# Elements of Khovanov Homology

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**Abstract**

*This talk is an introduction to Khovanov homology with emphasis on the combinatorial topology and skein theory. We discuss the meaning of Khovanov homology in the context of the diagrammatic understanding of the Jones polyomial via the bracket state sum model. Accordingly, we start with a quick introduction to the bracket polynomial, reformulating it and the Jones polynomial in a manner that paves the way for Khovanov homology. Then we show how interpreting the loop states of the bracket and surfaces that bound related states leads to the beautiful theory of Khovanov homology. We discuss how Frobenius algebras arise in this context and how they are central to the homology construction. We discuss applications to classical and virtual knot theory.*

**Keywords.** bracket polynomial, Khovanov homology, cube category, simplicial category, tangle cobordism, chain complex, chain homotopy , unitary transformation, quantum computing, quantum information theory, link homology, categorification.

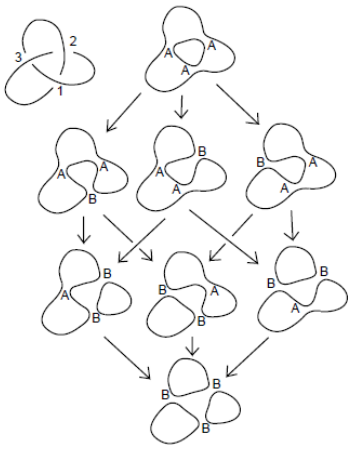


**Fig. 1. Bracket States and Khovanov Complex**

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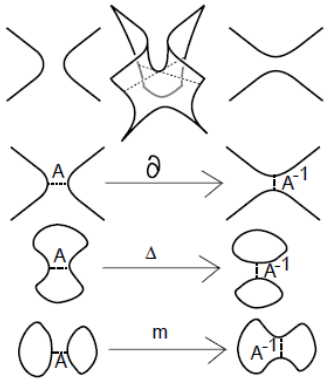


**Fig. 2. SaddlePoints and State Smoothings**


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# Word problem for virtual braid groups

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Joint work with P. Bellingeri and B. A. Cisneros de la Cruz [2].

Virtual braid groups were first defined by L. Kauffman [6] in terms of braid diagrams, but there are now other more topological and/or combinatorial viewpoints, such as in terms of Gauss diagrams [1], [3], or in terms of braids in thickened surfaces [3]. A complete and detailed definition will be given in the lecture. But, in order to give an int to the potential listener, an example of a braid diagram is given in Figure 1. The group operation is defined by concatenation of the diagrams.

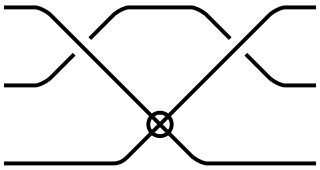

**Fig. 1.** A virtual braid diagram.

One can easily get a "natural" group presentation for $VB_n$ in terms of generators and relations from its definition in terms of virtual braid diagrams (see [5], [7]). In this presentation we have $2(n-1)$ generators, $\sigma_1, \dots, \sigma_{n-1}, \tau_1, \dots, \tau_{n-1}$, and the relations are the following.

$$\begin{array}{rl} \tau_i^2 = 1 & \text{for } 1 \leq i \leq n-1 \\ \sigma_i\sigma_j = \sigma_j\sigma_i\,,\ \sigma_i\tau_j = \tau_j\sigma_i\,,\ \text{and } \tau_i\tau_j = \tau_j\tau_i & \text{for } |i-j| \geq 2 \\ \sigma_i\sigma_j\sigma_i = \sigma_j\sigma_i\sigma_j\,,\ \sigma_i\tau_j\tau_i = \tau_j\tau_i\sigma_j\,,\ \text{and } \tau_i\tau_j\tau_i = \tau_j\tau_i\tau_j & \text{for } |i-j| = 1 \end{array}$$

We can deduce few properties of the group from this presentation. For instance, $VB_n$ contains the symmetric group $S_n$ (this is the subgroup generated by $\tau_1, \dots, \tau_{n-1}$) as well as the classical braid group $B_n$ (this is the subgroup generated by $\sigma_1, \dots, \sigma_{n-1}$). We can also deduce a solution to the word problem, but this is far from being obvious.

Recall that a *solution to the word problem* for a group $G$ generated by a set $S$ is an algorithm which, given a word $w$ over $S^{\pm 1}$, decides whether $w$ represents 1 in $G$ or not. A first solution to the word problem for $VB_n$ was shown in [4], but this has two main failures:

- it is quite theoretical and its implementation would be a hard question,
- its understanding requires a deep knowledge on Artin groups.

The goal of this lecture is to present a new solution, based on [2], easily implementable and whose understanding requires only little preliminary knowledge.

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# A new skein invariant for classical links from the Yokonuma–Hecke algebras

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This is joint work with M. Chlouveraki, J. Juyumaya and K. Karvounis.

One of the greatest accomplishments in knot theory and low-dimensional topology is the pioneering construction of the Jones polynomial by V. F. R. Jones in 1984. It made use for the first time of the Artin braid groups and their Markov equivalence via a Markov trace on the Temperley–Lieb algebras. It was easily computable thanks to the new diagrammatic skein methods developed by L. H. Kauffman. The *Homflypt polynomial* is a 2-variable generalization of the Jones polynomial, which was constructed with the use of the Ocneanu trace $\tau$ defined on the Iwahori–Hecke algebras of type $A$, $\mathrm{H}_n(q)$ [6]. Re-scaling $\tau$ according to the positive and negative stabilization yields the Homflypt polynomial $P(q,z)$.

Let $d, n \in \mathbb{N}$ and let $q$ be a non-zero complex number. The *Yokonuma–Hecke algebra* $\mathrm{Y}_{d,n}(q)$ of type $A$ can be obtained as a quotient of the group algebra over $\mathbb{C}$ of the modular framed braid group $(\mathbb{Z}/d\mathbb{Z})^n \rtimes B_n$ by the quadratic relation

$$g_i^2 = 1 + (q - q^{-1})e_i g_i \quad \text{for all } i = 1, \ldots, n-1,$$

where $g_1, \ldots, g_{n-1}$ are the images of the "braiding" generators of $B_n$, $t_1, \ldots, t_n$ denote the "framing" generators of $(\mathbb{Z}/d\mathbb{Z})^n$ and

$$e_i := \frac{1}{d} \sum_{s=0}^{d-1} t_i^s t_{i+1}^{d-s} \ , \quad \text{for all } i = 1, \ldots, n-1,$$

are idempotents in $\mathbb{C}[(\mathbb{Z}/d\mathbb{Z})^n]$. For $d = 1$, we have $e_i = 1$ and the algebra $\mathrm{Y}_{1,n}(q)$ coincides with the algebra $\mathrm{H}_n(q)$. J. Juyumaya defined a Markov trace $\mathrm{tr}_d$ on $\mathrm{Y}_{d,n}(q)$, depending on a parameter $z$, similarly to the Ocneanu trace, but also on $d-1$ parameters $x_1, \ldots, x_{d-1}$ corresponding to the framing generators and it is defined by the following rules:

$$\begin{array}{lrll}
(1) & \mathrm{tr}_d(ab) = \mathrm{tr}_d(ba) & a, b \in \mathrm{Y}_{d,n}(q) & \\
(2) & \mathrm{tr}_d(1) = 1 & 1 \in \mathrm{Y}_{d,n}(q) & \\
(3) & \mathrm{tr}_d(ag_n) = z\,\mathrm{tr}_d(a) & a \in \mathrm{Y}_{d,n}(q) & \text{(Markov property)} \\
(4) & \mathrm{tr}_d(at_{n+1}^k) = x_k\,\mathrm{tr}_d(a) & a \in \mathrm{Y}_{d,n}(q) & (1 \leqslant k \leqslant d-1).
\end{array}$$

Trying to re-scale $\mathrm{tr}_d$ according to the positive and negative stabilization of the framed braid equivalence, it turned out that $\mathrm{tr}_d$ is the only Markov trace known in literature that does not have straightforward re-scaling. In order to repeat a process similar to the construction of the Homflypt polynomial, the framing parameters $x_1, \ldots, x_{d-1}$ had to satisfy a non-linear system of equations, the so-called E–system [4]. As it was shown by P. Gérardin, the solutions of the E–system are parametrized by the non-empty subsets of $\mathbb{Z}/d\mathbb{Z}$ [4, Appendix]. Hence, for each solution of the E–system parametrized by a non-empty subset $D$ of $\mathbb{Z}/d\mathbb{Z}$, J. Juyumaya and S. Lambropoulou defined an invariant $\Gamma_{d,D}(q,z)$ for framed links [4]. Further, since $B_n$ embeds in $(\mathbb{Z}/d\mathbb{Z})^n \rtimes B_n$, and thus classical links are contained in the set of framed links (corresponding to the framed links with all framings equal to 0), the invariants $\Gamma_{d,D}$ restrict to invariants $\Delta_{d,D}$ for classical knots and links. For $d = 1$, we have $\mathrm{tr}_d = \tau$ and $\Delta_{1,\{0\}}(q,z) = P(q,z)$.

For the past years, we have been trying to compare the invariants $\Delta_{d,D}$, for $d > 1$, with the Homflypt polynomial. In a first attempt, M. Chlouveraki and S. Lambropoulou showed that there is no suitable choice of parameters that will make $\Delta_{d,D}$ coincide with the Homflypt polynomial, unless $q = \pm 1$ or $\mathrm{tr}_d(e_i) = 1$, which are both trivial conditions. It was also shown that there is no algebra homomorphism between the algebra $\mathrm{Y}_{d,n}(q)$ and the algebra $\mathrm{H}_n(q)$ which respects the trace, unless again $\mathrm{tr}_d(e_i) = 1$. However, despite these results, the invariants $\Delta_{d,D}$ could still be topologically equivalent to the Homflypt polynomial. Further,

although the framed link invariants $\Gamma_{d,D}$ satisfy a defining skein relation, this skein relation does not apply to the invariants $\Delta_{d,D}$ since it contains framed links. This fact has rendered a diagrammatic comparison with the Homflypt very difficult until now.

