

# Higher-Order Description Logics for Domain Metamodeling

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## Abstract

We investigate an extension of Description Logics (DL) with higher-order capabilities, based on Henkin-style semantics. Our study starts from the observation that the various possibilities of adding higher-order constructs to a DL form a spectrum of increasing expressive power, including domain metamodeling, i.e., using concepts and roles as predicate arguments. We argue that higher-order features of this type are sufficiently rich and powerful for the modeling requirements arising in many relevant situations, and therefore we carry out an investigation of the computational complexity of satisfiability and conjunctive query answering in DLs extended with such higher-order features. In particular, we show that adding domain metamodeling capabilities to *SHIQ* (the core of OWL 2) has no impact on the complexity of the various reasoning tasks. This is also true for *DL-Lite<sub>R</sub>* (the core of OWL 2 QL) under suitable restrictions on the queries.

## Introduction

Metamodeling allows one to treat concepts and properties as first-order citizens, and to see them as individuals whose properties can be asserted and reasoned upon. This feature is important in all applications where the need arises of modeling and reasoning about meta-concepts, i.e., concepts whose instances are themselves concepts, and meta-properties, i.e., relationships between meta-concepts.

It is well-known that in logic, and in Description Logics (DLs) in particular, higher-order constructs are needed for a correct representation of concepts and properties at the meta-level. However, the issue of devising suitable extensions to DLs for representing and reasoning about meta-level elements is largely unexplored. Recent research on this subject shows that there is a spectrum of meta-level modeling capabilities. Four points in this spectrum represent specific notable cases, which we now discuss.

*Domain modeling.* This is the simplest case of the spectrum, with no higher-order feature, and is actually the one addressed in most of the research on DLs.

*Metaquerying.* This is the case where the knowledge base does not contain any axiom regarding meta-concepts or

meta-roles, but the query language allows for using meta-concepts, so that concepts and roles in the knowledge base can match the variables in the query, and may thus be returned as answers to the query [Angiulli *et al.*, 2003]. This mechanism allows to express queries that are beyond first-order logic.

*Domain metamodeling.* This is the case where the language allows for using concepts and roles as predicate arguments, so that one can assert properties of concepts and roles, as if they were individuals. Domain metamodeling includes metaquerying as a special case. It is our opinion that higher-order features of this kind are sufficiently rich and powerful for the modeling requirements arising in many relevant situations. One of the most popular approaches to domain metamodeling, which is closely related to DLs, is HiLog [Chen *et al.*, 1993]. HiLog is a logic with a higher-order syntax, thus allowing predicates to appear as arguments in atomic formulae, but with a Henkin-style semantics, which implies that the expressive power of the language actually remains within first-order.

*Full metamodeling.* This is the most general case, where the modeling language allows not only for using concepts and roles as predicate arguments, but also for refining and extending the properties of the language operators, and to reason upon such properties. For instance, RDF and RDFS allow for stating properties not only on domain (meta-)elements, but also on the so-called built-in vocabulary (i.e., operators such as `rdf:type`) of the language.

In this paper, we investigate an extension of DLs with higher-order capabilities. We are especially interested in those features that allow us both to model and to query individuals, concepts, roles, meta-concepts and meta-roles with no limitations. Therefore, the extension that we study is geared towards domain metamodeling (thus including metaquerying). Specifically we provide the following contributions. First, we present syntax and semantics of an extension of DLs with domain metamodeling features (see Section 2). In particular, we show how, starting from any DL  $\mathcal{L}$ , one can define its higher-order version, called  $Hi(\mathcal{L})$ . From the syntax point of view, our approach stems from two ideas. On one hand, every modeling element can be seen simultaneously as an individual, as a concept, and as a role. On the other hand, since concepts in DLs are denoted not only by names, but also by complex expressions, every complex ex-

pression is a modeling element in our language. From the semantic point of view, we adopt a Henkin semantics, as in HiLog and RDF(S). Second, we carry out an investigation of the computational complexity of reasoning in DLs extended with higher-order features. By reasoning we mean not only logical implication, but also answering unions of conjunctive queries with metaquerying abilities. We show that adding domain metamodeling capabilities to expressive DLs, in particular to  $\mathcal{SHIQ}$  [Baader *et al.*, 2003], has no impact on the complexity of the various reasoning tasks, including satisfiability (Section 3), and conjunctive query answering (see Section 4). The situation is similar for the tractable DLs of the  $DL\text{-Lite}$  family [Calvanese *et al.*, 2007], under suitable restrictions on the queries (Section 5).

The idea of representing concepts and properties at the meta-level is an old one in Knowledge Representation and Computer Science. Semantic networks and early Frame-based systems incorporated specific mechanisms for representing concepts whose instances are themselves concepts [Lehmann, 1992; Attardi and Simi, 1981]. Conceptual modeling languages proposed in the 70's, such as TAXIS [Mylopoulos *et al.*, 1980], provided both the notion of meta-class, and suitable facilities for describing properties of operators on meta-classes. The notion of meta-class is also present in virtually all object-oriented languages, including modern programming languages.

The issue of extending DLs with higher-order constructs has been addressed only by few research papers. In [Badea, 1997], probably the first paper on this subject, the notion of “reification of concepts” is proposed as a means to express meta-level classes, but the paper does not address neither the issue of meta-roles, nor the issue of query answering. A more recent paper is [Colucci *et al.*, 2010] where second-order features with Henkin semantics are introduced in DLs to capture several forms of nonstandard reasoning. (Further references are dropped for preserving anonymity.) Other recent investigations, such as [Motik, 2007; Pan and Horrocks, 2006], address the issue of full metamodeling in the context of ontology languages, and therefore go beyond the scope of our work.

