

Combinatorial representation of tetrahedral chains

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Tetrahedral chains consisting of face-sharing regular tetrahedra in Euclidean three space are investigated. A parametrization of the chains by sequences of ordered reflections in barycentric coordinates is constructed and periodicity in their combinatorial structure is found. Periodicity along a chain is based on the structure of sequences of admissible triplets of integers and their cycling properties. The corresponding numerical invariants and an indexing role of a binary tetrahedral group are established.

1. Introduction

The simplest naturally ordered tetrahedral packing consists of an ordered sequence of regular tetrahedra glued together face to face as in the linear packing of a tetrahedral helix (Figure 1) introduced by H.S.M. Coxeter in [1]. Such tetrahedral structures, have been studied already by several authors [8–10, 12], are called *tetrahedral chains*.

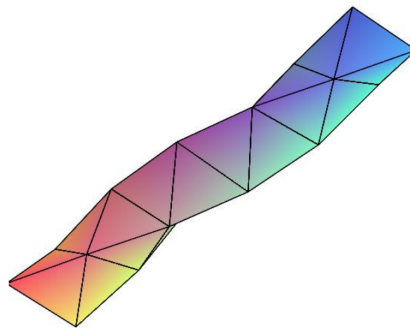


Figure 1: Tetrahelix.

Any tetrahedral chain consists of three types of simplest configurations of four consecutive tetrahedra called *tetrahedral units*. Two of these types are left and right tetrahedral short spirals, U, D , and the third type, F , is a flat configuration of four tetrahedra (Figure 2). The structure of a tetrahedral chain in D, F, U elementary units is written as a word like $UUDFUD \dots$.

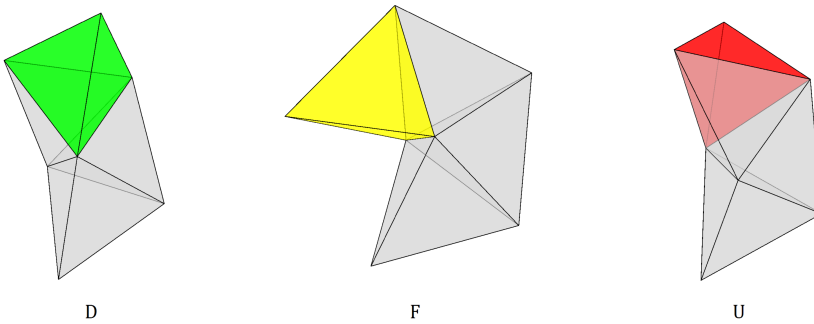


Figure 2: Tetrahedral units.

The three strands of the left or right oriented tetrahedral helix form a spiral with irrational slope. This is the reason for the effective density of tetrahedral chains (as proved by J.H.Mason [9]) and nonexistence of closed tetrahedral chains in Euclidean space (Figure 3).

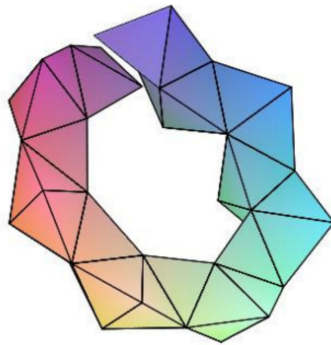


Figure 3: Semi-ring structure.

Let us assume that the gluing process of tetrahedra is ordered along a chain and each step of this process is realized by reflection in a particular

face of adjacent tetrahedron. To each tetrahedron we assign four reflections $R_i, i = 1, \dots, 4$, in the configurational three dimensional space V . Reflections R_i in V are represented by four corresponding reflect-morphisms $\bar{R}_i, i = 1, \dots, 4$, acting in the space of regular tetrahedra \mathcal{T} through a reflectional transformation of their vertices. Any tetrahedral chain of length $n + 1$ is uniquely represented by an initial tetrahedron T and an ordered sequence of n reflect-morphisms

$$\bar{R}_{i_1}, \dots, \bar{R}_{i_n}, \quad i_k \neq i_{k+1}, \quad k = 1, \dots, n - 1.$$

The fact that a tetrahedral chain is so rigid in 3-space and regular tetrahedra can not tile the space gives rise to several questions. The main question which we consider in this paper is the recognition of combinatorial and algebraic structures of tetrahedral chains. We want to investigate their geometric properties and determine the kind of shape information which is contained in the chain invariants of orthogonal transformations and re-numberings (cf. [8, 13]).

In Section 2 we introduce regular tetrahedra and affine reflections in their faces. Regular tetrahedra defined by four vertices are identified with elements of the tensor product of configurational three space and the four dimensional space of barycentric coordinates. Replacing all affine reflections of tetrahedra in faces by four linear reflections - reflect-morphisms, in barycentric four dimensional space, we uniquely encode all D, F, U elements of a chain by triplets of consecutive reflect-morphisms. Fixing enumeration of an initial tetrahedron (its vertices) we find that a reflect-morphism which reconstructs the adjacent tetrahedron by reflection along a chain, is denoted by the corresponding number of the reflected vertex. This way in Section 3 we parameterize a tetrahedral chain by the sequence of admissible triplets of integers $(k, j, i), k \neq j \neq i, 1 \leq k, j, i \leq 4$ and translate its geometric structure to purely combinatorial invariants of the re-numbering of the initial data. Thus the geometrical shape information of the chain is encoded by the sequence of admissible oriented triplets of integers displayed in Table 1. In Section 4 we investigate combinatorial properties of sequences of admissible triplets of integers and discuss notions of equivalence of representations. In particular we show that a complete invariant of chain equivalence is the sequence of signs $\{-1, 0, +1\}$ to which we reduce an admissible chain. In Section 5 all proper chains, i.e. chains which do not self-intersect, until their length equals 13 are listed and all proper chains centered around one common vertex with various branching orders are classified. There were found six proper chains centered around one vertex - icosi-clusters of maximal

length $n = 20$ and branching order $b = 1$. The periodic chains are investigated in Section 6 where it is proved that any periodic tetrahedral chain can be reconstructed by the composition of reflect-morphisms M and their powers M^m . The tetrahedral chains as sequences of D, F, U are replaced by compositions of the three corresponding permutations $\mathcal{L}_u, \mathcal{L}_d, \mathcal{L}_f$ of 12 elements set $\mathbb{I} = \{(\alpha, \beta) \in \Delta_4 \times \Delta_4 : \alpha \neq \beta\}, \Delta_4 = \{1, 2, 3, 4\}$. It is shown, that the permutations $\mathcal{L}_u, \mathcal{L}_d, \mathcal{L}_f$ of \mathbb{I} generate a tetrahedral group representation. And the non-periodic tetrahedral chains are indexed by elements of the tetrahedral group.

2. Tetrahedra in barycentric coordinates

A regular tetrahedron T in Euclidean 3-space is identified with the set of its four vertices $\{p_1, p_2, p_3, p_4\}, p_i \in \mathbb{R}^3$. We decompose T into four faces; $T = S_1 \cup \dots \cup S_4$, where we enumerate faces in such a way that the vertex p_i lies outside the plane defined by the face S_i . By (S_i, p_i) we denote an elementary pair of T . We also write $T = \{(S_1, p_1), \dots, (S_4, p_4)\}$. We denote by \mathcal{T} the space of regular tetrahedra in \mathbb{R}^3 , and in what follows we only consider regular tetrahedra. Let (p_1, p_2, p_3, p_4) be vertices of the tetrahedron T . We identify the space \mathcal{T} of regular tetrahedra with a subspace of the tensor product $\mathcal{T} \subset V \otimes U^*, U \equiv \mathbb{R}^4$, where V is a configurational vector space, $\dim V = 3$, and U is a space of barycentric coordinates $(\alpha_1, \dots, \alpha_4) \in \mathbb{R}^4$ contained in the canonical affine hyperplane $H = \{\sum_{i=1}^4 \alpha_i = 1\}$. Each tetrahedron $T \in \mathcal{T}$ defines the barycentric tetrahedral coordinates on V . For a regular tetrahedron $T \in \mathcal{T}$ we write $T = \sum_{i=1}^4 p_i \otimes e_i^*$, where $\{p_i\}$ satisfies the regularity equations, $\|p_i - p_j\| = \|p_k - p_l\|$ for $i \neq j, k \neq l$ and e_i^* is a canonical conjugate basis of $U^*, e_i^*(e_j) = \delta_{ij}$.