At this point computational packages were developed [2]. Computational data on several Homflypt-equivalent pairs of knots indicated that the invariants $\Delta_{d,D}$ do not distinguish those pairs either, leading us to the belief that the invariants $\Delta_{d,D}$ are topologically equivalent to the Homflypt polynomial. This belief was strengthened by the fact that Yokonuma–Hecke algebras are natural generalizations of Iwahori–Hecke algebras and the invariants $\Delta_{d,D}$ include the polynomial $P$ as a particular case. Consequently, in the case of *knots*, S. Jablan and K. Karvounis were able to formulate a concrete conjecture (cf. [2]), which is now a theorem. Namely,

**Theorem 1** *[1] If $K$ is a knot, then*

$$\Delta_{d,D}(q,z)(K) = \Delta_{1,\{0\}}(q,z|D|)(K) = P(q,z|D|)(K).$$

The proof of the above theorem requires the comparison of the trace $\tau$ with the specialized trace $\mathrm{tr}_{d,D}$, where $\mathrm{tr}_{d,D}$ is the notation we use for $\mathrm{tr}_d$ when the parameters $x_1,\ldots,x_{d-1}$ are specialized to the solution of the E–system parametrized by the non-empty subset $D$ of $\mathbb{Z}/d\mathbb{Z}$. Since we are only interested in classical knots and links, we need to compute $\mathrm{tr}_{d,D}$ only on the images of the elements of $B_n$ in the algebra $\mathrm{Y}_{d,n}(q)$. This process makes the framing generators $t_1,\ldots,t_n$ appear only in the form of the idempotents $e_i$. This led to the following Theorem, another important result, which was a conjecture of J. Juyumaya:

**Theorem 2** *[1] When computing $\mathrm{tr}_{d,D}$ on images of classical braids, the trace rule involving the framing generators,*

$$\mathrm{tr}_{d,D}(a\,t_{n+1}^k) = x_k\,\mathrm{tr}_{d,D}(a) \qquad a\in \mathrm{Y}_{d,n}(q) \quad (1\leqslant k\leqslant d-1),$$

*is replaced by two rules involving the idempotents $e_i$,*

$$\begin{aligned} \mathrm{tr}_{d,D}(ae_n) &= E_D\,\mathrm{tr}_{d,D}(a) \qquad a\in \mathrm{Y}_{d,n}(q)\\ \mathrm{tr}_{d,D}(ae_ng_n) &= z\,\mathrm{tr}_{d,D}(a) \qquad a\in \mathrm{Y}_{d,n}(q), \end{aligned}$$

*where $E_D := \mathrm{tr}_{d,D}(e_n) = 1/|D|$.*

So $\mathrm{tr}_{d,D}$ depends only on parameters $q$, $z$ and $E_D = 1/|D|$. As a consequence, we obtain that the invariants $\Delta_{d,D}$ are in fact parametrized by the natural numbers. Another important consequence of Theorem 2 is the ability to develop a program for computing the invariant $\Delta_{d,D}$ with much lower computational complexity. Such a program has been developed by K. Karvounis and it is available at `http://www.math.ntua.gr/~sofia/yokonuma`.

We next investigate the behaviour of the invariants $\Delta_{d,D}$ on *links*. Surprisingly, Theorem 2 does not hold for links, except in the case of disjoint unions of knots where an analogous result holds:

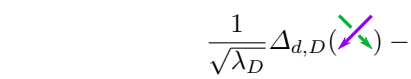
**Theorem 3** *[1] If $L$ is a disjoint union of $k$ knots, we have*

$$\Delta_{d,D}(q,z)(L) = E_D^{1-k}\Delta_{1,\{0\}}(q,z/E_D)(L) = E_D^{1-k}P(q,z/E_D)(L).$$

Further, even though the invariants $\Delta_{d,D}$ do not satisfy defining skein relations (as it is the case for the corresponding framed link invariants $\Gamma_{d,D}$), we discovered that the invariants $\Delta_{d,D}$ do satisfy a special skein relation, only on crossings of different components. Namely,

**Theorem 4** *[1] The following special skein relation holds for $\Delta_{d,D}$:*

$$\frac{1}{\sqrt{\lambda_D}}\Delta_{d,D}(\;) - \sqrt{\lambda_D}\Delta_{d,D}(\;) = (q-q^{-1})\,\Delta_{d,D}(\;),$$



*where different colors represent different components of a link and $\lambda_D := \frac{z-(q-q^{-1})E_D}{z}$.*

The above skein relation is derived from the skein relation of the invariants $\Gamma_{d,D}$ and is identical to the skein relation of the Homflypt polynomial considered at variables $q, \lambda_D$. This result led to the reveal of the behaviour of the invariants $\Delta_{d,D}$ on links. Namely, it led to Theorem 5, which states the following:

**Theorem 5** *[1] The value of $\Delta_{d,D}$ on a link $L$ is a linear combination of the Homflypt polynomial on $L$ and the Homflypt polynomials of disjoint unions of knots obtained by the skein relation.*

The intrinsic difference from the Homflypt polynomial on a link lies in the different values of $\Delta_{d,D}$ on the unlinks with more than one component in which the value $E_D$ appears. Theorem 5 was a strong indication that the invariants $\Delta_{d,D}$ might not be topologically equivalent to the Homflypt polynomial after all.

Finally, we reach the end of our quest, which is not the one that we expected when we started this research.

**Theorem 6** *[1] The Juyumaya-Lambropoulou invariants $\Delta_{d,D}$ are not topologically equivalent to the Homflypt polynomial.*

Indeed, in `http://www.indiana.edu/~linkinfo` one can find all 4.188 links with up to 11 crossings and the value of the Homflypt polynomial on them. We singled out 89 pairs with the same Homflypt value which are not the same as unoriented links. We computed the invariants $\Delta_{d,D}$ on all these pairs and we found that they distinguish six of them, given in Table 1. For one of these pairs, namely,

| Link notation | Braid word |
|---|---|
| $L11n358\{0,1\}$ | $\sigma_1\sigma_2^{-1}\sigma_3^{-1}\sigma_4^{-1}\sigma_3^2\sigma_5^{-1}\sigma_4\sigma_3^{-1}\sigma_2\sigma_1^{-1}\sigma_3^{-1}\sigma_2^{-1}\sigma_4^{-1}\sigma_3\sigma_2^{-3}\sigma_5\sigma_4\sigma_3^{-1}$ |
| $L11n418\{0,0\}$ | $\sigma_1^{-1}\sigma_2^{-1}\sigma_3\sigma_2^{-1}\sigma_3^{-1}\sigma_2\sigma_1^{-1}\sigma_3^{-2}\sigma_2\sigma_3^{-1}$ |

we give a diagrammatic proof using the special skein relation. Similar diagrammatic proofs should exist for the remaining 5 pairs.

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# Classification of Markov traces on Yokonuma–Hecke algebras

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The Yokonuma–Hecke algebra $Y_{d,n}$ (associated to the reductive group $GL_n$) is a quotient of the framed braid group and generalises the classical Iwahori–Hecke algebra used to obtain the HOMFLYPT polynomial.

In [3], Juyumaya introduced on $Y_{d,n}$ an analogue of the Ocneanu trace on the Iwahori–Hecke algebra. Given a solution of the so-called E-system, this trace was subsequently used by Juyumaya and Lambropoulou to produce isotopy invariants for framed links [4] and also for classical links [5]. Moreover, recent results [1] show that the invariants for classical links obtained from $Y_{d,n}$ are topological different than the HOMFLYPT polynomial.

The importance of the Yokonuma–Hecke algebras for topological consideration being now well-established, we are interested in understanding in details the space of Markov traces on the algebras $Y_{d,n}$. In other words we would like to have a classification of all Markov traces on $Y_{d,n}$ in order to construct as many invariants as possible.

Our starting point is a theorem stating that $Y_{d,n}$ is isomorphic to a direct sum of matrix algebras with coefficients in some classical Iwahori–Hecke algebras. Moreover, the isomorphism is given by explicit formulas. This allows us to translate our classification problem and to solve it.

As our main results, we obtain the desired classification and we provide an explicit description of all Markov traces on $Y_{d,n}$ in terms of Markov traces on classical Iwahori–Hecke algebras. We also identify in our classification the Markov traces used by Juyumaya and Lambropoulou for their invariants. We note that in our approach, there is no need to solve the E-system.

This is a joint work with Nicolas Jacon [2].

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# Framization of the Temperley-Lieb algebra

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The framization is a technique introduced by Juyumaya and Lambropoulou and consists in the construction of a non-trivial extension of a knot algebra by framing generators. The basic example of framization is the Yokonuma-Hecke algebra which can be considered as a framization of the Iwahori-Hecke algebra. In this talk we will discuss the concept and motivation behind the framization of the Temperley-Lieb algebra. We will present the invariants for framed and classical knots and links coming from the Framization of the Temperley-Lieb algebra which are not topologically equivalent to the Jones polynomial for the case of classical links.

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# Quotient algebras of mixed braid groups with two fixed strands

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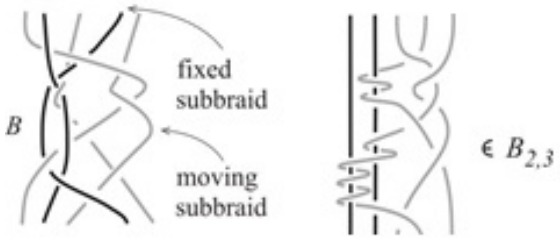
One way to talk about knots and links in a 3-manifold $M^3$ is to describe first the manifold itself in a convenient way, and then utilize this description in order to get a description of the knots and links in it.

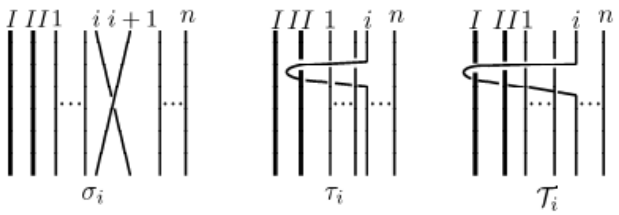
For example, any compact, connected, oriented (c.c.o.) 3-manifold $M^3$ can be thought of as the result of a finite number of Dehn-surgeries in the 3-sphere $S^3$ along a set of knots forming some link $L$ (all knots and links hereafter are considered oriented, and links will be used to mean both). Also, any link $K$ in $M^3$ can be isotoped to a new place $K'$ that lies inside the part of $M^3$ that belongs to $S^3$. Thus $K$ can be represented by the link $L \cup K' \in S^3$. Fixing $L$, these links can be used to express the topologic equivalence (ambient isotopy) of links in $M^3$ working solely in $S^3$: we isotope $L \cup K'$ to appear as the closure of some *mixed braid* $B_L \cup B_{K'}$ (like in the Figure below on the left), and we exhibit a set of Markov-style moves for the braid diagrams of these braids of $S^3$ that express the desired equivalence [6]. So the mixed braids in $S^3$ can encode the links in $M^3$ as isotopy classes, whereas their $B_L$ part encodes the manifold $M^3$ itself. Now braids in $S^3$ exhibit a rich algebraic structure due to their concatenation that turns into groups the sets $B_n$ consisting of the $n$-strand braids for $n \in \mathbb{N}$. So it makes sense to seek analogous algebraic structures for the mixed braids. For this, we first part these braids appropriately so that their $B_L$ part representing $M^3$ appears as a fixed subbraid in the first strands. Let $m$ be the number of *fixed* stands in $B_L$ in such a *parted mixed braid*, and let $n$ be the number of the remaining *moving* strands. Since concatenation in the set $C_{B_L(m,n)}$ of parted mixed braids in $m+n$ strands with $B_L$ as fixed part does not maintain $B_L$, this set cannot in general acquire automatically a nice algebraic structure. Nevertheless, after Artin combing any such braid becomes the concatenation of two parts. The top part is called *algebraic mixed braid*, it is the identity subbraid in its $n$ fixed strands and it contains braiding of its $m$ moving strands with each other and with the fixed ones. The bottom part consists of $B_L$ followed by $n$ identity strands to the right with no other linking of its strands. The set of algebraic mixed braids in $m+n$ strands with $m$ fixed ones is denoted $B_{m,n}$ (an element of $B_{2,3}$ is shown in the Figure below on the right) and becomes a group with the usual concatenation of braids, thus it is a subgroup of the usual braid group $B_{m+n}$ in $S^3$. It will cause no confusion if we call $B_{m,n}$ just as a mixed braid group. $C_{B_L(m,n)}$ is a coset of $B_{m,n}$ in $B_{m+n}$ [10]. Thus for a fixed $M^3$ and a fixed link $L \in S^3$ representing $M^3$, any element in $B_{m,n}$ represents unambiguously an element in $C_{B_L(m,n)}$, hence an oriented link in $M^3$. The equivalence of links in $M^3$ can be translated to Markov-type equivalence in $B_{m,n}$ as well. It is well established that similar considerations about mixed braid representation in $S^3$ of link structures in $M^3$ hold not only for c.c.o. but also for handlebodies and for complements of links in $S^3$ [3, 6, 10]




It has also been shown that the mixed-braid setting can be utilized in order to construct homfly-pt type invariants for oriented links in 3-manifolds $M^3$ whose braid structure is encoded by the groups $B_{1,n}$, like for example the solid torus [9] and the lens space $L(p,1)$ [3]. To achieve this, one mimics the original Jones construction of the classical homfly-pt polynomial for the oriented links in $S^3$ [2], first constructing appropriate algebras over the associated braid groups for the manifold, and then choosing an appropriate

"inductive" basis on them so that the construction of an Oceanu's Markov trace on their union would be possible, which subsequently could be used for the construction of the invariant. The construction of appropriate algebras and the discovery of appropriate "inductive" basis on them are both "hard" parts in this plan of constructing link invariants.

