FUNDAMENTAL GROUP ALGORITHM FOR LOW DIMENSIONAL TESSELLATED CW COMPLEXES.

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Abstract. We present a detailed description of a fundamental group algorithm based on Forman’s combinatorial version of Morse theory. We use this algorithm in a classification problem of prime knots up to 14 crossings.

1. Introduction

The aim of this paper is twofold. We present the mathematical details of the algorithm for computing a presentation of the fundamental group of a finite regular CW complex which was introduced in [2] and which is based on Forman’s combinatorial version of Morse theory [9]. We also present details of the performance of a C++ implementation of the algorithm. To assess the performance we systematically apply the algorithm to spaces arising as complements of prime knots on fourteen or fewer crossings and use the resulting fundamental group presentation, with standard low-index subgroup procedures, to distinguish between the knots.

1.1. Prior work. The combinatorially defined edge-path group of a connected simplicial complex K, due to Reidemeister, is well-known to be isomorphic to the fundamental group \( \pi_1(K) \) (see [27]). It is also well-known that this combinatorial definition and isomorphism extends to connected regular CW-spaces. In this paper we use the terms edge-path group and fundamental group interchangeably as synonyms. Several authors have described algorithms for implementing Reidemeister’s edge-path group. Rees and Soicher [26] use spanning trees and redundant relator searches in their description of an algorithm for finding a small finite presentation of the edge-path group of a 2-dimensional combinatorial cell complex; they implement their algorithm in GAP [12] for 2-dimensional simplicial clique complexes of graphs. Letscher [21] uses spanning trees and Tietze elimination/reduction of relators to compute edge-path groups from the 2-skeleta.

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of simplicial complexes arising from knot complements, the knots being produced from experimental data on protein backbones. Palmieri et al. [25] have implemented the edge-path group of simplicial complexes in Sage [28]; the implementation uses the 2-skeleton of the complex and calls GAP’s Tietze reduction/elimination procedures [12]. Kim et al. [18] describe an algorithm for the fundamental groups of 3-dimensional simplicial complexes; their algorithm, which makes use of 3-dimensional cells and the language of general CW-spaces, is applied to 3-dimensional tetrahedral meshes arising in computer vision.

We also mention that there is a large literature on the related problem of algorithmically determining a collection of shortest generating loops for the fundamental group of a space. The case of oriented combinatorial 2-manifolds is treated by Ericson and Whittlesey in [10]; their algorithm involves the computation of spanning trees.

1.2. Our contribution. Recall that a combinatorial vector field on a regular CW complex $X$ is a partition $V$ of cells of $X$ into singletons and doubletons such that each doubleton consists of a cell and one of its facets, that is, one of its faces of codimension 1. The singletons are called critical cells, the doubletons are called vectors. The combinatorial vector field is acyclic if the facet digraph of $X$, with direction reversed on edges in $V$, is acyclic. The algorithm we propose (Algorithm 3.1) inputs a connected finite regular CW complex $X$, constructs a homotopy equivalent CW complex $X'$ with potentially fewer cells, and outputs the finite presentation for $\pi_1(X)$ corresponding to the 2-skeleton of $X'$. The algorithm runs in linear time with respect to the number of cells in $X$ (see Theorem 3.2). However, its usefulness depends on the size of $X'$. We have no estimate for the number of cells in $X'$ other than it will be no greater than the number of cells in $X$. However, from several numerical experiments we see that $X'$ is usually significantly smaller than $X$.

At the heart of the algorithm is Forman’s theorem [9, Corollary 3.5] stating that an acyclic combinatorial vector field $V$ on a regular CW complex $X$ leads to another, homotopic, CW complex whose cells are in one-to-one correspondence with the critical cells of $V$. In order to justify the correctness of the algorithm we rework in an algorithmic, recursive spirit the proof of Forman’s theorem. We actually show that the vectors of $V$ may be quotiented out one by one until no vector is left.

We implemented the algorithm in C++ [4]. The implementation aims at large CW complexes arising from real-world data such as protein backbone complements or point-cloud data sets. However, in order to systematically study the performance of the algorithm, in this paper we apply it to a family of small cubical complexes arising as the complements of prime knots given in terms of efficient arc presentations [19]. We have chosen to work with this case, because it provides a large source of examples whose complexity can, to some extent, be measured by the number of crossings in the knots.
Recall that in [2] we proposed a computable, algebraic invariant of prime knots and used it to classify, up to mirror image, all prime knots up to 11 crossings. The invariant is constructed from low-index subgroups of the fundamental group of the complement of the knot with the index not exceeding 6. The C++ implementation of our algorithm enables fast computation of the presentation of the fundamental group. This lets us increase the classification in [2] from 801 knots up to 11 crossings to 59937 prime knots up to 14 crossings in the tabulation provided by Hoste, Thistlethwaite and Weeks in [16] and available from [19]. The C++ implementation shifted the computational barrier from the presentation of the fundamental group computations to the algebraic invariant computations. The latter are performed in GAP [12] and HAP [7].

The organization of the paper is as follows. In Section 2 we gather notation and preliminaries. In Section 3 we present a recursive approach to the discrete Morse theory. In Section 4 we study various reduction techniques. In Section 5 we present the algorithms. In Section 6 we apply the results of the paper to knot classification.

2. Preliminaries

2.1. Notation. Let \( \mathbb{N} := \{1, 2, 3, \ldots\} \) stand for the set of natural numbers, \( \mathbb{R} \) for the set of reals and let \( I \) denote the interval \([0, 1]\). We write \( f : X \rightarrow \top Y \) for a partial map from \( X \) to \( Y \), that is a map defined on a subset \( \text{dom} \; f \subset X \), called the domain of \( f \), and such that the set of values of \( f \), denoted \( \text{im} \; f \), is contained in \( Y \). Given a topological space \( X \) we write \( \text{cl} \; A \) for the closure of \( A \subset X \).

For \( n \in \mathbb{N} \) we write

\[
B^n := \{ x \in \mathbb{R}^n \mid ||x|| \leq 1 \},
S^{n-1} := \{ x \in \mathbb{R}^n \mid ||x|| = 1 \},
B^{n-1} := \{ x = (x_1, x_2, \ldots, x_n) \in S^{n-1} \mid x_n \leq 0 \},
B^{n-1}_+ := \{ x = (x_1, x_2, \ldots, x_n) \in S^{n-1} \mid x_n \geq 0 \},
\hat{B}^n := \{ x \in \mathbb{R}^n \mid ||x|| < 1 \}.
\]

Note that in particular \( B^1 = [-1, 1] \) and \( S^0 = \{-1, 1\} \). We extend this notation to \( n = 0 \) by setting

\[
\hat{B}^0 := B^0 := \{\ast\},
S^{-1} := \emptyset,
\]

where \( \ast \) is a unique point not belonging to any other set considered in this paper.

Let \( A \) be any set. An oriented element of \( A \) is \( a^\varepsilon := (a, \varepsilon) \) for \( \varepsilon \in \{-1, 1\} \) and \( a \in A \). We denote the set of oriented elements of \( A \) by \( \hat{A} \). We identify \( a^1 \) with \( a \) and we say that \( a \) and \( a^{-1} \) have mutually inverse orientation.
By a path in a topological space \( X \) we mean a continuous function \( \theta : B^1 = [-1,1] \to X \). We identify the oriented path \( \theta^1 \) with \( \theta \) and \( \theta^{-1} \) with the path
\[
B^1 \ni t \mapsto \theta(-t) \in X.
\]
We refer to \( \theta^{-1} \) as the inverse path of \( \theta \).

2.2. Directed multigraphs. Recall that a directed multigraph is a quadruple \( G = (V, E, e_-1, e_+1) \), where \( e_-1, e_+1 : E \to V \) are given maps. The set \( V \) is the set of vertices of \( G \), the set \( E \) is the set of edges of \( G \) and the maps \( e_-1, e_+1 \) assign to each edge its initial and terminal vertex respectively.

A path in \( G \) is a sequence of oriented edges \( \eta := e_1^1 e_2^2 \cdots e_n^n \) such that \( e_{k+1}(e_k) = e_{k-1}(e_{k+1}) \) for \( k = 1, \ldots, n - 1 \). The initial vertex of the path \( \eta \) is \( e_{-1}(e_1) \) and the terminal vertex of the path \( \eta \) is \( e_n(e_n) \). The path \( \eta \) is a cycle if the terminal and initial vertices coincide. The inverse of the path \( \eta \) is \( \eta^{-1} := e_{n-1}^e e_{n-2}^e \cdots e_1^e \).

Let \( \zeta \) be a path in \( G \) with the same initial and terminal vertices as an edge \( z \in E \). Moreover, assume that neither \( z \) nor \( z^{-1} \) appear in \( \zeta \). Let \( \eta \) be a path in \( G \). A \((z, \zeta)\)-substitution in \( \eta \), denoted \( S_{z, \zeta}(\eta) \), is the path obtained from \( \eta \) by replacing every occurrence of \( z \) in \( \eta \) by \( \zeta \) and every occurrence of \( z^{-1} \) in \( \eta \) by \( \zeta^{-1} \).

2.3. Quotient spaces. We recall from [6] some facts concerning quotient topological spaces. Given an equivalence relation \( R \) on a topological space \( X \), we denote by \( [x]_R \) the equivalence class of \( x \in X \) and by \( X/R \) the set of all equivalence classes of \( R \). Let \( \kappa_R : X \ni x \mapsto [x]_R \in X/R \) be the canonical projection. We drop the subscript \( R \) whenever the relation \( R \) is clear from context. The quotient topology on \( X/R \) consists of subsets \( A \subset X/R \) such that \( \kappa_R^{-1}(A) \) is open in \( X \).

**Proposition 2.1.** [6] Proposition 2.4.14 Assume \( R \) is an equivalence relation on \( X \) and \( S \) is an equivalence relation on \( X/R \). Then, \( X/R/S \) is homeomorphic to \( X/R_S \), where \( R_S \) is an equivalence relation on \( X \) defined by \( xR_S y \) if and only if \( \kappa_S(\kappa_R(x)) = \kappa_S(\kappa_R(y)) \).

Given a partial continuous map \( f : Y \to X \) such that \( \text{dom} \ f \) is closed in \( Y \) we define \( X \cup_f Y \) as the quotient space \( (X \cup Y)/R_f \) of the disjoint union \( X \sqcup Y \) by the equivalence relation \( R_f \) which identifies \( x \in \text{dom} \ f \) with \( f(x) \in X \). For \( z \in X \sqcup Y \) we denote by \( [z]_f \) the equivalence class of the relation \( R_f \). Note that if \( f \) is empty, then \( X \cup_f Y \) coincides with \( X \sqcup Y \).

In the special case when \( Y = B^n \) and \( \text{dom} \ f = S^{n-1} \) we say that \( X \cup_f Y \) results from \( X \) by gluing an \( n \) dimensional cell via the attaching map \( f \).

The relation \( R \) is called closed if the map \( \kappa_R \) is closed. The following proposition is a special case of [6] Proposition 2.4.9.

**Proposition 2.2.** The relation \( R \) is closed if and only if for any open \( U \) in \( X \) the set
\[
U_R := \{ x \in U \mid [x]_R \subset U \}
\]
is open in $X$.  

The following proposition is an easy consequence of Proposition 2.2.

**Proposition 2.3.** Assume $Y \subset X$ is closed and $R$ is a closed equivalence relation in $Y$. Then $\bar{R} := R \cup \text{id}_X$ is a closed equivalence relation on $X$.  

**Proposition 2.4.** Assume $X$ is a Hausdorff topological space and $R$ is a closed equivalence relation in $X$ with compact equivalence classes. Then $X/R$ is a Hausdorff space.