T defines the barycentric coordinate map $\mathbb{T} : H \rightarrow V, \mathbb{T}(\alpha) = \sum_{i=1}^4 p_i \otimes e_i^*(\alpha) = \sum_{i=1}^4 \alpha_i p_i$, where $\alpha = \sum_{i=1}^4 \alpha_i e_i \in H$, and geometrically $T = \mathbb{T}(H \cap \{\alpha_i \geq 0\})$. We see that any affine mapping $F : V \rightarrow V$ lifts to a linear transformation $M : U \rightarrow U$ of barycentric space preserving the hyperplane H , i.e. the following diagram commutes

$$\begin{array}{ccc}
 (U, H) & \xrightarrow{M} & (U, H) \\
 \downarrow \mathbb{T} & & \downarrow \mathbb{T} \\
 V & \xrightarrow{F} & V
 \end{array}$$

This diagram defines a barycentric representation of affine maps in V , where $M(H) = H$. To each F we uniquely associate a linear homogeneous

map in U preserving H . If $T \in \mathcal{T}$, $T = \sum_{i=1}^4 p_i \otimes e_i^*$, then its transformation by an affine mapping $F : V \rightarrow V$, $\bar{F}(T) = \sum_{i=1}^4 F(p_i) \otimes e_i^* \in \mathcal{T}$ is represented by a map M of barycentric space (U, H) through the commuting diagram above,

$$\mathbb{T}(M(\bullet)) = F(\mathbb{T}(\bullet))$$

and the affine action of F onto T can be expressed by a linear transformation M preserving H in the barycentric space. First we express uniquely $F(p_i)$ through $\{p_1, \dots, p_4\}$ in barycentric coordinates α_{ji} in such a way that $F(p_i) = \sum_{j=1}^4 \alpha_{ji} p_j$, $\sum_{j=1}^4 \alpha_{ji} = 1, i = 1, \dots, 4$. Then we write

$$\begin{aligned} (1) \quad F(\mathbb{T}(\alpha)) &= \sum_{i=1}^4 F(p_i) \otimes e_i^*(\alpha) = \sum_{i=1}^4 \sum_{j=1}^4 \alpha_{ji} p_j \otimes e_i^*(\alpha) \\ &= \sum_{j=1}^4 p_j \otimes \sum_{i=1}^4 \alpha_{ji} e_i^*(\alpha) = \mathbb{T}(M(\alpha)) \\ &= \sum_{i=1}^4 p_i \otimes e_i^*(M(\alpha)) = \sum_{i=1}^4 p_i \otimes M^*(e_i^*)(\alpha), \end{aligned}$$

where M^* is a conjugate mapping and we write $M = (\alpha_{ji})$.

Thus we have got the formula,

$$\sum_{i=1}^4 \sum_{j=1}^4 \alpha_{ji} p_j \otimes e_i^* = \sum_{j=1}^4 p_j \otimes \left(\sum_{i=1}^4 \alpha_{ji} e_i^* \right) = \sum_{j=1}^4 p_j \otimes M^*(e_j^*).$$

An ordered sequence $\{T^{(i)}\}_{i=0}^n$ of regular tetrahedra is called a *tetrahedral chain* if any pair of two consecutive tetrahedra have a common face.

We denote by s_i the center of S_i , $s_i = \frac{1}{3}(\sum_{j=1}^4 p_j - p_i)$. Four reflections R_i are defined uniquely by S_i and their orthogonals $s_i - p_i, 1 \leq i \leq 4$,

$$(2) \quad R_i(p) = p - 2 \frac{\langle p - s_i, s_i - p_i \rangle}{\langle s_i - p_i, s_i - p_i \rangle} (s_i - p_i),$$

where $\langle ., . \rangle$ denotes the inner product.

For a given tetrahedron T the *tetrahedral triangulation process* is attaching a copy of T to one of its faces. A natural step of the triangulation process is defined by reflection of the vertex p_i in the face S_i . The new attached tetrahedron is defined by three vertices lying on the face S_i and the reflected vertex $p_i^{(1)}$. We denote it by $T_i^{(1)}$ as it is uniquely determined

by an extra vertex $p_i^{(1)}$ after one step-reflection of triangulation process. The new attached tetrahedron $T_i^{(1)}$ has four vertices

$$\left\{ p_1^{(1)} = R_i(p_1), p_2^{(1)} = R_i(p_2), p_3^{(1)} = R_i(p_3), p_4^{(1)} = R_i(p_4) \right\},$$

where

$$R_i(p_j) = p_j, \quad j \neq i$$

as $p_j - s_i$ is orthogonal to $s_i - p_i$, and for $j = i$,

$$(3) \quad R_i(p_i) = p_i + 2(s_i - p_i),$$

that is,

$$(4) \quad R_i(p_j) = p_j^{(1)} = p_j + 2\delta_{ij} \left(\frac{1}{3} \sum_{k \neq i} p_k - p_j \right), \quad j = 1, \dots, 4.$$

We write $T_i^{(1)} = \bar{R}_i T$ where \bar{R}_i , acting in the space \mathcal{T} , is defined by reflection R_i (see 2) and it is called a *reflect-morphism* of \mathcal{T} , $\bar{R}_i^2 = id$.

Tetrahedral chains of lengths $1, 2, \dots, n$ are encoded and described in affine coordinates by compositions of $\bar{R}_i, i = 1, \dots, 4$:

$$\begin{aligned} T^{(0)} &= T, \\ T_{i_1}^{(1)} &= \bar{R}_{i_1} T, \\ T_{i_1 i_2}^{(2)} &= \bar{R}_{i_2} \bar{R}_{i_1} T, \quad i_1 \neq i_2, \\ &\dots \quad \dots \quad \dots \\ T_{i_1 i_2 \dots i_n}^{(n)} &= \bar{R}_{i_n} \dots \bar{R}_{i_2} \bar{R}_{i_1} T, \quad i_k \neq i_{k+1}, \quad k = 1, \dots, n - 1. \end{aligned}$$

The tetrahedral chain growth is defined by the reflect-morphisms \bar{R}_i (reflections) defined in (4) which operate in the space of regular tetrahedra \mathcal{T} . Each reflect-morphism defines a linear mapping operating on its second component;

$$(5) \quad \bar{R}_i : \mathcal{T} \rightarrow \mathcal{T}, \quad \bar{R}_i(v \otimes u^*) = v \otimes M_i^* u^*.$$

First we formulate the following useful

Lemma 2.1. *The reflect-morphism \bar{R}_i providing the tetrahedron $T_i^{(1)} = \bar{R}_i T$ by reflection of p_i in the face S_i is defined, by an operator M_i acting on barycentric space (U, H) , $M_i(H) = H$ by the following formula*

$$(6) \quad M_i^* e_k^* = e_k^* + \frac{2}{3}(1 - 4\delta_{ik})e_i^*, \quad M_i^{*2} = id,$$

where $1 \leq i, k \leq 4$.

Proof. We have

$$\begin{aligned} \bar{R}_i T &= \sum_{j=1}^4 p_j \otimes M_i^* e_j^* = \sum_{j=1}^4 p_j \otimes \left(e_j^* + \frac{2}{3}(1 - 4\delta_{ij})e_i^* \right) \\ &= \sum_{j=1}^4 p_j \otimes e_j^* + \sum_{l=1}^4 p_l \otimes \frac{2}{3}(1 - 4\delta_{il})e_i^* \\ &= \sum_{j=1}^4 p_j \otimes e_j^* + \left[\sum_{l=1}^4 \frac{2}{3}(1 - 4\delta_{il})p_l \right] \otimes e_i^* \\ &= \sum_{j=1}^4 p_j \otimes e_j^* + \left(\frac{2}{3} \sum_{l=1}^4 p_l - \frac{8}{3}p_i \right) \otimes e_i^* \\ &= \sum_{j=1}^4 p_j \otimes e_j^* + \left(\frac{2}{3} \sum_{k \neq i} p_k - 2p_i \right) \otimes e_i^* \\ &= \sum_{j=1}^4 p_j \otimes e_j^* + \sum_{j=1}^4 \left[2\delta_{ij} \left(\frac{1}{3} \sum_{k \neq i} p_k - p_j \right) \right] \otimes e_j^* \\ &= \sum_{j=1}^4 \left(p_j + 2\delta_{ij} \left(\frac{1}{3} \sum_{k \neq i} p_k - p_j \right) \right) \otimes e_j^* = \sum_{j=1}^4 p_j^{(1)i} \otimes e_j^*. \end{aligned}$$