Finally, we remark that *punning*, i.e., using the same name for different elements of the ontology (for example, an individual and a concept), has been introduced in OWL 2<sup>1</sup>, as a consequence of recognizing the importance of domain metamodeling<sup>2</sup>. While punning can be treated trivially in classical reasoning tasks over the DL ontology, it poses interesting problems in the context of query processing. In particular, if variables are not typed a priori, punning introduces the kind of metaquerying studied in our work. Indeed, the DL query language presented in this paper is the first one (to our knowledge) that exploits punning in queries, since it allows for expressing joins involving variables which simultaneously denote both individuals and predicates.

## Higher-order Description Logics

In this section, we show how, starting from a DL  $\mathcal{L}$ , one can define its higher-order version, called  $Hi(\mathcal{L})$ . In partic-

ular, we refer to a specific DL, namely  $\mathcal{SHIQ}$  (the core of OWL 2), and detail the higher-order DL  $Hi(\mathcal{SHIQ})$ .

Before delving into  $Hi(\mathcal{L})$ , we present some preliminary definitions. Every traditional DL  $\mathcal{L}$  is characterized by a set  $OP(\mathcal{L})$  of *operators*, used to form concept and role expressions, and a set of  $MP(\mathcal{L})$  of *meta-predicates*, used to form assertions. Each operator and each meta-predicate have an associated arity. If symbol  $S$  has arity  $n$ , then we write  $S/n$  to denote such symbol and its arity. For  $\mathcal{SHIQ}$ , we have:

$$\begin{aligned} OP(\mathcal{SHIQ}) &= \{Inv/1, And/2, Not/1\} \cup \\ &\quad \{AtLeastQ_n/2 \mid n \in \mathbb{N}\} \\ MP(\mathcal{SHIQ}) &= \{Inst_C/2, Inst_R/3, Isa_C/2, Isa_R/2, Tran/1\}. \end{aligned}$$

We assume that the reader is familiar with  $\mathcal{SHIQ}$ . Therefore, the intuitive meaning of all the above symbols should be clear. Their semantics will be given shortly.

**Syntax.** We assume the existence of two disjoint, countably infinite alphabets:  $\mathcal{S}$ , the set of *names*, and  $\mathcal{V}$ , the set of *variables*. The building blocks of a  $Hi(\mathcal{L})$  knowledge base are assertions, which in turn are based on expressions. We define the set of *expressions*, denoted by  $\mathcal{E}_{\mathcal{L}}(\mathcal{S})$ , over the alphabet  $\mathcal{S}$  for  $Hi(\mathcal{L})$  inductively as follows:

- if  $E \in \mathcal{S}$  then  $E \in \mathcal{E}_{\mathcal{L}}(\mathcal{S})$ ;
- if  $C/n \in OP(\mathcal{L})$  and  $E_1, \dots, E_n \in \mathcal{E}_{\mathcal{L}}(\mathcal{S})$  then  $C(E_1, \dots, E_n) \in \mathcal{E}_{\mathcal{L}}(\mathcal{S})$ .

A  $Hi(\mathcal{L})$  *assertion* over  $\mathcal{E}_{\mathcal{L}}(\mathcal{S})$  is a statement of the form  $M(E_1, \dots, E_n)$  where  $M \in MP(\mathcal{L})$ ,  $n \geq 0$  is the arity of  $M$ , and for every  $1 \leq i \leq n$ ,  $E_i \in \mathcal{E}_{\mathcal{L}}(\mathcal{S})$ . A  $Hi(\mathcal{L})$  *knowledge base (KB)* is a set of assertions over  $\mathcal{E}_{\mathcal{L}}(\mathcal{S})$ . Thus, an assertion is simply an application of a meta-predicate to a set of expressions. Intuitively, an assertion is an axiom that predicate over a set of individuals, concepts or roles.

**Example 1** Suppose that the alphabet  $\mathcal{S}$  contains the names *Cours*, *Teaches*, *Full*, *GradCourse*, *UnivConcept*, *ObsoleteConcept*, *John*, and *DefinedBy*. Then the following are  $Hi(\mathcal{SHIQ})$  assertions:

$$\begin{aligned} &Isa_C(GradCourse, \\ &\quad And(Course, Not(AtLeastQ_2(Inv(Teaches)), Full))) \\ &Inst_C(And(Course, \\ &\quad Not(AtLeastQ_2(Inv(Teaches)), Full))), UnivConcept) \\ &Inst_R(UnivConcept, John, DefinedBy) \\ &Inst_R(Not(ObsoleteConcept), John, DefinedBy) \end{aligned}$$

The first assertion states that every graduate course is taught by at most one full professor. The second assertion says that concept  $And(Course, Not(AtLeastQ_2(Inv(Teaches)), Full))$  is an instance of concept *UnivConcept* (which is therefore a meta-concept). Finally, the meaning of the third and the fourth assertions is that concepts *UnivConcept* and  $Not(ObsoleteConcept)$  have been introduced in the KB by *John*.  $\square$

Next, we introduce the notion of query, which relies on the notion of “atom”. Intuitively, an atom is constituted by a meta-predicate applied to a set of arguments, where each argument is either an expression or a variable. Formally, we define the set  $\tau(\mathcal{S}, \mathcal{V})$  of *terms* over  $\mathcal{S}$  and  $\mathcal{V}$  to be  $\mathcal{E}_{\mathcal{L}}(\mathcal{S}) \cup \mathcal{V}$ . Terms of the form  $\mathcal{E}_{\mathcal{L}}(\mathcal{S})$  are called *ground*. We define an *atom* to be constituted by the application of a meta-predicate in  $MP(\mathcal{L})$  to a set of terms, and we call an atom *ground* if no variable occurs in it. Note that a ground atom has the same

<sup>1</sup>[http://www.w3.org/2007/OWL/wiki/OWL\\_Working\\_Group](http://www.w3.org/2007/OWL/wiki/OWL_Working_Group)

<sup>2</sup><http://www.w3.org/2007/OWL/wiki/Punning>

form of an assertion. An atom whose meta-predicate is  $Isa_C$  or  $Isa_R$  is called an *ISA-atom*, while we call *instance-atom* an atom whose meta-predicate is  $Inst_C$  or  $Inst_R$ .