We are currently working with the mixed braid groups $B_{2,n}$ which are related to links in handlebodies of genus two, in the complement of the 2-unlink and in the connected sums $L(p,1)\#L(q,1)$. As an appropriately related sequence of algebras to carry over the above plan for a knot invariant construction, we have defined for every $n$ the quotient algebra $\mathcal{H}_{2,n}(q)$ of $\mathbb{Z}[q^{\pm}]B_{2,n}$ over the quadratic skein relations $g_i^2 = (q-1)g_i + q \cdot 1, i = 1,2,\ldots,n-1$ of the classical Iwahori-Hecke algebra $\mathcal{H}_n(q)$ for the images $g_i$ of the braiding generators $\sigma_i$ shown in the Figure below. And we have spotted an appropriate "inductive" basis $\Lambda_n = \Pi_1\Pi_2\cdots\Pi_n P_1 P_2 \cdots P_n g$ for this algebra, where $g \in \mathcal{H}_n(q)$ and $P_i, \Pi_i$ are finite products of the loopings $\tau_i^{\pm 1}$ and $\tau_i^{\pm 1}, \mathcal{T}_i^{\pm 1}$ respectively (these loopings are shown in the Figure below). Notice that the indices of the $\tau_i^{\pm 1}, \mathcal{T}_i^{\pm 1}$'s in each product $\Pi_1\Pi_2\cdots\Pi_n, P_1P_2\cdots P_n$ are ordered from left to right in increasing order. We have proved that $\Lambda_n$ is a spanning set of $\mathcal{H}_{2,n}(q)$ and our next goal is to prove that it is also linearly independent.




$\sigma_i$ $\tau_i$ $\mathcal{T}_i$

Establishing that $\Lambda$ forms a spanning set of $\mathcal{H}_{2,n}(q)$ is not straightforward because the application of the quadratic relation may result at expressing an element via itself. In general, for any braid $w \in B_{2,n}$, we can use Artin combing to separate it in three consecutive parts $w_1, w_2, w_3$ containing respectively the braiding of the first fixed strand with all the others, of the second fixed strand with all the others, and of all "moving" strands. $w_3$ is subjected to the "canonical" form of the classical Hecke algebra $\mathcal{H}_n(q)$, given by V.F.R. Jones [2], and $w_2$ is also subjected to the "canonical" form of the generalized Hecke algebra $\mathcal{H}_{1,n}(q)$ given in [9]. The two fixed strands of $w_1$ can be straightened so that the moving strands are braided solely with the fixed ones, and then $w_1$ can be written as a finite product of the $\mathcal{T}_i, \tau_i$'s. To have our result, we need to show that $w_1$ is written (suppressing coefficients) as $\sum(\Pi_1\Pi_2\cdots\Pi_n)G$ where $G$ is a finite product of $g_i$'s, and $\Pi_i$ is for all $i$ a finite product of only the loopings $\mathcal{T}_i^{\pm 1}, \tau_i^{\pm 1}$. $G$ can be subsequently pushed at the end of each term in the sum expressing the original $w$ without affecting the desired form in the final sum expressing $w$. "Pushing" $t_i$ to the right of $t_j$ in a product $t_it_j$ with $i > j$ and $t_i \in \{\mathcal{T}_i^{\pm 1}, \tau_i^{\pm 1}\}, t_j \in \{\mathcal{T}_j^{\pm 1}, \tau_j^{\pm 1}\}$ or pushing $g_i$ to the right of a product $g_i\mathcal{T}_j^{\pm 1}, g_i\tau_j^{\pm 1}$ we use the obvious "exchange positions" relations, like for example $g_i\mathcal{T}_i = q^{-1}\mathcal{T}_{i+1}g_i + (q^{-1}-1)\mathcal{T}_{i+1}$. These rules express the original product as a sum of the desired form. Considering products of three loopings introduces us to the existence of recursive phenomena since the original product can sometimes be expressed in terms of a sum containing itself. Then the exact coefficients in this sum become important, and fortunately we can solve the equation at hand and express the original product in the desired canonical form in every individual example. Expanding on this observation, we prove that all words $\tau_M^{\epsilon}\mathcal{T}_M^{-\epsilon}\bar{t}_m^{\zeta}$ for $\bar{t}_m \in \{\mathcal{T}_m^{\pm 1}, \tau_m^{\pm 1}\}$, $m < M$ and $\epsilon, \zeta \in \{-1, 1\}$ can be written as a sum in the desired canonical form. Then the proof that all $w_1$ acquire such a form, is completed by an induction argument for a stronger result which deals with additional information about the indices in the monomials that appear in the desired sum. The induction is on the pair $(k(w_1), d(w_1))$, where $k(w_1)$ is the number of loopings $\mathcal{T}_m^{\pm 1}, \tau_m^{\pm 1}$ appearing in a product form of $w_1$, and $d(w_1)$ is the difference of the greatest from the lowest index appearing in these loopings.

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# Representation theory of framisations of knot algebras

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Yokonuma–Hecke algebras were introduced by Yokonuma in the 1960's in the context of Chevalley groups, as generalisations of Iwahori–Hecke algebras. Recently, Juyumaya and Lambropoulou used these algebras in order to construct invariants for framed knots, that is, knots with differently coloured strands. Their idea arose from the fact that the Yokonuma–Hecke algebra of type $A$ is a quotient of the framed braid group algebra, in the same way that the Iwahori–Hecke algebra of type $A$ is a quotient of the classical braid group algebra. In this spirit, we can say that the Yokonuma–Hecke algebra is a "framisation" of the Iwahori–Hecke algebra. The technique of framisation has been since then applied to other algebras with applications in knot theory, such as Temperley–Lieb algebras. In this talk, we will discuss the representation theory of the Yokonuma–Hecke algebra of type $A$ and of new algebras obtained as framisations of knot algebras. We will see how the study of the representation theory of these objects gave rise to the definition of some new algebras and knot invariants, as well as connections with the already existing ones.

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# The HOMFLYPT skein module of the lens spaces $L_{p,1}$

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In this talk I recall the definition of HOMFLYPT skein modules [6], which extend the HOMLFYPT polynomial [1, 5] from links in $S^3$ to links in arbitrary orientable 3-manifolds. Then I present the methods that we have used to compute this skein module for the lens spaces $L_{p,1}$ [3]. In particular the notion of arrow diagrams from [4] for links in $S^1 \times F$ ($F$ oriented surface) is presented and extended to links in oriented Seifert manifolds [5]. Then the computation of the HOMFLYPT skein module of the solid torus from [4, 8] is translated into the language of arrow diagrams. Based on this, a function $H$ is constructed from arrow diagrams of links in $L_{p,1}$ to a free module with a basis $\mathcal{B}_p$. In fact, $H$ induces an isomorphism between the HOMLFYPT skein module of $L_{p,1}$ and this free module. Some proofs will be given and my coauthor will explain in a subsequent talk how the invariance of $H$ under Reidemeister moves is proven.

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# The isomorphism function from $\mathcal{S}_3(L_{p,1})$ to the free module

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In order to prove that the HOMFLYPT skein module of $L_{p,1}$ is freely generated, we construct a function $H$ from the set of arrow diagrams in $L_{p,1}$ to a free module generated by a set $B_p$. We argue that $H$ induces a function that respects the HOMFLYPT relation, is invariant under the Reidemeister moves and is invariant under the slide move arising from the surgery in the definition of $L_{p,1}$. Thus, this function is an isomorphism between the HOMFLYPT skein module and the free module generated by $B_p$.

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# The Homflypt skein module of $L(p, 1)$ via braids

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## Abstract

In this talk we will first present algebraic mixed braid classification of links in any c.c.o. 3-manifold $M$ obtained by rational surgery along a framed link in $S^3$ and we will focus on the case where $M = L(p, q)$. Then, we will present a new basis, $\Lambda$, for the Homflypt skein module of the solid torus, which topologically is compatible with the handle sliding moves and is appropriate for computing skein modules of arbitrary c.c.o. 3-manifolds. Finally, using $\Lambda$, we will present a basis for the Homflypt skein module of the lens spaces $L(p, 1)$ and discuss current work toward the computation of the Homflypt skein module of $L(p, q)$ in general.

Skein modules of 3-manifolds have become very important algebraic tools in the study of 3-manifolds. Their properties renders topological information about the 3-manifolds. Skein modules are quotients of free modules over ambient isotopy classes of knots and links in a 3-manifold by properly chosen skein relations. A skein module of a 3-manifold $M$ based on the Homflypt skein relation is called *Homflypt skein module* of $M$ and is denoted by $S(M)$. For the lens spaces $L(p, q)$, obtained from $S^3$ by rational surgery along the unknot with rational surgery coefficient $p/q$, we have the following:

**Conjecture 0.1 (Przytycki)** *The Homflypt skein module of the lens spaces $L(p, q)$ is free and isomorphic to the symmetric tensor algebra over the module spanned by conjugacy classes of non trivial elements of the fundamental group.*

In [10] $S(\mathrm{ST})$ has been recovered using algebraic means. More precisely, the generalized Hecke algebra of type B, $\mathrm{H}_{1,n}(q)$, is introduced and a unique Markov trace is constructed on these algebras, leading to a universal invariant for links in ST. The defining relation of the skein module $S(\mathrm{ST})$ is reflected into the quadratic relation of $\mathrm{H}_{1,n}(q)$. In the algebraic language of [10] the basis of $S(\mathrm{ST})$ is given in open braid form by a set $\Lambda'$ and ST is considered as the complement of an unknot. The elements in $\Lambda'$ are all conjugates, so they are consistent with the trace property and they enable the definition of the trace via simple inductive rules. In this talk we present a new basis, $\Lambda$, for the Homflypt skein module of the solid torus, which topologically is compatible with the handle sliding moves. For finding the basis $\Lambda$ we start with the well-known basis $\Lambda'$ of $S(\mathrm{ST})$ and an appropriate linear basis $\Sigma_n$ of the algebra $\mathrm{H}_{1,n}$. We then convert elements in $\Lambda'$ to sums of elements in $\Sigma_n$. Then, using conjugation and the stabilization moves, we convert these elements to sums of elements in $\Lambda$ by managing gaps in the indices, by ordering the exponents of the looping elements and by eliminating braiding tails in the words. Further, we define total orderings on the sets $\Lambda'$ and $\Lambda$ and, using these orderings, we relate the two sets via a block diagonal matrix, where each block is an infinite lower triangular matrix with invertible elements in the diagonal. Using this matrix we prove linear independence of the set $\Lambda$, thus $\Lambda$ is a basis for $S(\mathrm{ST})$.

