangles

\mathcal{O}, \{[0,0,1],[2,7,0],[7,2,2]\}, \{[0,0,1],[2,7,2],[7,2,0]\}, \{[0,2,0],[5,7,2],[7,0,1]\},

\{[0,5,0],[5,0,2],[7,7,1]\}, \{[0,5,2],[5,0,0],[7,7,1]\}, \{[0,7,1],[2,0,0],[7,5,2]\}, \{[0,7,1],[2,0,2],[7,5,0]\},

so \omega(\mathcal{O}) = 8. It turns out that \alpha_0(\mathcal{O}) = 48, \alpha(\mathcal{O}) = 144, \beta(\mathcal{O}) = 40 and \gamma(\mathcal{O}) = 0. Formula (\ref{eq:omega}) becomes

N(\mathcal{O}, k) = 24(k - 1)(k - 6)^2, \quad k \geq 7.

It turns out the this factorization is not accidental and the following alternative to (\ref{eq:omega}) is true.

\textbf{Theorem 2.1.} Given \mathcal{O}, one of the objects mentioned before, and B_{m,n,p} the smallest box containing a translation of \mathcal{O} (m \geq n \geq p), we let u = m - n, v = n - p, and

\Delta = \omega(\mathcal{O})(k - m + 1)(k - n + 1)(k - p + 1).

Then the number of distinct objects in the cube B_{k,k,k} (k \geq m), obtained from \mathcal{O} by all possible integer translations and symmetries is equal to

(2) \quad N(\mathcal{O}, k) = \begin{cases} 
\Delta & \text{if } u = v = 0, \\
3\Delta & \text{if } u \text{ or } v \text{ is } 0, \\
6\Delta & \text{if } u \text{ and } v > 0.
\end{cases}

\textbf{Proof.} The case u = v = 0 implies \omega(\mathcal{O}) = \alpha_0(\mathcal{O}) = \alpha(\mathcal{O}) and \beta(\mathcal{O}) = \gamma(\mathcal{O}) = 0 because there is no room to shift the orbit Orbit(\mathcal{O}’) inside of B_{m,m,m}. The formula follows from (\ref{eq:omega}).

Let us look into the case u > 0 and v > 0. We begin by observing that each integer translation of the box B_{m,n,p} in all possible ways inside B_{k,k,k} will give \omega(\mathcal{O}) more copies of \mathcal{O}. There is no overlap between these copies because neither one of them can be inside of two distinct translations of B_{m,n,p}. This is due to the minimality of m, n and p. We get \Delta such copies by counting all possible translations. Since m, n and p are all distinct, the box B_{m,n,p} can be positioned first with the biggest of its dimensions along one of the directions given by the axis of coordinates, that is
three different ways, and for each such position the next largest dimension can be positioned along
the two remaining directions. The minimality of \( m, n \) and \( p \) makes the six different situations
 generate distinct objects. This explains the factor of six that appears in (2) for this situation.

In the last case, the box \( B_{m,n,p} \) has two of its dimensions the same, so there are only three
possibilities to arrange the box before one translates it. To see that we get all possible translates
and symmetries of \( O \) by this counting, we can start with one copy \( O' \). Construct the minimum box
around it. In terms of its position and dimensions, we know in what of the six or three cases we are.

We transform it into the standard standard position, \( B_{m,n,p} \), and look at the corresponding object,
\( O'' \). The transformations involved form a group of transformations generated by the permutations
of the coordinates, the reflections into the axes and integer translations. Every transformation in
this group, say \( g = \tau \circ \sigma \circ \pi \) with \( \pi \) a permutation, \( \sigma \) a reflection or a composition of reflections
and \( \tau \) a translation, which satisfies \( g(O) = O'' \) determines a representation \((s_1 \circ s_2)(O) = O''\) with
\( s_1 \in S_b, s_2 \in S_6 \) as in the definition of \( \omega(O) \). This can be done by taking \( s_2 = \pi \) and \( s_1 = \tau \circ \sigma \). This
is true again because of the minimality of the box \( B_{m,n,p} \), i.e. there is only one integer translation
that takes a reflected box \( B'_{m,n,p} \) into \( B_{m,n,p} \).

This new way of counting is more efficient from a computational point of view because \( \omega \)
is simply no bigger than 48, as opposed to the previous situation when \( \alpha, \beta \) and \( \gamma \) could turn out to
be big numbers and so the number of iterations for computing them would be also large. Roughly
speaking, this counting factors out fast the problem with the integer translations.

As an example, let us consider

\[
OC_2 = \{[0, 0, 1], [0, 3, 4], [1, 4, 0], [3, 0, 4], [4, 1, 0], [4, 4, 3]\}.
\]

The minimal box here is \( B_{4,4,4} \) and after rotating \( OC_2 \) in all possible ways (Figure 2 (b)) we get
\( \omega(OC_2) = 4 \).