**Proof:** Let $[x] \neq [y]$ be two equivalence classes of $R$. Since they are compact and $X$ is a Hausdorff space, we can find disjoint open sets $U, V$ in $X$ such that $[x] \subset U$ and $[y] \subset V$. By Proposition 2.2, $U_R$ and $V_R$ are open in $X$. It follows that $\kappa(U_R)$, $\kappa(V_R)$ are disjoint, open in $X/R$. Obviously, they are neighbourhoods respectively of $[x]$ and $[y]$. Hence, $X/R$ is a Hausdorff space. \hfill $\Box$

Given $A \subset \bar{X}$ we denote by $X/A$ the quotient space $X/R_A$, where

$$R_A := \{(x, y) \in X^2 \mid x = y \text{ or } x \in A \text{ and } y \in A\}.$$  

2.4. **Finite CW complexes.** In this paper by a CW complex we always mean a finite CW complex. Here we recall its definition. Let $K$ be a Hausdorff topological space. A finite CW structure on $K$ is a pair $(\mathcal{K}, \{\varphi_\sigma\}_{\sigma \in \mathcal{K}})$ such that $\mathcal{K}$ is a finite family of subsets of $K$ and:

- **(CW0)** Each element $\sigma \in \mathcal{K}$ is a subset of $K$ homeomorphic to $B^n$ for some $n \geq 0$. The subset $\sigma$ is referred to as an $n$-cell. The number $n$ is called the dimension of $\sigma$ and denoted $|\sigma|$. The dimensions provide a filtration $K^j := \bigcup \{ \sigma \in \mathcal{K} \mid |\sigma| \leq j \}$.

- **(CW1)** The family $\mathcal{K}$ is a decomposition of $K$, i.e. $K = \bigcup \mathcal{K}$ and any two different elements of $\mathcal{K}$ are disjoint.

- **(CW2)** Each $\varphi_\sigma$ is a continuous map $\varphi_\sigma : B^{|\sigma|} \to K$ mapping $B^{|\sigma|}$ homeomorphically onto $\sigma$ and $\varphi_\sigma(S^{|\sigma|-1}) \subset K^{|\sigma|-1}$. The map $\varphi_\sigma$ is called the characteristic map of $\sigma$.

A finite CW complex (cf. [5] Section I.3) is a triple $(K, \mathcal{K}, \{\varphi_\sigma\}_{\sigma \in \mathcal{K}})$ such that $(\mathcal{K}, \{\varphi_\sigma\}_{\sigma \in \mathcal{K}})$ is a finite CW structure on $K$. It is convenient to slightly abuse the language and refer to $K$ as the CW complex, assuming that the CW structure is given implicitly.

The CW complex is called regular if each $\varphi_\sigma : B^{|\sigma|} \to K$ is a homeomorphism onto its image.

By the boundary of a cell $\sigma$ we mean the set $\text{Bd} \sigma := \text{cl} \sigma \setminus \sigma$. We say that a cell $\tau$ is a face of a cell $\sigma$ if $\tau \cap \text{cl} \sigma \neq \emptyset$. The face is proper if $\tau \neq \sigma$. The face is a facet if $|\tau| = |\sigma| - 1$. A 0-dimensional cell is called a vertex.

We refer to the collection of facets of a cell $\sigma$ as its combinatorial boundary and we denote it by $\text{bd} \sigma$. It is also convenient to consider the collection of cells whose facet is $\sigma$. This collection is called the combinatorial coboundary of $\sigma$ and is denoted $\text{cbd} \sigma$. Note that if $\sigma$ is a 1-cell, then...
bd \sigma = \{ \varphi(-1), \varphi(1) \}. In the case of a 1-cell these two facets (or one if \varphi(-1) = \varphi(1)) are referred to as the \textit{endpoints} of \sigma.

A cell is \textit{top-dimensional} if it is not a proper face of a higher dimensional cell. The CW structure and CW complex are called \textit{pure} if all top-dimensional cells have the same dimension. We will refer to the closure of a top-dimensional cell as a \textit{toplex}. It is easily seen that a CW complex is the union of its toplexes.

A union \( L := \bigcup L \) of a subfamily \( L \subset K \) such that \( L \) is closed in \( K \) is called a \textit{subcomplex} of \( K \). A subcomplex is a CW complex with its CW structure consisting of \( L \) with the same characteristic maps as in \( K \). Note that, in particular, every vertex is a subcomplex. Also, \( \bigcup K^j \) is a subcomplex, called the \textit{j-skeleton} of \( K \).

Since by [10, Theorem 1.4.10] the closure of a cell in a regular CW complex is a subcomplex, we have the following proposition.

\textbf{Proposition 2.5.} If cells \( \sigma, \tau \) in a regular CW complex satisfy \( \tau \cap \text{cl} \sigma \neq \emptyset \), then \( \tau \subset \text{cl} \sigma \), i.e. \( \tau \) is a face of \( \sigma \). \( \square \)

As a consequence of Proposition 2.5 we obtain the following proposition.

\textbf{Proposition 2.6.} Assume \( \tau \) is a proper face of \( \sigma \) in a regular CW complex \( X \). Then \( \tau \) is a facet of a face of \( \sigma \).

\textbf{Proof:} Set \( n := |\sigma| \). Since \( X \) is regular, \( \text{Bd} \sigma \) is homeomorphic to \( S^{n-1} \). Let \( k := |\sigma| - |\tau| \). Since \( \tau \) is a proper face of \( \sigma \) we have \( k > 0 \). We proceed by induction on \( k \). If \( k = 1 \) the claim is obvious. Thus, assume \( k > 1 \). Let \( x \in \tau \) and consider a shrinking sequence of open balls in \( \text{Bd} \sigma \) centered at \( x \). All these balls are homeomorphic to \( B^{n-1} \) and none of these balls is contained in \( \tau \), because otherwise \( |\tau| = n - 1 \) and \( k = 1 \). Thus, there exists a sequence \( \{ x_j \} \subset \text{Bd} \sigma \setminus \tau \) converging to \( x \). By passing to a subsequence, if necessary, we may assume that the sequence is contained in a cell \( \sigma' \subset \text{Bd} \sigma \). It follows that \( \tau \cap \text{cl} \sigma' \neq \emptyset \) and, by the regularity of \( X \), \( \tau \) is a face of \( \sigma' \). The conclusion now follows from the induction assumption, because \( |\sigma'| - |\tau| < k \). \( \square \)

\textbf{Proposition 2.7.} ([10] Proposition 1.5.17) A finite CW complex is a metrizable topological space. \( \square \)

Note that if \( h : B^n \to B^n \) is a homeomorphism, then \( h \) maps homeomorphically \( \tilde{B}^n \) onto \( \tilde{B}^n \) and \( S^{n-1} \) onto \( S^{n-1} \). In consequence, if \( \varphi_\sigma \) is a characteristic map, then so is \( \varphi_\sigma \circ h \). Thus, we can freely substitute homeomorphisms into characteristic maps without loosing the CW structure. In particular, in the characteristic map \( \varphi_\sigma \) we can replace \( B^n \) by any set homeomorphic to \( B^n \).

Let \( \sigma \) be a top-dimensional cell of \( K \). Then \( K \setminus \sigma \) is easily seen to be a subcomplex of \( K \) and \( K \) results from \( K \setminus \sigma \) by gluing \( B^{|\sigma|} \) via the attaching map \( \theta_\sigma := \varphi_\sigma|S^{|\sigma| - 1} \).
Let $\sigma = (\sigma_j)_{j=1}^k$ be an admissible ordering of the cells of $K$, i.e., an ordering of all cells in $K$ such that each cell is preceded by its faces. For $j = 1, 2, \ldots, k$ set

$$\Sigma_j := \bigcup_{i=1}^j \sigma_i.$$  

It is not difficult to prove that each $\Sigma_j$ is closed in $K$, hence a subcomplex of $K$ and $\Sigma_j$ results from $\Sigma_{j-1}$ by gluing the cell $\sigma_j$ via the attaching map $\theta_{\sigma_j} = \varphi_{\sigma_j} \mid S^{[\sigma_j]}$. 

One easily verifies that an admissible ordering always exists on a finite CW complex. Moreover, when $L$ is a subcomplex of $K$, then one can choose the ordering in such a way that $L = \Sigma_l$ for some $l \leq k$. Thus, we have the following standard result.

**Proposition 2.8.** Each finite CW-complex can be constructed recursively by attaching a cell to a subcomplex. □

We will use also the following fact which is a special case of [20, Theorem 11.11].

**Theorem 2.9.** Assume $X_1, X_2$ are homotopy equivalent spaces and $h : X_1 \to X_2$ is a homotopy equivalence. If maps $f_1 : S^{n-1} \to X_i$ are such that $f_2 = h \circ f_1$, then the spaces $X_1 \cup f_1 B^n$ and $X_2 \cup f_2 B^n$ are homotopy equivalent. □

2.5. Oriented CW complexes. Our fundamental group algorithm of a CW complex $X$ is based on a theorem reducing the computation to a group generated by the 1-cells with relators provided by the 2-cells. To present the theorem in detail, we recall the definition of the orientation of an $n$-cell $\sigma$ in $X$. For $n = 0$ it is just an element of $\{-1, 1\}$. For $n > 0$ it is an equivalence class in the homotopy equivalence relation of the characteristic map $\varphi_{\sigma} : (B^n, S^{n-1}) \to (\text{cl} \sigma, \text{Bd} \sigma)$ considered as a map of pairs. By [13, Corollary 2.5.2] there are precisely two orientations for each cell. An oriented CW complex is a CW complex with a fixed orientation for every its cell.

Assume $K$ is an oriented 2-dimensional CW complex. By an edge in $K$ we mean an oriented 1-cell. An edge $\tau$, as each 1-cell, has two endpoints $\varphi_{\tau}(-1)$ and $\varphi_{\tau}(1)$. The orientation allows us to distinguish between them. The first is called the initial vertex of $\tau$ and denoted $e_-(\tau)$, the other is called the terminal vertex of $\tau$ and denoted $e_+(\tau)$. Thus, the CW structure of the 1-skeleton of $K$ may be considered as a directed multigraph. A characteristic map of an edge is a characteristic map $\varphi_{\tau}$ of the associated 1-cell which induces the chosen orientation of the edge.

Consider now a 2-cell $\sigma$. There is a closed path $\tau_1, \tau_2, \ldots, \tau_n$ in the directed multigraph of edges such that the homotopy class of the attaching map $\theta_{\sigma}$ contains a map $\theta : S^1 \to K^1$ such that $S^1 = \bigcup_{j=1}^n I_j$ and $\theta_{I_j}$ is the characteristic map of the edge $\tau_j$ (see [13, Proposition 3.1.1 and 3.1.2]). The loop $\tau_1, \tau_2, \ldots, \tau_n$ is called the homotopically boundary of $\sigma$. We have the following theorem.
Theorem 2.10. ([13] Proposition 3.1.7 and Theorem 3.1.8) Assume $K$ is a connected CW complex with precisely one vertex. Then, the fundamental group of $K$ depends only on the 2-skeleton of $K$. Moreover, up to an isomorphism it is the group generated by the edges of $K$ with arbitrarily selected orientation of $K$ and homotopical boundaries of all 2-cells as relators.

3. Discrete Morse theory

3.1. Reduction pairs. We say that a facet $\alpha_0$ of an $n$-cell $\alpha_1$ is regular if $\varphi_{\alpha_1}(S^{n-1})$ is a subcomplex of $K$, $\varphi_{\alpha_1}|_{B^n_0}$ is the characteristic map of $\alpha_0$, and $\varphi_{\alpha_1}(B^n_0) \cap \alpha_0 = \emptyset$.

Note that in a regular CW complex each facet is automatically regular.

We say that $\alpha := (\alpha_0, \alpha_1)$ is a reduction pair in a CW complex $K$ if $\alpha_0$ is a regular facet of $\alpha_1$. The following proposition is straightforward.