□

In local coordinates we have the following matrix form of M_i ,

$$M_1 = \begin{pmatrix} -1 & \frac{2}{3} & \frac{2}{3} & \frac{2}{3} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}^T, \quad M_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{2}{3} & -1 & \frac{2}{3} & \frac{2}{3} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}^T,$$

$$M_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{2}{3} & \frac{2}{3} & -1 & \frac{2}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}^T, \quad M_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \frac{2}{3} & \frac{2}{3} & \frac{2}{3} & -1 \end{pmatrix}^T.$$

Using M_i in barycentric space U we can write the n -th tetrahedron in a chain by composition of barycentric coordinate maps,

$$(7) \quad \mathbb{T}_{i_1 \dots i_n}^{(n)} = \mathbb{T}M_{i_1} \cdots M_{i_n}.$$

Acting on vertices $\{p_1, p_2, p_3, p_4\}$, \bar{R}_i is represented by the transpose of M_i . As an example we show the matrix form of the \bar{R}_1 - action.

$$\bar{R}_1 \left(\sum_{i=1}^4 p_i \otimes e_i^* \right) = \sum_{i=1}^4 p_i^{(1)_1} \otimes e_i^*,$$

where

$$\begin{pmatrix} p_1^{(1)_1} \\ p_2^{(1)_1} \\ p_3^{(1)_1} \\ p_4^{(1)_1} \end{pmatrix} = \begin{pmatrix} -1 & \frac{2}{3} & \frac{2}{3} & \frac{2}{3} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{pmatrix},$$

then the composition of reflect-morphisms acting on the tetrahedra reads,

$$T_{i_1 \dots i_n}^{(n)} = \bar{R}_{i_n} \cdots \bar{R}_{i_1} T.$$

3. Coding in the triplets of consecutive steps

The mapping prescribing an affine center point of a tetrahedron; $C : \mathcal{T} \rightarrow V$,

$$C(T) = \mathbb{T} \left(\frac{1}{4} \sum_{l=1}^4 e_l \right) = \sum_{i=1}^4 p_i \otimes e_i^* \left(\frac{1}{4} \sum_{l=1}^4 e_l \right) = \frac{1}{4} \sum_{i=1}^4 p_i,$$

and the corresponding vectors joining centers of two consecutive tetrahedra in a chain are defined by

$$\begin{aligned} x_r &= C(T^{(r)} - T^{(r-1)}) = c^{(r)} - c^{(r-1)} \\ &= ((\bar{R}_{i_r} - Id)\bar{R}_{i_{r-1}} \cdots \bar{R}_{i_1} T)(\alpha_c), \quad 1 \leq r \leq n, \end{aligned}$$

where $c^{(r)}$ is the center of a tetrahedron $T^{(r)}$,

$$c^{(r)} = C(T^{(r)}) = \mathbb{T}^{(r)}(\alpha_c), \quad n = 0, 1, \dots,$$

and $\alpha_c = \frac{1}{4} \sum_{l=1}^4 e_l$. The skeleton of the tetrahedral chain is a broken line built from consecutive segments, intervals $|x_r|$ joining the consecutive centers (Figure 4),

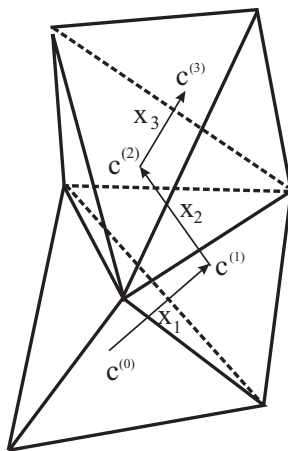


Figure 4: The orientation unit.

The three consecutive tetrahedra or two skeleton segments define an orientation plane spanned by two vectors x_{r+2} and x_{r+1} . The corresponding tetrahedron $T_{i_{r+1}i_{r+2}i_{r+3}}^{(r+3)} = \bar{R}_{i_{r+3}} T_{i_{r+1}i_{r+2}}^{(r+2)}$ follow from the orientation tetrahedral unit, consisting of the three consecutive tetrahedra,

$$T^{(r)}, \quad T_{i_{r+1}}^{(r+1)} = \bar{R}_{i_{r+1}} T^{(r)}, \quad T_{i_{r+1}i_{r+2}}^{(r+2)} = \bar{R}_{i_{r+2}} \bar{R}_{i_{r+1}} T^{(r)}.$$

The three possible consecutive reflections $\bar{R}_{i_{r+1}}, \bar{R}_{i_{r+2}}, \bar{R}_{i_{r+3}}$ of an initial tetrahedron $T^{(r)}$ extend the initial tetrahedron to an oriented quadruple of four tetrahedra and determine the three skeleton segments $x_{r+1}, x_{r+2}, x_{r+3}$.

Definition 3.1. The three units F, U, D of a tetrahedral chain, built from four consecutive tetrahedra are defined by three possible orientations of the three consecutive skeleton segments,

$$(8) \quad F : \quad T^{(r+3)}; \quad \det(x_{r+1}, x_{r+2}, x_{r+3}) = 0$$

$$(9) \quad U : \quad T^{(r+3)}; \quad \det(x_{r+1}, x_{r+2}, x_{r+3}) > 0$$

$$(10) \quad D : \quad T^{(r+3)}; \quad \det(x_{r+1}, x_{r+2}, x_{r+3}) < 0.$$

The initial value for continuation of the triangulation process, at each step of a process, is defined by $T^{(r)}$ with $r \geq 0$. A tetrahedral chain with fixed orientation in a space, i.e. with coordinates prescribed to each vertex of the chain, is written in the form of a word, e.g. $F \cdots FU \cdots UD \cdots D \cdots$.

The initial configuration of three consecutive tetrahedra $T^{(0)}, T_{i_1}^{(1)}, T_{i_1 i_2}^{(2)}$, where $T^{(0)} = T$, establishes the exact position of a chain in \mathbb{R}^3 . However the distribution of elements F,D,U along the word defines its geometric structure uniquely. In the symbolic description of a chain (invariant under $SO(3)$ symmetries) we do not consider this initial configuration of the three consecutive tetrahedra and so we ignore its geometric position.

Proposition 3.2. *At each element of a tetrahedral chain, say $T^{(r+3)}$, its position, F, U, D is defined uniquely by the triplet of three consecutive tetrahedra $T^{(r)}, T^{(r+1)}, T^{(r+2)}$ and one of the three reflect-morphisms acting on $T^{(r+2)}$.*

Proof. At each step of the triangulation process of a tetrahedral chain we have three preceding operations by reflect-morphisms,

$$\begin{aligned} T_k^{(r+1)} &= \bar{R}_k T^{(r)} \\ T_{kj}^{(r+2)} &= \bar{R}_j \bar{R}_k T^{(r)} \\ T_{kji}^{(r+3)} &= \bar{R}_i \bar{R}_j \bar{R}_k T^{(r)}. \end{aligned}$$

Let $T^{(r)} = \sum_{l=1}^4 p_l \otimes e_l^*$. Then we have,

$$\begin{aligned} T_k^{(r+1)} &= \bar{R}_k T^{(r)} = T^{(r)} + \frac{8}{3} (c^{(r)} - p_k) \otimes e_k^*, \\ T_{kj}^{(r+2)} &= \bar{R}_j \bar{R}_k T^{(r)} = T^{(r+1)} + \frac{8}{3} \left(\frac{5}{3} c^{(r)} - p_j - \frac{2}{3} p_k \right) \otimes e_j^*, j \neq k \\ T_{kji}^{(r+3)} &= \bar{R}_i \bar{R}_j \bar{R}_k T^{(r)} \\ &= T^{(r+2)} + \frac{8}{3} \left(\left(\frac{5}{3} + \beta_{ik} \right) c^{(r)} - p_i - \frac{2}{3} p_j - \beta_{ik} p_k \right) \otimes e_i^*, \end{aligned}$$

for $\beta_{ik} = \frac{1}{9}(10 - 24\delta_{ik}), i \neq j$

Now we distinguish separately the three configurations depending on the last reflect-morphism \bar{R}_i . Assuming $c^{(r)} = \frac{1}{4} \sum_{i=1}^4 p_i = 0$ we get,

$$(F) : i = k, x_{r+1} = -\frac{2}{3}p_k, x_{r+2} = -\frac{2}{3}\left(p_j + \frac{2}{3}p_k\right), x_{r+3} = -\frac{4}{9}\left(p_j + \frac{5}{6}p_k\right)$$

$$(U) : i \neq k, x_{r+1} = -\frac{2}{3}p_k, x_{r+2} = -\frac{2}{3}\left(p_j + \frac{2}{3}p_k\right),$$

$$x_{r+3} = -\frac{2}{3}\left(p_i + \frac{2}{3}p_j + \frac{10}{9}p_k\right), \quad \det(p_k, p_j, p_i) < 0$$

$$(D) : i \neq k, x_{r+1} = -\frac{2}{3}p_k, x_{r+2} = -\frac{2}{3}\left(p_j + \frac{2}{3}p_k\right),$$

$$x_{r+3} = -\frac{2}{3}\left(p_i + \frac{2}{3}p_j + \frac{10}{9}p_k\right), \quad \det(p_k, p_j, p_i) > 0.$$

These configurations uniquely determine the three possible elements of the tetrahedral chain. \square

Definition 3.3. A triplet of integers (k, j, i) , $1 \leq i, j, k \leq 4$ such that $k \neq j \neq i$ is called an admissible triplet. The set of all admissible triplets we denote by A .