![Figure 2 (a): OC2 octahedron](image1)

![Figure 2 (b): Four octahedrons in the box](image2)
The idea of calculations is basically the same as in [12], in which we have constructed a list of irreducible cubes that are used to generate all the other cubes in \( B_{k,k,k} \). Here, we are using Theorem 1.1 to construct a similar list of irreducible regular hexahedrons. As expected, an irreducible regular hexahedron is one whose coordinates cannot be obtained from a strictly smaller one with vertices in \( \mathbb{Z}^3 \) by integer dilations and translations. One simple consequence of Theorem 1.1 is the next corollary.

**Corollary 2.2.** The sides of every irreducible regular octahedron in \( \mathbb{Z}^3 \) are of the form

\[
(2k - 1)\sqrt{2}
\]

with \( k \in \mathbb{N} \).

We used the same way of finding the parameterizations of the equilateral triangles as in [12]:

\[
\begin{align*}
\overrightarrow{OP} &= m \zeta - n \eta, \\
\overrightarrow{OQ} &= n \zeta - (n - m) \eta,
\end{align*}
\]

with \( \zeta = (\zeta_1, \zeta_2, \zeta_3), \eta = (\eta_1, \eta_2, \eta_3) \),

\[
\begin{align*}
\zeta_1 &= -\frac{rac + dbs}{q}, \\
\zeta_2 &= \frac{das - bcr}{q}, \\
\zeta_3 &= r, \\
\eta_1 &= -\frac{db(s - 3r) + ac(r + s)}{2q}, \\
\eta_2 &= \frac{da(s - 3r) - bc(r + s)}{2q}, \\
\eta_3 &= \frac{r + s}{2},
\end{align*}
\]

where \( q = a^2 + b^2 \) and \( (r, s) \) is a suitable solution of \( 2q = s^2 + 3r^2 \) that makes all the numbers in (4) integers. The sides-lengths of \( \triangle OPQ \) are equal to \( d \sqrt{2(m^2 - mn + n^2)} \) and the triangle can be completed to a regular tetrahedron (in space) with integer coordinates if and only if \( k^2 = m^2 - mn + n^2 \) for some \( k \in \mathbb{Z} \). Related to this fact we have the following proposition.
**Proposition 2.3.** For a prime \( p > 3 \), the number of irreducible regular octahedrons in \( \mathbb{Z}^3 \) (up to translations and symmetries) having side lengths equal to \( p\sqrt{2} \), is at most \( \pi \epsilon(p) + 1 \), where

\[
\pi \epsilon(p) = \frac{\Lambda(p) + 24 \Gamma_2(3p^2)}{48},
\]

with \( \Lambda \) and \( \Gamma \) defined as in \([11]\).

The exact number of such objects is yet a big mystery to us.