Proposition 3.1. If $L$ is a subcomplex of $K$ and $\alpha$ is a reduction pair in $L$, then $\alpha$ is a reduction pair in $K$. \qed

3.2. Discrete vector fields. A discrete vector field $V$ on the CW structure $K$ is a partition of $K$ into singletons and doubletons such that each doubleton, when ordered by dimension, forms a reduction pair. By a critical cell of $V$ we mean a cell $\alpha \in K$ such that $\{\alpha\}$ is a singleton in $V$. We denote the set of critical cells of $V$ by $\text{crit}_V$. By pairing the lower dimensional cell with the higher dimensional cell in every doubleton of $V$ we may and will consider $V$ as an injective partial self-map $V: K \rightarrow K$ such that $K$ is the disjoint union of $\text{dom}_V$, $\text{im}_V$ and $\text{crit}_V$ and for each $\alpha \in \text{dom}_V$ the pair $(\alpha, V(\alpha))$ is a reduction pair. We will call such a reduction pair a vector of $V$.

With $V$ we associate a directed graph, $G_V$. Its vertices are the cells of $K$ and edges go from each cell $\sigma$ to each of its facets $\tau$ with orientation reversed if $\sigma = V(\tau)$. If $G_V$ is acyclic, the discrete vector field $V$ is called acyclic. In this case the graph $G_V$ induces a partial order on the cells in $K$. In particular, for each cell $\sigma \in K$ there is a minimal cell less than or equal to $\sigma$ in this partial order. We say about such a cell that it is inferior to $\sigma$.

Assume now that $K$ is a regular CW complex with a CW structure $K$. An algorithm constructing an acyclic discrete vector field on $K$ is presented in Table 1. It is a simplified version of the algorithm proposed in [14, 15], based on the method of coreductions [23].

For a CW structure $K$ let $M(K)$ denote the maximal cardinality of $\text{bd} \sigma$ and $\text{cbd} \sigma$ over all $\sigma \in K$.

Theorem 3.2. Assume Algorithm 3.1 in Table 1 is called with $K$ containing a CW structure of a non-empty, regular, connected finite CW complex $K$. The algorithm always stops, returning an acyclic vector field on $K$. Moreover, on return $C$ contains the respective set of critical cells with precisely one critical cell in dimension zero. If the data structure used to store the
Algorithm 3.1. discreteVectorField(CW structure $\mathcal{K}$)

$V := L := C := \emptyset$;
while $\mathcal{K} \neq \emptyset$ do
  if $L = \emptyset$ then
    $n := \min \{ q \mid \mathcal{K}^q \neq \emptyset \}$;
    move an element $r$ from $\mathcal{K}^n$ to $C$;
    for each $u \in (\mathcal{K} \cap \text{cbd} r) \setminus L$ do enqueue $u$ in $L$;
  else
    $\sigma :=\text{dequeue}(L)$;
    if $\mathcal{K} \cap \text{bd} \sigma = \{ \tau \}$ then
      remove $\tau$ and $\sigma$ from $\mathcal{K}$ and insert $(\tau, \sigma)$ to $V$;
      for each $u \in (\mathcal{K} \cap \text{cbd} \tau) \setminus L$ do enqueue $u$ in $L$;
    else if $\mathcal{K} \cap \text{bd} \sigma = \emptyset$ then
      for each $u \in (\mathcal{K} \cap \text{cbd} \sigma) \setminus L$ do enqueue $u$ in $L$;
  return $V$;

Table 1. Discrete Vector Field by coreduction method

$CW$ complex provides iteration over the boundary and coboundary of a cell as well as removing a cell in $O(M)$ time with $M := M(\mathcal{K})$, then the algorithm runs in $O(M^2 \text{card} \mathcal{K})$ time.

Proof: Observe that if an element $\tau \in \mathcal{K}$ contributes its coboundary elements to $L$ as an element of a coreduction pair $(\tau, \sigma)$, then it is removed from $\mathcal{K}$, so it may never again contribute in this role. Similarly, if an element $\sigma$ with zero boundary contributes its coboundary elements to $L$, it may never again do so, because it is not in the coboundary of any element, so it may not reappear in $L$. Therefore, each element of $S$ may appear in $L$ at most $2M$ times. It follows that the while loop is passed at most $2M \text{card} \mathcal{K}$ times. In particular, the algorithm always stops and its complexity is $O(M^2 \text{card} \mathcal{K})$.

Let $\mathcal{K}_j$, $C_j$ and $V_j$ denote respectively the contents of variable $\mathcal{K}$, $C$ and $V$ on leaving the $j$th pass of the while loop for $j > 0$ and the initial values of these variables for $j = 0$. We will show by induction in $j$ that $V_j$ is an acyclic vector field on $\mathcal{K}$ with $\mathcal{K}_j \cup C_j$ as the set of its critical cells. This is obvious for $j = 0$, because $V_0 = \emptyset$, so every cell is critical. Thus, assume the claim holds for $k < j$. It is obvious that $V_j$ is a discrete vector field on $\mathcal{K}$. We only need to prove that $V_j$ is acyclic. This is evident if $V_j = V_{j-1}$, thus assume $V_j \neq V_{j-1}$. Then $V_j = V_{j-1} \cup \{ (\tau, \sigma) \}$ for some reduction pair $(\tau, \sigma)$. Assume $V_j$ is not acyclic. Then, there exists a cycle $s_0, t_0, s_1, t_1, \ldots, s_n, t_n, s_0$ in $G_{V_j}$ such that $(t_i, s_i) \in V_j$ and $t_i$ is a facet of $s_{(i+1) \text{mod} n}$. In particular, $t_n \in \text{bd} s_0$. Since by induction assumption $V_{j-1}$ is acyclic, precisely one of the pairs $(t_i, s_i)$ is the pair appearing in $V_{j-1}$ on the $j$th pass of the while loop. Without loss of generality we may assume that this is the pair $(t_0, s_0)$. 
Thus, we have $K_{j-1} \cap \text{bd} s_0 = \{ t_0 \}$. In particular, $t_0 \in K_{j-1}$. Since the pair $(t_1, s_1) \in V_j - 1$, it must have been included in the vector field on an earlier pass of the while loop, say $k$th pass with $k < j$. Thus, $K_{k-1} \cap \text{bd} s_1 = \{ t_1 \}$. But $t_0 \notin \text{bd} s_1$, therefore $t_0 \notin K_{k-1}$. However, the sequence $(K_i)$ is clearly decreasing, hence $t_0 \notin K_{j-1}$, a contradiction. This proves that $V_j$ is acyclic for every $j$. In particular, the vector field returned by the algorithm is acyclic. Since after the last pass of the while loop $K = \emptyset$, its critical cells are all stored in $C$.

We still need to prove that $C$ contains precisely one vertex. First observe that for each $j$ the union of the cells in set $A_j := C_j \cup \text{dom} V_j \cup \text{im} V_j$ is a closed subcomplex of $K$. Indeed, this is obviously true for $j = 0$, because $A_0 = \emptyset$. Now, arguing by induction, we see that $A_{j+1} \setminus A_j$ is either empty, or a critical cell in $C_{j+1}$ whose boundary is in $A_j$, or a doubleton $\{ \tau, \sigma \}$ such that $(\tau, \sigma)$ is a reduction pair satisfying $K_j \cap \text{bd} \sigma = \{ \tau \}$, i.e. $bd \sigma \setminus A_j = \{ \tau \}$. Thus, in each case $\bigcup A_j$ is closed, because $\bigcup A_{j-1}$ is closed by induction argument.

Observe that on the very first pass of the while loop a vertex, say $v$, is removed from $K$ and moved to $C$. Thus, we only need to show that this never happens again. Assume the contrary. Let $w$ be another vertex moved to $C$ and assume this happens on the $j$th pass of the while loop. Since $K$ is connected, there is a path $v = v_0, e_0, v_1, e_1, \ldots, e_m = w$ such that each $e_i$ is a 1-cell with endpoints in vertices $v_i$ and $v_{i+1}$. Without loss of generality we may assume that $v_i \in C$ implies $v_i = v$ or $v_i = w$. Since $\bigcup A_{j-1}$ is closed and $v_m \notin A_{j-1}$, we see that also $e_m \notin A_{j-1}$. We will show that also $v_{m-1} \notin A_{j-1}$. If not, then $e_m$ would have been placed on $L$ and then removed together with $v_m$ as a reduction pair before the $j$th pass of the while loop. Arguing by induction, we see that $v_0 \notin A_{j-1}$, a contradiction.

3.3. Quotients of reduction pairs. For a reduction pair $\alpha$ we write $K_\alpha := \text{cl} \alpha_1$, $\varphi_\alpha := \varphi_\alpha$, $|\alpha| := |\alpha_1|$, $K_\alpha^- := \varphi_\alpha(B_0^\alpha)$, $K_\alpha^+ := \varphi_\alpha(B_1^\alpha)$, $K_\alpha^- := K \setminus \alpha_1 \setminus \alpha_0$. Set

$$K_\alpha := \{ \tau \in K \mid \tau \subset K_\alpha \},$$

$$K_\alpha^+ := K_\alpha \setminus \{ \alpha_0, \alpha_1 \}.$$

Lemma 3.3. We have $K_\alpha = \bigcup K_\alpha$ and $K_\alpha^+ = \bigcup K_\alpha^+$. In particular, $K_\alpha$ and $K_\alpha^+$ are subcomplexes of $K$.

Proof: Obviously $\bigcup K_\alpha \subset K_\alpha$. To prove the opposite inclusion take an $x \in K_\alpha$. If $x \in \alpha_1$, then $x \in \bigcup K_\alpha$, because $\alpha_1 \subset K_\alpha$. Otherwise, $x \in \varphi_\alpha(S^{|\alpha|-1})$. By assumption (i) of the definition of a regular facet we have $x \in \tau$ for some cell $\tau \subset \varphi_\alpha(S^{|\alpha|-1})$. But $\varphi_\alpha(S^{|\alpha|-1}) \subset K_\alpha$, hence $x \in \bigcup K_\alpha$. This proves the first equality.

We have

$$K_\alpha = \varphi_\alpha(B_0^\alpha) = \varphi_\alpha(B_0^\alpha) \cup \varphi_\alpha(B_1^\alpha) \cup \varphi_\alpha(B_1^\alpha) = \alpha_1 \cup \alpha_0 \cup K_\alpha^+.$$
But $\alpha_1 \cap K_+ = \emptyset$ by the definition of a cell and $\alpha_0 \cap K_+ = \emptyset$ by the definition of the reduction pair. Therefore,

$$K_+^\alpha = K_\alpha \setminus \alpha_1 \setminus \alpha_0 = \bigcup K_+^\alpha,$$

which shows that $K_\alpha$ is a subcomplex of $K$. □

Let $\chi = (\chi_1, \chi_2) : B^{[\alpha]} \to B^{[\alpha]} - 1 \times I$ be a homeomorphism such that

$$\chi(B_{-}^{[\alpha]}) = B^{[\alpha]} - 1 \times \{1\} \cup S^{[\alpha]} - 1 \times I,$$
$$\chi(B_{+}^{[\alpha]}) = B^{[\alpha]} - 1 \times \{0\}.$$

Set $\chi_\alpha := \varphi_\alpha \circ \chi^{-1}$.

Define the map $f_\alpha : K_\alpha \to K_+^\alpha$ by

$$f_\alpha(x) := \begin{cases} \chi_\alpha(\chi_1(\varphi_\alpha^{-1}(x)), 0) & \text{if } x \in \alpha_1 \cup \alpha_0, \\ x & \text{otherwise.} \end{cases}$$

It is not difficult to check that $f_\alpha$ is well defined and continuous.

**Proposition 3.4.** The map $f_\alpha$ is a retraction of $K_\alpha$ onto $K_+^\alpha$, i.e. $f_\alpha|_{K_+^\alpha} = \text{id}_{K_+^\alpha}$. Moreover, it is a homotopy inverse of the inclusion map $K_+^\alpha \subset K_\alpha$.