A *higher-order conjunctive query (HCQ)* of arity  $n$  is an expression of the form  $q(x_1, \dots, x_n) \leftarrow a_1, \dots, a_m$  where  $q$ , called the query predicate, is a symbol that does not belong to  $\mathcal{S} \cup \mathcal{V}$ , every  $x_i$  belongs to  $\mathcal{V}$ , every  $a_i$  is a (possibly non-ground) atom, and all variables  $x_1, \dots, x_n$  occur in some  $a_j$ . The variables  $x_1, \dots, x_n$  are called the *free variables* (or distinguished variables) of the query, while the other variables occurring in  $a_1, \dots, a_m$  are called *existential variables*. A *higher-order union of conjunctive queries (HUCQ)* of arity  $n$  is a set of HCQs of arity  $n$  with the same query predicate. A HCQ/HUCQ is called *Boolean* if it has no free variable.

**Example 2** Referring to the alphabet mentioned in Example 2, the following is a HCQ:

$$q(x) \leftarrow Inst_C(x, y), Inst_R(y, John, DefinedBy)$$

Intuitively, the query asks for the instances of all the concepts in the KB defined by John. In our case, the answer will be simply  $\{GradCourse, Not(AtLeastQ_2(Inv(Teaches), Full))\}$ .

**Example 3** Consider now the case where we want to ask for the instances of all the concepts  $y$  such that the expression  $Not(y)$  is a concept in the knowledge base defined by John. The natural formulation of this query would be:

$$q(x) \leftarrow Inst_C(x, y), Inst_R(Not(y), John, DefinedBy)$$

However, according to our syntax for queries, variables cannot appear as arguments within terms, and therefore the above is *not* a query in  $Hi(SHIQ)$ . See also the conclusions.  $\square$

**Semantics.** The semantics of  $Hi(\mathcal{L})$  is based on the notion of interpretation structure. An *interpretation structure* is a triple  $\Sigma = \langle \Delta, \mathcal{I}_c, \mathcal{I}_r \rangle$  where: (i)  $\Delta$  is a non-empty (possibly countably infinite) set; (ii)  $\mathcal{I}_c$  is a function that maps each  $d \in \Delta$  into a subset of  $\Delta$ ; and (iii)  $\mathcal{I}_r$  is a function that maps each  $d \in \Delta$  into a subset of  $\Delta \times \Delta$ . In other words,  $\Sigma$  treats every element of  $\Delta$  simultaneously as: (i) an individual; (ii) a unary relation, i.e., a concept, through  $\mathcal{I}_c$ ; and (iii) a binary relation, i.e., a role, through  $\mathcal{I}_r$ .

An *interpretation* over  $\Sigma$  is a pair  $\mathcal{I} = \langle \Sigma, \mathcal{I}_o \rangle$ , where  $\Sigma = \langle \Delta, \mathcal{I}_c, \mathcal{I}_r \rangle$  is an interpretation structure, and  $\mathcal{I}_o$  is a function that maps: (i) each element of  $\mathcal{S}$  to a single domain object of  $\Delta$ ; and (ii) each element  $C/n \in OP(\mathcal{L})$  to an  $n$ -ary function  $C^{\mathcal{I}_o} : \Delta^n \rightarrow \Delta$  that satisfies the conditions characterizing the operator  $C/n$ . In particular, the conditions for the operators in  $OP(SHIQ)$  are the following:

1. for each  $d_1 \in \Delta$ , if  $d = Inv^{\mathcal{I}_o}(d_1)$  then  $d^{\mathcal{I}_r} = (d_1^{\mathcal{I}_r})^{-1}$ ;
2. for each  $d_1, d_2 \in \Delta$ , if  $d = And^{\mathcal{I}_o}(d_1, d_2)$  then  $d^{\mathcal{I}_c} = d_1^{\mathcal{I}_c} \cap d_2^{\mathcal{I}_c}$ ;
3. for each  $d_1 \in \Delta$ , if  $d = Not^{\mathcal{I}_o}(d_1)$  then  $d^{\mathcal{I}_c} = \Delta - d_1^{\mathcal{I}_c}$ ;
4. for each  $d_1, d_2 \in \Delta$  and  $n \in \mathbb{N}$ , if  $d = AtLeastQ_n(d_1, d_2)$  then  $d^{\mathcal{I}_c} = \{e \mid \exists e_1, \dots, e_n \text{ s.t. } e_i \neq e_j \text{ for } i \neq j, \text{ and } \forall i \text{ s.t. } 1 \leq i \leq n, \langle e, e_i \rangle \in d_1^{\mathcal{I}_r} \text{ and } e_i \in d_2^{\mathcal{I}_c}\}$ .

We extend  $\mathcal{I}_o$  to expressions in  $\mathcal{E}_{\mathcal{L}}(\mathcal{S})$  inductively as follows: if  $C/n \in OP(\mathcal{L})$ , then  $(C(E_1, \dots, E_n))^{\mathcal{I}_o} = C^{\mathcal{I}_o}(E_1^{\mathcal{I}_o}, \dots, E_n^{\mathcal{I}_o})$ . To interpret non-ground terms, we

need assignments over interpretations. An *assignment*  $\mu$  over  $\langle \Sigma, \mathcal{I}_o \rangle$  is a function  $\mu : \mathcal{V} \rightarrow \Delta$ .