3. The Maple Code

We wrote the code using the Maple Software and so we took advantage of the built-in commands available for a various number of functions. The beginning is pretty standard:

```maple
> restart:with(numtheory):with(plots):

Step 1. The next three procedures calculate all possible values of \( k \), then the parameters \( m, n \), and finally the normal vector \((a, b, c)\). The values of \( k \) are determined by using a characterization theorem for the quadratic form involved here, i.e. all values of \( k \) less than \( n \) such that \( k \) is of the form a product of primes of the form \( 3\ell + 1 \), \( \ell \geq 2 \) or \( k = 1 \).

> kvalues:=proc(n)
    local i,j,k,L,a,p,q,r,m,mm;
    L:={};mm:=floor((n+1)/2);
    for i from 2 to mm do
        a:=ifactors(2*i-1);
        k:=nops(a[2]);r:=0;
        for j from 1 to k do
            m:=a[2][j][1]; p:=m mod 3;
            if m=3 then r:=1 fi;
            if r=0 and p=2 then r:=1 fi;
        od;
        if r=0 then L:=L union {2*i-1};fi;
    od; L:=L union {1}; L:=convert(L,list);
    end:

For example, \( kvalues(100) = [1, 7, 13, 19, 31, 37, 43, 7^2, 61, 67, 73, 79, 7(13), 97] \).

Next, we are interested in the solutions \((m, n)\) of the equation \( k^2 = m^2 - mn + n^2 \), which are primitive in the sense that \( \gcd(m, n) = 1 \), \( m > 0 \), \( n > 0 \), and \( 2m < n \). We apply this procedure to only those \( k \)'s which are the output of \( kvalues \).
> listofmn:=proc(k)
local a,b,i,nx,x,m,n,L;
x:=[isolve(k^2=m^2-m*n+n^2)];
x:=nops(x); L:={};
for i from 1 to nx do
  if lhs(x[i][1])=m then a:=rhs(x[i][1]); b:=rhs(x[i][2]);
  else b:=rhs(x[i][1]); a:=rhs(x[i][2]); fi;
  if gcd(a,b)=1 and a>=0 and b>0 and 2*a<b then L:=L union {[a,b]};fi;
od;
end:

A prime of the form $3\ell + 1$ has a unique primitive decomposition as described, for example, $\text{listofmn}(79) = \{[40,91]\}$ since $79^2 = 40 - 40(91) + 91^2$ and 79 is a prime. In general, the number of solutions is equal to $2^{\omega(k)-1}$ where $\omega(k)$ is the number of distinct factors of $k$ which are of the form $3\ell + 1$. This choice of $m$ and $n$ helps identify the irreducible octahedrons: all the other solutions $(m, n)$ of the equation $k^2 = m^2 - mn + n^2$ lead to the same regular octahedron. We included the case $a = 0$ to obtain the output $\{[0,1]\}$ for $\text{listofmn}(1)$ which is necessary later on.

> abcsol:=proc(d)
local i,j,k,m,u,x,y,sol,cd;sol:={};
for i from 1 to d do
  u:=[isolve(3*d^2-i^2=x^2+y^2)];k:=nops(u);
  for j from 1 to k do
    if rhs(u[j][1])>=i and rhs(u[j][2])>=i then
      cd:=gcd(gcd(i,rhs(u[j][1])),rhs(u[j][2]));
      if cd=1 then sol:=sol union {sort([i,rhs(u[j][1]),rhs(u[j][2])])};fi;fi;
od;
end:

For $d = 17$, for instance, the procedure $\text{abcsol}$ gives the four solutions: $[1, 5, 29]$, $[7, 17, 23]$, $[11, 11, 25]$ and $[13, 13, 23]$. We observe that two of them have the property that $a = b$, in which case, we know (see [12]) that the formulae (4) simplify quite a bit.

**Step 2.** The next seven procedures implement the new way of finding $r$ and $s$ which appear in the parametrization (4). It is followed by the calculation of the of the parametrization of
equilateral triangles \( \{1\} \) and only one regular octahedron is constructed based on Theorem 1.1. This octahedron is then translated minimally into the positive octant and the minimal cube containing it is computed.

For a prime \( p \) of the form \( 6\ell + 1 \), there exists an unique decomposition \( p = x^2 + 3y^2 \) which is calculated next.

\[
\text{uniquedecomposition} := \text{proc}(p) \\
\text{if } p=2 \text{ then } \text{out} := [1, 1]; \text{ fi;}
\text{ if } p>2 \text{ then } s := \text{isolve}(p=x^2+3*y^2); \text{ out1} := \text{abs(rhs(s[1][1]))}; \text{ out2} := \text{abs(rhs(s[1][2]))};