**Proof:** The fact that $f_\alpha$ is a retraction is an elementary calculation. To see that $f_\alpha$ is a homotopy equivalence, define a homotopy $h : K_\alpha \times I \to K_+^\alpha$ by

$$h(x, t) := \begin{cases} \chi_\alpha(\chi_1(\varphi_\alpha^{-1}(x)), t\chi_2(\varphi_\alpha^{-1}(x))) & \text{if } x \in \alpha_1 \cup \alpha_0, \\ x & \text{otherwise.} \end{cases}$$

It is not difficult to check that $h$ is well defined, continuous and $h_0 = f_\alpha$, $h_1 = \text{id}_{K_+^\alpha}$.

Define an equivalence relation $R_\alpha$ in $K$ by

$$R_\alpha := \{(x, y) \in K^2 \mid x = y \text{ or } x, y \in K_\alpha \text{ and } f_\alpha(x) = f_\alpha(y)\}.$$

Let $[x]_{\alpha}$ denote the equivalence class of $x$ with respect to $R_\alpha$ and let $\kappa_\alpha : K \owns x \mapsto [x]_{\alpha} \in K/R_\alpha$ denote the quotient map.

**Proposition 3.5.** The space $K/R_\alpha$ is Hausdorff.

**Proof:** Note that $[x]_{\alpha} = f_\alpha^{-1}(f_\alpha(x))$, therefore the equivalence classes of $R$ are compact. Since $K$ is Hausdorff and $K_\alpha$ is closed in $K$, in view of Proposition 2.4 and Proposition 2.3 it is enough to verify that the restriction of $R_\alpha$ to $K_\alpha$ is closed. By Proposition 2.2 it suffices to show that for any $U$ open in $K_\alpha$ the set $U_R$ is open in $K_\alpha$. Assume this is not true. Then, for some $x \in U_R$ no neighbourhood $V$ of $x$ satisfies $V \subset U_R$. Thus, Proposition 2.7 allows us to select a sequence $x_n \to x$ such that $[x_n]_R \not\subset U$. Let $y_n \in [x_n] \setminus U$. Passing to a subsequence, if necessary, we may assume that $y_n \to y \in K \setminus U$. Since $y_n \in [x_n]$, we have $f_\alpha(x_n) = f_\alpha(y_n)$. Thus, $f_\alpha(x) = f_\alpha(y)$. It follows that $[x]_R = [y]_R$. In consequence $y \in U$, a contradiction. □

Set $\kappa_\alpha^+ := \kappa_\alpha|_{K_+^\alpha}$. 
Lemma 3.6. The restriction $\kappa_\alpha^\lambda := \kappa_{\alpha|K_\alpha^\lambda} : K_\alpha^\lambda \rightarrow K/R_\alpha$ is a continuous bijection.

Proof: The map $\kappa_\alpha^\lambda$ is continuous as a restriction of a continuous map. To show that $\kappa_\alpha^\lambda$ is surjective, take an $x \in K$. If $x \notin K_\alpha$, then $\kappa_\alpha(x) = [x]_\alpha$. Hence, assume $x \in K_\alpha$. Since $f_\alpha$ is a retraction onto $K_\alpha^+$, we have $f_\alpha(x) = f_\alpha(f_\alpha(x))$. Thus $[x]_\alpha = [f_\alpha(x)]_\alpha = \kappa_\alpha^+|_{f_\alpha(x)}$, which shows that $\kappa_\alpha^+$ is surjective. Assume in turn that $[x_1]_\alpha = [x_2]_\alpha$ for some $x_1, x_2 \in K$. Then $f_\alpha(x_1) = f_\alpha(x_2)$. If either $x_1$ or $x_2$ is not an element of $K_\alpha$, then both classes are singletons, hence $x_1 = x_2$. Thus, assume that $x_1, x_2 \in K_\alpha^+$. Since $f_\alpha$ is a retraction onto $K_\alpha^+$, we have $x_1 = f_\alpha(x_1) = f_\alpha(x_2) = x_2$, which shows that $\kappa_\alpha^+$ is injective. \hfill $\square$

Lemma 3.7. The restrictions $\kappa_{\alpha|K_\alpha^+}$ and $\kappa_{\alpha|K \setminus K_\alpha}$ are homeomorphisms onto their images.

Proof: By Lemma 3.6 both maps are continuous bijections. Since $K_\alpha$ is compact and $K/R_\alpha$ is Hausdorff, the first restriction is a homeomorphism onto $K_\alpha^+$. To see that the other restriction is a homeomorphism observe that equivalence classes in $K \setminus K_\alpha$ are singletons, therefore $\kappa_\alpha^{-1}(\kappa_\alpha(U)) = U$ for any $U \subset K \setminus K_\alpha$. In particular, for any open set $U \subset K \setminus K_\alpha$ its image $\kappa_\alpha(U)$ is open, which shows that also the other restriction is a homeomorphism. \hfill $\square$

3.4. Collapses. We call the quotient space $K/R_\alpha$ an $\alpha$-collapse of $K$ and write briefly $\kappa_\alpha$ for the quotient map $\kappa_{R_\alpha}$.

By performing a collapse we do not change the homotopy type and stay in the class of CW complexes, as the following theorem shows.

Theorem 3.8. The quotient space $K/R_\alpha$ is a CW-complex with CW structure $\{(\kappa_\alpha(\sigma))_{\sigma \in K \setminus \{a_1, a_0\}}$, $\{(\kappa_\alpha \circ \varphi_\sigma)_{\sigma \in K \setminus \{a_1, a_0\}}\}$. Moreover, the complexes $K$ and $K/R_\alpha$ are homotopy equivalent.

Proof: First recall that by Proposition 3.5 $K/R_\alpha$ is a Hausdorff space. Let $\sigma \in K \setminus \{a_1, a_0\}$. In order to prove property (CW0) of the definition of CW complex it suffices to show that $\kappa_\alpha(\sigma)$ is homeomorphic to $\sigma$. By Lemma 3.3 the set $K_\alpha^+$ is a subcomplex, therefore either $\sigma \subset K_\alpha^+$ or $\sigma \subset K \setminus K_\alpha$. Thus, by Lemma 3.7 in both cases $\kappa_\alpha(\sigma)$ is homeomorphic to $\sigma$, as required. Properties (CW1) and (CW2) are straightforward.

By Proposition 2.8 a complex $K$ may be obtained from $K_\alpha$ by consecutively gluing a sequence $(\sigma_j)$ of cells via the attaching maps $\theta_{\sigma_j}$. It is not difficult to observe that applying to $K_\alpha/R_\alpha$ the same sequence of gluings but with attaching maps $\kappa_\alpha \circ \theta_{\sigma_j}$ we obtain the complex $K/R_\alpha$. Therefore, the conclusion follows by induction from Theorem 2.9 and Theorem 3.8. \hfill $\square$

Proposition 3.9. If $L$ is a subcomplex of $K$, then $\kappa_\alpha(L)$ is a subcomplex of $K/R_\alpha$. \hfill $\square$
Let $\mathcal{V}$ be an acyclic vector field on $\mathcal{K}$. Choose $\alpha_0, \alpha_1 \in \mathcal{V}$ such that $\alpha_1 = \mathcal{V}(\alpha_0)$. Then $\alpha := (\alpha_0, \alpha_1)$ is a reduction pair. Define a partial map $\mathcal{V}_\alpha : K/R_\alpha \to K/R_\alpha$ by

$$
\text{dom} \mathcal{V}_\alpha := \{ \kappa_\alpha(\sigma) \mid \sigma \in \text{dom} \mathcal{V} \setminus \{\alpha_0\} \},
$$

$$
\mathcal{V}_\alpha(\kappa_\alpha(\sigma)) := \kappa_\alpha(\mathcal{V}(\sigma)).
$$

**Theorem 3.10.** If $\mathcal{V}$ is acyclic, then $\mathcal{V}_\alpha$ is a well defined discrete vector field on $K/R_\alpha$ and it is also acyclic.

**Proof:** To show that $\mathcal{V}_\alpha$ is a well defined discrete vector field on $K/R_\alpha$ consider $\beta_0 \in \text{dom} \mathcal{V} \setminus \{\alpha_0\}$ and let $\beta_1 := \mathcal{V}(\beta_0)$. Then, $\beta := (\beta_1, \beta_0)$ is a reduction pair in $K$. Moreover, $\beta \neq \alpha$. Thus, $\beta_1, \beta_0 \in K_\alpha$. Since by Lemma 3.6 $\kappa_\alpha$ is injective on $K_\alpha$, we see that $\mathcal{V}_\alpha$ is injective and $\text{dom} \mathcal{V}_\alpha \cap \text{im} \mathcal{V}_\alpha = \emptyset$. Hence, we only need to show that $\kappa_\alpha(\beta_0)$ is a regular facet of $\kappa_\alpha(\beta_1)$ in $K_\alpha$. Note that (i) follows from Proposition 3.9 and (ii) from Lemma 3.6. To prove (iii) assume the contrary. Then, $\kappa_\alpha(\beta_0) \neq \emptyset$. Hence, we can choose an $x \in K_\beta^+$ and a $y \in \beta_0$ such that $x \neq y$ and $\kappa_\alpha(x) = \kappa_\alpha(y)$. Since $\kappa_\alpha$ is bijective on $K_\alpha$, we have $x, y \in K_\alpha$ and either $x$ or $y$ is not in $K_\beta^+$. But $y \in \alpha_0 \cup \alpha_1$ implies $\beta_0 = \alpha_0$ or $\beta_0 = \alpha_1$ and contradicts $\alpha \neq \beta$. Thus, $x \notin K_\beta^+$, i.e. either $x \in \alpha_1$ or $x \in \alpha_0$. Consider $x \in \alpha_1$. Then $\alpha_1 \cap K_\beta^+ \neq \emptyset$ which implies $K_\alpha \subset K_\beta^+$ and

$$
\emptyset \neq \beta_0 \cap K_\alpha^+ \subset \beta_0 \cap K_\beta^+ \subset \beta_0 \cap K_\alpha \subset \beta_0 \cap K_\beta^+,
$$

a contradiction. Consider $x \in \alpha_0$. Then, $\beta_0 \cap K_\alpha^+$ and $\alpha_0 \cap K_\beta^+$, i.e. $\alpha_0$ is a facet of $\beta_1$ and $\beta_0$ is a facet of $\alpha_1$. Thus, $\alpha_0, \alpha_1, \beta_0, \beta_1, \alpha_0$ is a cycle in $G_\mathcal{V}$, a contradiction again. This completes the proof that $\mathcal{V}_\alpha$ is a well defined discrete vector field on $K/R_\alpha$.

We still need to prove that $\mathcal{V}_\alpha$ is acyclic. Assume it is not. Then, we have a cycle

$$
\kappa_\alpha(\beta_0^i), \kappa_\alpha(\beta_1^i), \kappa_\alpha(\beta_0^{i+1}), \kappa_\alpha(\beta_1^{i+1}), \ldots, \kappa_\alpha(\beta_0^n), \kappa_\alpha(\beta_1^n), \kappa_\alpha(\beta_0^0)
$$

such that $\beta^i := (\beta_0^i, \beta_1^i) \neq \alpha$, $\kappa_\alpha(\beta_0^i)$ is a regular facet of $\kappa_\alpha(\beta_1^i)$ and $\kappa_\alpha(\beta_0^{i+1})$ is a facet of $\kappa_\alpha(\beta_1^i)$. Since $\beta_0^i, \beta_1^i \subset K_\beta$, and $K_\beta$ is a compact subset of $K_\alpha$, we see from Lemma 3.6 that $\kappa_\alpha|_{K_\beta}$ is a homeomorphism, hence $\beta_0^i$ is a regular facet of $\beta_1^i$. If $\text{cl} \beta_1^i \cap K_\alpha = \emptyset$ for all $i$, then

$$
(1) \quad \beta_0^1, \beta_1^1, \beta_0^2, \beta_1^2, \ldots, \beta_0^n, \beta_1^n, \beta_0^1
$$

is a cycle in $G_\mathcal{V}$, because $\kappa_\alpha$ restricted to $K \setminus K_\alpha$ is a homeomorphism onto its image. Hence, assume that $\beta_0^{i+1}$ is not a facet of $\beta_1^i$ for some $i$ but $\kappa_\alpha(\beta_0^{i+1}) \subset \text{cl} \kappa_\alpha(\beta_1^i)$. This is only possible if $\alpha_0$ is a facet of $\beta_1^i$ and $\beta_0^{i+1}$ is a facet of $\alpha_1$. Thus, we can insert $\alpha_0, \alpha_1$ between $\beta_0^{i+1}$ and $\beta_1^i$ in (1) obtaining a cycle in $G_\mathcal{V}$, a contradiction.