$S(\mathrm{ST})$ plays an important role in the study of Homflypt skein modules of arbitrary c.c.o. 3-manifolds, since every c.c.o. 3-manifold can be obtained by integral surgery along a framed link in $S^3$ with unknotted components. In particular, the new basis $\Lambda$ is appropriate for computing the Homflypt skein module of the lens spaces.

We will then provide algebraic mixed braid classification of links in any c.c.o. 3-manifold $M$ obtained by rational surgery along a framed link in $S^3$. We do this by representing $M$ by a closed framed braid in $S^3$ and links in $M$ by closed mixed braids in $S^3$. We will first give the analogue of the Reidemeister theorem for links in $M$ and then give geometric formulations of the mixed braid equivalence using the $L$-moves and the braid

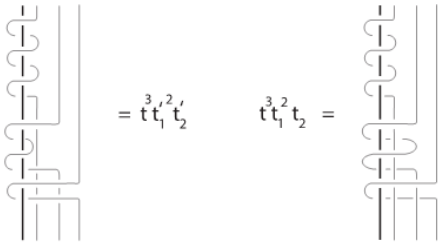


**Fig. 1.** Elements in $\Lambda'$ and $\Lambda$.

band moves. Finally we will formulate the algebraic braid equivalence in terms of the mixed braid groups $B_{m,n}$, using cabling and the parting and combing techniques for mixed braids. Our results set a homogeneous algebraic ground for studying links in 3-manifolds and in families of 3-manifolds using computational tools. We will provide concrete formulas of the braid equivalences in lens spaces.

Finally, we will present a basis for the Homflypt skein module of the lens spaces $L(p,1)$ using the braid approach. We will first show the connection between $S(\mathrm{ST})$ and $S(L(p,1))$ and in particular, we will show that $S(L(p,1))$ is obtained from $S(\mathrm{ST})$ by considering relations coming from the braid band move on elements in the basis $\Lambda$, where the braid band move is performed on every moving strand of each element. We then solve an infinite system of equations coming from the braid band moves, by showing that the system splits into self-contained subsystems and that each subsystem admits unique solution. This led to the following basis for $S(L(p,1))$:

$$B_{p,1} = \{t^{k_0} t_1^{k_1} \dots t_m^{k_m}, : m \in \mathbb{N}, p > k_0 > k_1 > \dots > k_m \in \mathbb{N}^*\} \cup \{\emptyset\}.$$

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# Entanglements in Molecular Simulations of Polymers

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## 1 Introduction

Entanglements among long macromolecular chains govern the flow behavior of polymer melts and shape the mechanical properties of products obtained from plastics processing operations. Recent developments in statistical mechanics-based computer simulation algorithms have enabled sampling detailed molecular configurations of polymer melts which are equilibrated at all length scales. These configurations have served as a starting point for topological analysis of entanglements. Here we briefly discuss (a) connectivity-altering Monte Carlo algorithms for the equilibration of long-chain polymer melt models; (b) the CReTA algorithm for analyzing topological constraints on chains in these models and results obtained therefrom for various chemical constitutions; (c) aspects of the time evolution of topological constraints in linear and crosslinked polymer melts as obtained from molecular dynamics simulations, on the basis of which a distribution of persistences or "strengths" of entanglements can be quantified; (d) a mesoscopic Brownian Dynamics/kinetic Monte Carlo (BD/kMC) simulation approach which utilizes the picture of an entanglement network to predict melt viscoelastic properties.

## 2 Connectivity-altering Monte Carlo Algorithms for Polymer Melts

The importance of topological constraints among chains in shaping the peculiar rheological properties of long-chain polymers was recognized early in polymer science. Reptation theory, pioneered by de Gennes and Doi and Edwards [1], envisions that a linear chain in a melt is confined by "entanglements" with its surroundings into a tube, along which its "primitive path" executes Brownian motion. This picture has been very successful in explaining experimental observations on chain dynamics and melt viscoelasticity and their dependence on chain length and architecture. Molecular simulations offer the possibility of observing entanglements directly. Their application, however, was hampered by the very broad spectra of correlation times characterizing polymer motion in melts (from sub-femtoseconds to seconds), the upper range of these times exceeding the longest times that can be simulated by atomistic molecular dynamics (MD) by six orders of magnitude. A breakthrough in this area has been the development of connectivity-altering Monte Carlo algorithms [4]. These are capable of boldly sampling the long length-scale conformational properties of chains (e.g., the end-to-end distance and the radius of gyration) and thereby achieving full equilibration of systems of industrial relevance. Their application has led to excellent predictions for chain dimensions, volumetric properties, and molecular packing for a wide variety of chemical constitutions. For chemically complex polymers, a useful strategy is to first coarse-grain into a model invoking fewer degrees of freedom and smoother effective potentials, equilibrate at the coarse-grained level, and then reverse-map back to the detailed atomistic level [3].

## 3 Topological Analysis of Polymer Melt Configurations

Well-equilibrated long-chain melt configurations constitute an excellent starting point for studying entanglements. A number of algorithms have been developed for this purpose [4–6]. In the Contour Reduction Topological Analysis (CReTA) algorithm, the contour length of all chains in a melt configuration are shrunk simultaneously through linearizing Monte Carlo moves, under the constraint that no two chains are allowed

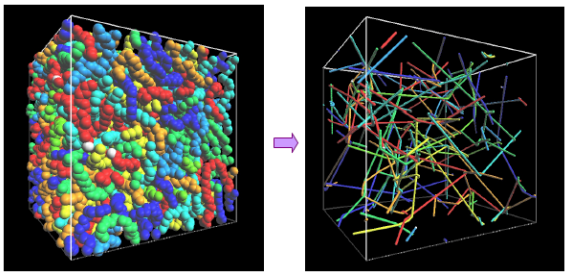

**Fig. 1.** Atomistic configuration of a C1000 melt at 450 K and 1 atm (left) and corresponding reduced network obtained by application of the CReTA algorithm (right). Chain ends, which remain fixed during the reduction process, are shown as white spheres on the left.

to cross themselves. When chain contour lengths are no longer diminishing, chain thickness is reduced and the process starts anew. Chain ends are kept fixed throughout the reduction process, which terminates when a prescribed thickness (e.g., 0.5 Å ) is reached. Chains are ultimately reduced to zig-zag lines coming together at topological constraints with coordination number 4 (see Figure 1). These lines are analogous to Edwards's "primitive paths". From their mean contour length, estimates of the entanglement tube diameter $d$ and of the molar mass between entanglements $M_e$ have been obtained for a variety of chemical constitutions. These estimates are in excellent agreement with experimental evidence.

## 4 Temporal Evolution of the Entanglement Network and Strength of Entanglements

Anogiannakis et al. [7] have undertaken a study of the evolution of the entanglement network as time elapses. To this end they have simulated atomistic polyethylene models with MD and analyzed every recorded configuration along the trajectory with CReTA. They have conducted their analysis on perfect elastomeric systems, where every chain is terminally linked to two crosslink points. In such systems release of the entanglement constraints through chain diffusion is impossible. An interesting finding from this study is that topological constraints, as determined via the CReTA algorithm, come on and off ("blink") in a system at equilibrium. One can use the fraction of time a constraint is active as a measure of the "strength" of that constraint. The distribution of strengths is quite broad, with only the strongest constraints being able to support stress and contribute to $M_e$ as measured experimentally.

## 5 Mesoscopic Simulation of Melt Viscoelastic Properties

One can use the information extracted from static and dynamic topological analysis of atomistically simulated melts in order to construct mesoscopic simulation models to track the dynamics of melts and rubbers over times on the order of milliseconds to seconds, which are inaccessible to MD. Such hierarchies of atomistic and mesoscopic modeling are very promising for addressing polymer melt rheology in a predictive fashion, with all parameters extracted from chemical constitution and macromolecular architecture. The polymer is represented as a set of coarse-grained beads connected by "entropy springs" along chain contours and a set of "slip springs" connecting different chains, whose ends are capable of hopping from bead to bead. Bead motion is tracked with Brownian Dynamics (BD), while hops of the slip spring ends along the contours of the chains they connect, creation and destruction processes at chain ends, are tracked with a kinetic Monte Carlo (kMC) scheme. The mesoscopic model, with all parameters extracted from atomistic simulation, can predict the dynamics of cis-1,4 polyisoprene melts in good agreement with experiment (see Figure 2). One aspect which sets this model apart from similar models is that it is based on an explicit expression for the free energy of the system as a function of the mesoscopic degrees of freedom.

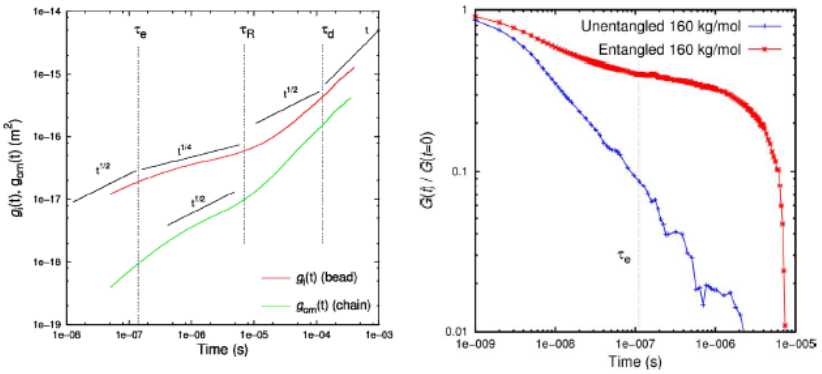


**Fig. 2.** Dynamical predictions of mesoscopic BD/kMC method for entangled melts of linear monodisperse cis-1,4 polyisoprene. Left: mean square displacement of beads, $g_i(t)$, and of chain centers of mass, $g_{\rm cm}(t)$, as functions of time $t$ in a melt of molar mass 50 kg/mol. Results exhibit the crossovers expected from reptation theory. Right: Stress relaxation modulus $G(t)$ in a melt of molar mass 160 kg/mol (entangled), clearly exhibiting a plateau over a range of time scales. Deactivating the slip springs in the simulation (unentangled) leads to a $G(t)$ decaying with time as $t^{-1/2}$, as expected from the Rouse model.