We are now ready to interpret terms in  $Hi(\mathcal{L})$ . Given an interpretation  $\mathcal{I} = \langle \Sigma, \mathcal{I}_o \rangle$  and an assignment  $\mu$  over  $\mathcal{I}$ , we define the function  $(\cdot)^{\mathcal{I}_o, \mu} : \tau(\mathcal{S}, \mathcal{V}) \rightarrow \Delta$  as follows:

- if  $t \in \mathcal{S}$  then  $t^{\mathcal{I}_o, \mu} = t^{\mathcal{I}_o}$ ;
- if  $t \in \mathcal{V}$  then  $t^{\mathcal{I}_o, \mu} = \mu(t)$ ;
- if  $t$  is of the form  $C(t_1, \dots, t_n)$ , then  $t^{\mathcal{I}_o, \mu} = C^{\mathcal{I}_o}(t_1^{\mathcal{I}_o, \mu}, \dots, t_n^{\mathcal{I}_o, \mu})$ .

Satisfaction of an assertion with respect to an interpretation  $\mathcal{I}$  and an assignment  $\mu$  over  $\mathcal{I}$  is based on the semantics of the meta-predicates in  $MP(\mathcal{L})$ . For the meta-predicates in  $SHIQ$ , satisfaction in  $\mathcal{I}, \mu$  is defined as follows:

- $\mathcal{I}, \mu \models Inst_C(E_1, E_2)$  if  $E_1^{\mathcal{I}_o, \mu} \in (E_2^{\mathcal{I}_o, \mu})^{\mathcal{I}_c}$ ;
- $\mathcal{I}, \mu \models Inst_R(E_1, E_2, E_3)$  if  $(E_1^{\mathcal{I}_o, \mu}, E_2^{\mathcal{I}_o, \mu}) \in (E_3^{\mathcal{I}_o, \mu})^{\mathcal{I}_r}$ ;
- $\mathcal{I}, \mu \models Isa_C(E_1, E_2)$  if  $(E_1^{\mathcal{I}_o, \mu})^{\mathcal{I}_c} \subseteq (E_2^{\mathcal{I}_o, \mu})^{\mathcal{I}_c}$ ;
- $\mathcal{I}, \mu \models Isa_R(E_1, E_2)$  if  $(E_1^{\mathcal{I}_o, \mu})^{\mathcal{I}_r} \subseteq (E_2^{\mathcal{I}_o, \mu})^{\mathcal{I}_r}$ ;
- $\mathcal{I}, \mu \models Tran(E)$  if  $(E^{\mathcal{I}_o, \mu})^{\mathcal{I}_r}$  is a transitive relation.

A  $Hi(\mathcal{L})$  KB  $\mathcal{H}$  is satisfied by  $\mathcal{I}$  if all the assertions in  $\mathcal{H}$  are satisfied by  $\mathcal{I}$ .<sup>3</sup> As usual, the interpretations  $\mathcal{I}$  satisfying  $\mathcal{H}$  are called the *models* of  $\mathcal{H}$ . A  $Hi(\mathcal{L})$  KB  $\mathcal{H}$  is *satisfiable* if it has at least one model.

Let  $\mathcal{I}$  be an interpretation and  $\mu$  an assignment over  $\mathcal{I}$ . A Boolean HCQ  $q$  of the form  $q \leftarrow a_1, \dots, a_n$  is *satisfied* in  $\mathcal{I}, \mu$  if every assertion  $a_i$  is satisfied in  $\mathcal{I}, \mu$ . A Boolean HUCQ  $Q$  is *satisfied* in  $\mathcal{I}, \mu$  if there exists a Boolean HCQ  $q \in Q$  that is satisfied in  $\mathcal{I}, \mu$ . A Boolean HUCQ  $Q$  is satisfied in  $\mathcal{I}$ , written  $\mathcal{I} \models Q$ , if there exists an assignment  $\mu$  over  $\mathcal{I}$  such that  $Q$  is satisfied in  $\mathcal{I}, \mu$ . Given a Boolean HUCQ  $Q$  and a  $Hi(\mathcal{L})$  KB  $\mathcal{H}$ , we say that  $Q$  is *logically implied* by  $\mathcal{H}$  (denoted by  $\mathcal{H} \models Q$ ) if for each model  $\mathcal{I}$  of  $\mathcal{H}$  there exists an assignment  $\mu$  such that  $Q$  is satisfied by  $\mathcal{I}, \mu$ .

Given a non-Boolean HUCQ  $q$  of the form  $q(t_1, \dots, t_n) \leftarrow a_1, \dots, a_m$ , a grounding substitution of  $q$  is a substitution  $\theta$  such that  $t_1\theta, \dots, t_n\theta$  are ground terms. We call  $t_1\theta, \dots, t_n\theta$  a grounding tuple. The set of *certain answers* to  $q$  in  $\mathcal{H}$  is the set of grounding tuples  $t_1\theta, \dots, t_n\theta$  that make the Boolean query  $q\theta \leftarrow a_1\theta, \dots, a_m\theta$  logically implied by  $\mathcal{H}$ . Notice that, in general, the set of certain answers may be infinite even if the KB is finite. Therefore, it is of interest to define suitable notions of safety, which guarantee that the set of answers is bounded. This issue, however, is beyond the scope of the present paper.

Indeed, in this paper, we focus on Boolean queries only, so as to address the computation of certain answers as a decision problem. Also, in our analysis, we measure the computational complexity in three different ways: with respect to the size of the whole KB (*KB complexity*), with respect to the size of the part of the KB formed by the assertions involving only the meta-predicates  $Inst_C/2, Inst_R/3$  (*instance complexity*), and with respect to the size of the KB and the query together (*combined complexity*).

### Satisfiability in $Hi(SHIQ)$

In this section we study the computational characterization of KB satisfiability in the higher-order DL  $Hi(SHIQ)$ .

<sup>3</sup>We do not need to mention assignments here, since all assertions in  $\mathcal{H}$  are ground.