\text{ if out1}^2 + 3*\text{out2}^2 = p \text{ then } \text{out} := [\text{out1}, \text{out2}]; \text{ else } \text{out} := [\text{out2}, \text{out1}]; \text{ fi;}
\text{ fi; out; end:}
\]

For \( p = 2 \) this procedure has the needed output \([1, 1]\). As an example, \text{uniquedecomposition}(2011) = [44, 5] since 2011 is a prime and 2011 = 44^2 + 3(5^2). The next procedure is calculating the factorization in \( \mathbb{Z}[^3\sqrt{3}] \) of a number of the form \( u + v\sqrt{3}i \).

\[
\text{factoroverEisensteinintegers} := \text{proc}(u, v)
\text{ local i, N, M, k, a, x, f1, f2, g, y1, y2, L, NN, MM, uu, vv;}
\text{ a := sqrt(3)*I; NN := gcd(u, v); uu := u/NN; vv := v/NN; N := uu}^2+3*vv^2; x := uu+vv*a; M := ifactors(N); k := nops(M[2]);
\text{ for i from 1 to k do}
\text{ f1 := M[i][1]; f2 := M[i][2];}
\text{ if f1 > 2 then}
\text{ g := uniquedecomposition(f1);} \quad \text{ else } \quad g := [1, 1]; f2 := 1;
\text{ fi;}
\text{ y := expand(rationalize(x/(g[1]+a*g[2]))));}
\text{ y1 := Re(y); y2 := type(y1, integer);}
\text{ if y2 = true then L[i] := [g[1]+a*g[2], f2]; else}
\text{ L[i] := [g[1]-a*g[2], f2];}
\text{ fi;}
\text{ od; [NN, seq(L[i], i = 1 .. k)], expand(NN*product(L[i][1]^L[i][2], ii = 1 .. k))]; end:}
\]

As a simple example here, the following decomposition is obtained for \( u = 13 \) and 17:

\[
(1 + I\sqrt{3})(2 + I\sqrt{3})(5 - 2I\sqrt{3}) = 13 + 17I\sqrt{3}.
\]
Perhaps one word of caution is necessary at this point. The decomposition in general is not unique in the usual sense since \(4 = 2(2) = (1 + \sqrt{3})(1 - \sqrt{3})\). As in the example shown, we go for the second representation when something like this happens. We are interested in this decomposition because it provides suitable values for \(r\) and \(s\) that we find next. This turns out to be the greatest common divisor between \(A + I\sqrt{3}B\) and \(2q\) with \(A = ac, B = bd\) and \(q = a^2 + b^2\) (see [12]).

\[
> \text{findgcd}:=\text{proc}(A,B,q) \\
> \text{local a,i,j,f,f1,f2,common,m,qq,fac,nfac,s,rs,P; a:=sqrt(3)*I;} \\
> f:=\text{factoroverEisensteinintegers}(A,B); m:=\text{nops}(f)-1; \\
> \text{common:=gcd}(f[1],2*q); \quad \text{qq:=2*q/common^2; P:=common;} \\
> \text{fac:=ifactors(qq);nfac:=nops(fac[2]);} \\
> \text{for i from 1 to nfac do} \\
> \quad \text{f1:=fac[2][i][1];f2:=fac[2][i][2];} \\
> \quad \text{if f1=2 then f2:=1;fi;} \\
> \quad \text{s:=uniquedecomposition(f1);} \\
> \quad \text{for j from 1 to m do} \\
> \quad \quad \text{if s[1]+a*s[2]=f[j][1] then} \\
> \quad \quad \quad \text{P:=P*(s[1]+a*s[2])^\text{min}(f[j][2],f2)}; \quad \text{fi;} \\
> \quad \quad \text{if s[1]-a*s[2]=f[j][1] then} \\
> \quad \quad \quad \text{P:=P*(s[1]-a*s[2])^\text{min}(f[j][2],f2)}; \quad \text{fi;} \\
> \quad \text{od;} \\
> \text{od;} \text{P:=expand(P);rs:=[Re(P),Im(P)/sqrt(3)];} \\
> [rs,A*rs[1]+3*B*rs[2] \text{ mod } 2*q,A*rs[2]-B*rs[1] \text{ mod } 2*q]; \text{end:}
\]

In the case we have seen before, where \(d = 17\), if we take \(a = 1, b = 5\) and \(c = 29\), then we have \(A = ac = 29, B = bd = 85\) and \(q = a^2 + b^2 = 26\). The procedure above gives \(r = -1\) and \(s = 7\) and checks that \(As + 3Br \equiv 0 \pmod{2q}\) and \(Ar - Bs \equiv 0 \pmod{2q}\). These two conditions are enough to insure that the expressions in [4], all give integer values for the coordinates of \(\eta\) and \(\zeta\).

In the next procedure we use the \(r\) and \(s\) determined earlier and construct an irreducible regular octahedron in \(Z^3\), given a vector \((a, b, c)\) and the possible values for \((m, n)\) in the decomposition of \(k^2 = m^2 - mn + n^2\). We are using simple formulae which can be derived easily from Figure 1(b), thinking that the point \(H\) is the origin, \(T[1], T[2]\) and \(T[3]\) are the points \(M, N\) and \(L\). Then the other three vertices are simply given by the addition of every two of these there vectors. Although there are six possible equilateral triangles that one may start with in this construction, one can see that in the end, essentially the same regular octahedron (up to symmetries and translations) is obtained.