A sequence $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_m)$ of reduction pairs in $\mathcal{K}$ is called *admissible* if the associated collection $\{\alpha_1, \alpha_2, \ldots, \alpha_m\}$ of reduction pairs is a
discrete vector field. Obviously, given a discrete vector field \( \mathcal{V} \), any ordering of its elements is admissible. Assuming \( \mathcal{V} \) is acyclic and fixing an ordering \( \alpha \), we can use Theorem 3.10 to recursively apply collapses of reduction pairs in \( \alpha \). By Theorem 3.8, the resulting space is a CW complex homotopy equivalent to the original complex \( K \). We call it the Morse complex of the vector field \( \mathcal{V} \) and denote \( K/\mathcal{V} \). This is some abuse of language, because the construction depends on the ordering \( \alpha \) but we assume the ordering is implicit. Summarizing, we get the following fundamental result of discrete Morse theory.

**Corollary 3.11.** Let \( K \) be a finite CW complex and \( \mathcal{V} \) an acyclic discrete vector field on the CW structure \( \mathcal{K} \) of \( K \). Then, the complexes \( K \) and \( K/\mathcal{V} \) are homotopy equivalent.

\[ \square \]

4. Reductions.

4.1. **External collapses.** We say that the reduction pair \( \alpha \) is free if \( K/\alpha \) is a subcomplex of \( K \).

**Theorem 4.1.** If \( \alpha \) is free then the complexes \( K \) and \( K/\alpha \) are homotopy equivalent.

**Proof:** We know from Lemma 3.6 that the restriction \( \kappa_{\alpha|K/\alpha} \) is a continuous bijection onto \( K/R_\alpha \). Thus, it is a homeomorphism, because \( K/\alpha \), as a subcomplex, is compact. Hence, the conclusion follows from Theorem 3.8.

When \( \alpha \) is free, we say that \( K/\alpha \) is an external collapse of \( K \). Otherwise we say that \( K/R_\alpha \) is an internal collapse of \( K \). On the algorithmic side external collapses are advantageous, because to compute them it is enough to remove the reduction pair from the list \( \mathcal{K} \) of cells of \( K \). Thus, it is convenient to make as many external collapses as possible. We say that \( K \) collapses onto the subcomplex \( L \) if there exists a sequence of subcomplexes \( L = L_0 \subset L_1 \subset \ldots \subset L_m = K \) such that \( L_{j-1} \) is an external collapse of \( L_j \). Note that for convenience we admit the case when \( m = 0 \), i.e. \( L = K \).

An immediate consequence of Proposition 3.4 is the following proposition.

**Proposition 4.2.** If \( K \) collapses onto a subcomplex \( L \) then the inclusion \( L \subset K \) is a homotopy equivalence.

\[ \square \]

4.2. **Collapsible subcomplexes.** Complex \( K \) is called collapsible if it collapses onto a vertex.

**Theorem 4.3.** Assume \( L \) is a collapsible subcomplex of \( K \). Then, \( K \) and \( K/L \) are homotopy equivalent.

**Proof:** Let \( L_0 \subset L_{m-1} \subset \ldots \subset L_0 = L \) be a sequence of subcomplexes of \( L \) such that \( L_j \) is an external collapse of \( L_{j-1} \) by a reduction pair \( \alpha_j \).
and \( L_m = \{*\} \) consists only of a vertex. Let \( \kappa_j : L_j \to L_j/R_{\alpha_j} \) be the quotient map and let \( \kappa_* := \kappa^m \circ \kappa^{m-1} \circ \cdots \kappa^1 \). By Proposition 3.1 each \( \alpha_j \) is a reduction pair in \( K \). Thus, by Theorem 4.1 \( K \) is homotopy equivalent to

\[ K/R_{\alpha_1}/R_{\alpha_2} \cdots/R_{\alpha_m} \]

and by Proposition 2.1 this space is homeomorphic to \( K/R_* \), where \( R_* \) is a relation on \( X \) defined by \( xR_*/y \) if and only if \( \kappa_*(x) = \kappa_*(y) \). But \( \kappa_* \) is constant on \( L \) and a homeomorphism on \( K \setminus L \). Hence, \( K/R_* \) and \( K/L \) are homeomorphic, and consequently \( K \) and \( K/L \) are homotopy equivalent. \( \square \)

**Theorem 4.4.** Assume \( K \) is a regular CW complex and \( L \) is a subcomplex with CW structure \( \mathcal{L} \subset \mathcal{K} \). Then, \( K \) collapses onto \( L \) if and only if there exists an acyclic discrete vector field on \( \mathcal{K} \) such that \( \text{crit} \mathcal{V} = \mathcal{L} \).

**Proof:** Assume first \( K \) collapses onto \( L \). Then, we have subcomplexes \( L = L_0 \subset L_1 \subset \ldots \subset L_m = K \) such that \( L_{j-1} \) is an external collapse of \( L_j \) resulting from removing a reduction pair \( \alpha^j \). It is straightforward to verify that the collection \( \{\alpha^1, \alpha^2, \ldots, \alpha^n\} \) is an acyclic discrete vector field on \( \mathcal{K} \) whose set of critical cells is precisely \( \mathcal{L} \).

To prove the opposite implication assume \( \mathcal{V} \) is an acyclic discrete vector field on \( \mathcal{K} \) such that \( \text{crit} \mathcal{V} = \mathcal{L} \). Let \( n \) be the cardinality of \( \mathcal{K}\setminus\mathcal{L} \). We proceed by induction on \( n \). For \( n = 0 \) the conclusion is trivial. Thus, consider the case \( n > 0 \). Then, we can choose a non-critical cell in \( \sigma \in \mathcal{K} \). Since \( \mathcal{V} \) is acyclic, we can choose a cell \( \tau \) which is inferior to \( \sigma \), that is \( \tau \) is a minimal cell less than or equal to \( \sigma \) in the partial order induced by \( \mathcal{V} \). We claim that \( \tau \) is not a critical cell of \( \mathcal{V} \). To see this consider a path \( \tau = \tau_0, \tau_1, \ldots, \tau_m = \sigma \) in \( G_{\mathcal{V}} \). Since \( \tau \) is inferior to \( \sigma \), such a path obviously exists. If \( \tau \) is critical, then we consider the smallest index \( k \) such that \( \tau_{k-1} \) is critical and \( \tau_k \) is not critical. Since the partial order induced by \( G_{\mathcal{V}} \) goes against the facet partial order only for the vectors of \( \mathcal{V} \), we have \( \tau_k \in \text{dom} \mathcal{V} \) and \( \tau_k \subset \text{cl} \tau \subset L \), because \( \tau \), as a critical cell, is a subset of \( L \) and \( L \) as a subcomplex is closed. It follows that \( \tau_k \) is critical, a contradiction. Therefore \( \tau \in \text{dom} \mathcal{V} \). Let \( K' := K \setminus \tau \setminus \mathcal{V} (\tau) \). To prove that \( K' \) is closed, assume the contrary. Then, there exists an \( x \in \text{cl} K' \setminus K' \). Hence, \( x \in \tau \cap \mathcal{V} (\tau) \) and \( x \in \text{cl} \sigma' \) for some cell \( \sigma' \subset K' \). By Proposition 2.5 \( \tau \) is a face of \( \sigma' \) and by Proposition 2.6 \( \tau \) is a facet of a facet \( \sigma'' \) of \( \sigma' \). Thus \( \sigma'' \) precedes \( \tau \) in the partial order induced by \( G_{\mathcal{V}} \), and consequently \( \tau \) is not inferior to \( \sigma \). This contradiction shows that \( K' \) is a subcomplex of \( K \) and consequently \( K \) collapses onto \( K' \). By induction assumption \( K' \) collapses onto \( L \). Therefore, \( K \) collapses onto \( L \). \( \square \)

As an immediate consequence of Theorem 4.4 we obtain the following corollary.

**Corollary 4.5.** A regular CW complex is collapsible if and only if it admits a discrete vector field whose set of critical cells consists of precisely one vertex. \( \square \)
4.3. Redundant configurations. Let \( K \) be a regular CW complex, \( L \) its subcomplex and \( \mathcal{K} \) and \( \mathcal{L} \) the corresponding CW structures. We refer to the pair \((K,L)\) as a configuration. We say that the configuration \((K,L)\) is redundant if there exists a discrete vector field \( \mathcal{V} \) on \( K \) such that \( \text{crit} \mathcal{V} = \mathcal{L} \). We say that subcomplexes \( L, M \) of \( K \) form a redundant decomposition of \( K \) if \( K = L \cup M \) and the configuration \((M,L \cap M)\) is redundant.

**Theorem 4.6.** Assume subcomplexes \( L \) and \( M \) of a regular CW complex \( K \) form a redundant decomposition. Then, the inclusion \( L \subset K \) is a homotopy equivalence.

**Proof:** Let \( \mathcal{V} \) be a discrete vector field on \( M \) such that \( \text{crit} \mathcal{V} \) consists of the cells in \( L \cap M \). Extend it to all cells in \( K \) by making all cells not in the domain of \( \mathcal{V} \) critical. It follows from Theorem 4.4 that \( K \) collapses onto \( L \), thus we get the assertion from Proposition 4.2. \( \square \)

The advantage of Theorem 4.6 is twofold. We may use it to reduce the complex without changing its homotopy type by removing a subcomplex from a redundant decomposition. We may also simplify the complex by quotienting out a maximal collapsible subcomplex. We can construct such a subcomplex \( L \subset K \) by starting from a vertex and recursively adding to \( L \) a subcomplex \( M \) such that \( L \) and \( M \) form a redundant decomposition of \( L \cup M \). However, to make it work in practice we need a quick method to test for redundant configurations.

This is possible in the setting of tessellations discussed next.

4.4. Tessellated spaces and lattice complexes. We say that a CW structure \( \mathcal{K} \) on a pure, regular CW complex \( X \), finite or not, is a tessellation if the closures of any two top-dimensional cells \( \sigma_1, \sigma_2 \) in \( \mathcal{K} \) are isomorphic, i.e. there exists a homeomorphism \( h: \text{cl} \sigma_1 \rightarrow \text{cl} \sigma_2 \) mapping cells onto cells. A CW complex is a tessellated CW complex if its CW structure is a tessellation. Obviously, every pure subcomplex of a tessellated space is a tessellated space.

