Research Networking Programmes

Short Visit Grant ☐ or Exchange Visit Grant ☒

(please tick the relevant box)

Scientific Report

The scientific report (WORD or PDF file – maximum of eight A4 pages) should be submitted online within one month of the event. It will be published on the ESF website.

Proposal Title: Applied Computational Group Theory

Application Reference N°: 4474

1) Purpose of the visit

Visit Herbert Edelsbrunner's group at IST Vienna, investigate potential applications of computational group theory to topics in applied topology, work on a graduate-level textbook on Computational Homotopy.

2) Description of the work carried out during the visit

I worked on:

(i) developing and implementing algorithms for computing the fundamental group of a finite regular CW-space and applying the algorithms to complements of protein backbone knots (joint work with Marian Mrozek et al.);

(ii) applying computational homology algorithms to the classification of homotopy 2-types of order up to 128 (joint work with Le Van Luyen);

(iii) writing a textbook on Computational Homotopy;

(iv) attending the weekly geometry and topology seminar at the IST;

(v) co-editing a special volume on applied and computational topology for the Springer journal "Applicable Algebra in Engineering, Communication and Computing". See following pages for further details

3) Description of the main results obtained

See following pages for details

4) Future collaboration with host institution (if applicable)

I plan to extend my stay at the IST to cover the period 4 November 2013 to 30 June 2014

5) Projected publications / articles resulting or to result from the grant *(ESF must be acknowledged in publications resulting from the grantee's work in relation with the grant)*

[1] "Computing fundamental groups from point clouds", P. Brendel, P. Dlotko, G. Ellis, M. Juda and M. Mrozek, 18 pages, to be submitted to AAECC. (Available from http://hamilton.nuigalway.ie/preprints/fundamental.pdf)

[2] "Homotopy 2-types of low order", G. Ellis and Le V.L., 9 pages, submitted to Experimental Mathematics. (Available from http://hamilton.nuigalway.ie/preprints/2t.pdf)

[3] "Computational Homotopy", poster to be presented at the workshop on Topological Systems at the IMA in Minnesota, 3-7 March 2014. (Available from http://hamilton.nuigalway.ie/preprints/IMAposter.pdf)

[4] "Computational Homotopy", textbook, in preparation.

6) Other comments (if any)

I would like to thank the ESF for its support.

2 Description of the work carried out during the visit

Since arriving at IST Austria on 4 November 2013 I have been working mainly on the following topics:

1. Developing and implementing algorithms for computing the fundamental group of a finite regular CW-space, applying the algorithms to complements of protein backbone knots and other knots, and writing up the research as an article for publication. This is joint work with Marian Mrozek (Krakow), who visited IST in December, and other members of his group.
2. Applying computational homology algorithms to the classification of homotopy 2-types of order up to 128 and writing up the research for publication. This is joint work with Le Van Luyen (Galway).
3. Writing the first two chapters of a textbook on Computational Homotopy and developing code to provide suitable examples for the book.
4. Attending the weekly geometry and topology seminar run by Herbert Edelsbrunner's group at the IST.
5. Co-editing a special volume on applied and computational topology for the Springer journal "Applicable Algebra in Engineering, Communication and Computing".

3 Description of the main results obtained

3.1 Fundamental groups

The main theorem obtained is the following.

Theorem 1. *For a knot* $K: S^1 \to \mathbb{R}^3$ *define* $G(K) = \pi_1(\mathbb{R}^3 \setminus K)$. *The knot invariant*

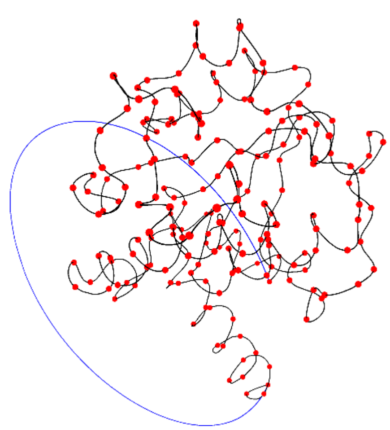
$$I^{[6,1,1]}(G(K)) = \{S_{ab} \ : \ S \leq G(K), |G(K) : S| \leq 6\}$$

distinguishes, up to mirror image, between ambient isotopy classes of all prime knots that admit planar diagrams with eleven or fewer crossings.