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# Models of Knotting and Linking in Polymeric Systems

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**Abstract.** Polymeric systems are modeled by collections of mathematical curves that are entangled due to the effects of knotting or linking, both local and global. This mutual interference is implicated in large-scale effects making their characterization and quantification an objective of substantial interest. Several mathematical streams are brought together: (1) the knotting linking of closed chains encountered in classical knot theory and its application to study topoisomerase mechanisms [1]; (2) knotting and linking of open chains used to characterize aspects of, for example, protein structures [2–4]; (3) the ergodic sampling of open and closed chains with specified thickness (recent results of Laura Plunkett [5] and Kyle Chapman [6]) and, (4) the periodic linking measures used to study entanglement in periodic boundary condition (PBC) models of polymer melts [7, 8]. The first derives from the application of knot polynomial invariants (A polynomial invariant of oriented links [9] and quantification of linking inspired by the Gauss linking number, the second concerns their extension to open chains, the third addresses both the need for rigorous mathematical methods and the desire to properly generate large samples of chains with specified thickness, while the fourth (work of Eleni Panagiotou) provides a rigorous method for the mathematical linking analysis of large complex systems of chains, e.g. polymer melts or vortex filaments in fluid flow.

**Keywords:** knots, links, thickness, ergodic simulation, DNA, polymer melt

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# A study of the entanglement in systems of curves with Periodic Boundary Conditions

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**Abstract.** The entanglement of filaments arises in many physical systems such as polymer melts, polymer gels, proteins and fluid flows [1,2,4,5]. In these systems open or closed filaments attain complex conformations from which they cannot escape in the timescales of interest, affecting their mechanical properties. In this talk we review some of the ways by which one may quantify and extract entanglement information from a physical system using tools from knot theory.
We use a classical measure of entanglement, the Gauss linking number, to define the *linking fingerprint* of filaments and apply this measure to study the local entanglement of proteins and topoisomerases.
For the simulation of polymer melts, polymer gels and fluid flows, Periodic Boundary Conditions (PBC) are often used (see Figure 1). We define the *periodic linking number* as a measure of entanglement for two oriented curves in a system employing PBC [6]. We mention some of its properties for open and closed chains and we discuss two applications: First, we apply this measure of linking to assess the extend of entanglement of linear chains in a melt and we study the effect of CReTA (Contour Reduction Topological Analysis) algorithm on the entanglement of polyethylene chains [3]. Our results show that the new linking measure is consistent for the original and reduced systems. Next, we apply the periodic linking number to study the entanglement in Olympic gels and we measure the probability of percolation for confined and non-confined systems for the first time.

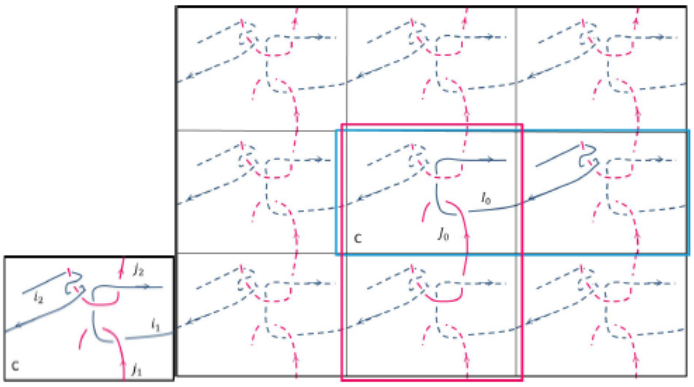


**Fig. 1.** A cartoon image of the simulation cell $C$ and a portion of the periodic system it generates in the case of open chains in a system with 2PBC. Left: The central cell $C$. The *generating chain* $i$ (resp. $j$) is composed by the blue (resp. red) arcs in $C$, ie. the arcs $i_1, i_2$ ($j_1, j_2$, resp.). Right: The *free chain* $I$ (resp. $J$) is the set of dotted blue (resp. red) chains in the periodic system. Highlighted are parent images $I_0$ and $J_0$ and the highlighted blue and red cells are their *minimal unfoldings*.

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# Threading of ring poly(ethylene oxide) molecules by linear chains or other rings in the melt: molecular dynamics simulations followed by a geometric analysis

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We address the issue of topological interactions in blends of ring - linear polyethylene oxide (PEO) melts with a focus on cyclic threading by linear molecules [1], [2].

Our approach entails three main steps. First, detailed molecular dynamics (MD) simulations are performed with model PEO melts characterized by molecular weights $M$ up to 20,000 g/mole for times up to one microsecond to get a large number of fully equilibrated atomistic configurations at the conditions of interest ($P$=1atm and $T$=413K). Second, the accumulated trajectories are reduced to ensembles of primitive paths (PPs) by applying the so called CReTA algorithm (Contour Reduction Topological Analysis) [3] for the static analysis of uncrossability constraints in linear polymer systems; the method is adapted here to the case of ring polymers presenting no chain ends. Third, we geometrically analyze the reduced ensemble of PPs using vector calculus to identify ring-ring and ring-linear threading events and compute their characteristic time scales [1].

We will present numerical results for: a) the relationship between the percentage of rings chains that are threaded by other rings or linear chains and degree of contamination of the melt in linear chains, b) the characteristic survival times of the two types of threadings (ring-ring and ring-linear), and c) their effect on individual ring molecule dynamics and conformational properties.

It turns out that, in particular, ring threading by linear molecules is so strong that it leads to a dramatic reduction of ring diffusivity and orientational relaxation rendering the system's overall dynamics highly heterogeneous. The conformational properties, on the other hand, remain practically unaffected.

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# Chain Size and Shape Dependence of the Tendency for Entanglement in Linear Polymer Melts

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In concentrated solutions and melts, long polymer chains intertwine with one another. At a mesoscopic length scale the material structure resembles an entangled 'spaghetti' of threadlike objects with open ends. This entangled state is considered to be fundamentally responsible for the dynamical and viscoelastic properties of polymer liquids and the large-scale deformation properties (crazing, strain hardening) of glassy polymers. From a technological point of view the understanding of the microscopic mechanisms that govern these properties is important for the design of new polymeric materials.

A successful conceptual framework embodying the 'spaghetti' picture at a molecular level is offered by tube model theories [1]. The latter postulate that the mutual uncrossability of polymer chains generates topological constraints, generally called entanglements, which effectively restrict individual chain conformations in a curvilinear tubelike region surrounding each chain. Large-scale motion is promoted via reptation [11], an effective one dimensional diffusion of a chain along its tube axis. The axis corresponds to a coarse-grained representation of the real chain which neglects small length scale conformational fluctuations, and it is called the primitive path.

In earlier work we have presented [2, 3] a Contour Reduction Topological Analysis algorithm (CReTA) which coarse grains a dense system of polymer chains to the mesoscopic level of a corresponding system of primitive paths (PPs). The latter are constructed as shortest paths which are under the same topological constraints as the original chains. The algorithm fixes chain ends in space, and by prohibiting chain crossing minimizes (shrinks) simultaneously the contour lengths of all chains, until they become sets of rectilinear strands coming together at the nodal points of a network. The nodal points are effective localization points of the topological constraints (TCs) each chain is subjected to. Spatially, they are defined as contact points between shortest path conformations which block further contour reduction and form a microscopic Local Link (LL) (see Fig. 1 and ref [6]).

Using the CReTA algorithm we have analysed entangled samples of Polyethylene (PE) [2] and Polystyrene (PS) [7]. For each system we have available an equilibrium ensemble of configurations of different topologies, generated by the application of connectivity altering Monte Carlo methods [4]. The resulting Kuhn length of PPs provides an excellent estimate of the molar mass between entanglements and of the entanglement tube diameter extracted from plateau modulus measurements. Thus, the ensemble average topology (or mutual threading of polymer chains) of our systems is representative of the real polymers, PE and PS, we studied.

Here, our aim is to examine at a microscopic level the tendency for entanglement of individual chains, in connection with their size and shape in the concentrated state of a melt. A similar problem has been studied by Rawdon et al. [5] who look into the effect of knotting on the shape of single chain, cyclic polymers, modeled as random isosegmental polygons. It was shown that random polygons forming different knot types reach asymptotic shapes that are distinct from the ensemble average shape. For the same chain length, more complex knots are, on average, more spherical than less complex knots, i.e., a correlation between knot type and chain shape was observed.

In a polymer melt, for a given chain length, instantaneous chain conformations can take very different sizes and shapes. The average size (radius of gyration) is determined by random-walk statistics, and the average shape is a prolate ellipsoid. Moreover, each chain is entangled with many other surrounding chains ('the matrix') in a complicated, difficult to describe manner. Do we expect any correlation between the degree of entanglement (which plays the role of knot type) of a chain with the matrix, and the specific shape and size it adopts in the 'spaghetti' state of the melt? A quantitative answer to this question is mathematically

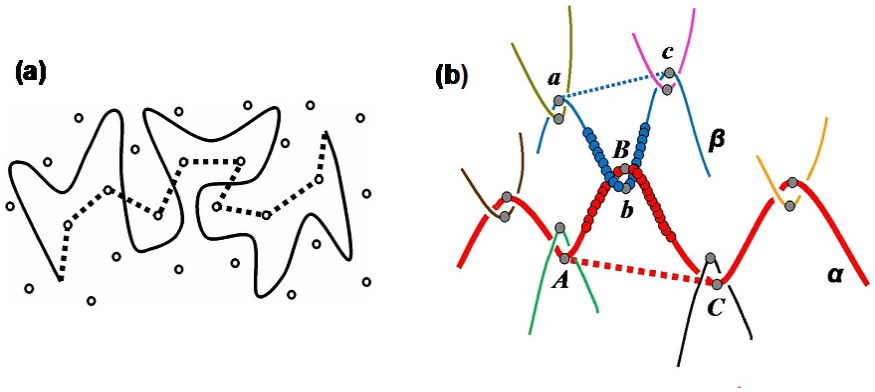


**Fig. 1.** (a) Schematic representation of a test chain (solid line) lying on a plane, which is conformationally restricted by other chains (circles), with local orientations perpendicular to the plane. The primitive path (dashed line) is the shortest path constructed by keeping chain ends fixed and continuously shrinking the chain contour, up to the point that topological (uncrossability) constraints, generated from the bodies of other chains, block further contour reduction. (b) Network nodes, local links, and the topological criterion satisfied by local links. PPs are composed of consecutive beads. Parts ABC and abc, of chains $\alpha, \beta$, respectively, constrain each other and are sketched with a bead structure. All other parts are sketched with contour lines. The beads which 'carry' a TC are colored gray. They mark the points along the PPs where a suitably defined curvature shows a local maximum. Each TC bead is pairwise associated with a TC bead along the PP of a mutually constrained chain. Thus, chain ends and TC bead pairs partition a chain into consecutive strands. In order to decide if a TC bead pair defines a local link we apply a topological criterion at the bead level. For each pair, such as (B,b) between chains $\alpha, \beta$, we construct the composite strands ABC and abc. The ends of these strands are virtually connected, and then we check if the strand ABC crosses the area enclosed by the virtual segment ac and the beads along abc. Similarly, we examine if the strand abc crosses the area enclosed by the virtual segment AC and the beads along ABC. In this way, we examine twice if the ABC and abc rings concatenate. If at least one of these checks is successful, the TC bead pair (B,b) is promoted to a network node (Local Link), otherwise it is discarded.

intractable, since for chains with open ends true topological invariants do not exist, not mentioning the multi-chain nature of the problem.