> findpar:=proc(a,b,c,mm,nn)
local q,d,r,s,rs,A,B,k,mx,my,mz,my,nu,mv,nv,mw,nw,
u,v,w,x,y,z,T,R1,R2,DD,E,F;
q:=a^2*b^2;k:=sqrt(mm^2-mm*nn+nn^2);d:=sqrt((a^2+b^2+c^2)/3);A:=a*c;B:=b*d;
rs:=findgcd(A,-B,q);r:=rs[1][2]; s:=rs[1][1]
mx:=-(d*b*(3*r+s)+a*c*(r-s))/(2*q);nx:=-(r*a*c+d*b*s)/q;
my:=(d*a*(3*r+s)-b*c*(r-s))/(2*q);ny:=(r*b*c-d*a*s)/q;mz:=(r-s)/2;nz:=r;
u:=mu;mv:=ny;mw:=nz;nu:=nx-mx;nv:=ny-my;nw:=nz-mz;
\ni:=mu*mm-nu*nn; v:=mv*mm-nv*nn; w:=mw*mm-nw*nn;
x:=mx*mm-nx*nn; y:=my*mm-ny*nn; z:=mz*mm-nz*nn;
R1:=((x+u-2*a*k)/3,(v+y-2*b*k)/3,(z+w-2*c*k)/3);
R2:=((x+u+2*a*k)/3,(v+y+2*b*k)/3,(z+w+2*c*k)/3);
if R1[1]=floor(R1[1]) then T:=[[u,v,w],[x,y,z],R1]; else
T:=[[u,v,w],[x,y,z],R2];
fi;
DD:=[T[1][1]+T[2][1],T[1][2]+T[2][2],T[1][3]+T[2][3]];E:=[T[1][1]+T[3][1],T[1][2]+T[3][2],T[1][3]+T[3][3]];F:=[T[2][1]+T[3][1],T[2][2]+T[3][2],T[2][3]+T[3][3]];[T[1],T[2],T[3],DD,E,F];
end:

Since for \( k = 2011 \) we get \( \text{listofmn}(k) = \{880, 2301\} \), we checked to see what regular octahedron is obtained for \( \text{findpar}(1,1,1,880,2301) \): \([2301, -1421, -880], [880, -2301, 1421], [2401, 100, 1521], [3181, -3722, 541], [4702, -1321, 641], \) and \([3281, -2201, 2942]\). Since the set \( \text{abcsol}(2011) \) has 336 elements in it, there are essentially at most 337 irreducible regular octahedra in \( \mathbb{Z}^3 \) with side lengths equal to \( 2011\sqrt{2} \) as we pointed out in Proposition 2.3. Next, we have a short function for subtracting two vectors \( U \) and \( V \).

subtrv:=proc(U,V)
> local W;
W[1]:=U[1]-V[1];W[2]:=U[2]-V[2];W[3]:=U[3]-V[3];[W[1],W[2],W[3]];
end:

In order to compare various octahedrons it is easier if they are all translated to the positive octant in such a way each plane of coordinates contains at least a vertex of the octahedron. This is accomplished with the next routine.

> tmttopqoctahedron:=proc(T)


local i, a, b, c, v, C;
    a := min(T[1][1], T[2][1], T[3][1], T[4][1], T[5][1], T[6][1]);
    b := min(T[1][2], T[2][2], T[3][2], T[4][2], T[5][2], T[6][2]);
    c := min(T[1][3], T[2][3], T[3][3], T[4][3], T[5][3], T[6][3]);
    v := [a, b, c]; C := {subtrv(T[1], v), subtrv(T[2], v), subtrv(T[3], v),
                       subtrv(T[4], v), subtrv(T[5], v), subtrv(T[6], v)};
end:

So, for instance, the octahedron mentioned earlier of sides lengths $2011 \sqrt{2}$ becomes: $[2401, 1521, 3822], [3822, 2401, 1521], [2301, 0, 1421], [1521, 3822, 2401], [0, 1421, 2301]$, and $[1421, 2301, 0]$. The smallest cube $C_m = [0, m]^3$ containing an octahedron positioned in the positive octant as specified earlier is computed in the following procedure.

> mscofmoctahedron := proc(Q)
    local a, b, c, T;
    T := convert(Q, list);
    a := max(T[1][1], T[2][1], T[3][1], T[4][1], T[5][1], T[6][1]);
    b := max(T[1][2], T[2][2], T[3][2], T[4][2], T[5][2], T[6][2]);
    c := max(T[1][3], T[2][3], T[3][3], T[4][3], T[5][3], T[6][3]);
    max(a, b, c);
end:

Step 3. In our construction of these octahedrons we end up with essentially the same octahedron if we proceed from a different face of it. To eliminate the possibility of counting an octahedron twice or more than one time, we would like to have a way of distinguishing between octahedra and so an invariant to translation and symmetries, like the side lengths, will be good. Such an invariant is the set of $k$ values which are given by the four pairs of opposite (parallel) faces of a regular octahedron. We must have

$$\ell = d_1 k_1 \sqrt{2} = d_2 k_2 \sqrt{2} = d_3 k_3 \sqrt{2} = d_4 k_4 \sqrt{2}.$$ 