We start by defining a translation  $\Pi$  from  $Hi(SHIQ)$  to  $SHIQ$ . First, we define three injective functions  $\nu_O : \mathcal{E}_{SHIQ}(\mathcal{S}) \rightarrow \mathcal{S}^o$ ,  $\nu_C : \mathcal{E}_{SHIQ}(\mathcal{S}) \rightarrow \mathcal{S}^c$ , and  $\nu_R : \mathcal{E}_{SHIQ}(\mathcal{S}) \rightarrow \mathcal{S}^r$ , where  $\mathcal{S}^o$ ,  $\mathcal{S}^c$  and  $\mathcal{S}^r$  are three mutually disjoint alphabets of names, each one disjoint from  $\mathcal{S}$ . Then, we inductively define two functions  $\tau_C$  and  $\tau_R$  as follows:

- if  $S \in \mathcal{S}$ , then  $\tau_C(S) = \nu_C(S)$  and  $\tau_R(S) = \nu_R(S)$ ;
- $\tau_C(Not(E)) = Not(\tau_C(E))$ ;
- $\tau_C(And(E_1, E_2)) = And(\tau_C(E_1), \tau_C(E_2))$ ;
- $\tau_C(AtLeastQ_n(E_1, E_2)) = AtLeastQ_n(\tau_C(E_1), \tau_C(E_2))$ ;
- $\tau_R(Inv(E)) = Inv(\tau_R(E))$ .

Now, let  $Expr(\mathcal{H})$  denote the set of ground expressions occurring in  $\mathcal{H}$  (notice that every subexpression of an expression occurring in  $\mathcal{H}$  also belongs to  $Expr(\mathcal{H})$ ). Then, given a  $Hi(SHIQ)$  KB  $\mathcal{H}$ , we inductively define the  $SHIQ$  KB  $\Pi(\mathcal{H})$  as follows:

1. if  $Not(E) \in Expr(\mathcal{H})$ , then  $\nu_C(Not(E)) \equiv \tau_C(Not(E)) \in \Pi(\mathcal{H})$ ;
2. if  $Inv(E) \in Expr(\mathcal{H})$ , then  $\nu_R(Inv(E)) \equiv \tau_R(Inv(E)) \in \Pi(\mathcal{H})$ ;
3. if  $And(E_1, E_2) \in Expr(\mathcal{H})$ , then  $\nu_C(And(E_1, E_2)) \equiv \tau_C(And(E_1, E_2)) \in \Pi(\mathcal{H})$ ;
4. if  $AtLeastQ_n(E_1, E_2) \in Expr(\mathcal{H})$ , then  $\nu_C(AtLeastQ_n(E_1, E_2)) \equiv \tau_C(AtLeastQ_n(E_1, E_2)) \in \Pi(\mathcal{H})$ ;
5. if  $Inst_C(E_1, E_2) \in \mathcal{H}$ , then  $\nu_C(E_1)(\nu_O(E_2)) \in \Pi(\mathcal{H})$ ;
6. if  $Inst_R(E_1, E_2, E_3) \in \mathcal{H}$ , then  $\nu_R(E_1)(\nu_O(E_2), \nu_O(E_3)) \in \Pi(\mathcal{H})$ ;
7. if  $Isa_C(E_1, E_2) \in \mathcal{H}$ , then  $\nu_C(E_1) \sqsubseteq \nu_C(E_2) \in \Pi(\mathcal{H})$ ;
8. if  $Isa_R(E_1, E_2) \in \mathcal{H}$ , then  $\nu_R(E_1) \sqsubseteq \nu_R(E_2) \in \Pi(\mathcal{H})$ ;
9. if  $Tran(E) \in \mathcal{H}$ , then  $Tran(\nu_R(E)) \in \Pi(\mathcal{H})$ .

Informally, the above translation provides a  $SHIQ$  KB  $\Pi(\mathcal{H})$  in which for every ground term  $E$  occurring in  $\mathcal{H}$  (notice that  $E$  may be a subterm of another term occurring in  $\mathcal{H}$ ) there exists a concept name  $\nu_C(E)$  (and a role name  $\nu_R(E)$ ) that is defined, through the use of the function  $\tau_C$  (respectively,  $\tau_R$ ) as equivalent to the term  $E$  seen as a concept (respectively, role) expression.

Based on the above translation, we get our first result, namely a reduction of KB satisfiability in  $Hi(SHIQ)$  to KB satisfiability in  $SHIQ$ .

**Theorem 4** *A  $Hi(SHIQ)$  KB  $\mathcal{H}$  is satisfiable iff the  $SHIQ$  KB  $\Pi(\mathcal{H})$  is satisfiable.*

From the above theorem, and the computational characterization of KB satisfiability in  $SHIQ$  [Baader *et al.*, 2003], we are able to provide the computational characterization of KB satisfiability in  $Hi(SHIQ)$ .

**Theorem 5** *KB satisfiability in  $Hi(SHIQ)$  is EXPTIME-complete w.r.t. KB complexity, and coNP-complete w.r.t. instance complexity.*

### Query answering in $Hi(SHIQ)$

In this section we study query answering in  $Hi(SHIQ)$ . In particular, we restrict our attention to a specific class of HUCQs, which we call *guarded*. For the definition of this class of queries, we need the notions of object position, concept position, and role position, whose goal is to characterize the various argument positions in atoms and terms. If we use symbol **O** to mark object positions, symbol **C** to mark

concept positions, and symbol **R** to mark role positions, then we have:  $Inst_C(\mathbf{O}, \mathbf{C})$ ,  $Inst_R(\mathbf{O}, \mathbf{O}, \mathbf{R})$ ,  $Isa_C(\mathbf{C}, \mathbf{C})$ ,  $Isa_R(\mathbf{R}, \mathbf{R})$ ,  $Tran(\mathbf{R})$ ,  $Not(\mathbf{C})$ ,  $And(\mathbf{C}, \mathbf{C})$ , and  $Inv(\mathbf{R})$ .

Now, a HCQ  $q$  is called *guarded* if, for every variable  $x$  occurring in an ISA-atom of  $q$ ,  $x$  also occurs in a concept or role position of an instance-atom of  $q$ . A HUCQ is called guarded is every HCQ  $q$  in  $Q$  is guarded.