By Proposition 3.2, to each admissible triplet of integers encoding one of the F, U, D elements of a chain we associate a corresponding triplet of reflect-morphisms,

$$(k, j, i) \mapsto (\bar{R}_k, \bar{R}_j, \bar{R}_i).$$

As it is seen from the proof of Proposition 3.2 to complete orientation in the directed chain of tetrahedra and define especially the U and D chain elements we need to orient at least one tetrahedron of the chain. This means that if we fix the sign, say $\det[p_1, p_2, p_3] > 0$, then the orientation is defined for all other admissible triplets. In what follows we will assume this orientation for the initial tetrahedron. By straightforward calculation (for standard tetrahedron inscribed in the unit sphere) based on the proof of Proposition 3.2 we get the following result,

Proposition 3.4. *Assume that the normalization conditions, $\sum_{i=1}^4 p_i = 0$, and $\det(p_1, p_2, p_3) > 0$, are satisfied. Then the classes of admissible triplets representing the first step u, d , and f chain oriented elements are displayed in Table 1 .*

d	f	u
$\det(x_1, x_2, x_3) = -32\sqrt{3}/243$	$\det(x_1, x_2, x_3) = 0$	$\det(x_1, x_2, x_3) = 32\sqrt{3}/243$
(k, j, i)	(k, j, i)	(k, j, i)
$(1, 2, 3)$	$(3, 2, 3)$	$(3, 2, 1)$
$(1, 3, 4)$	$(4, 3, 4)$	$(4, 3, 1)$
$(1, 4, 2)$	$(4, 2, 4)$	$(2, 4, 1)$
$(2, 1, 4)$	$(1, 2, 1)$	$(4, 1, 2)$
$(2, 3, 1)$	$(4, 1, 4)$	$(1, 3, 2)$
$(2, 4, 3)$	$(3, 1, 3)$	$(3, 4, 2)$
$(3, 1, 2)$	$(3, 4, 3)$	$(2, 1, 3)$
$(3, 2, 4)$	$(2, 1, 2)$	$(2, 3, 4)$
$(3, 4, 1)$	$(1, 3, 1)$	$(1, 4, 3)$
$(4, 1, 3)$	$(1, 4, 1)$	$(3, 1, 4)$
$(4, 2, 1)$	$(2, 4, 2)$	$(1, 2, 4)$
$(4, 3, 2)$	$(2, 3, 2)$	$(4, 2, 3)$

Table 1: Classification of admissible triplets.

Each tetrahedron of a tetrahedral chain is given by reflection of the previous one. At each step of determining of the D, F, U positions we have to normalize the initial conditions (initial tetrahedron) as it is described in Proposition 3.4, and follow the part of the proof of Proposition 3.2. Indeed if the initial tetrahedron, say $T^{(r)}$, was oriented by $\det[p_1, p_2, p_3] > 0$, then the next one $T^{(r+1)}$, serving as an initial for the next step of determination of the D, F, U elements, is given as a reflection of a previous one, so after normalization of its coordinates, $\sum_{i=1}^4 p_i = 0$ we get the opposite orientation of the initial condition, i.e. $\det[p_1, p_2, p_3] < 0$. And this orientation changes at each even step of our construction. Thus choosing an admissible triplet, say for D in the second step we choose it from the u column of admissible triplets of Table 1. In the next step (odd) of this procedure the initial data orientation comes to the first one, i.e. $\det[p_1, p_2, p_3] > 0$, and we use the Table 1 as it is. This is the reason why we denoted the admissible triplets by lower case characters f, u, d . And f corresponds to the geometric form F along the chain, but u and d interchange D and U along the chain depending on orientation of the local initial data.

To avoid this varying initial orientation data along the triangulation process we introduce, using duality concept defined below, the notion of an *adjoint word* in the lower case characters of admissible triplets.

Definition 3.5. To each tetrahedral chain written in the form of word W (possibly infinite), for example

$$W = UUDDUUFFU \dots$$

we associate uniquely a new word $\bar{W} = I(W)$ which is called an *adjoint word*. The adjoint word is defined by replacing each character U (or D) by d (or u respectively) if it is in an even position of the word W . All F characters are replaced by f in its adjoint form, for example (resp.)

$$I(W) = \bar{W} = udduudffu \dots$$

I is a duality between the spaces of admissible words, one written in the capital characters and the another one written in the lower case characters.

Reducing the word characters along the chain to the ones listed in Table 1 which are the first step characters represented numerically we show that each tetrahedral chain can be uniquely represented by a sequence of admissible triplets of integers. This sequence of triplets is defined by an initial triplet and the triplets of Table 1.

4. Numerical invariants of the tetrahedral chains

Any tetrahedral chain is described as a composition of admissible ordered triplets representing the corresponding characters D, F, U of a defining word, e.g. for $UUDFD$ we have $I(UUDFD) = uddf d$ and respectively,

$$(3, 4, 2) \rightarrow (4, 2, 1) \rightarrow (2, 1, 4) \rightarrow (1, 4, 1) \rightarrow (4, 1, 3).$$

and

$$T_{3421413}^{(7)} = \bar{R}_3 \bar{R}_1 \bar{R}_4 \bar{R}_1 \bar{R}_2 \bar{R}_4 \bar{R}_3 T.$$

Each admissible triplet (i_1, i_2, i_3) is a mapping from an ordered set $\Delta_3 = \{1, 2, 3\}$ to the set $\Delta_4 = \{1, 2, 3, 4\}$ denoted by $f_{i_1 i_2 i_3}$, $f_{i_1 i_2 i_3}(j) = i_j \in \Delta_4, j = 1, 2, 3$. There is a natural action of the direct product of symmetric groups $S_4 \times S_3$ in the space of such mappings,

$$(\xi, \sigma).f_{i_1 i_2 i_3} = \xi \circ f_{i_1 i_2 i_3} \circ \sigma, \quad \xi \in S_4, \sigma \in S_3.$$

The set of all mappings f into admissible triplets, i.e. $f_{i_1 i_2 i_3}(\Delta_3) \in A$ we denote by \mathcal{A} . Obviously \mathcal{A} is not preserved by the above defined group action.

Now we fix an orientation of a chain choosing a reference triplet (i, j, k) , $i \neq j \neq k \neq i$. We call this triplet positive. One can easily see that any mapping $f_{i_1 i_2 i_3} \in \mathcal{A}$ can be reconstructed from the reference mapping f_{ijk} by the group action, i.e.

$$f_{i_1 i_2 i_3} = \xi \circ f_{ijk} \circ \sigma.$$

- Lemma 4.1.**
1. If $i_1 \neq i_2 \neq i_3 \neq i_1$, $f_{i_1 i_2 i_3}(s) \in \{i, j, k\}$, $1 \leq s \leq 3$, then there is a uniquely defined $\sigma \in S_3$ such that $f_{i_1 i_2 i_3} = (id, \sigma).f_{ijk}$.
 2. If $i_1 \neq i_2 \neq i_3 \neq i_1$, $\{i_1, i_2, i_3\} \neq \{i, j, k\}$, then there are uniquely defined, transposition $\tau \in S_4$ and permutation $\sigma \in S_3$ such that $f_{i_1 i_2 i_3} = (\tau, \sigma).f_{ijk}$.

Proof. The case 1.) is straightforward as an image set of $f_{i_1 i_2 i_3}$ is equal to $\{i, j, k\}$. In the case 2.) there are three possibilities $\{i_1, i_2, i_3\} = \{i, j, l\}$, $\{i_1, i_2, i_3\} = \{i, l, k\}$, and $\{i_1, i_2, i_3\} = \{l, j, k\}$, where $\{l\} = \Delta_4 - \{i, j, k\}$. In each of these cases there is one of the transpositions τ_{kl} , τ_{jl} , τ_{il} such that the image of $f_{i_1 i_2 i_3}$ is equal to $\tau_* \circ f_{ijk}$, where τ_* denotes one of the permutations τ_{kl} , τ_{jl} and τ_{il} . Then there is a uniquely defined element $\sigma \in S_3$ such that $f_{i_1 i_2 i_3} = \tau_* \circ f_{ijk} \circ \sigma$. □

On the basis of Lemma 4.1 and straightforward checking, we get a new numerical characteristic of admissible triplets.