For our analysis we need measures of size, shape and entanglement. Chain size is characterized by the radius of gyration, while chain shape is obtained from the eigenvalues of the radius of gyration tensor. The degree of entanglement of each chain is characterized by the length of its PP [8] or by the number of microscopic Local Links it forms with the matrix. Our quantitative analysis shows that microscopically, in a melt of given chemical constitution, there is negligible, if any, dependence of the tendency for entanglement on chain shape. Short chains show a relatively decreased tendency for entanglement with decreasing chain size, which for longer chains becomes negligible. Thus, in a polymer melt the degree of a entanglement of a long polymer chain is determined only by its length and not by its size and/or shape. A simple but mathematically non-rigorous explanation for this counter-intuitive result will be given.

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# Extending Topological Surgery to Natural Processes

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Topological surgery occurs in natural phenomena where two points are selected, forces are applied and the manifold in which they occur changes type. More specifically, in [1], we observed that 1-dimensional surgery happens during DNA recombination and magnetic reconnection, while 2-dimensional surgery happens in the formation of tornadoes, Falaco Solitons [2], cell mitosis and in the formation of black holes [3]. Inspired by such phenomena, we introduce in [1] new theoretical concepts which enhance the formal definition of topological surgery with the observed dynamics, thus making the static topological process of surgery an intrinsic and dynamic property of many natural phenomena. More precisely, we introduce local forces caused by an attracting center. Furthermore, we define the notion of solid topological surgery where the interior is filled in. For example, solid 2-dimensional surgery on a 3-ball is defined as 2-dimensional surgeries on the whole continuum of concentric spheres, and surgery on the center is defined to be a circle, see Figure 1. We also embed 2-dimensional topological surgery in the 3-sphere for modelling phenomena which involve more intrinsically the ambient space.

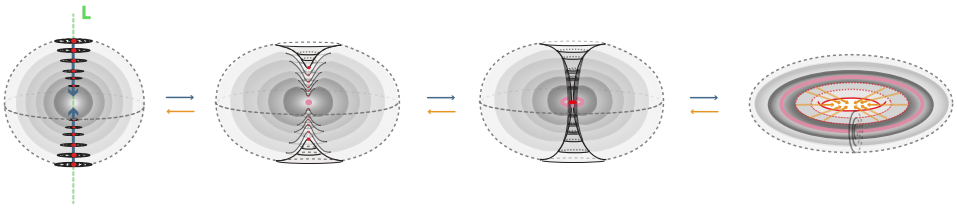


**Fig. 1.** Solid 2-dimensional surgery on a 3-ball.

On the other hand, we observed in [4] that the trajectories of the 3-dimensional generalization of the classical Lotka-Volterra system presented in [5] perform solid 2-dimensional topological surgery. With a slight perturbation of parameters, a nesting of spherical trajectories turn into a nesting of toroidal trajectories through a hole drilling process along a slow manifold L and the central steady point turns into a steady limit circle. This system is proposed as a model for solid 2-dimensional surgery and as a starting point for connecting the Hopf bifurcation with topological surgery. We hope that through this study the topology and dynamics of many natural phenomena will be better understood.

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# Molecular Simulation of Ionic Liquids: Structure, Dynamics and Permeability Properties

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**Abstract.** Ionic liquids (ILs) are organic salts that are in the liquid state at room temperature. ILs exhibit a unique combination of properties that renders them ideal for use in a wide range of applications. In the present work, ILs are studied by means of molecular simulation aiming at the investigation of the molecular mechanisms and the prediction of the IL properties.

**Keywords:** ionic liquids, molecular simulation, physical properties

## 1 Introduction

Ionic liquids are characterized by extremely low vapor pressures, thermal stability, good electrolytic and solvation properties, non-flammability, chemical tunability and easy recycling. In combination with the aforementioned properties, several ILs exhibit also an unexpectedly large $CO_2$ absorption capacity and selectivity [1] and are, therefore, classified among the most attractive candidate sorbents for $CO_2$ capture and separation from post-combustion flue gases. The chemical diversity in the molecular structure of the ions involved affects directly the physicochemical properties of the ILs, thus enabling the tuning of the properties of an IL by making moderate changes in ions chemical formula and structure.

## 2 Methodology and results

The present work focuses on the molecular simulation of imidazolium-based ionic liquids and their permeability and selectivity to gases using optimized and validated classical force fields. Long molecular dynamics (MD) simulations of the $[C_nmim^+][TF_2N^-]$ and $[C_nmim^+][TCM^-]$ ILs families have been performed at various temperatures and at atmospheric pressure in order to calculate the thermodynamic, structural and transport properties of the pure ILs, exploring, simultaneously, the intrinsic characteristics and mechanisms of the systems under study at the atomistic level [2] [3]. Predictions on density extracted from molecular dynamics simulations are in very good agreement with experimental data. The calculated radial distribution functions between the ions centers of mass revealed that ILs exhibit organization at much longer distances compared with conventional liquids with the anion-cation interaction being stronger than the other two interactions at all temperatures. The effect of the alkyl tail length on these properties was also investigated and tail aggregation phenomena, which become more evident for the longer alkyl chain lengths, were detected by calculating radial distribution functions between different sites on the ions. The ions translational motion was analyzed along specific axes in order to investigate anisotropy phenomena in the ions diffusion while the presence of heterogeneities in the dynamics was investigated by detecting deviations from the expected Gaussian behaviour. Ions self-diffusion coefficients were calculated in the Fickian regime using the Einstein relation and shear viscosity calculations were performed using the Green-Kubo relation. The predicted diffusivities are in very good agreement with experimental measurements for the cation. Gas permeability was studied by performing additional very long MD simulations for the prediction of gas diffusivity while gas solubility has been calculated in the infinite dilution regime using the Widom test particle insertion method. All gases appear to have comparable diffusivities in each IL system studied and for that, the solubility is expected to control the selectivity properties of these ILs, a fact that is also supported by experimental results [4].

## 3 Conclusions

Very long MD simulations of several tens of nanoseconds, were performed in a wide temperature range, and at atmospheric pressure in order to study the thermodynamic, structural, dynamic and transport properties of imidazolium-based ILs. The temperature effect was thoroughly studied, as well as, the influence of the anion and the cations alkyl chains length in the properties under investigation. The microscopic mechanisms that govern the spatial organization and the dynamical behaviour of these systems were thoroughly investigated. The predictesthermodynamic, transport and permeability properties are in good agreement with the available experimental data.

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# On ($p$-)almost direct products and residual properties of pure braid groups of surfaces

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It is well known that pure braid groups are residually nilpotent, but all known proofs do not extend to pure braid groups on surfaces. However, in the case of surfaces with non empty boundary, the residual nilpotence of these groups can be verified constructing embeddings in some Torelli groups. The case of closed surface is more complicated: one possible solution implies the structure of ($p$-)almost direct product of these groups. After a short survey on pure braid groups of surfaces, I will explain the notion of ($p$)-almost direct product, its consequences on residual proporties and I-adic filtrations and possible applications to finite type invariants for (surface) braids.

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# Infinite loop spaces, Steenrod, Dyer-Lashof and Dickson algebras

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**Abstract**

The $k$-th stable and unstable homotopy groups $\pi_k^s(X)$ and $\pi_k(X)$ are related by means of a stabilization process involving the homotopy groups of $\Sigma^n X$. The iterated loop spaces $\Omega^n X$ have the property that $\pi_k(\Omega^n X) = \pi_{k+n}(X)$ and the stabilization functor $Q = \Omega^\infty \Sigma^\infty$ has the property $\pi_k(QX) = \pi_k^s(X)$. If $S^0$ is the zero sphere, then $\pi_*\left(QS^0\right)$ are the stable homotopy groups of spheres. One needs to compute $H^*\left(QS^0, \mathbb{Z}/p\mathbb{Z}\right)$ as an algebra over the Steenrod algebra.

Let $\Sigma_\infty = \varinjlim \Sigma_n$ be the infinite symmetric group and $B\Sigma_\infty$ its classifying space. There exists a natural map between $B\Sigma_\infty$ and $Q_0 S^0$. A Theorem of Quillen ( [**?**]) and, independently, Barratt and Priddy ( [1]), shows that the (co)-homology of $Q_0 S^0$ is isomorphic to that of $B\Sigma_\infty$. We give an alternative perspective on this result using modular invariants. The role of modular invariant theory contributes important information for the cohomology of finite groups. The Dickson algebras play a basic role in describing the cohomology rings of the symmetric groups.

Let $D = \bigoplus_{k \geqslant 1} D_k^+$ be the Steenrod module generated by the Dickson algebra monomials of positive degree of any length and $SD = \bigoplus_{k \geqslant 1} SD_k^+$ a certain submodule. For $p = 2$, they coincide. $SD_k$ is a certain subalgebra of the ring of invariants of the general linear group generated by certain elements. In the frame of this work an explicit basis for $H^*(B\Sigma_\infty, \mathbb{Z}/p\mathbb{Z})$ can be constructed in terms of Dickson invariants ( [4]).

Let $\mathcal{A}$ denote the mod $p$ Steenrod algebra and $R$ the mod $p$ Dyer-Lashof algebra. The Dyer-Lashof algebra $R$, a Hopf algebra of homology operations on infinite loop spaces, is a component coalgebra $R = \bigoplus_{n \geqslant 0} R[n]$ with respect to the length of the operations. We consider the category of connected cocomutative positively graded coalgebras. In our case the opposite of the Steenrod algebra acts on our coalgebra and $R[n]$ becomes an unstable $\mathcal{A}$-coalgebra. In this work we compare $R[n]$ with a cofree unstable $\mathcal{A}$-coalgebra. A cofree unstable $\mathcal{A}$-coalgebra of finite type is isomorphic to the dual of a free unstable $\mathcal{A}$-algebra.

Following Madsen, Mui proved that the hom dual of $R[n]$ is isomorphic to the classical Dickson algebra $D_n$, for $p = 2$, as $\mathcal{A}$-algebras ( [6]). Naturally, the Peterson conjecture comes on stage. The Peterson conjecture is about the global structure of the classical Dickson algebra as an unstable algebra over the Steenrod algebra. This conjecture was solved by Pengelley, Peterson and Williams for $p = 2$ ( [7]). They proved that the classical Dickson algebra is a free unstable algebra on a certain cyclic module, modulo one additional relation.

We are interested in the $p$ odd case. Following May ( [2]), we proved that the hom dual of $R[n]$ is isomorphic to a particular subalgebra, $SED_n$, of the extended Dickson algebra $ED_n$ as $\mathcal{A}$-algebras ( [3]). Hence this case is also related to the Peterson conjecture ( [8]).

We prove that $R[n]$ is isomorphic to a subcoalgebra of a cofree unstable $\mathcal{A}$-coalgebra on two cogenerators. Dually, $R[n]^*$ is isomorphic to a free unstable $\mathcal{A}$-algebra on a module generated by two elements $\mu$ and $u$ modulo certain relations, this is our main result. An unstable module $\mathcal{M}(\mu, u)$ is defined on two generators $\mu$ and $u$ under certain relations. Following Steenrod an unstable algebra $\mathcal{Q}(\mu, u)$ is defined on the module $\mathcal{M}(\mu, u)$. It is the quotient of a free unstable algebra ( [5]).