We start our analysis of query answering by showing that answering guarded HUCQs is coNP-hard w.r.t. KB complexity (actually, w.r.t. instance complexity only) and  $\Pi_2^p$ -hard w.r.t combined complexity, as soon as the DL admits the  $Inst_C$ ,  $Inst_R$  and  $Isa_C$  meta-predicates (and even if the DL does not allow for any logical operator).

**Theorem 6** *Let  $\mathcal{L}$  be a DL such that  $MP(\mathcal{L})$  contains the meta-predicates  $Inst_C$ ,  $Inst_R$  and  $Isa_C$ . Answering guarded HUCQs over  $Hi(\mathcal{L})$  KBs is coNP-hard w.r.t. instance complexity, and  $\Pi_2^p$ -hard w.r.t. combined complexity, even if  $OP(\mathcal{L}) = \emptyset$ .*

The coNP lower bound stated in the theorem is obtained through a reduction from 3-CNF unsatisfiability, while the  $\Pi_2^p$  lower bound is proved through a reduction from 2-QBF. Both reductions exploit the possibility of defining a HUCQ where one disjunct asks for an instance of a concept named  $C$ , and another disjunct checks containment of  $C$  into other concepts. Since in every model in which  $C$  is empty,  $C$  is contained into every concept, this query forces a form of “reasoning by cases” over the models of the KB (i.e., different variable assignments must be considered in different models). Actually the proof uses a KB formed by instance assertions only.

This theorem implies that answering guarded HUCQs is intractable w.r.t. instance (and KB) complexity not only in  $Hi(SHIQ)$ , but in *all* the DLs currently studied, since all DLs comprise the meta-predicates  $Inst_C$ ,  $Inst_R$  and  $Isa_C$ .

We now provide a technique for query answering over  $Hi(SHIQ)$  KBs, which is based on the reduction to  $SHIQ$  provided by the function  $\Pi()$  defined for KB satisfiability. For query answering, however, the function  $\Pi()$  must be extended to account for expressions occurring in the query; moreover, we also need to define a translation  $\pi$  of HUCQs. Such functions are defined below.

Let  $Q$  be a HUCQ. We say that  $Q$  is a *metaground* HUCQ if it does not contain any variable in concept or role position. Moreover, we say that  $Q$  is an *instance* HUCQ if it only contains instance-atoms. We denote by  $Expr(Q)$  the set of ground expressions occurring in a HUCQ  $Q$ . Let  $q$  be a HCQ and let  $e_1, \dots, e_k$  be the ground expressions occurring as arguments of ISA-atoms in  $q$ . We define inductively the set of expressions  $conj_{ISA}(q)$  as follows:

$$\begin{aligned} \mathcal{C}_1 &= \{e_1, \dots, e_k\} \\ \mathcal{C}_{i+1} &= \{And(e, e_0) \mid e \in \mathcal{C}_i \text{ and } e_0 \in \mathcal{C}_1\} \\ conj_{ISA}(q) &= \mathcal{C}_k \end{aligned}$$

Informally,  $conj_{ISA}(q)$  denotes the set of all the possible conjunctions of ground expressions occurring as arguments of ISA-atoms in  $q$ . We are now ready to define the set of ground expressions  $Expr(\mathcal{H}, Q)$  as follows:

$$Expr(\mathcal{H}, Q) = Expr(\mathcal{H}) \cup Expr(Q) \cup \bigcup_{q \in Q} conj_{ISA}(q)$$

$Expr(\mathcal{H}, Q)$  constitutes the set of ground expressions that we use for grounding metavariables. Notice that  $Expr(\mathcal{H}, Q)$  has size polynomial in the size of  $\mathcal{H}$ .

Let  $q$  be a HCQ. An  $\mathcal{H}$ -metaground instantiation of  $q$  is a HCQ obtained from  $q$  by replacing every variable occurring in at least one concept or role position with an expression of  $Expr(\mathcal{H}, q)$ . Given a HCQ  $q$ , we define  $metaground(q, \mathcal{H})$  as the HUCQ corresponding to the union of all the  $\mathcal{H}$ -metaground instantiations of  $q$ . If there are no ground terms occurring in  $\mathcal{H}$  (i.e.,  $\mathcal{H}$  is empty), we define  $metaground(q, \mathcal{H})$  to be the HCQ obtained from  $q$  by replacing all variables occurring in concept and role positions with any name in  $\mathcal{S}$ . Given a HUCQ  $Q$ , we define  $metaground(Q, \mathcal{H}) = \bigcup_{q \in Q} metaground(q, \mathcal{H})$ .

Given a metaground HUCQ  $Q$ , we denote by  $\pi(Q, \mathcal{H})$  the standard UCQ obtained from  $metaground(Q, \mathcal{H})$  by: (i) replacing every ground term  $E$  occurring as an argument in object position of an atom in  $Q$  with  $\nu_O(E)$ ; (ii) replacing every ground term  $E$  occurring as an argument in concept position of an atom in  $Q$  with  $\nu_C(E)$ ; (iii) replacing every ground term  $E$  occurring as an argument in role position of an atom in  $Q$  with  $\nu_R(E)$ . Finally, given a  $Hi(SHIQ)$  KB  $\mathcal{H}$  and a HUCQ  $Q$ , we denote by  $\Pi(\mathcal{H}, Q)$  the  $SHIQ$  KB obtained starting from  $\Pi(\mathcal{H})$  and adding, for every ground term  $E$  that occurs in  $metaground(Q, \mathcal{H})$  and does not occur in  $\mathcal{H}$ , the inclusion assertions generated by the first 5 items in the definition of  $\Pi(\mathcal{H})$  above.