Proposition 4.2. *To each admissible triplet $f_{i_1 i_2 i_3}$ we associate uniquely its sign Λ , i.e. there is a mapping $\Lambda : \mathcal{A} \rightarrow \{-1, 0, +1\}$, such that*

1. $\Lambda(f_{ijk}) = +1$
2. If $i_1 \neq i_2 \neq i_3 \neq i_1$, $f_{i_1 i_2 i_3}(s) \in \{i, j, k\}$, $1 \leq s \leq 3$, then $f_{i_1 i_2 i_3} = (id, \sigma).f_{ijk}$ and $\Lambda(f_{i_1 i_2 i_3}) = \text{sgn}(\sigma)$.
3. If $i_1 \neq i_2 \neq i_3 \neq i_1$, $\{i_1, i_2, i_3\} \neq \{i, j, k\}$, then $f_{i_1 i_2 i_3} = (\tau_*, \sigma).f_{ijk}$ and $\Lambda(f_{i_1 i_2 i_3}) = \text{sgn}(\tau_*)\text{sgn}(\sigma) = -\text{sgn}(\sigma)$.
4. If $i_1 = i_3$, $\Lambda(f_{i_1 i_2 i_3}) = 0$.

As a formal notion for Λ we propose its representation as the sign of the determinant built by the three vertices of the initial tetrahedron of the tetrahedral chain, i.e. the positive reference triplet means $\det(p_i, p_j, p_k) > 0$

($\text{sgn}(\det(p_i, p_j, p_k)) = +1$), and

$$\Lambda(f_{i_1 i_2 i_3}) = \text{sgn}(\det(p_{i_1}, p_{i_2}, p_{i_3})).$$

Now we investigate the properties of Λ represented by this determinant and stated in Proposition 4.2. We show that

$$\begin{aligned} \Lambda(f_{i_1 i_2 i_3}) &= \text{sgn}(\det(p_{i_1}, p_{i_2}, p_{i_3})) = \Lambda(\xi \circ f_{ijk} \circ \sigma) \\ &= -\text{sgn}(\sigma)\text{sgn}(\det(p_i, p_j, p_k)). \end{aligned}$$

Indeed,

$$\begin{aligned} &\det(p_{\xi \circ f_{ijk} \circ \sigma(1)}, p_{\xi \circ f_{ijk} \circ \sigma(2)}, p_{\xi \circ f_{ijk} \circ \sigma(3)}) \\ &= \text{sgn}(\sigma) \det(p_{\xi \circ f_{ijk}(1)}, p_{\xi \circ f_{ijk}(2)}, p_{\xi \circ f_{ijk}(3)}) \\ &= \text{sgn}(\sigma) \det(p_{\xi(i)}, p_{\xi(j)}, p_{\xi(k)}) = \text{sgn}(\sigma) \det(p_i, p_j, p_l), \end{aligned}$$

because we choose (as an example) $\xi = \tau_{kl}$. And taking $p_l = -(p_i + p_j + p_k)$ we get

$$\begin{aligned} \text{sgn}(\sigma) \det(p_i, p_j, p_l) &= \text{sgn}(\sigma) \det(p_i, p_j, -p_i - p_j - p_k) \\ &= -\text{sgn}(\sigma) \det(p_i, p_j, p_k). \end{aligned}$$

In the sequence of admissible triplets defining a tetrahedral chain for a given triplet of the sequence the two last numbers of this triplet repeat in the subsequent triplet in the same order. To each tetrahedral chain W_n we associate the chain of admissible triplets.

Definition 4.3. The chain of admissible triplets

$$\dots \xrightarrow{\tilde{L}_*} (i_1, i_2, i_3) \xrightarrow{\tilde{L}_*} (i_2, i_3, i_4) \xrightarrow{\tilde{L}_*} (i_3, i_4, i_5) \xrightarrow{\tilde{L}_*} \dots,$$

where \tilde{L}_* is defined by the corresponding transposition $\tau_* \in S_4$, maximal order element (maximal cycle) γ of S_3 and the unique relation

$$(11) \quad f_{i_{r+2} i_{r+3} i_{r+4}} = \tau_* \circ f_{i_{r+1} i_{r+2} i_{r+3}} \circ \gamma,$$

is called an admissible chain and we denote it by Q_n .

Action of the above defined pairs $(\tau_*, \gamma) \in S_4 \times S_3$ preserves the space of admissible mappings \mathcal{A} . The relation of sign of Λ in an admissible sequence

reads

$$\Lambda(f_{i_2i_3i_4}) = \Lambda(\tau_* \circ f_{i_1i_2i_3} \circ \gamma) = -\text{sgn}(\gamma)\Lambda(f_{i_1i_2i_3}).$$

In the space of all finite admissible chains of triplets we introduce the following equivalence,

Definition 4.4. Two admissible chains Q_n and Q'_n

$$\begin{aligned} Q_n &= \cdots \xrightarrow{\tilde{L}_*} (i_{r+1}, i_{r+2}, i_{r+3}) \xrightarrow{\tilde{L}_*} (i_{r+2}, i_{r+3}, i_{r+4}) \\ &\qquad \qquad \qquad \xrightarrow{\tilde{L}_*} (i_{r+3}, i_{r+4}, i_{r+5}) \xrightarrow{\tilde{L}_*} \cdots, \\ Q'_n &= \cdots \xrightarrow{\tilde{L}_*} (j_{r+1}, j_{r+2}, j_{r+3}) \xrightarrow{\tilde{L}_*} (j_{r+2}, j_{r+3}, j_{r+4}) \\ &\qquad \qquad \qquad \xrightarrow{\tilde{L}_*} (j_{r+3}, j_{r+4}, j_{r+5}) \xrightarrow{\tilde{L}_*} \cdots, \end{aligned}$$

are equivalent, $Q_n \sim Q'_n$, if there exists $\xi \in S_4$ such that $f_{i_{k+1}i_{k+2}i_{k+3}} = \xi \circ f_{j_{k+1}j_{k+2}j_{k+3}}$ for $k = 0, \dots, n - 1$.

To each admissible chain, say Q_n , we associate its sign sequence

$$\Lambda(Q_n) = \{\Lambda(f_{i_1i_2i_3}), \dots, \Lambda(f_{i_ni_{n+1}i_{n+2}})\}.$$

Proposition 4.5. *The sign sequence is a numerical invariant, i.e.*

$$\Lambda(Q_n) = \Lambda(Q'_n) \text{ if and only if } Q_n \sim Q'_n.$$

Thus the sign sequences corresponding to the admissible sequences are in 1-1 correspondence with the tetrahedral chains. There is a natural correspondence of these two sequences,

$$\begin{array}{ccccccccc} \cdots & \xrightarrow{\tilde{L}_*} & \mathcal{A} & \xrightarrow{\tilde{L}_*} & \mathcal{A} & \xrightarrow{\tilde{L}_*} & \mathcal{A} & \xrightarrow{\tilde{L}_*} & \cdots \\ \Lambda \downarrow & & \Lambda \downarrow & & \Lambda \downarrow & & \Lambda \downarrow & & \Lambda \downarrow \\ \cdots & \xrightarrow{\tilde{S}_*} & G & \xrightarrow{\tilde{S}_*} & G & \xrightarrow{\tilde{S}_*} & G & \xrightarrow{\tilde{S}_*} & \cdots \end{array}$$

where $G = \{-1, 0, +1\}$ and \tilde{S}_* is an operator $G \rightarrow G$ corresponding to \tilde{L}_* .

5. Geometric characteristics

All finite regular tetrahedral chains or equivalently the finite words consisting of D, F, U or by duality u, d, f characters are denoted by $\Gamma_{\mathcal{T}}$. It is a

collection of chains $C_n \in \Gamma_{\mathcal{T}}(n)$ of length $n, n \in \mathbb{N}$, $\Gamma_{\mathcal{T}} = \bigcup_{n \in \mathbb{N}} \Gamma_{\mathcal{T}}(n)$. All chains which do not self-intersect form a subspace of $\Gamma_{\mathcal{T}}$. We call them *proper tetrahedral chains* and denote by $\mathcal{C}_{\mathcal{T}}$, $\mathcal{C}_{\mathcal{T}} = \bigcup_{n \in \mathbb{N}} \mathcal{C}_{\mathcal{T}}(n) \subset \Gamma_{\mathcal{T}}$, where $\mathcal{C}_{\mathcal{T}}(n)$ are proper tetrahedral chains of length n .