So, knowing $\ell$ and the $d_i$’s will give us $k_i$’s. The set $\{k_1, k_2, k_3, k_4\}$ is clearly and invariant to translations and the symmetries we have talked about at the beginning of the paper. Hence, two octahedra with different sets of $k$-values will be essentially different. We determine these $k$-values from the first three points given in the procedure findpar. The following calculation finds $d/gcd(a, b, c)$, given $(a, b, c)$ such that $a^2 + b^2 + c^2 = 3d^2$.

> unitvector := proc(U)
    local i, j, k, l, x;
i:=U[1]; j:=U[2]; k:=U[3];
l:=gcd(gcd(i,j),k); x:=(i^2+j^2+k^2)/(3*l^2);
sqrt(x); end:

Then we need a routine to add three vectors.

> addvec:=proc(U,V,W)
local X;
X[1]:=U[1]+V[1]+W[1]; X[2]:=U[2]+V[2]+W[2]; X[3]:=U[3]+V[3]+W[3];
[X[1],X[2],X[3]]; end:

The next function is multiplying a scalar with a vector.

> multbyfactorv:=proc(v,k)
local w; w[1]:=v[1]*k; w[2]:=v[2]*k; w[3]:=v[3]*k;
[w[1],w[2],w[3]]; end:

The Euclidean distance between to points is needed later.

> distance:=proc(A,B)
local C; C:=subtrv(A,B); sqrt(C[1]^2+C[2]^2+C[3]^2); end:

As we said before, in the procedure that follows, T is the list of the first three vertices given by findpar.

> fourkvalues:=proc(T)
local N1,N2,N3,N4,x,length;
length:=distance(T[1],T[2])/sqrt(2);
N1:=unitvector(addvec(T[1],T[2],T[3]));
N2:=unitvector(addvec(T[1],T[2],multbyfactorv(T[3],-3)));
N3:=unitvector(addvec(T[1],T[3],multbyfactorv(T[2],-3)));
N4:=unitvector(addvec(T[3],T[2],multbyfactorv(T[1],-3)));
{length/N1,length/N2,length/N3,length/N4};
end:

For the octahedron in Step 2, we have the set of k-values, \{1,2011\}, as expected since 2011 is a prime.

**Step 4.** In this step we calculate the orbit of an octahedron T within the reduced cube. The procedure orbitbox1 is taking care only of the eight possible symmetries.

> orbitbox1:=proc(T)
local i,k,T1,a,b,c,x,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11,T12,T13,T14,T15,T16,T17,T18,
T19,T20,T21,T22,T23,T24,S,Q;
Q:=convert(T,list);
    a:=max(Q[1][1],Q[2][1],Q[3][1],Q[4][1],Q[5][1],Q[6][1]);
    b:=max(Q[1][2],Q[2][2],Q[3][2],Q[4][2],Q[5][2],Q[6][2]);
    c:=max(Q[1][3],Q[2][3],Q[3][3],Q[4][3],Q[5][3],Q[6][3]);
T1:=T;
T2:={seq([Q[i][1],Q[i][2],c-Q[i][3]],i=1..6)};
T3:={seq([a-Q[i][1],Q[i][2],Q[i][3]],i=1..6)};
T4:={seq([a-Q[i][1],b-Q[i][2],Q[i][3]],i=1..6)};
T5:={seq([a-Q[i][1],b-Q[i][2],c-Q[i][3]],i=1..6)};
T6:={seq([a-Q[i][1],Q[i][2],c-Q[i][3]],i=1..6)};
T7:={seq([Q[i][1],b-Q[i][2],Q[i][3]],i=1..6)};
T8:={seq([a-Q[i][1],b-Q[i][2],c-Q[i][3]],i=1..6)};
S:={T1,T2,T3,T4,T5,T6,T7,T8};
S;
end:

The next procedure implements Theorem 2.1 in our situation where the objects of interest are octahedrons.

> orbitbox:=proc(T,p)
    local S,Q,TT,a,b,c,m,SS,i,d,u,v,w,y,mm,nn,x,k;
    Q:=convert(T,list);
    a:=max(Q[1][1],Q[2][1],Q[3][1],Q[4][1],Q[5][1],Q[6][1]);
    b:=max(Q[1][2],Q[2][2],Q[3][2],Q[4][2],Q[5][2],Q[6][2]);
    c:=max(Q[1][3],Q[2][3],Q[3][3],Q[4][3],Q[5][3],Q[6][3]);
    d:=max(a,b,c);u:=d-a;v:=d-b;w:=d-c;
    TT[1]:={seq([Q[i][3],Q[i][2],Q[i][1]],i=1..6)};
    TT[2]:={seq([Q[i][2],Q[i][3],Q[i][1]],i=1..6)};
    TT[3]:={seq([Q[i][1],Q[i][3],Q[i][2]],i=1..6)};
    TT[4]:={seq([Q[i][2],Q[i][1],Q[i][3]],i=1..6)};
    TT[5]:={seq([Q[i][3],Q[i][1],Q[i][2]],i=1..6)};
    S:=orbitbox1(TT[1]);
    for i from 1 to 5 do
        S:=S union orbitbox1(TT[i]);
    od;
    S:=convert(S,list);m:=nops(S);SS:={};
    for i from 1 to m do
        if S[i][1][1]<=a and S[i][2][1]<=a and S[i][3][1]<=a and S[i][4][1]<=a and S[i][5][1]<=a and S[i][6][1]<=a
            and S[i][1][2]<=b and S[i][2][2]<=b and S[i][3][2]<=b and S[i][4][2]<=b and S[i][5][2]<=b and S[i][6][2]<=b
            and S[i][1][3]<=c and S[i][2][3]<=c and S[i][3][3]<=c and S[i][4][3]<=c and S[i][5][3]<=c and S[i][6][3]<=c
            and S[i][1][1]>0 and S[i][2][1]>0 and S[i][3][1]>0 and S[i][4][1]>0 and S[i][5][1]>0 and S[i][6][1]>0
            and S[i][1][2]>0 and S[i][2][2]>0 and S[i][3][2]>0 and S[i][4][2]>0 and S[i][5][2]>0 and S[i][6][2]>0