A special way to define a tessellation is to consider a lattice \( L \subseteq \mathbb{R}^n \), i.e. an additive subgroup of \( \mathbb{R}^n \) generated by some choice of \( n \) linearly independent vectors \( V_L = \{v_1, \cdots, v_n\} \). Any \( v \in L \) determines a Dirichlet–Voronoi cell

\[
D_L(v) := \{ x \in \mathbb{R}^n \mid ||v - x|| \leq ||w - x|| \ \forall w \in L \}.
\]

For \( x \in \mathbb{R}^n \) set

\[
\chi_L(x) := \{ v \in L \mid x \in D_L(v) \}
\]

and define an equivalence relation \( R \subset \mathbb{R}^n \times \mathbb{R}^n \) by \( xRy \) if and only if \( \chi_L(x) = \chi_L(y) \). One can show that the equivalence classes of this relation provide a CW structure of \( \mathbb{R}^n \) which is a tessellation. We call it a lattice tessellation and denote it \( \mathcal{K}_L \). When \( V_L \) consists of \( n \) orthogonal vectors, the sets \( D_L(v) \) are \( n \)-dimensional hypercubes and the tessellation is the classical cubical decomposition of \( \mathbb{R}^n \). By identifying \( \mathbb{R}^n \) with the hyperplane

\[
\{(x_1, \ldots, x_{n+1}) \in \mathbb{R}^{n+1} : x_1 + \cdots + x_{n+1} = 0\}
\]
and taking as $V_L$ the set $v_1 = (1-n, 1, 1, \ldots, 1, 1)$, $v_2 = (1, 1-n, 1, \ldots, 1, 1)$, $\ldots$, $v_n = (1, 1, 1, \ldots, 1-n, 1)$ we obtain a tessellation of $\mathbb{R}^n$ consisting of $n$-dimensional permutahedra.

A pure, finite CW complex whose CW structure is a subfamily of a lattice tessellation will be called a lattice CW complex. Lattice CW complexes may be easily and efficiently stored in bitmaps.

Fix a lattice $L$. Two top-dimensional cells in $K_L$ are called neighbours if the intersection of their closures is non-empty. Consider a top-dimensional cell $\sigma \in K_L$ and a lattice CW complex $K$ with its CW structure $K \subset K_L$.

Observe that $K \setminus \sigma$ and $\text{cl} \sigma$ are also lattice CW complexes. Their intersection is a subcomplex of $X$. We will call it the contact complex of $\sigma$ and $K$. Note that this makes sense both if $\sigma \subset K$ and $\sigma \cap K = \emptyset$.

Let $N_K(\sigma)$ denote the set of neighbours of $\sigma$ contained in $K$. Then

$$(K \setminus \sigma) \cap \text{cl} \sigma = \bigcup \{ \text{cl} \sigma \cap \text{cl} \tau \mid \tau \in N_K(\sigma), \tau \neq \sigma \},$$

i.e. the contact space is uniquely determined by the neighbours of $\sigma$ in $K$.

The toplex $\text{cl} \sigma$ is said to be redundant in $K$ if the configuration $(\text{cl} \sigma, K \setminus \sigma \cap \text{cl} \sigma)$ is redundant. If $\sigma$ has $k$ neighbours, then there are $2^k$ configurations to test for redundancy. Since all toplexes in a lattice tessellation are isomorphic, tests done for one toplex may be reused for other toplexes. Even better, for reasonably small number of neighbours we can test all configurations of a toplex for redundancy and store them in a lookup table for later quick redundancy tests. The number of neighbours for a cubical tessellation in $\mathbb{R}^n$ is $3^n - 1$. The number of neighbours for a permutahedral tessellation in $\mathbb{R}^n$ is $2^{n+1} - 2$. Thus, the lookup tables may be computed and stored in less than 1GB of memory for cubical tessellations up to dimension 3, requiring $2^{26}$ bits or $2^{23}$ bytes in dimension 3 and for permutahedral tessellations up to dimension 4, requiring $2^{30}$ bits or $2^{27}$ bytes in dimension 4.

5. Reduction algorithms.

5.1. Shaving and collapsing. Two reduction algorithms based on redundancy tests are presented in Tables 2 and 3. The first, often called shaving, removes redundant toplexes as long as they exist. The second constructs a possibly large collapsible subcomplex.

**Theorem 5.1.** Algorithm 5.1 applied to a collection of toplexes representing a lattice space always stops and returns a homotopy equivalent subcomplex with no redundant toplexes.

**Proof:** The conclusion follows immediately from Theorem 4.6. □

**Theorem 5.2.** Algorithm 5.2 applied to a collection of toplexes representing a lattice space always stops and returns a collapsible subcomplex. The resulting quotient complex is homotopy equivalent to the complex on input.

**Proof:** The conclusion follows immediately from Theorem 4.6 and Theorem 4.3. □
Algorithm 5.1. shaving(collection of toplexes $K$)

$Q := \emptyset$;

while there exists a redundant toplex $\sigma$ in $K$ do

remove $\sigma$ from $K$;

enqueue $N_K(\sigma)$ in $Q$;

while $Q \neq \emptyset$ do

$\sigma$=dequeue($Q$);

if $\sigma$ is a redundant in $K$ do

remove $\sigma$ from $K$;

enqueue $N_K(\sigma)$ in $Q$;

return $K$;

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
\textbf{Algorithm 5.1.} shaving & \textbf{Table 2.} Shaving \\
\hline
\end{tabular}
\end{table}

Algorithm 5.2. collapsibleSubset(collection of toplexes $K$)

$C := Q := \emptyset$;

choose any toplex $\sigma$ in $K$ and insert it into $C$;

enqueue $N_K \setminus C(\sigma)$ in $Q$;

while $Q \neq \emptyset$ do

$\sigma$:=dequeue($Q$);

if $\sigma$ is redundant in $C$ do

insert $\sigma$ into $C$;

enqueue $N_K \setminus C(\sigma)$ in $Q$;

return $C$;

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
\textbf{Algorithm 5.2.} collapsibleSubset & \textbf{Table 3.} Collapsible subset construction \\
\hline
\end{tabular}
\end{table}

5.2. $C$-structures. In order to obtain an algorithm based on acyclic vector fields and Theorem 2.10 it is convenient to consider the following concept.

Let $C$ be a finite set decomposing into the disjoint union $C = C_0 \cup C_1 \cup C_2$. By a $C$-structure we mean a quadruple $(C, e_{-1}, e_{+1}, d)$ such that $(C_0, C_1, e_{-1}, e_{+1})$ is a directed multigraph and $d : C_2 \rightarrow \text{Cycles}(C_1)$, where $\text{Cycles}(C_1)$ stands for the set of cycles in $C_1$.

We write $|c| = j$ if and only if $c \in C_j$.

For $c \in C$ we define its boundary by

$$\text{bd } c := \begin{cases} 
\emptyset & \text{if } |c| = 0, \\
\{e_{-1}(c), e_{+1}(c)\} & \text{if } |c| = 1, \\
\{e_1, e_2, \ldots, e_n\} & \text{if } |c| = 2 \text{ and } d(c) = e_1^{\epsilon_1} e_2^{\epsilon_2} \cdots e_n^{\epsilon_n}.
\end{cases}$$
With every $C$-structure $C$ we associate a 2-dimensional CW complex $K$ defined as follows. For each $c \in C$ we have a formal cell $\langle c \rangle := B^{\circ |c|} \times \{c\}$. However, to simplify notation, in the sequel we identify $\langle c \rangle$ with $c$. Let

$$K^j := \bigcup \{ c \in C \mid |c| \leq j \}.$$  

For $c \in C_1$ and $t \in B^1$ we define the characteristic map $\varphi_c : B^1 \to K^1$ by

$$\varphi_c(t) := \begin{cases} (t, c) & \text{if } t \in B^1, \\ e_1(c) & \text{otherwise.} \end{cases}$$

To define the characteristic map $\varphi_c : B^2 \to K^2$ for a $c \in C_2$ assume $d(c) = e_1^{c_1} e_2^{c_2} \cdots e_n^{c_n}$ and take an $x \in B^2$. Set

$$\varphi_c(x) := \begin{cases} (x, c) & \text{if } x \in B^{\circ 2}, \\ \varphi^t_k \left( \frac{n \pi}{k} - k \right) & \text{if } x = e^{2\pi ti} \text{ and } \frac{2\pi ti}{n} k \leq t \leq \frac{2\pi ti}{n} (k + 1). \end{cases}$$

It is not difficult to verify that the cells $c$ together with the characteristic maps $\varphi_c$ define a CW complex. We denote it by $CW(C)$. Conversely, given a finite, regular, 2-dimensional CW complex $K$ it is straightforward to obtain a $C$-structure $C$ such that $CW(C)$ is isomorphic to $K$.

Given a reduction pair $(\alpha_0, \alpha_1)$ in $CW(C)$ we define a $C$-structure $C'$ as follows. Let $C' := C \setminus \{\alpha_0, \alpha_1\}$. To define $e'_1 : C'_1 \to C'_0$ and $d' : C'_2 \to \text{Cycles}(C'_1)$, consider first the case $|\alpha_1| = 1$. By the definition of a reduction pair $\alpha_0$ is a regular facet of $\alpha_1$. This implies that $bd \alpha_1$ consists of precisely two elements one of which is $\alpha_0$. Let $\alpha_0^*$ be the other. Set

$$e'_1(c) := \begin{cases} \alpha_0^* & \text{if } e(c) = \alpha_0, \\ e(c) & \text{otherwise}, \end{cases}$$

$$d'(c) := d(c).$$

Consider the case $|\alpha_1| = 2$. Since $\alpha_0$ is a regular facet of $\alpha_1$, the facet $\alpha_0$ appears precisely once in the cycle $d(\alpha_1) = e_1^{c_1} e_2^{c_2} \cdots e_n^{c_n}$. Without loss of generality we may assume that $\alpha_0 = e_1$. Let $\alpha_0^* := (e_2^{c_2} e_3^{c_3} \cdots e_n^{c_n})^{-c_1}$. Then $\alpha_0^*$ and $\alpha_0$ have the same initial and terminal vertex. Moreover, $\alpha_0$ does not appear in $\alpha_0^*$. Set

$$d'(c) := S_{\alpha_0, \alpha_0^*}(d(c)),$$

where $S_{\alpha_0, \alpha_0^*}$ denotes the $\alpha_0, \alpha_0^*$ substitution in $d(c)$.

It is not difficult to verify that $(C', e'_1, e'_2, d')$ is a $C$-structure. We call it the $\alpha$-collapse of $C$. One easily verifies the following proposition.

**Proposition 5.3.** The CW complex $CW(C')$ associated with the $\alpha$-collapse $C'$ is homeomorphic to the quotient complex $CW(C)/R_\alpha$. \qed

Algorithm 5.3 computing a presentation of the homotopy group of a regular CW complex $K$ represented as a collection of top-dimensional cells is presented in Table 4.
Algorithm 5.3. fundGroup(collection of toplexes K)
K := shaving(K);
A := collapsibleSubset(K);
C := C-structure of K/A;
V := discreteVectorField(C);
for each α ∈ V do
    assign to C the α-collapse of C;
return (C_1, d(C_2));

Table 4. Fundamental group presentation of a regular CW complex.

Theorem 5.4. Assume Algorithm 5.3 is called with a collection of top cells of a CW structure of a lattice space K. It always stops and returns a presentation, up to an isomorphism, of the fundamental group of K.

Proof: The theorem follows immediately from Theorem 5.1, Theorem 5.2, Theorem 3.2, Theorem 3.8, Proposition 5.3, Theorem 3.10 and Theorem 2.10.

6. Application to knot classification.

6.1. Knot classification. Recall that two knots K, K' ⊂ \( \mathbb{R}^3 \) are equivalent \([22, 11]\) if there exists a homeomorphism \( f : \mathbb{R}^3 \to \mathbb{R}^3 \) such that \( K' = f(K) \). They are orientation equivalent \([22]\) or isotopic \([11]\) if the homeomorphism is an ambient isotopy of knots, that is it is isotopic to the identity. Gordon and Luecke \([11]\) prove that K, K' are equivalent if and only if the complements \( \mathbb{R}^3 \setminus K \) and \( \mathbb{R}^3 \setminus K' \) are homeomorphic. Thus, topological invariants of the complements of knots may be used to distinguish between non-equivalent knots. They cannot be used to distinguish between non-isotopic knots. But, by a result of Fisher \([8]\) two equivalent but non-isotopic knots differ only by the mirror image.