One of the geometric properties of tetrahedral chains is their clustering characteristic. First we introduce the notion of vertex order. If p is a common vertex for a number of tetrahedra we call this number an order of vertex p . Vertex order is a function $P : V_{C_n} \rightarrow \mathbb{N}$ defined on an ordered sequence of vertices V_{C_n} of chain C_n which to each vertex $p \in V_{C_n}$ along the chain C_n associate its order $P(p)$. In the same way we define an edge order function $G : E_{C_n} \rightarrow \mathbb{N}$ defined on an ordered sequence of edges E_{C_n} . $G(l)$ is the number of tetrahedra which share an edge $l, l \in E_{C_n}$. We can easily check the following

Lemma 5.1. *1. The total vertex order $\tilde{V} = \sum_{p \in V_{C_n}} P(p)$ for a chain does not depend on a form of the chain and for the chain of length n it is equal to $4n$.*

2. A maximal vertex order of the proper tetrahedral chain is 20 and all chains of length 20 with such vertex of maximal order are called icosi-clusters (icosihedral clusters). The distribution of values of the vertex order function along the chain defines uniquely up to orientation the geometric shape of the chain, i.e. if two functions P_1 and P_2 associated to two chains of the same length are equal then their shapes are identical up to orientation.

Remark 5.2. If the vertex order function along a chain is less than or equal to 4, then the chain is a tetrahelix with U or D orientation. In this case the level sets of an edge order function $G, G^{-1}(1), G^{-1}(2), G^{-1}(3)$ form the three helices built from external edges, two broken helices made of edges of order two and the central broken spiral.

On each space $\mathcal{C}_{\mathcal{T}}(n) \subset \Gamma_{\mathcal{T}}(n)$ of the proper tetrahedral chains of length n , we have the clustering function $Cl : \mathcal{C}_{\mathcal{T}}(n) \rightarrow \mathbb{N}$,

$$Cl(C_n) = \sum_{p \in V_{C_n}} \max(0, P(p) - 4).$$

We see that the clustering function vanishes on the tetrahelix and has a maximal value for the chains consisting of a number of icosi-clusters, say m , and completed by a k -cluster (the chain composed of one common vertex of order k) with $k = n \pmod{20m}, k < 20$.

For small n we can classify all proper tetrahedral chains of length n . Up to $n = 7$ a selfintersection appears only for FFF part of the chain. If

$8 \leq n \leq 10$ the selfintersected chains appear in chains with one common vertex, i.e. if all tetrahedra of a chain have a common vertex. The cases $n \geq 11$ add to the above possibilities the chains which are selfintersecting in long distance geometric structures.

Proposition 5.3. *The numbers of proper chains A_n of length $n \leq 13$ are listed in the following table.*

n	3	4	5	6	7	8	9	10	11	12	13
A_n	1	3	9	26	76	218	628	1802	5146	14670	41734

Table 2: Proper tetrahedral chains.

In the tetrahedral triangulation process of a proper chain at each final tetrahedron one may have at most three possibilities to attach the next tetrahedron. If we replace tetrahedrons by the equal tightly packed spheres, then the process of attaching the new tetrahedron corresponds to gluing an appropriate sphere and use the computational methods (cf. [5]). Thus we see that every tetrahedron along a chain has its *branching order* which is the number b , $0 \leq b \leq 3$ of possible concurrent continuations of the chain at the given tetrahedron. The zero branching order terminates the chain, i.e. each of the three attached tetrahedra intersect the chain. An example of zero branching order chain written in the form $UUFFDDUUFFDDUUFFDDDDUDDUDDUDDDDFDDDUUUUFDUUUUUUFFDDDDD$, is shown in Figure 5. The branching order of the final tetrahedron in a chain is called the *branching order of the chain*. If the branching order of a chain is one, then at its final tetrahedron there is only one possibility of continuation of the chain.

Such chains with branching order one, form the basic units with substantially reduced space of possible configurations. Classification of proper chains with all tetrahedra having a fixed common vertex and fixed branching order is given in the following,

Theorem 5.1. *The proper tetrahedral chains with all tetrahedra sharing one fixed geometrical vertex, with different branching orders $b = 1, 2$ and 3 are listed in Table 3.*

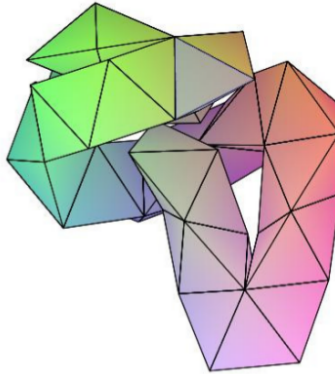


Figure 5: Example of chain with zero branching order

$b \backslash n$	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	<i>total</i>
1	0	0	0	0	0	1	2	6	9	19	38	49	69	79	71	34	6	383
2	0	0	1	4	6	10	24	46	78	113	137	153	132	85	36	6	0	831
3	2	4	6	9	16	27	38	48	55	56	50	35	22	12	2	0	0	380
<i>total</i>	2	4	7	13	22	38	64	100	142	188	225	237	223	176	109	40	6	1594

Table 3: Table of chains sharing one common vertex.

Example 5.4. The first listing of short proper chains centered at one fixed vertex with $4 \leq n \leq 8$ reads as follows:

$n = 4$: F, D

$n = 5$: $FF, FD, DU, DF,$

$n = 6$: $FFD, FDF, FDU, DUF, DUD, DFF, DFU$

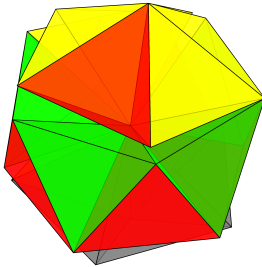
$n = 7$: $FFDF, FF DU, FDF F, FDFU, FDUF, FDUD, DUFF,$
 $DUFD, DUDF, DUDU, DFFU, DFUF, DFUD$

$n = 8$: $FFDFU, FFDF F, FFDUD, FDFFU, FDFUD, FDFUF,$
 $FDUFD FDUDU, FDUDF, DUFFD, DUFDU, DUFDF,$
 $DUDFU, DUDFF DUDUD, DUDUF, DFFUF, DFFUD,$
 $DFUFD, DFUFF, DFUDU, DFUDF.$

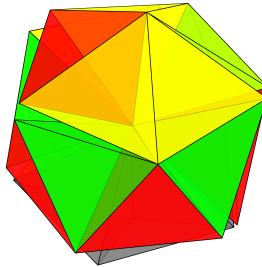
Remark 5.5. 1. The shortest proper tetrahedral chain (cluster) centered at one fixed vertex of branching order $b = 1, n = 9$, is given by the code $UDFUDF$.

2. The icosi-clusters are listed in the following 6 codes (examples see Figure 6):

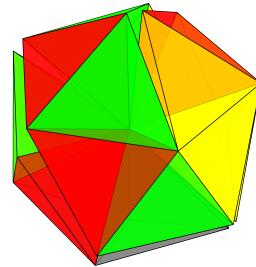
$FFUFFDUDUDFFUFFDU, FFUFFDUDUDUDFFUFF$
 $UFFDFFUDUDUFFDFU, UFFDUDFFUFFDUDFFU$
 $UDFFUFFDUDFFUFFDU, UDFUFFDUDUDFFUFF.$



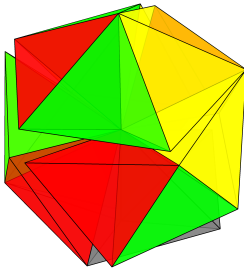
FFUFFDUDUDUDFFUFF



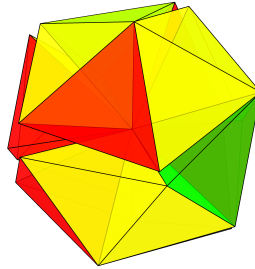
FFUFFDUDUDFFUFFDU



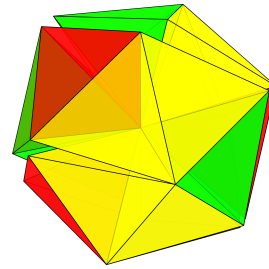
UDFUFFDUDUDFFUFF



UDFUFFDUDFFUFFDU



UFFDUDFFUFFDUDFFU



UFFDFFUDUDUFFDFU

Figure 6: Six different configurations of icosi-clusters $n = 20, b = 1$.