            and S[i][1][3]>0 and S[i][2][3]>0 and S[i][3][3]>0 and S[i][4][3]>0 and S[i][5][3]>0 and S[i][6][3]>0
            then SS:=SS union {S[i]}; fi;
    od;
    nn:=nops(SS);
    nn:=(k+w)*(k+w+1)*(k+w+1);
    if nops(y)=3 then x:=6*mm*nn;fi;
    if nops(y)=2 then x:=3*mm*nn;fi;
    if nops(y)=1 then x:=mm*nn;fi;
    [x,SS,nops(SS),[u,v]]; end:

The next two routines calculate the orbit of an octahedron within its minimal cube $C_m$. This orbit has at most 48 elements and it is needed in the process of elimination of octahedrons that
have already appeared in the construction. In comparison with the previous orbit, it is bigger and
invariant to all the symmetries.

> orbitloctahedron:=proc(T)
local i,k,T1,a,b,c,x,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11,T12,T13,T14,
T15,T16,T17,T18,T19,T20,T21,T22,T23,T24,S,Q,d,a1,b1,c1;
Q:=convert(T,list);
d:=mscofmoctahedron(T);
T1:=T;
T2:={seq([Q[k][2],Q[k][3],Q[k][1]],k=1..6)};
T3:={seq([Q[k][1],Q[k][3],Q[k][2]],k=1..6)};
T4:={seq([Q[k][1],Q[k][2],d-Q[k][3]],k=1..6)};
T5:={seq([Q[k][2],Q[k][3],d-Q[k][1]],k=1..6)};
T6:={seq([Q[k][1],Q[k][3],d-Q[k][2]],k=1..6)};
T7:={seq([Q[k][2],d-Q[k][3],Q[k][1]],k=1..6)};
T8:={seq([Q[k][1],d-Q[k][3],Q[k][2]],k=1..6)};
T9:={seq([Q[k][1],Q[k][3],d-Q[k][2]],k=1..6)};
T10:={seq([d-Q[k][1],Q[k][2],Q[k][3]],k=1..6)};
T11:={seq([d-Q[k][2],Q[k][3],Q[k][1]],k=1..6)};
T12:={seq([d-Q[k][1],Q[k][3],Q[k][2]],k=1..6)};
T13:={seq([Q[k][1],d-Q[k][2],d-Q[k][3]],k=1..6)};
T14:={seq([Q[k][2],d-Q[k][3],d-Q[k][1]],k=1..6)};
T15:={seq([Q[k][1],d-Q[k][3],d-Q[k][2]],k=1..6)};
T16:={seq([d-Q[k][1],d-Q[k][2],Q[k][3]],k=1..6)};
T17:={seq([d-Q[k][2],d-Q[k][3],Q[k][1]],k=1..6)};
T18:={seq([d-Q[k][1],d-Q[k][3],Q[k][2]],k=1..6)};
T19:={seq([d-Q[k][1],Q[k][2],d-Q[k][3]],k=1..6)};
T20:={seq([d-Q[k][2],Q[k][3],d-Q[k][1]],k=1..6)};
T21:={seq([d-Q[k][1],Q[k][3],d-Q[k][2]],k=1..6)};
T22:={seq([d-Q[k][1],d-Q[k][2],d-Q[k][3]],k=1..6)};
T23:={seq([d-Q[k][2],d-Q[k][3],d-Q[k][1]],k=1..6)};
T24:={seq([d-Q[k][1],d-Q[k][3],d-Q[k][2]],k=1..6)};
S:={T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11,T12,T13,T14,T15,T16,
T17,T18,T19,T20,T21,T22,T23,T24};
S; end:
Step 5. At this point we are ready to build a list of minimal, irreducible octahedrons. With each entry we keep, in order, \( d \), the value \( m \) which is the size of the minimal cube \( C_m \), the six vertices of the octahedron, the \( k \)-values and the corresponding vector \((a, b, c)\). In the end, another list is created in a new procedure, to get the list of all corresponding reducible cubes needed in a calculation for a given dimension \( n \). The construction is a little complicated because there are octahedrons for which all \( k \)-values are different of 1.
\begin{verbatim}
d:=mscofmoctahedron(p0);
tnel:=tnel+1;
fi;
fi;
od;
LL:=[seq(L[i],i=1..nel),seq(NL[j],j=nel+1..tnel)];
fi;LL,orb;
end:

To generate all the other octahedrons we have to magnify the irreducible ones.

\texttt{> multbyfactoroctahedron:=proc(T,k)
local i,NT,Q;NT:=\{\};
Q:=convert(T,list);
for i from 1 to 6 do
NT:=NT union \{multbyfactorv(Q[i],k)\};
od;NT; end:

The procedure \textit{ExtendList} is used recursively in the next loop to generate the list needed to calculate all octahedrons in $C_N$ for a certain value $N$.

\texttt{> ExtendListuptoN:=proc(N)
local i,j,k,l,kv,kvn,NN,L,Orb::array,mn,nmn,E,n,ii;
kv:=kvalues(N);kvn:=nops(kv);
NN:=floor((N+1)/2);
L:=[ ];Orb:=array(1..2*NN+1);
for ii from 1 to 2*NN+1 do
Orb[ii]:={};
od;
for i from 1 to kvn do
k:=kv[i];mn:=listofmn(k);nmn:=nops(mn);
for j from 1 to nmn do
for l from 1 to NN+1 do
n:=2*l-1;
E:=ExtendList(n,N,L,mn[j][1],mn[j][2],Orb);
L:=E[1];
for ii from 1 to 2*NN+1 do
Orb[ii]:=E[2][ii];
end:
\end{verbatim}
we get only two essentially different octahedrons of side lengths 19

Let us observe that although there are four primitive solutions for

\[ a b c s o l (19) = \{ 5, 23, 23, 11, 11, 29, 13, 17, 25, 11, 11, 31 \} \]