Now we restrict our attention to queries that are both *metaground* and *instance*, for which we can easily prove:

**Lemma 7** *Let  $\mathcal{H}$  be a  $Hi(SHIQ)$  KB, and let  $Q$  be a metaground instance HUCQ. Then,  $\mathcal{H} \models Q$  iff  $\Pi(\mathcal{H}, Q) \models \pi(Q, \mathcal{H})$ .*

Based on the known computational characterization of answering “standard” UCQs, i.e., both *metaground* and *instance* UCQs, in  $SHIQ$  [Glimm *et al.*, 2007; Calvanese *et al.*, 2008; Ortiz *et al.*, 2008], we immediately get:

**Theorem 8** *Answering metaground instance HUCQs over  $Hi(SHIQ)$  KBs is coNP-complete w.r.t. instance complexity, EXPTIME-complete w.r.t. KB complexity, and 2-EXPTIME-complete w.r.t. combined complexity.*

We can extend this result to the whole class of instance HUCQs. First, we show the following key property, which holds for the whole class of guarded HUCQs.

**Theorem 9** *Let  $\mathcal{H}$  be a  $Hi(SHIQ)$  KB, and let  $Q$  be a guarded HUCQ.  $\mathcal{H} \models Q$  iff  $\mathcal{H} \models metaground(Q, \mathcal{H})$ .*

*Proof (sketch).* One direction (if  $\mathcal{H} \models metaground(Q, \mathcal{H})$  then  $\mathcal{H} \models Q$ ) is trivial. The proof of the other direction is quite involved. First, the following property (\*) can be shown: if  $\mathcal{H} \models Q$  then  $\mathcal{H} \models metaground(Q)$ , where  $metaground(Q)$  is the query obtained from  $Q$  through the meta-grounding of the meta-variables over the set of all expressions of the language (not only those terms occurring in  $Expr(\mathcal{H}, Q)$ ). Now suppose  $\mathcal{H} \models Q$ . If  $\mathcal{H} \not\models metaground(Q, \mathcal{H})$ , then there exists a model  $\mathcal{I}$  for  $\mathcal{H}$  such that  $\mathcal{I} \models metaground(Q)$  and  $\mathcal{I} \not\models metaground(Q, \mathcal{H})$ . It is now possible to define a model  $\mathcal{I}'$  for  $\mathcal{H}$  which is essentially the disjoint union of a countably infinite number of

copies of  $\mathcal{I}$ , in which the function  $\mathcal{I}'_o$  is defined in such a way that  $\mathcal{I}' \not\models metaground(Q)$ , which contradicts the above property (\*). Consequently,  $\mathcal{H} \models metaground(Q, \mathcal{H})$ .  $\square$

Lemma 9, and Theorems 7, 8 allow us to immediately derive the computational characterization of query answering in  $Hi(SHIQ)$  for the whole class of instance HUCQs.

**Theorem 10** *Answering instance HUCQs over  $Hi(SHIQ)$  KBs is coNP-complete w.r.t. instance complexity, EXPTIME-complete w.r.t. KB complexity, and 2-EXPTIME-complete w.r.t. combined complexity.*

In order to go beyond instance HUCQs, and answer guarded HUCQs in  $Hi(SHIQ)$ , we now define a technique which reduces this problem to answering standard UCQs in  $SHIQ$ . In the following, we call *intensional (or, TBox) assertion* every assertion using one of the meta-predicates  $Isa_C$ ,  $Isa_R$ , and  $Tran$ . Moreover, given a KB  $\mathcal{H}$  and a HUCQ  $Q$ , we define  $TA_{\mathcal{H}, Q}$  to be the set of all intensional assertions in  $SHIQ$  that can be obtained from the set of ground terms occurring in  $Expr(\mathcal{H}, Q)$ .

Let  $\mathcal{T}'$  be a subset of  $TA_{\mathcal{H}, Q}$ . We say that  $\mathcal{T}'$  is *coherent with  $\mathcal{H}$*  iff  $\mathcal{T} \subseteq \mathcal{T}'$ , where  $\mathcal{T}$  is the set of TBox assertions occurring in  $\mathcal{H}$ , and  $\mathcal{T}' \cup \mathcal{H} \not\models \alpha$  for every  $\alpha \in TA_{\mathcal{H}, Q} - \mathcal{T}'$ . Then, we denote by  $IntEval(Q, \mathcal{H}, \mathcal{T}')$  the metaground instance HUCQ  $Q'$  obtained starting from  $Q' = metaground(Q, \mathcal{H})$  and then evaluating every intensional assertion over  $\mathcal{T}'$  as follows:

- if  $\alpha$  is an intensional assertion occurring in a HCQ  $q \in Q'$  and  $\alpha \in \mathcal{T}'$ , then eliminate  $\alpha$  from  $q$ ;
- if  $\alpha$  is an intensional assertion occurring in a HCQ  $q \in Q'$  and  $\alpha \notin \mathcal{T}'$ , then eliminate  $q$  from  $Q'$ .

Finally, we define  $KB_{SHIQ}(\mathcal{H}, \mathcal{T}', Q)$  as the  $SHIQ$  KB<sup>4</sup> obtained starting from  $\mathcal{K}' = \Pi(\mathcal{H}', Q)$  (where  $\mathcal{H}' = \mathcal{T}' \cup \mathcal{H}$ ) and then adding to  $\mathcal{K}'$  the following assertions for every TBox assertion  $\alpha \in TA_{\mathcal{H}, Q} - \mathcal{T}'$ :

- if  $\alpha = Isa_C(E_1, E_2)$  then add to  $\mathcal{K}'$  the ABox assertions  $\nu_C(E_1)(n)$  and  $\nu_C(Not(E_2))(n)$ , where  $n$  is a new individual name in  $\mathcal{K}'$ ;
- if  $\alpha = Isa_R(E_1, E_2)$  then add to  $\mathcal{K}'$  the TBox assertion (role disjointness)  $\nu_R(E_2) \sqsubseteq \neg Aux_i$ , where  $i$  is such that  $Aux_i$  is a new role name in  $\mathcal{K}'$ , and the ABox assertions  $\nu_R(E_1)(n_1, n_2)$  and  $Aux_i(n_1, n_2)$ , where  $n_1, n_2$  are new individual names in  $\mathcal{K}'$ ;
- if  $\alpha = Tran(E)$  then add to  $\mathcal{K}'$  the TBox assertion (role disjointness)  $\nu_R(E) \sqsubseteq \neg Aux_i$ , where  $i$  is such that  $Aux_i$  is a new role name in  $\mathcal{K}'$ , and the ABox assertions  $\nu_R(E)(n_1, n_2)$ ,  $\nu_R(E)(n_2, n_3)$  and  $Aux_i(n_1, n_3)$ , where  $n_1, n_2, n_3$  are new individual names in  $\mathcal{K}'$ .