3. Table 3 displays numbers of all proper tetrahedral chains whose tetrahedra share one geometrically fixed point as a vertex. This way we get part of the clusters, namely those which have a fixed orientation. Table 3 extended by numbers of all chains having codes with U replaced by D and vice versa completes the set of all proper tetrahedral chains with one common vertex.

6. Periodic tetrahedral chains

A tetrahedral chain is called periodic if the configuration of elements F, U, D in the defining word, $D \cdots DU \cdots UF \cdots$ is periodic. Any periodic tetrahedral chain is uniquely defined by its period which forms the shortest finite tetrahedral chain written in the form of word, say $W_m = UDFU \cdots DU$, of length m . We will call this word the *basic period* of a periodic tetrahedral chain.

In the reflect-morphism representation of a chain for each of D, F, U unit along the chain we need two preceding reflect-morphisms which define an admissible triplet of integers. Thus the period in a numerical characterization of a periodic tetrahedral chain by its sequence of admissible triplets corresponds to the shortest cycle of the triplets which continues repeating along a sequence. The cycle of triplets is directly represented by reflect-morphisms and finally by their composition. This cycle forms a principal operator which is a 4×4 matrix for a periodic chain. In this section we show the existence of such a matrix for a periodic chain and display some of its properties.

To construct a coordinate representation of a periodic chain, i.e. the reflect-morphism composition for a cycle of admissible triplets, we define the corresponding *adjoint defining sequence* of a periodic tetrahedral chain and its *adjoint period*.

We observe that the shortest word W_m is a period of a tetrahedral chain W if its adjoint word \bar{W}_m is also period for an adjoint defining sequence \bar{W} . We notice that if the length of a basic period W_m is even, then the adjoint word $\bar{W}_m = I(W_m)$ is also a basic period for an adjoint defining sequence. Obviously the doubled basic period is a period for the adjoint defining sequence in the case of odd length of the basic period.

Let us assume the positive orientation of an initial tetrahedron $T = \{p_1, p_2, p_3, p_4\}$, i.e., $\det[p_1, p_2, p_3] > 0$, then using Table 1 for any two indices i_1, i_2 , $i_1 \neq i_2, 1 \leq i_1, i_2 \leq 4$ we associate uniquely an integer $i_3, 1 \leq i_3 \leq 4$ such that (i_1, i_2, i_3) is an admissible triplet of the fixed type " d, f, u ". Thus we have defined the natural mappings $L_u, L_d, L_f : \mathbb{I} \rightarrow \Delta_4$, where $\Delta_4 = \{1, 2, 3, 4\}$ and $\mathbb{I} = \{(\alpha, \beta) \in \Delta_4 \times \Delta_4 : \alpha \neq \beta\}$.

Any word W_m of length m can be represented as a composition of $m + 2$ reflect-morphisms $\bar{R}_{i_{m+2}} \cdots \bar{R}_{i_1}$. A sequence of indices i_1, \dots, i_{m+2} is defined by the sequence of L_* -mappings (i.e. L_u, L_d or L_f) directly corresponding to the sequence of characters in the dual word \bar{W}_m .

Example 6.1. As an example the L_* -sequence for $W_m = UDFU \cdots DU$ and $\bar{W}_m = uud \cdots dd$ reads,

$$\begin{aligned} L_u(i_1, i_2) &= i_3, \\ L_u(i_2, i_3) &= i_4, \\ L_f(i_3, i_4) &= i_5, \\ L_d(i_4, i_5) &= i_6, \\ &\dots \dots \dots \\ L_d(i_{m-1}, i_m) &= i_{m+1}, \\ L_d(i_m, i_{m+1}) &= i_{m+2}. \end{aligned}$$

For any pair of initial integers (i_1, i_2) from \mathbb{I} the remaining indices $i_k, k = 3, \dots, m + 2$ are uniquely defined by Table 1.

Taking the reflect-morphisms representation of a periodic tetrahedral chain with W_m to be a period we see that the corresponding composition $\bar{R}_{i_{m+2}} \cdots \bar{R}_{i_1}$ does not necessarily continue periodically along a chain. It would be so if the L_* -sequence, i.e. ordered (according to \bar{W}_m) collection of mappings L_u, L_d, L_f is cyclic, i.e., if $i_1 = i_{m+1}, i_2 = i_{m+2}$.

Example 6.2. This fact may be easily seen for the three basic periodic chains,

$$\begin{aligned} U \text{ periodic} &: U \cdots U \cdots, \\ D \text{ periodic} &: D \cdots D \cdots, \\ F \text{ periodic} &: F \cdots F \cdots. \end{aligned}$$

In the first two cases the period is a word of two characters, UU, DD . In U (and D) periodic chains the defining numerical sequences are cyclic after four iterations of the L_* -sequence, $L_u L_d, L_u L_d$,

$$\begin{aligned} L_u(i_1, i_2) &= i_3, & L_d(i_2, i_3) &= i_4, \\ L_u(i_3, i_4) &= i_1, & L_d(i_4, i_1) &= i_2, & (i_1, i_2) &\in \mathbb{I}, \end{aligned}$$

which reads in numerical characters

$$I(UUUUUU \cdots) = ududud \cdots, \quad I(DDDDDD \cdots) = dududu \cdots$$

as displayed in Table 4. Obviously the L_* -sequence $L_f L_f$ for the period of F - periodic chain is cyclic, i.e. $L_f(i_1, i_2) = i_1, L_f(i_2, i_1) = i_2, (i_1, i_2) \in \mathbb{I}$.

Corollary 6.3. *Examples of cycles of admissible triplets defining U and D periodic tetrahedral chains are displayed in Table 4.*

U -chains	D -chains
$(3, 2, 1) \rightarrow (2, 1, 4) \rightarrow (1, 4, 3) \rightarrow (4, 3, 2)$	$(2, 1, 4) \rightarrow (1, 4, 3) \rightarrow (4, 3, 2) \rightarrow (3, 2, 1)$
$(4, 3, 1) \rightarrow (3, 1, 2) \rightarrow (1, 2, 4) \rightarrow (2, 4, 3)$	$(3, 1, 2) \rightarrow (1, 2, 4) \rightarrow (2, 4, 3) \rightarrow (4, 3, 1)$
$(2, 4, 1) \rightarrow (4, 1, 3) \rightarrow (1, 3, 2) \rightarrow (3, 2, 4)$	$(4, 1, 3) \rightarrow (1, 3, 2) \rightarrow (3, 2, 4) \rightarrow (2, 4, 1)$
$(3, 4, 2) \rightarrow (4, 2, 1) \rightarrow (2, 1, 3) \rightarrow (1, 3, 4)$	$(4, 2, 1) \rightarrow (2, 1, 3) \rightarrow (1, 3, 4) \rightarrow (3, 4, 2)$
$(4, 1, 2) \rightarrow (1, 2, 3) \rightarrow (2, 3, 4) \rightarrow (3, 4, 1)$	$(1, 2, 3) \rightarrow (2, 3, 4) \rightarrow (3, 4, 1) \rightarrow (4, 1, 2)$
$(4, 2, 3) \rightarrow (2, 3, 1) \rightarrow (3, 1, 4) \rightarrow (1, 4, 2)$	$(2, 3, 1) \rightarrow (3, 1, 4) \rightarrow (1, 4, 2) \rightarrow (4, 2, 3)$
$(1, 4, 3) \rightarrow (4, 3, 2) \rightarrow (3, 2, 1) \rightarrow (2, 1, 4)$	$(4, 3, 2) \rightarrow (3, 2, 1) \rightarrow (2, 1, 4) \rightarrow (1, 4, 3)$
$(1, 2, 4) \rightarrow (2, 4, 3) \rightarrow (4, 3, 1) \rightarrow (3, 1, 2)$	$(2, 4, 3) \rightarrow (4, 3, 1) \rightarrow (3, 1, 2) \rightarrow (1, 2, 4)$
$(1, 3, 2) \rightarrow (3, 2, 4) \rightarrow (2, 4, 1) \rightarrow (4, 1, 3)$	$(3, 2, 4) \rightarrow (2, 4, 1) \rightarrow (4, 1, 3) \rightarrow (1, 3, 2)$
$(2, 1, 3) \rightarrow (1, 3, 4) \rightarrow (3, 4, 2) \rightarrow (4, 2, 1)$	$(1, 3, 4) \rightarrow (3, 4, 2) \rightarrow (4, 2, 1) \rightarrow (2, 1, 3)$
$(2, 3, 4) \rightarrow (3, 4, 1) \rightarrow (4, 1, 2) \rightarrow (1, 2, 3)$	$(3, 4, 1) \rightarrow (4, 1, 2) \rightarrow (1, 2, 3) \rightarrow (2, 3, 4)$
$(3, 1, 4) \rightarrow (1, 4, 2) \rightarrow (4, 2, 3) \rightarrow (2, 3, 1)$	$(1, 4, 2) \rightarrow (4, 2, 3) \rightarrow (2, 3, 1) \rightarrow (3, 1, 4)$

Table 4: Cycles of admissible triplets defining U and D periodic tetrahedral chains.