we get only two essentially different octahedrons of side lengths \( 19 \sqrt{2} \). We also need to take into account the reducible octahedrons.
dd:=d*j;lc:=nops(LL);
LL:=LL union {{L[i][1]*j,dd,CC,L[i][4]};
    j:=j+1;
    od;
    fi;
i:=i+1;
od;
convert(LL,list);
end:

> LL:=ExtendListuptoNmultiples(20,L):

The program is taking the previous list and inflates only the octahedrons needed:
LL := [[3, 6, [3, 3, 6], [3, 3, 0], [3, 6, 3], [0, 3, 3], [6, 3, 3], [3, 0, 3]], {1}],
[2, 4, [[2, 2, 4], [2, 2, 0], [2, 4, 2], [0, 2, 2], [4, 2, 2], [2, 0, 2]], {1}],
[7, 14, [[7, 7, 14], [7, 7, 0], [7, 14, 7], [0, 7, 7], [14, 7, 7], [7, 0, 7]], {1}],
[6, 12, [[6, 6, 12], [6, 6, 0], [6, 12, 6], [0, 6, 6], [12, 6, 6], [6, 0, 6]], {1}],
[5, 10, [[5, 10, 5], [0, 5, 5], [5, 5, 10], [5, 5, 0], [10, 5, 5], [5, 0, 5]], {1}],
[4, 8, [[4, 0, 4], [4, 4, 0], [4, 4, 8], [4, 8, 4], [0, 4, 4], [8, 4, 4]], {1}],
[10, 20, [[10, 10, 20], [10, 10, 0], [10, 20, 10], [0, 10, 10], [10, 0, 10], [20, 10, 10]], {1}],
[9, 18, [[9, 9, 18], [9, 9, 0], [9, 18, 9], [0, 9, 9], [18, 9, 9], [9, 0, 9]], {1}],
[8, 16, [[8, 8, 16], [8, 8, 0], [8, 16, 8], [0, 8, 8], [16, 8, 8], [8, 0, 8]], {1}],
[15, 20, [[0, 15, 20], [0, 0, 5], [15, 0, 20], [5, 20, 0], [20, 20, 15], [20, 15, 0]], {1, 3}],
[12, 16, [[0, 12, 16], [4, 16, 0], [16, 4, 0], [0, 0, 4], [12, 0, 16], [16, 16, 12]], {1, 3}],
[9, 12, [[0, 9, 12], [0, 0, 3], [0, 9, 12], [12, 12, 9], [3, 12, 0], [12, 3, 0]], {1, 3}],
[6, 8, [[2, 8, 0], [8, 8, 6], [8, 2, 0], [0, 8, 0], [6, 0, 8], [0, 0, 2]], {1, 3}],
[10, 20, [[8, 0, 8], [14, 10, 0], [8, 20, 8], [0, 10, 2], [16, 10, 14], [2, 10, 16]], {1}]

**Step 6.** Finally we are adding up the contribution of each octahedron located in the union of
the two lists created earlier.

> addupnew:=proc(N,L,LL)
local i,j,k,nc,mm,m,d,C,CC,x,dd,nt; nc:=0; m:=nops(L); i:=1;
while i<=m do
    d:=L[i][2];
    if d<=N then


x:=orbitbox(L[i][3],N)[1];
nc:=nc+x;
fi; i:=i+1;

od;
m:=nops(LL);
i:=1;
while i<=m do
d:=LL[i][2];
if d<=N then
x:=orbitbox(LL[i][3],N)[1];
nc:=nc+x;
fi; i:=i+1;

od;
nc;end:
The next command produces the sequence we are looking for.
>NO:=[seq([k,addupnew(k,L,LL)],k=1..100)];

So, the first one hundred terms of A178797 are:

[1, 0], [2, 1], [3, 8], [4, 32], [5, 104], [6, 261], [7, 544], [8, 1000], [9, 1696], [10, 2759], [11, 4296], [12, 6434], [13, 9352], [14, 13243], [15, 18304], [16, 24774], [17, 32960], [18, 43223], [19, 55976], [20, 71752], [21, 90936], [22, 113973], [23, 141312], [24, 173436], [25, 210960], [26, 254587], [27, 305000], [28, 364406], [29, 432824], [30, 511421], [31, 600992], [32, 702556], [33, 817200], [34, 946131], [35, 1090392], [36, 1251238], [37, 1430072], [38, 1629391], [39, 1850064], [40, 2094276], [41, 2363616], [42, 2659813], [43, 2984600], [44, 3341660], [45, 3731720], [46, 4156689], [47, 4618480], [48, 5119292], [49, 5661600], [50, 6248705], [51, 6882808], [52, 7568126], [53, 8306520], [54, 9104339], [55, 9962320], [56, 10888762], [57, 11882896], [58, 12949661], [59, 14090952], [60, 15311286], [61, 16613736], [62, 18001975], [63, 19479680], [64, 21052826], [65, 22724576], [66, 24500175], [67, 26383240], [68, 28387456], [69, 30510616], [70, 32758963], [71, 35136544], [72, 37656214], [73, 40317328], [74, 43125329], [75, 46085496], [76, 49207224], [77, 52493112], [78, 55954267], [79, 59592272], [80, 63415296], [81, 67428832], [82, 71642127], [83, 76059704], [84, 80701546], [85, 85565064], [86, 90662451], [87, 95997360], [88, 101592122], [89, 107443264], [90, 113561009], [91, 119951832], [92, 126644136], [93, 133629672], [94, 140916757], [95, 148513712], [96, 156444624], [97, 164706400], [98, 173308509], [99, 182260568], [100, 191575248]

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COUNTING ALL REGULAR OCTAHEDRONS IN \{0, 1, ..., n\}³

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