Let \( T \) be an invariant of topological spaces, that is \( T(X) = T(Y) \) if X and Y are homeomorphic. Then, obviously \( T(\mathbb{R}^3 \setminus K) = T(\mathbb{R}^3 \setminus K') \) if K and K' are equivalent. We say that T classifies a family of knots \( K \) if for any two non-equivalent knots K, K' ∈ \( K \) we have \( T(\mathbb{R}^3 \setminus K) \neq T(\mathbb{R}^3 \setminus K') \). Note that if the family \( K \) is finite and the invariant T is algorithmically computable, then, at least theoretically, one can verify if T classifies \( K \) in finite computation. A natural candidate for a good T is the fundamental group. Unfortunately, by the results of Novikov \([24]\) and Boone \([1]\), in general it is not possible to decide algorithmically from finite presentations of two groups if they are non-isomorphic. However, this finite presentation may be used to compute some further, algorithmically decidable, invariants. This is the path we used in \([2]\). Recall that given a knot \( K \subset \mathbb{R}^3 \), using Algorithm 5.3 we can compute
a presentation of the fundamental group $G_K := \pi(D^3 \setminus M_K)$, where $D^3$ is a cubical ball in $\mathbb{R}^3$ containing the knot $K$ and $M_K$ is a cubical neighbourhood of $K$ containing $K$ as a deformation retract. Using this presentation and the GAP software library, we can compute some algebraic invariants of $G_K$. In particular, given integers $n, c \geq 1, m \geq 0$ we study in [2] the invariant $I[n,c,m](K)$. It is defined by

$$I[n,c,m](K) := \left\{ H_m(S/\gamma_{c+1} S, \mathbb{Z}) : S \leq G_K, |G_K : S| \leq n \right\},$$

where $H_m(G, \mathbb{Z})$ denotes the integral homology of group $G$ and $\gamma_k G$ is defined recursively by $\gamma_1 G := G$, $\gamma_{k+1} G := [\gamma_k G, G]$. Trying to balance the computational expenses between the cost of computing the invariant $I[n,c,m](K)$ and its ability to distinguish between knots we chose the invariant $I^n(K)$ with $c = m = 1$ and varying $n$. Using a GAP implementation of Algorithm 5.3 we provide in [2] a computer assisted proof of the following result.

**Theorem 6.1.** The invariant $I^n(K)$ distinguishes, up to mirror image, between ambient isotopy classes of all prime knots that admit planar diagrams with eleven or fewer crossings.

6.2. **Classifying index.** Using a C++ implementation of Algorithm 5.3 and an improved strategy of computing the classifying invariant we are able to strengthen Theorem 6.1 (see Theorem 6.3 below). The computational challenge of this extension lies, in particular, in the exponential growth of the number $N(c)$ of prime knots with $c$ crossings. Prime knots up to 16 crossing were tabulated by Hoste, Thistlethwaite and Weeks in [16]. The number of such knots for a given $n$ is presented in Table 5. In our computations we used the Hoste-Thistlethwaite tabulation available from [19].

There are only 801 prime knots up to 11 crossings but 59937 prime knots up to 14 crossings. The additional challenge is in the cost of computing the invariant $I^n$, particularly when $n$ grows. An observation we made is that for most knots relatively low values of $n$ suffice to distinguish them from other knots. But, some knots require relatively high values of $n$. Thus, in order to decrease the computational cost, it makes sense to take as the classifying invariant the pair $(n, I^n(K))$ for a possibly low $n$ selected individually for each knot. Assuming the invariant classifies a family of knots $K$, given a knot $K \in K$ we refer to $n$ in the invariant $(n, I^n(K))$ as the classifying index.

\[
\begin{array}{|c|c|c|c|c|c|c|c|}
\hline
\text{c} & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
\hline
N(c) & 1 & 1 & 2 & 3 & 7 & 21 & 49 \\
\hline
\end{array}
\]

\[
\begin{array}{|c|c|c|c|c|c|c|c|}
\hline
\text{c} & 10 & 11 & 12 & 13 & 14 & 15 & 16 \\
\hline
N(c) & 165 & 552 & 2176 & 9988 & 46972 & 253293 & 1388705 \\
\hline
\end{array}
\]

**Table 5.** The growth of the number of prime knots $N(c)$ with the number of crossings $c$. 
Algorithm 6.1. classify(collection of knots $\mathcal{K}$)

$Q :=$ empty queue; // to process $(K, n)$
$A :=$ empty set; // $(K, n)$ added to $Q$
$I :=$ empty dictionary; // $I[i]$ is a list of $(K, n)$, s.t. $i = I^n(K)$
$C :=$ empty dictionary; // $C[K]$ final invariant for $K$
$D :=$ empty dictionary; // $D[i] = K$ iff $C[K] = i$
$N := 0; // classifying index$

foreach $K \in \mathcal{K}$ do
    enqueue $(K, 2)$ in $Q$;
    insert $(K, 2)$ into $A$;
while $Q$ is non-empty do
    $(K, n) :=$ dequeue $(Q)$;
    $N := \max(N, n)$;
    $i := I^n(K)$;
    if $i$ is not a key in $I$ then
        $I[i] :=$ empty list;
        append $(K, n)$ to list $I[i]$;
        $D[i] := K$;
        $C[K] := (n, i)$;
    else
        append $(K, n)$ to list $I[i]$;
        remove key $i$ from $D$;
    foreach $(\bar{K}, \bar{n}) \in I[i]$ do

(*) remove $\bar{K}$ from $C$;
if $(\bar{K}, \bar{n} + 1) \notin A$ then
(**) enqueue $(\bar{K}, \bar{n} + 1)$ in $Q$;
insert $(\bar{K}, \bar{n} + 1)$ into $A$;
return $(C, D, N)$;

Table 6. Classification algorithm.

of $K$. By the classifying index of the family $\mathcal{K}$ we mean the maximum of all classifying indexes of individual knots $K \in \mathcal{K}$. The idea of classifying indexes leads to Algorithm 6.1 presented in Table 6. Note that the while loop in Algorithm 6.1 is potentially infinite. But, we have the following theorem.

Theorem 6.2. Assume Algorithm 6.1 starts with a collection of knots $\mathcal{K}$ on input and stops. Then, the triple $(C, D, N)$ on output, consisting of dictionaries $C$, $D$ and an integer $N$, has the following features.

(a) The integer $N$ is the classifying index of $\mathcal{K}$.
(b) The keys of $C$ are all knots in $\mathcal{K}$.
(c) The keys of \( D \) constitute a collection of invariants \( I^n(K) \), one per each knot \( K \in K \). Given an invariant \( i \) in the keys of \( D \), the associated value \( D[i] \) is the unique knot in \( K \) such that \( C[K] = (n, I^n(K)) = (n, i) \). Then, the number \( n \) is the classifying index of \( K \).

(d) Both dictionaries \( C \) and \( D \) are injective. In particular, for any two knots \( K, L \in K \) the invariants \( C[K] \) and \( C[L] \) are different.

**Proof:** Given a variable \( x \) in Algorithm 6.1 we let \( x^{(l)} \) denote the state of \( x \) after \( l \) iterations of the while loop. In particular, for \( l = 0 \) this is the state just before entering the while loop. We will show by induction that for every \( l \geq 0 \) we have the following properties:

(i) \( A^{(l)} = \bigcup_{k=0}^{l} Q^{(k)} \),
(ii) the sequence \( \{n^{(i)}\}_{i=1}^{l} \) is not descending,
(iii) \( (K^{(l)}, n^{(l)}) \neq (K^{(l')}, n^{(l')}) \) for each \( l' < l \),
(iv) for each \( K \in K \) the value of \( C^{(l)}[K] \) is set if and only if \( K \in K \setminus L^{(l)} \),

\[ L^{(l)} := \{ K \in K \mid \exists n \in \mathbb{N}, (K, n) \in Q^{(l)} \} \],

(v) \( C^{(l)} \) and \( D^{(l)} \) are injective,
(vi) the value \( D^{(l)}[i] \) is the unique \( K \in K \) such that

\[ C^{(l)}[K] = (n, I^n(K)) = i. \]

First observe that dictionaries \( C^{(0)}, D^{(0)}, I^{(0)} \) are empty, \( A^{(0)} \) is equal to \( Q^{(0)} \) because of the first for loop, \( Q^{(0)} \) contains only pairs \((K, 2)\) for every \( K \in K \), \( L^{(0)} = K \), \( n^{(0)} \) is not defined, \( n^{(1)} = 2 \) and \( n^{(j)} \geq 2 \) for every \( j \geq 1 \). In particular, properties [iii][vi] are trivially satisfied for \( l = 0 \). Thus, fix \( l > 0 \) and assume the conditions are satisfied for \( k < l \).

To prove [ii] observe that in course of the \( l \)th iteration of the while loop we add an element to \( A \) if and only if we add it to \( Q \) and we never remove elements from \( A \). This proves [ii].

By the induction assumption \( n^{(k)} \geq n^{(k-1)} \) for \( k < l \). Hence, in order to prove [ii] we only need to show that \( n^{(l)} \geq n^{(l-1)} \). The inequality is obvious when \( n^{(l-1)} = 2 \). Thus, assume that \( n^{(l-1)} > 2 \). Then, \( n^{(l-1)} \) and consequently also \( n^{(l)} \) enter the queue \( Q \) in pair with a respective knot inside the while loop. Hence, there exist \( k \) and \( k' \) such that \( l > k > k' \), \( n^{(l)} = n^{(k)} + 1 \) and \( n^{(l-1)} = n^{(k')} + 1 \). From the induction assumption \( n^{(k)} \geq n^{(k')} \), therefore \( n^{(l)} = n^{(k)} + 1 \geq n^{(k')} + 1 = n^{(l-1)} \).

To prove [iii] let \( l' < l \) be such that \( (K^{(l)}, n^{(l)}) = (K^{(l')}, n^{(l')}) \). This obviously cannot happen if \( n^{(l)} = 2 \). Thus, for \( l \) there exists a \( k < l \) and for \( l' \) there exists a \( k' < l' \) such that

\[ (K^{(l)}, n^{(l)}) \in Q^{(k)} \setminus Q^{(l)} \]

and

\[ (K^{(l')}, n^{(l')}) \in Q^{(k')} \setminus Q^{(l')}. \]
Without loss of generality we may assume that $k' < k$. In the $k$th iteration line (**) is executed with $(K^{(l)}), n^{(l)}) \not\in A^{(k)}$. However,

$$(K^{(l)}, n^{(l)}) = (K^{(l')}, n^{(l')}) \in Q^{(k')} \subset A^{(k')} \subset A^{(k)},$$
a contradiction.

Now we prove (iv). Assume to the contrary that there exists a $K \in \mathcal{K} \setminus \mathcal{K}^{(l)}$ such that $C^{(l)}[K]$ is not set. Then, on the $l$th pass of the while loop line (*) is executed with $K^{(l)} = K$. Indeed, if $K \not\in \mathcal{L}^{(l-1)}$, then $C^{(l-1)}[K]$ is set and the algorithm executes line (*) by the induction assumption. If $K \in \mathcal{L}^{(l-1)}$, then $K = K^{(l)}$ and the algorithm executes the else branch, because $C^{(l)}[K]$ is not set. In particular, $(K, n)$ with $n = n^{(l)}$ is processed as one of the elements of $\Gamma^{(l)}[i]$ in the second foreach loop. If the algorithm executes line (**), then $K \in \mathcal{K}^{(l)}$, a contradiction. Otherwise $(K, n + 1) \in A^{(l-1)}$ and consequently $(K, n + 1) \in Q^{(l')}$ for some $l' < l$. Because of the assumption $(K, n + 1)$ also is not in $Q^{(l)}$. Hence, $K = K^{(l')}$ and $n + 1 = n^{(l')} > n^{(l)} = n$ for some $l''$ such that $l' < l'' < l$. This contradicts (ii).