Example 6.4. Using the cycles of Table 4 the numerical representation for U - periodic tetrahedral chains with the initial $(i_1, i_2) = (3, 2)$ is written in the form

$$L_u(3, 2) = 1, L_d(2, 1) = 4, L_u(1, 4) = 3, L_d(4, 3) = 2.$$

And the corresponding composition defining the principal operator $M_U = \bar{R}_4 \bar{R}_1 \bar{R}_2 \bar{R}_3$ reconstructs this periodic chain geometrically.

For L_* -sequence of U (D resp.) periodic tetrahedral chain we associate a corresponding operator $M_U = \bar{R}_{i_4} \cdots \bar{R}_{i_1}$ (M_D resp.) such that the U - periodic chain is a composition of M_U (M_D resp.). Here $M_F = \bar{R}_{i_2} \bar{R}_{i_1}$.

Recall $\mathbb{I} = \{(\alpha, \beta) \in \Delta_4 \times \Delta_4 : \alpha \neq \beta\}$, $\#\mathbb{I} = 12$. Any two consecutive indexes i_k, i_{k+1} determine uniquely the third one i_{k+2} for an element of the chain of type D, F, U , and so on for subsequent pair i_{k+1}, i_{k+2} . Then we naturally define the corresponding maps

$$(12) \quad \mathcal{L}_u, \mathcal{L}_d, \mathcal{L}_f : \mathbb{I} \rightarrow \mathbb{I},$$

$\mathcal{L}_*(i_1, i_2) = (i_2, L_*(i_1, i_2)), * \in \{d, f, u\}$. $\#\mathbb{I} = 12$ and on the basis of Table 1 \mathcal{L}_* are bijections of \mathbb{I} .

For any word W_m of length m we define the mapping $\mathcal{L}_{W_m} : \mathbb{I} \rightarrow \mathbb{I}$, $\mathcal{L}_{W_m}(i_1, i_2) = (i_{m+1}, i_{m+2})$ which is a composition of bijections, $\mathcal{L}_u, \mathcal{L}_d, \mathcal{L}_f$ in the order of the adjoint word \bar{W}_m .

$$\mathcal{L}_* \cdots \mathcal{L}_*(i_1, i_2) = (i_{m+1}, i_{m+2}).$$

This composition of bijections will be called the \mathcal{L} -sequence.

Example 6.5. Any word, say $W_5 = DUUFD$, is represented by \mathcal{L} -sequence. Taking its adjoint word $I(DUUFD) = ddufd$ we write

$$\mathcal{L}_{W_5} = \mathcal{L}_d \mathcal{L}_f \mathcal{L}_u \mathcal{L}_d \mathcal{L}_d.$$

(i_1, i_2)	(1, 2)	(1, 3)	(1, 4)	(2, 1)	(2, 3)	(2, 4)	(3, 1)	(3, 2)	(3, 4)	(4, 1)	(4, 2)	(4, 3)
$\mathcal{L}_{W_5}(i_1, i_2)$	(1, 3)	(1, 4)	(1, 2)	(2, 4)	(2, 1)	(2, 3)	(3, 2)	(3, 4)	(3, 1)	(4, 3)	(4, 1)	(4, 2)

Table 5: Table of the mapping \mathcal{L}_{dduufd} .

There is a natural question, whether any periodic tetrahedral chain, with period W_m is represented by a principal operator M_{W_m} , i.e. a finite composition of reflect-morphisms defined by a cycling \mathcal{L} -sequence \mathcal{L}_{W_m} , such that $\mathcal{L}_{W_m}(i_1, i_2) = (i_1, i_2)$. If we have the principal operator M_{W_m} for a periodic chain, then any part of the chain of length kn is represented by ordered composition of reflect-morphism in $M_{W_m}^k$.

Theorem 6.1. *For any periodic tetrahedral chain with a period W_m there exists a principal operator $M_{W_m} : \mathcal{T} \rightarrow \mathcal{T}$ consisting of a composition of reflect-morphisms $\bar{R}_i, i = 1, \dots, 4$, defined by a cycling composition of a numerical representation \mathcal{L}_{W_m} .*

Proof. To each period W_m we prescribe uniquely a bijection \mathcal{L}_{W_m} of the twelve-element set \mathbb{I} . $\mathcal{L}_{W_m} \in S_{12}$, and as an element of the symmetric group has a finite order, say k such that $\mathcal{L}_{W_m}^k = id_{\mathbb{I}}$. Thus for any pair $(i_1, i_2) \in \mathbb{I}$ after $mk + 2$ steps we get a cycle property. \square

A collection of \mathcal{L} -sequences is denoted by $\Gamma_{\mathcal{L}}$. To each element of $\Gamma_{\mathcal{T}}$ which can be treated also as an adjoint word, we associate uniquely a composition of reflect-morphisms $\bar{R}_{i_n} \cdots \bar{R}_{i_1}$ representing the corresponding configuration of d, f, u elements in a chain. By construction of the sequence of

numbers i_1, \dots, i_n in the reflect-morphism representation (see Section 2) the elements of $\Gamma_{\mathcal{T}}$ are indexed uniquely by the finite \mathcal{L} -sequences belonging to $\Gamma_{\mathcal{L}}$. These sequences are built of three bijections $\mathcal{L}_u, \mathcal{L}_d, \mathcal{L}_f$ which are elements of the permutation group S_{12} , i.e there is a well defined map $\Gamma_{\mathcal{T}} \rightarrow \Gamma_{\mathcal{L}}$ of finite words of $\Gamma_{\mathcal{T}}$ into the space of finite formal sequences of these three bijections. Taking the final composition of the corresponding \mathcal{L} - sequence elements as elements of the permutation group S_{12} , we get the *indexing map*, $\Phi : \Gamma_{\mathcal{L}} \rightarrow S_{12}$. To each tetrahedral chain an indexing map Φ associates bijection $\mathbb{I} \rightarrow \mathbb{I}$. Image of an indexing map Φ is called the indexing space of $\Gamma_{\mathcal{T}}$.

Theorem 6.2. *The indexing space of $\Gamma_{\mathcal{T}}$ is a tetrahedral group. $\Phi(\Gamma_{\mathcal{T}})$ is a tetrahedral subgroup of S_{12} generated by three elements,*

$$\mathcal{L}_u, \quad \mathcal{L}_d, \quad \mathcal{L}_f$$

with the relations

$$(13) \quad \mathcal{L}_u^3 = id, \quad \mathcal{L}_d^3 = id, \quad \mathcal{L}_f^2 = id, \quad (\mathcal{L}_u \mathcal{L}_d)^2 = id.$$

Elements $\mathcal{L}_u, \mathcal{L}_d$, with relations $\mathcal{L}_u^3 = id, \mathcal{L}_d^3 = id, (\mathcal{L}_u \mathcal{L}_d)^2 = id$ generate the tetrahedral group T of 12 elements.

$$T = \{id, \mathcal{L}_u, \mathcal{L}_d, \mathcal{L}_u^2, \mathcal{L}_d^2, \mathcal{L}_d \mathcal{L}_u, \mathcal{L}_u \mathcal{L}_d, \mathcal{L}_u^2 \mathcal{L}_d, \mathcal{L}_u \mathcal{L}_d^2, \mathcal{L}_d^2 \mathcal{L}_u, \mathcal{L}_d \mathcal{L}_u^2, \mathcal{L}_u \mathcal{L}_d^2 \mathcal{L}_u\}.$$

Example 6.6. To each tetrahedral chain, defined by a word W_m , the indexing map Φ associates a reduced word being an element of a tetrahedral group generated by $\mathcal{L}_u, \mathcal{L}_d, \mathcal{L}_f$ with the relations. For the word $W_6 = UFUFDD$ we have $I(W_6) = ufufdu$ and $\Phi(I(W_6)) = \mathcal{L}_u \circ \mathcal{L}_d \circ \mathcal{L}_f \circ \mathcal{L}_u \circ \mathcal{L}_f \circ \mathcal{L}_u = \mathcal{L}_u^2$. And finally an indexing word is equal to UD .

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