This theorem was obtained by developing and implementing software for computing fundamental groups of regular CW-spaces, and for constructing regular CW-spaces that model knot complements. To describe this software we illustrate how it can be used to compute aperipheral system

$$\begin{array}{rcl} \pi_1(\partial K) \cong \langle a, b | aba^{-1}b^{-1} \rangle & \to & \pi_1(\mathbb{R}^3 \setminus K) \cong \langle x, y | xyx = yxy \rangle \\ a & \mapsto & x^{-2}yx^2y \\ b & \mapsto & x \end{array}$$

for the knot $\kappa: S^1 \to \mathbb{R}^3$ determined by the alpha carbon atoms in the backbone of the Thermophilus protein.



```
gap> K:=ReadPDBfileAsPurePermutahedralComplex("1V2X.pdb");
Pure permutahedral complex of dimension 3.

gap> C:=ComplementOfPureComplex(K);
Pure permutahedral complex of dimension 3.

gap> C:=ZigZagContractedPureComplex(C);
Pure permutahedral complex of dimension 3.

gap> Y:=PermutahedralComplexToRegularCWComplex(C);;
Regular CW-space of dimension 3

gap> i:=BoundaryPairOfPureRegularCWComplex(Y);
Map of regular CW-spaces

gap> CriticalCellsOfRegularCWComplex(Source(i));
[ [ 2, 1 ], [ 2, 1331 ], [ 1, 9951 ], [ 1, 31415 ],
  [ 0, 22495 ], [ 0, 25646 ] ]

gap> phi:=FundamentalGroup(i,22495);
[ f1, f2 ] -> [ f1^-3*f2*f1^2*f2*f1, f1 ]

gap> RelatorsOfFpGroup(Source(phi));
[ f1*f2^-1*f1^-1*f2 ]

gap> RelatorsOfFpGroup(Target(phi));
[ f1^-1*f2^-1*f1*f2*f1*f2^-1 ]
```

3.2 Classification of homotopy types

In this joint project with Le Van Luyen we initiated a classification of homotopy types of connected CW-spaces X with $\pi_n X = 0$ for $n \neq 1, 2$. The homotopy type of X is called a *homotopy* 2*-type*. It is well-known that such a homotopy type can be modelled by a group homomorphism $\partial\colon M \to P$ and group action $(p, m) \mapsto {}^p m$ of P on M satisfying

1. $\partial({}^p m) = p(\partial m)p^{-1}$
2. ${}^{\partial m} m' = m m' m^{-1}$

for $p \in P, m, m' \in M$. Such a homomorphism and action constitute a *crossed module*. The model is such that $\pi_n X \cong \pi_n(\partial)$ for $n = 1, 2$ where one defines $\pi_1(\partial) = P/\mathrm{im}\,\partial$ and $\pi_2(\partial) = \ker\partial$. A *morphism* of crossed modules $\phi_*\colon(\partial\colon M \to P) \to (\partial'\colon M' \to P')$ consists of two group homomorphisms $\phi_1\colon P \to P'$, $\phi_2\colon M \to M'$ that satisfy $\partial'\phi_2(m) = \phi_1\partial(m)$, $\phi_2({}^p m) = {}^{\phi_1 p}\phi_2(m)$ for $m, m' \in M, p \in P$. A morphism induces canonical homomorphisms $\pi_n(\phi_*)\colon \pi_n(\partial) \to \pi_n(\partial')$ for $n = 1, 2$. The morphism ϕ_* is said to be an *isomorphism* if ϕ_n is an isomorphism for $n = 1, 2$. The morphism ϕ_* is said to be a *quasi-isomorphism* if $\pi_n(\phi_*)$ is an isomorphism for $n = 1, 2$. Two crossed modules ∂, ∂' are said to be *quasi-isomorphic* if there exists a sequence of quasi-isomorphisms $\partial \to \partial_1 \leftarrow \partial_2 \to \partial_3 \leftarrow \cdots \to \partial_n \leftarrow \partial'$ of arbitrary length n. We write $\partial \simeq \partial'$ to denote that ∂ is quasi-isomorphic to ∂'. Note that $\simeq$ is an equivalence relation on crossed modules; the corresponding equivalence classes are called *quasi-isomorphism classes*. We emphasize that two crossed modules ∂, ∂' could be quasi-isomorphic without the existence of any quasi-isomorphism directly between ∂ and ∂'.

Mac Lane and Whitehead showed that there is a one-one correspondence between homotopy 2-types and quasi-isomorphism classes of crossed modules. We define the *order* of a crossed module

$\partial\colon M \to P$ to be the product $|\partial| = |M| \times |P|$ of the orders of the groups M, P. We define the *order* of a quasi-isomorphism class of crossed modules to be the least order of any crossed module in the class. We define the *order* of a homotopy 2-type X to be the order of the corresponding quasi-isomorphism class of crossed modules. A homotopy 2-type X can also be represented by the fundamental group $\pi_1 X$, the $\pi_1 X$-module $\pi_2 X$ and a cohomology class $\kappa \in H^3(\pi_1 X, \pi_2 X)$ known as the *Postnikov invariant*. The Postnikov invariant κ is the trivial cohomology class if and only if the homotopy 2-type can be represented by a crossed module $\partial\colon M \to P$ with $\partial = 0$. In this case we deem the homotopy 2-type, and also the quasi-isomorphism type, to be *trivial*.