Another aspect is to approximate $H^*(Q_0 S^0)$ by certain subalgebras defined by Dickson algebras. Let $D^\#$ and $SD^\#$ be the corresponding abelian restricted Lie algebras. Here the Lie bracket is zero. There exists a monomorphism $i : SD \to H^*(Q_0 S^0)$ which is not an $\mathcal{A}$-module map. The map $i$ provides an algebra generating set for $H^*(Q_0 S^0)$. Let $V\left(SD^\#\right)$ be the universal enveloping algebra on $SD^\#$. It turns out that $H^*(Q_0 S^0)$ is isomorphic to a free $\mathcal{A}$-algebra generated by Dickson subalgebras of various length. The isomorphism described above is not an isomorphism of Steenrod modules. We wish to approximate that

difference. Certain subalgebras $C^k$ of the universal enveloping algebra $V\left(SD^{\#}\right)$ are defined and their images $(A^k)$ filter $H^*(Q_0S^0)$. The interesting point is that certain quotients of those $\mathcal{A}$-algebras are isomorphic with free Steenrod algebras generated by certain Dickson submodules.

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# Constructing Class Invariants

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The ring class field of imaginary quadratic orders, can be generated by evaluating the $j$-invariant at certain algebraic integers. In a series of articles A. Gee and P. Stevenhagen developed a method based on Shimura reciprocity law in order to to check if a modular function is a class invariant. So far there were few classes of such functions known. Our aim is to describe a systematic method to give whole vector spaces of class functions.

Let $\Gamma(N)$ be the kernel of the map $\mathrm{SL}(2,\mathbb{Z}) \mapsto \mathrm{SL}\left(2,\mathbb{Z}/N\mathbb{Z}\right)$. The group $\mathrm{SL}(2,\mathbb{Z})$ acts on the upper half plane $\mathbb{H}$ in terms of linear fractional transformations and is known to be generated by the elements $S : z \mapsto -\frac{1}{z}$ and $T : z \mapsto z+1$.

The candidates for class invariants are modular functions of level $N$ which can be seen as elements in the function field $F_N$ of the modular curves $X(N)$, defined over the number fields $\mathbb{Q}(\zeta_N)$. The group $\Gamma(N)/\{\pm 1\}$ acts on $F_N$, and also the group $\left(\frac{\mathbb{Z}}{N\mathbb{Z}}\right)^* \cong \mathrm{Gal}(\mathbb{Q}(\zeta_N)/\mathbb{Q})$ acts on the Fourier coefficients of elements in $F_N$.

We have an action of the group $\mathrm{GL}\left(2,\frac{\mathbb{Z}}{N\mathbb{Z}}\right)$ on $F_N$ that fits in the following short exact sequence.

$$1 \to \mathrm{SL}\left(2,\mathbb{Z}/N\mathbb{Z}\right) \to \mathrm{GL}\left(2,\mathbb{Z}/N\mathbb{Z}\right) \xrightarrow{\det} \left(\mathbb{Z}/N\mathbb{Z}\right)^* \to 1.$$

A. Gee and P. Stevenhagen [2] proved the following theorem based on the work of Shimura:

**Theorem 1.** *Let $\mathcal{O} = \mathbb{Z}[\theta]$ be the ring of integers of an imaginary quadratic number field $K$ of discriminant $d < -4$. Suppose that a modular function $h \in F_N$ does not have a pole at $\theta$ and $\mathbb{Q}(j) \subset \mathbb{Q}(h)$. Denote by $x^2 + Bx + C$ the minimum polynomial of $\theta$ over $\mathbb{Q}$. Then there is a subgroup $W_{N,\theta} \subset \mathrm{GL}\left(2,\frac{\mathbb{Z}}{N\mathbb{Z}}\right)$ with elements of the form:*

$$W_{N,\theta} = \left\{ \begin{pmatrix} t - Bs & -Cs \\ s & t \end{pmatrix} \in \mathrm{GL}\left(2,\frac{\mathbb{Z}}{N\mathbb{Z}}\right) : t\theta + s \in (\mathcal{O}/N\mathcal{O})^* \right\}.$$

*The function value $h(\theta)$ is a class invariant if and only if the group $W_{N,\theta}$ acts trivially on $h$.*

Since every element in $\mathrm{SL}(2,\mathbb{Z}/N\mathbb{Z})$ can be written as a word in $S, T$ we obtain a function $\rho$

$$\left(\frac{\mathcal{O}}{N\mathcal{O}}\right)^* \xrightarrow{\phi} \mathrm{GL}(2,\mathbb{Z}/N\mathbb{Z}) \longrightarrow \mathrm{GL}(V), \qquad \overset{\rho}{\frown} \tag{0.1}$$

where $\phi$ is the natural homomorphism given by theorem 1.

The map $\rho$ defined in eq. (0.1) in previous section is not a homomorphism but a cocycle

$$\rho(\sigma\tau) = \rho(\tau)\rho(\sigma)^\tau \tag{0.2}$$

and gives rise to a class in $H^1(G, \mathrm{GL}(V))$, where $G = (\mathcal{O}/N\mathcal{O})^*$. The restriction of the map $\rho$ in the subgroup $H = \ker(\det\phi) \subset G$ is a homomorphism.

We will consider the polynomial algebra $A := \mathbb{Q}(\zeta_N)[e_1,\ldots,e_m]$, acted in by the group $H$ acts on this algebra in terms of the linear representation $\rho$. Classical invariant theory provides us with effective methods (Reynolds operator method,linear algebra method in order to compute the ring of invariants $A^H$. Also there is a well defined action of the quotient group $G/H \cong \mathrm{Gal}(\mathbb{Q}(\zeta_N)/\mathbb{Q})$ on $\mathbb{Q}(\zeta_N)[e_1,\ldots,e_m]^H$.

Define the vector space $V_n$ of invariant polynomials of given degree $n$:

$$V_n := \{F \in \mathbb{Q}(\zeta_N)[e_1,\ldots,e_m]^H : \deg F = n\}.$$

The action of $G/H$ on $V_n$ gives rise to a cocycle

$$\rho' \in H^1(\mathrm{Gal}(\mathbb{Q}(\zeta_N))/\mathbb{Q}), \mathrm{GL}(V_n)).$$

The multidimensional Hilbert 90 theorem asserts that the above cohomology group is trivial, so there is an element $P \in \mathrm{GL}(V_n)$ such that

$$\rho'(\sigma) = P^{-1}P^{\sigma}. \tag{0.3}$$

A modification of the Glasby-Howlett probabilistic algorithm can be used in order to compute the matrix $P$. Let $v_1, \ldots, v_\ell$ be a basis of $V_n$ consisted of $H$-invariant elements. By a simple computation $w_i := v_i P^{-1}$ are also $G/H$ invariant. Therefore theorem 1 implies

**Proposition 1.** *Consider the polynomial ring $\mathbb{Q}(\zeta_N)[e_1, \ldots, e_m]$ and the vector space $V_n$ of $H$-invariant homogeneous polynomials of degree $n$. If $P$ is a matrix such that eq. (0.3) holds, then the images of a basis of $V_n$ under the action of $P^{-1}$ are class invariants.*

This method can be applied to the modular functions of level $24N$ called *generalized Weber functions*:

$$\nu_{N,0} := \sqrt{N}\frac{\eta \circ \begin{pmatrix} N & 0 \\ 0 & 1 \end{pmatrix}}{\eta} \text{ and } \nu_{k,N} := \frac{\eta \circ \begin{pmatrix} 1 & k \\ 0 & N \end{pmatrix}}{\eta}, 0 \leqslant k \leqslant N-1, \tag{0.4}$$

All known so far class invariants are special cases of polynomials of $\nu_{k,N}$.

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# On Algebraic Modeling of Computational Structures

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Algebraic specifications, is one of the most well known families of formal methods. In the Thalis project we worked towards the unification of the well-known algebraic specification language CafeOBJ [1] with the strong theorem prover Athena [2] within a common interface. Also, we developed further the Institution based formal specification theory and applied techniques from algebraic specifications for the modeling and verification of specific application domains.

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# Towards the integration of Athena with CafeOBJ using tool support

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Formal methods are mathematical techniques that provide powerful means for analyzing systems behavior and can prove really helpful for preventing design errors at an early stage of development. The need for the specification and verification of software and hardware system properties increases as more and more complex systems are built and used in critical domains.

Algebraic specification languages such as CafeOBJ [1, 2], Maude [3] and CASL [4] have well-known advantages for modeling and reasoning about digital systems. The specifications are relatively simple, readable and writable, and can be executed and automatically analyzed in various other ways to provide valuable information to the modelers. Sometimes however, it is useful to use more conventional theorem proving systems to automate the verification process and to ensure the soundness of the proofs. To this end, we propose a framework of integration of CafeOBJ with Athena [6, 7] and a common interface.

CafeOBJ provides mechanized implementations of Observational Transition Systems (OTSs), a species of behavioral specifications, that allow users to specify distributed systems using multi-sorted conditional equational logic with subsorting. The specifications are executable via rewriting, which is useful for building up computational intuitions about the underlying system. In addition, CafeOBJ allows users to compose proof scores that establish certain invariant properties, typically by induction.

Athena is a system based on general polymorphic multi-sorted first-order logic. It integrates computation and deduction, allows for readable and highly structured proofs, guarantees the soundness of results that have been proved, and also has built-in mechanisms for general model-checking and theorem-proving, as well as seamless connections to state-of-the-art external systems for both.

By integrating these two methodologies we wish to combine the strengths of CafeOBJ, most notably succinct, composable, executable specifications based on conditional equational logic with those of Athena, namely, structured and readable proofs, and greater automation both for proof and for counterexample discovery.

We illustrate our approach through a simple algorithm that is often used to illustrate OTSs in CafeOBJ. In our mutex example there is a set of processes, each of which is executing code. At any point in time (i.e, at any system state), a process is either in some critical section of the code or in some remainder (non-critical) section. When a process $p$ enters its critical section, the resulting state becomes locked. When $p$ exits the critical section, the resulting state is unlocked. For $p$ to enter its critical section in some state $s$, $p$ must be *enabled* in $s$. A process $p$ is enabled in $s$ iff $p$ is in its remainder section in $s$ and $s$ is not locked. This is, therefore, the effective condition of the enter state transition for a given process. The effective condition of the exit transition is for the process to be in its critical section. We have two observer functions, one that takes a state $s$ and a process id $p$ and tells us what section of the code $p$ is executing in $s$ (critical or remainder), and a function that takes a state $s$ and tells us whether $s$ is locked.

The developed interface takes as input an OTS-based specification written in CafeOBJ and automatically produces an Athena specification. The output specification in our example is demonstrated below.