Assume in turn that $C^{(l)}[K]$ is set and $K \in \mathcal{L}^{(l)}$. If $C^{(l-1)}[K]$ is set, then by the induction assumption $K \not\in \mathcal{L}^{(l-1)}$. Thus, the algorithm executes line (**) in the $l$th iteration with $K_1 = K$. In particular, it also executes line (*), a contradiction. If $C^{(l-1)}[K]$ is not set, then $K^{(l)} = K$. Let $n := n^{(l)}$. Since $K \in \mathcal{L}^{(l)}$ and the algorithm stops, there is a $k > l$ such that $K^{(k)} = K$. Without loss of generality we may assume that $k$ is minimal with this property. By (ii) we have $n^{(k)} \geq n^{(l)}$ and by (iii) $n^{(k)} > n^{(l)}$. It cannot be $n^{(k)} = n^{(l)} + 1$, because on the $l$th pass of the while loop the else branch is not executed. Thus, $n^{(k)} > n^{(l)} + 1$. It follows that there exists a $p < k$ such that $K^{(p)} = K$ and $n^{(k)} > n^{(p)} + 1$. Therefore, $n^{(p)} > n^{(l)}$ and by (ii) $p > l$. Consequently, the number $k$, contrary to its choice, is not minimal.

Now we prove (v). It follows easily from the induction assumption that if $C^{(l)}$ is not injective, then there exists a $k < l$ such that

$$C^{(l)}[K^{(l)}] = C^{(l)}[K^{(k)}] = C^{(k)}[K^{(k)}].$$

It means that

$$(n^{(l)}, i^{(l)}) = (n^{(k)}, i^{(k)}).$$

We set $C[K]$ only in the then branch of the first if statement. Hence, $i^{(l)} \not\in I^{(l-1)}$. But in the $k$th branch of the while loop we set $C[K^{(k)}]$. Therefore, $i^{(k)} \in I^{(k)}$. We do not delete elements from $I$. Thus, since $k \leq l - 1$, we have $i^{(l)} = i^{(k)} \in I^{(l-1)}$, a contradiction.

Again from the induction assumptions, if $D^{(l)}$ is not injective, then there exists a $k < l$ such that

$$K^{(l)} = D^{(l)}[i^{(l)}] = D^{(l)}[i^{(k)}] = K^{(k)},$$

and $i^{(l)} \neq i^{(k)}$. Since $K^{(l)} = K^{(k)}$, we have $i^{(l)} = I^n(K^{(l)}) = I^n(K^{(k)}) = i^{(k)}$, a contradiction.
To prove (vi) let $i, K$ be such that $D^{(l)}[i] = K$. Since $D$ is injective, we see that $K$ is unique. If $D^{(l)}[i] = D^{(l-1)}[i]$ then (2) follows from the induction assumption. Otherwise, the algorithm sets $D$ in the $l$th iteration. Thus, it also sets $C[K]$ to $(n, i)$.

To finish the proof first observe that assertion (a) is obvious. Let $l^{\star}$ denote the final pass of the while loop. Then, $Q(l^{\star}) = \emptyset$. Thus, we get from (iv) that the keys of $C$ are all knots in $\mathcal{K}$. This proves assertion (b). Assertion (c) follows from (vi) and assertion (d) from (v). □

Given a family $\mathcal{K}$ of prime knots and an integer $c$ we denote by $\mathcal{K}_c$ the subfamily of these knots in $\mathcal{K}$ whose minimal planar diagram requires $c$ crossings and we set $\mathcal{K}_{\leq c} := \bigcup_{i \leq c} \mathcal{K}_i$. Let HTW denote the family of 1 701 936 prime knots tabulated by Hoste, Thistlethwaite and Weeks in [16] and available from [19]. We have the following extension of Theorem 6.1.

**Theorem 6.3.** The invariant $I^n(K)$ distinguishes, up to mirror image, between ambient isotopy classes of all prime knots in $\text{HTW}_{\leq 14}$ and the classifying index of this family is 7.

**Proof:** Apply Algorithm 6.1 to the family HTW$_{\leq 14}$. The algorithm stops, returning 7 as the classifying index of the family. Hence the result follows from Theorem 6.1. □

The same way we can determine the classifying index for HTW$_{\leq c}$ with $c \leq 14$. The results are presented in Table 7. Figure 1 presents the grouping of classifying indexes of individual knots. Tables 8, 9 and 10 indicate that for most knots their classifying index is relatively low.

### Table 7. Classifying indexes $N(c)$ for the family HTW$_{\leq c}$ with $c \leq 14$.  

| $c$ | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|-----|---|---|---|---|---|---|---|----|----|----|----|----|
| $N(c)$ | 2 | 2 | 3 | 3 | 3 | 5 | 5 | 6  | 6  | 7  | 7  |    |

6.3. **Limitations of the method.** Recall that during the computations of the $I^n$ invariant of a knot $K$ we first build a finite presentation of the fundamental group $G$ of $\mathbb{R}^3 \setminus K$ and construct the family $S^n(G)$ of the subgroups of index $n$ of $G$.

Since each subgroup of index $n$ of a finitely generated group $G$ corresponds to a homomorphism $G \rightarrow S_n$, the number of such subgroups is bounded from above by $(n!)^g$ where $g$ is the number of generators in $G$. We cannot bound the number from below. Thus, we can influence the computational time of constructing $S^n(G)$ only via $g$. Therefore, since $g$ is not greater than the number of critical cells of the constructed discrete vector fields, it is important to minimize this number. The problem of computing $S^n(G)$ is well studied in the literature. A good source of references is [3].
Figure 1. The image shows knots separation in HTW $\leq 14$ by the invariant $I^n$. The middle white circle represents all knots in HTW $\leq 10$. The first ring counting from inside presents arcs grouping knots with the same invariant with classifying index 2. The length of the coloured arc represents the group size. The following rings show groups for the classifying indexes 3, 4 and 5. We can see how the groups split. Also, it is visible that the classifying index exceeds 3 only for a small number of knots.

The problem of computing the optimal number of critical cells is NP-complete [17]. In the construction of the discrete vector field we use greedy algorithms. They usually behave very well for homology computation, where the difference of one more or less critical cell has no significant consequence for the total computational complexity. However, in the case of the $I^7$ invariant, one more critical cell may increase the total computation time from minutes to days. The most time-consuming knot we encountered is $K_{14,38437}$ presented in Figure 2. For this knot the computations of $I^7(K)$ vary between a few minutes and 52 days, depending on the method used to construct the discrete vector field (coreductions, reductions) and the order of cells in the data structure. The best method and order varies from knot to knot. Since
algorithm 5.3 proposed in this paper computes a group presentation in a small fraction of time needed for the low-index subgroup computation, a reasonable strategy to minimize the total computation time is to test a few methods for each knot in the search of the possibly small number of critical cells.

The problem is additionally complicated by the Tietze transformations used to simplify the group presentation. It turns out that the number of generators after transformations depends on some qualitative properties of the constructed discrete vector field. In Table 11 we show the number of generators and relators before and after Tietze transformations in the case of four different strategies for the construction of the discrete vector field for knot $K_{14,38437}$. Only in one case we get 3 generators and only in this case we are able to compute $I^7(K)$ in several minutes. Our conclusion

Table 8. Distribution of $I^n(K)$ computations for HTW$_{\leq 12}$. The entry in the $c$th row and $n$th column gives the number of knots $K \in$ HTW$_c$ for which it was necessary to compute the $I^n(K)$ in order to guarantee classification in HTW$_{\leq 12}$.

| $c \backslash n$ | 2    | 3    | 4    | 5    | 6    |
|-----------------|------|------|------|------|------|
| 3               | 1 (100%) | 1 (100%) | 0 (0%) | 0 (0%) | 0 (0%) |
| 4               | 1 (100%) | 1 (100%) | 1 (100%) | 0 (0%) | 0 (0%) |
| 5               | 2 (100%) | 2 (100%) | 2 (100%) | 2 (100%) | 0 (0%) |
| 6               | 3 (100%) | 3 (100%) | 3 (100%) | 2 (67%) | 0 (0%) |
| 7               | 7 (100%) | 7 (100%) | 6 (86%) | 3 (43%) | 0 (0%) |
| 8               | 21 (100%) | 21 (100%) | 14 (67%) | 10 (48%) | 1 (5%) |
| 9               | 49 (100%) | 49 (100%) | 30 (61%) | 19 (39%) | 1 (2%) |
| 10              | 165 (100%) | 165 (100%) | 110 (67%) | 75 (45%) | 1 (1%) |
| 11              | 552 (100%) | 552 (100%) | 355 (64%) | 225 (41%) | 10 (2%) |
| 12              | 2176 (100%) | 2156 (99%) | 1151 (53%) | 727 (33%) | 31 (1%) |

Table 9. Distribution of $I^n(K)$ computations for HTW$_{\leq 13}$. The entry in the $c$th row and $n$th column gives the number of knots $K \in$ HTW$_c$ for which it was necessary to compute the $I^n(K)$ in order to guarantee classification in HTW$_{\leq 13}$.

| $n \backslash c$ | 2    | 3    | 4    | 5    | 6    | 7    |
|-----------------|------|------|------|------|------|------|
| 3               | 1 (100%) | 1 (100%) | 0 (0%) | 0 (0%) | 0 (0%) | 0 (0%) |
| 4               | 1 (100%) | 1 (100%) | 1 (100%) | 1 (100%) | 0 (0%) | 0 (0%) |
| 5               | 2 (100%) | 2 (100%) | 2 (100%) | 2 (100%) | 0 (0%) | 0 (0%) |
| 6               | 3 (100%) | 3 (100%) | 3 (100%) | 2 (67%) | 0 (0%) | 0 (0%) |
| 7               | 7 (100%) | 7 (100%) | 7 (100%) | 3 (43%) | 0 (0%) | 0 (0%) |
| 8               | 21 (100%) | 21 (100%) | 16 (76%) | 12 (57%) | 1 (5%) | 0 (0%) |
| 9               | 49 (100%) | 49 (100%) | 40 (82%) | 24 (49%) | 1 (2%) | 0 (0%) |
| 10              | 165 (100%) | 165 (100%) | 142 (86%) | 93 (56%) | 6 (4%) | 0 (0%) |
| 11              | 552 (100%) | 552 (100%) | 474 (86%) | 301 (55%) | 15 (3%) | 0 (0%) |
| 12              | 2176 (100%) | 2176 (100%) | 1692 (78%) | 1004 (46%) | 48 (2%) | 0 (0%) |
| 13              | 9988 (100%) | 9972 (100%) | 7198 (72%) | 4426 (44%) | 293 (3%) | 2 (0%) |
Table 10. Distribution of $I^n(K)$ computations for $HTW_{\leq 14}$. The entry in the $c$th row and $n$th column gives the number of knots $K \in HTW_c$ for which it was necessary to compute the $I^n(K)$ in order to guarantee classification in $HTW_{\leq 14}$.

**Figure 2.** Knot $K_{14,38437}$.

is that the number of generators does not determine the efficiency of the transformations.

Nevertheless, for the calculations it is important to perform shaving and collapsibleSubset steps even for knots given as arc presentation [19]. Without the geometric simplifications we cannot get less than 4 generators for the knot in Figure 2. The steps are also important for applications, where knots are placed in a big cubical grid, e.g. 3D pictures of proteins.

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Table 11. Number of generators (g) and relators (r) before and after Tietze transformations for knot $K_{14,38437}$.

| Method                      | Before Tietze | After Tietze |
|-----------------------------|---------------|--------------|
| Reductions, cells order A   | g=4, r=4      | g=4, r=3     |
| Reductions, cells order B   | g=4, r=4      | g=3, r=2     |
| Coreductions, cells order A | g=6, r=6      | g=4, r=3     |
| Coreductions, cells order B | g=14, r=14    | g=4, r=3     |

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