Intuitively,  $KB_{SHIQ}(\mathcal{H}, \mathcal{T}', Q)$  is such that, if  $\alpha \in TA_{\mathcal{H}, Q} - \mathcal{T}'$ , then  $\alpha$  is forced to be false in every model of  $KB_{SHIQ}(\mathcal{H}, \mathcal{T}', Q)$ . The following theorem (whose proof relies on Theorem 9) reduces answering guarded HUCQs in  $Hi(SHIQ)$  to answering standard UCQs in  $SHIQ$ .

**Lemma 11** *Let  $\mathcal{H}$  be a  $Hi(SHIQ)$  KB, and let  $Q$  be a guarded HUCQ. Then,  $\mathcal{H} \models Q$  iff there exists a subset  $\mathcal{T}'$  of  $TA_{\mathcal{H}, Q}$  such that  $\mathcal{T}'$  is coherent with  $\mathcal{H}$ , and  $KB_{SHIQ}(\mathcal{H}, \mathcal{T}', Q) \models \pi(IntEval(Q, \mathcal{H}, \mathcal{T}'), \mathcal{H})$ .*

<sup>4</sup>Actually,  $KB_{SHIQ}(\mathcal{H}, \mathcal{T}', Q)$  is a  $SHIQ$  KB with role disjointness assertions. However, adding this kind of axioms to  $SHIQ$  does not change the complexity of query answering.

Based on Lemma 11, and Theorems 7, 8, we get the computational characterization of answering guarded HUCQs in  $Hi(SHIQ)$ .

**Theorem 12** *Answering guarded HUCQs over  $Hi(SHIQ)$  KBs is coNP-complete w.r.t. instance complexity, EXPTIME-complete w.r.t. KB complexity, and 2-EXPTIME-complete w.r.t. combined complexity.*

### Tractable cases

The results presented in the previous section show that (guarded) query answering in the higher-order version of  $SHIQ$  is computationally no worse than query answering in standard (first-order)  $SHIQ$ . However, since all the basic reasoning tasks in  $SHIQ$  are already intractable, it is impossible to identify a tractable subclass of HUCQs in the higher-order version of  $SHIQ$ . So, we look at DLs in which standard reasoning is tractable, to see whether tractability is preserved in the higher-order extension of such logics. We focus in particular on  $DL-Lite_{\mathcal{R}}$ , a well-known DL of the  $DL-Lite$  family [Calvanese *et al.*, 2007], which is the core of OWL 2 QL. The higher-order extension of  $DL-Lite_{\mathcal{R}}$ , which we call  $Hi(DL-Lite_{\mathcal{R}})$ , is immediately obtained as in the case of  $SHIQ$ .

First, due to Theorem 6, it follows that answering guarded HUCQs in  $Hi(DL-Lite_{\mathcal{R}})$  is in general intractable. That is, for general guarded HUCQs, query answering is computationally harder than answering standard UCQs (w.r.t. all the three complexity measures considered in this paper).

On the other hand, following the line of reasoning used for Theorem 10, we can immediately show that answering instance HUCQs in  $Hi(DL-Lite_{\mathcal{R}})$  has the same complexity as answering standard UCQs in  $DL-Lite_{\mathcal{R}}$ :

**Theorem 13** *Answering instance HUCQs over  $Hi(DL-Lite_{\mathcal{R}})$  KBs is in  $AC^0$  w.r.t. instance complexity, in PTIME w.r.t. KB complexity, and NP-complete w.r.t. combined complexity.*

We now complement the previous tractability result, by considering the class of *ISA-ground* HCQs, defined as follows: a HCQ  $q$  is *ISA-ground* if all its ISA-atoms are ground. Observe that the class of ISA-ground HCQs is more general than the class of instance HCQs. The technique for answering instance HUCQs (based on the grounding of the metavariables) can be easily extended to handle the presence of ISA-ground atoms in a HCQ. Essentially, first the ISA-ground atoms are evaluated over the KB; then, if some of the ISA-ground atoms is not entailed by the KB, then the query is obviously false; if otherwise all such atoms are entailed by the KB, the rest of the HCQ (which corresponds to an instance HCQ) is evaluated according to the technique described in the previous section. Thus we can prove:

**Theorem 14** *Answering ISA-ground HCQs over  $Hi(DL-Lite_{\mathcal{R}})$  KBs is in  $AC^0$  w.r.t. instance complexity, in PTIME w.r.t. KB complexity, and NP-complete w.r.t. combined complexity.*

Finally, we remark that the above techniques can be used to prove analogous results for other tractable DLs: e.g., the above techniques immediately show tractability of answering instance HUCQs and ISA-ground HCQs also in the higher-order extension of  $\mathcal{EL}$ .

## Conclusions

The research presented here can be continued along different lines. First, while the query answering algorithm presented in here is suited for the class of guarded HUCQs, it is of interest to address query answering for the whole class of HUCQs. Also, more metamodeling features can be added to the query language. In particular, one might wonder whether the query answering method described in this paper can be extended to deal with the case where variables can appear freely within the terms in the query atoms. Unfortunately, our first investigation on this subject shows that allowing for a more flexible use of variables in the queries easily leads to undecidability of query answering.

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