In this project we developed two computer functions, both of which have been implemented by the Le Van Luyen in the HAP package for the computer algebra system GAP. The first function lists representatives for all the quasi-isomorphism classes of crossed modules of a given order $m \le 127$, $m \ne 32, 64, 81, 96$. The second function inputs a user-defined crossed module (of order possibly greater than 127) and tries to return numbers (m, k) that identify the least order m of any quasi-isomorphic crossed module and a catalogue number k that uniquely identifies the quasi-isomorphism class of the input; it certainly succeeds if the input is of order $\le 127, \ne 32, 64, 81, 96$. We have used the implementation of these two functions, and related functions, to compile Table 1. The table uses the notation:

$I2(m)$	$=$	number of isomorphism classes of crossed modules of order m.
$Q2(m)$	$=$	number of homotopy 2-types of order m
	$=$	number of quasi-isomorphism classes of order m.
$T2(m)$	$=$	number of trivial homotopy 2-types of order m.

It is an easy exercise to see that $I2(p) = Q2(p) = T2(p) = 2$ for p a prime and so we omit prime values of m from the table. It is also easy to show that for primes $p < q$ we have $I2(pq) = Q2(pq) = T2(pq) = 6$ when p divides $q - 1$ and $I2(pq) = Q2(pq) = T2(pq) = 4$ when p does not divide $q - 1$ and so these values of m are also omitted from the table. (To establish the formulae one uses that: the cyclic group of order p can act non-trivially on the cyclic group of order q precisely when p divides $q-1$; the only groups of order p or order pq with p not dividing $q-1$ are the cyclic groups; the only groups of order pq with p dividing $q - 1$ are the cyclic group and one non-abelian semi-direct product of cyclic groups.) The table suggests the general formulae:

$I2(m) - 1 = Q2(m) = T2(m) = 5$ for $m = p^2$;
$I2(m) - 4 = Q2(m) = T2(m) = 14$ for $m = p^3, p \ge 3$;
$I2(m) - 2 = Q2(m) = T2(m) = 18$ for $m = 4p, p \ge 5, p \equiv 1 \bmod 4$;
$I2(m) - 2 = Q2(m) = T2(m) = 16$ for $m = 4p, p \ge 5, p \equiv 3 \bmod 4$;

and more complicated formulae for the cases $m = q^2 p, q \ge 3$ and $m = pqr$ with p, q, r distinct primes. These formulae can be verified for a good range of m using the above mentioned computer functions.

3.3 Textbook on computational homotopy

The first draft of the first two chapters of a textbook on *Computational Homotopy* were completed. The table of contents is appended below.

m	1	4	8	9	12	16	18	20	24	25	27	28	30	32	36	40	42
$I2(m)$	1	6	18	6	20	62	22	20	73	6	18	18	20	251	78	72	26
$Q2(m)$	1	5	14	5	18	43	19	18	61	5	14	16	20	A	63	60	26
$T2(m)$	1	5	14	5	18	42	19	18	61	5	14	16	20	152	63	60	26

m	44	45	48	49	50	52	54	56	60	63	64	66	68	70	72
$I2(m)$	18	12	296	6	22	20	81	68	77	18	1276	20	20	20	325
$Q2(m)$	16	10	224	5	19	18	65	56	73	16	B	20	18	20	251
$T2(m)$	16	10	220	5	19	18	65	56	73	16	697	20	18	20	251

m	75	76	78	80	81	84	88	90	92	96	98	99	100	102	104
$I2(m)$	14	18	26	302	64	90	66	76	18	1446	22	12	87	20	72
$Q2(m)$	12	16	26	230	C	84	54	66	16	D	19	10	71	20	60
$T2(m)$	12	16	26	226	44	84	54	66	16	971	19	10	71	20	60

m	105	108	110	112	114	116	117	120	121	124	125	126	128
$I2(m)$	12	308	26	270	26	20	18	342	6	18	18	102	9120
$Q2(m)$	12	238	26	202	26	18	16	302	5	16	14	92	?
$T2(m)$	12	238	26	198	26	18	16	302	5	16	14	92	4668

$$158 \leq A \leq 171,\ 727 \leq B \leq 831,\ 45 \leq C \leq 46,\ 996 \leq D \leq 1052$$

Table 1:

Contents