The generated specification can be fed directly to Athena and the user can then proceed with the verification of the properties of interest. One such property in the mutex algorithm is that at most one process can be in its critical section at any given time. Using Athena a completely automatic proof by structural induction can be obtained and then a more detailed proof in natural-deduction style which is also automatically checked for soundness.

```
datatype Label := rs | cs
assert Label-axioms := (datatype-axioms  "Label")
define L := ?L:Label
domain Pid
define I := ?I:Pid
structure Sys := init | (try1 Sys Pid)| (exit Sys Pid)
declare pc: [Sys Pid] -> Label
declare locked: [Sys] -> Boolean
define S := ?S:Sys
define I := ?I:Pid
define J := ?J:Pid
define c-try := lambda (S I) (((pc S I) = rs ) and (not locked S))
define c-exit := lambda (S I) ((pc S I) = cs )
assert* axioms :=
[((pc init I) = rs)
((locked init) = false)
((pc (try1 S I) J ) = cs if ((I  = J ) and (c-try S I)))
((pc (try1 S I) J ) = (pc S J) if (not ((I  = J ) and (c-try S I))))
((locked (try1 S I)) = true if (c-try S I))
((try1 S I) = S if (not c-try S I))
((pc (exit S I) J ) = rs if ((I  = J ) and (c-exit S I)))
((pc (exit S I) J ) = (pc S J) if (not ((I  = J ) and (c-exit S I))))
((pc (exit S I) J ) = (pc S J) if ((not (I  = J )) and (not
c-exit S I)))
((locked (exit S I)) = false if (c-exit S I))
((exit S I) = S if (not c-exit S I))]
```

As a future work we plan to conduct more case studies using the proposed methodology and to investigate possible connections with othe tools, like Hets [8] for example. Our approach could be used as a vehicle for integrating other algebraic specification methods (such as Maude) with more conventional theorem-proving systems based on first- or higher-order logic.

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# Cafe2JML: Integrating Behavioral Algebraic Specifications with Design by Contract

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In the last decade, an increased interest for the development of Design by Contract (DbC) [1] languages for Java and C# has been noticed (JML [2], Cofoja [3], Spec# [4]). These languages mainly aim to verify an implementation against its specification. The corner stone idea of this approach is that the class's methods and the clients (programs) that invoke them have a contract between them, i.e. a specification which defines their obligations and requirements [5]. Contracts are defined in the programming language itself and can be translated into executable code by the compiler. Most of these languages provide a wide range of tools to ensure that the implementation satisfies the specification, like run-time assertion checks (RAC), unit test generation, static verification (SV) and formal verification tools. On the other hand specification languages independent of a particular implementation language are being developed for almost thirty years now. In the family of algebraic specification languages the research and applications of OBJ, BOBJ, CafeOBJ, Maude, CASL, etc. have been more than active. These languages are used to verify the system's design abstracting away from the implementation details. Thus any implementation (model) satisfying the design will preserve the verified properties.

Both approaches have their merits and downsides. From a programmer's point of view DbC languages are preferable because their syntax is closer to the programming language, thus easier to learn, and can be used without dealing with difficult mathematical concepts [2]. However, it is very difficult to verify the correct behavior of complex systems with such languages [6] and even more difficult to create verifying compilers for all useful combinations of languages and platforms. From a design engineer's or a mathematician's point of view algebraic specification languages that focus on the verification of the design of an application, instead of its code are preferable because they nearly always leads to greater conceptual clarity of the system and also because, as it has been argued, the main sources of errors in software are in areas other than code, namely, requirements, specification, and design [7]. However, enforcing conformance of the implementation to the design decisions is largely an open problem for these type of languages since manual verification, if at all possible, is impractical for many projects [8].

| Questions | JML | OTS/CafeOBJ | Cafe2jml |
|---|---|---|---|
| Can the language be used to model the logical structure and organization of OO programs? | ✓ | ✓ | ✓ |
| Can arbitrarily-large programs be represented abstractly, uncluttered by implementation minutiae? | | ✓ | ✓ |
| Can we verify the conformance of an implementation to a design specification ? | ✓ | | ✓ |
| Can we verify high level security and/or behavioral properties of the system? | | ✓ | ✓ |
| Can we verify the behavior of heterogeneous (infinite) state systems? | | ✓ | ✓ |
| Can conflicts between design and implementation be detected automatically? | ✓ | | ✓ |

**Table 1.** Central Questions

In this paper we attempt to combine these two approaches and hopefully adopt the strengths of both while minimizing their weaknesses. To this end, we address the problem of developing verified critical software systems by proposing a methodology, which can be summarized to the following steps:

1. The design of the system is specified using a Behavioral Algebraic Specification language and its behavior is formally verified by a design engineer [9].
2. Next, the specification, which was verified in the previous step, is translated to a DbC specification.
3. The DbC specification is used by a programmer to create a compliant program. Because there are many such programs optimization of the code is possible.
4. Finally, using existing DbC tools like [10] the program is verified against the DbC specification.

Using the proposed methodology we can derive an optimized program that satisfies the desired (complex) safety properties. As the DbC language we use the Java Modeling Language (JML) and as the Behavioral Algebraic specification methodology we use Observational Transition Systems (OTS) defined in CafeOBJ [11] terms. However, the proposed methodology can be applied to various combinations of other such languages. The reason for using JML is mainly the number of tools available, while we use OTS/CafeOBJ because the method has been applied successfully in a plethora of cases for the verification of design, and also because it provides an object oriented approach to specification with natural support for inheritance and object composition. In order to clarify the scope and goals of our work, in table 1 we pose and answer some questions (taken from [9] and adapted to the design of critical object oriented systems) that we believe a software development methodology of critical systems must enjoy.

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# Towards Formal Open Standards: the Case of RSS

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Open standardization seems to be very popular among software developers as it makes the standard's adoption by the software engineering community easier and smoother. All open standards are accompanied by a specification document that is available for anyone to see. That document, usually written in natural language format, is an explicit set of requirements -set out by the standard setting organization- that are to be satisfied by the standard's design [1]. However such specification documents are usually accompanied by some issues:

- Verbosity: Such documents can be huge in size (for instance, the Dicom specification [2] spans a total of 4900 pages),
- Lack of clarity: It is sometimes difficult to use language in a precise and unambiguous way without making the document wordy and difficult to read. The built-in ambiguity of natural language can lead to misunderstandings.
- Requirements amalgamation: Several different requirements may be expressed together as a single requirement, so to discover the consequence of a change, you may have to look at every requirement rather than at just a group of related requirements. Also, since a natural language requirements specification is over-flexible, you can say the same thing in completely different ways, leaving it up to the reader to find out when requirements are the same and when they are distinct.
- Requirements confusion: A standard's specification does not necessarily prove that the standard is working as intended. It might be verified to comply with a specification but this does not, by itself, indicate that it is fit for any particular use. The ones who use or specify the standard are the ones responsible to consider the choice of available specifications, specify the correct one, enforce compliance, and use the standard correctly. Some validation of suitability is necessary.

The problems that can come up due to the above reasons can make requirements specifications that are written in natural language prone to misunderstandings and errors. Most of the times, these errors are only discovered during later phases of the software development process and may then be very expensive to resolve [3].

The term "formal methods" is used to refer to any activities that rely on mathematical representations of software including formal system specification, specification analysis and proof, transformational development, and program verification. All these activities are dependent on the formal specification of the software [3]. While formal methods allow for more precision, clarity and provide a property verification backbone, the popularity of them is not that high, as the industry seems to have little motivation to move into this territory.

In this paper the authors present i) the idea of applying formal specification techniques to open standards' specifications, creating an "Open Formal Standard", and ii) an example of a formal specification of the RSS v2.0 open standard. The authors provide evidence for the advantages of the open standards formal specification over natural language documentations: Formal specifications are more concise, less ambiguous,

more complete with respect to the original documentation and also executable and reusable as they support module inheritance. The merging of formal specification methods and open standards allows i) a more concrete standard design; ii) an improved understanding of the environment under design; iii) an enforced certain level of precision into the specification [4, 5], and also iv) provides software engineers with extended property checking/verification capabilities, especially if they use any algebraic specification language. The authors showcase how the RSS standard can be formally specified using an algebraic specification language and demonstrate how can that be beneficial.

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# Fixed Point Logics as Institutions

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## Abstract

It has been already proved that several logics are institutions [3], [14], such as **PL** - Propositional calculus, **FOL** - First Order Logic, $\boldsymbol{FOL^1}$ - Single-sorted logic, $\boldsymbol{FOL^+}$ - Positive First Order Logic, **UNIV** - Universal setences in first order logic, **HCL** - Horn clause logic, **EQL** - Equational logics, $(\Pi \cup \Sigma)^0_n$, **SOL** - Second order logic, $\boldsymbol{FOL_{\infty,\omega}}, \boldsymbol{FOL_{\alpha,\omega}}$ - infinitary logics , **MFOL** - Modal (first order) logic.
Finite model theory is the study of logics on classes of finite structures. One of the central issues in finite model theory is the relationship between logical definability and computational complexity. The expressive power of First Order Logic (FOL) is weak to express several properties on finite structures, like connectivity on finite graphs. Another critical issue is that first-order logic is not closed under inductive definition. For example, consider the notion of a connected component of a graph. We define this concept inductively. Let $v$ a vertex of a graph $G$ and $P_0(v) = \{v\}$, for each $n \in \mathbb{N}$ we define $P_n = \{x \in G \mid G \models R(x, y) \text{for some y} \in P_{n-1}(v)\}$. If $G$ is finite graph then for some $m$ $P_m(v) = P_{m+1}(v)$. In this case $P_m(v)$ is the connected component of $v$ in $G$. Although first-order logic can define the sets $P_m$ for each $m \in \mathbb{N}$, it cannot define the notion of a connected component. Hence first-order logic is not closed under inductive definitions. A methodology that can be followed in order to construct Logics with greater expressive power than FOL, includes Logics which extend the FOL allow inductive definitions.
A way of modeling recursive definitions is to incorporate an explicit fixed point operator. Logics following this approach are called fixed-point logics. We consider logics that include various fixed-point operators. These logics are minimal extensions of first-order logic that are closed under inductive definitions.
There is more than one way to make the notion of inductive definition precise. Each corresponds to a different fixed-point operator.

1. Least Fixed Point Logic ($\boldsymbol{LFP}$)
2. Monotone Fixed Point Logic ($\boldsymbol{MFP}$)
3. Inflationary Fixed Point Logic ($\boldsymbol{IFP}$)
4. Partial Fixed Point Logic ($\boldsymbol{PFP}$)

In our paper we plane to prove that $\boldsymbol{LFP}$ and $\boldsymbol{MFP}$ are institutions.

## Future Research

The development of institution-independent model theory been used for developing general results about compactness [6], axiomatizability [14], elementary chains [4], interpolation [8], [5], definability [10], completeness [11], [17], generating a big array of novel concrete results in actual unconventional, or even in conventional well studied logics. Moreover, the institution-independent approach to model theory makes the access to highly difficult model theoretic results considerably easier, an example being the Keisler-Shelah isomorphism theorem. Continuing from the aforementioned we will through institution theory study the finite model theory and the properties of logics that expand upon the expressiveness of first order logic. The interconnection of institution theory and descriptive complexity offers a large field of research, in the sense that it forms a connecting link between abstract categorical model theory and computability. We could for example view basic theorems like that of Fagin [15], [16] in categorical terms, or generalise within the limits of institution theory the Ehrenfeucht-Fraisse Games, which provides a sound and complete method for delineating the expressive power of logics in the finite.

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