

# Query Answering in Object Oriented Knowledge Bases in Logic Programming: Description and Challenge for ASP

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**Abstract.** Research on developing efficient and scalable ASP solvers can substantially benefit by the availability of data sets to experiment with. `KB.Bio_101` contains knowledge from a biology textbook, has been developed as part of Project Halo, and has recently become available for research use. `KB.Bio_101` is one of the largest KBs available in ASP and the reasoning with it is undecidable in general. We give a description of this KB and ASP programs for a suite of queries that have been of practical interest. We explain why these queries pose significant practical challenges for the current ASP solvers.

## 1 Introduction

The `KB.Bio_101` represents knowledge from a textbook used for advanced high school and introductory college biology courses [19]. The KB was developed by SRI as part of their work for Project Halo<sup>3</sup> and contains a concept taxonomy for the whole textbook and detailed rules for 20 chapters of the textbook. SRI has tested the educational usefulness of this KB in the context of an intelligent textbook called *Inquire*<sup>4</sup>.

The `KB.Bio_101` was originally developed using a knowledge representation and reasoning system called Knowledge Machine (KM) [9]. To express `KB.Bio_101` in answer set programming (ASP) required us to define a conceptual modeling layer called *Object Oriented Knowledge Base* or OOKB [6]. The goal of this paper is not to introduce OOKB as a more complete specification and analysis of formal properties of OOKBs are available elsewhere [6]. OOKB is of more general interest as it supports conceptual modeling primitives that are commonly found in description logic (DL) family of languages such as a facility to define classes and organize them into a hierarchy, define partitions, ability to define relations (also known as slots) and organize them into a relation hierarchy, support for domain, range and qualified number constraints, support for defining sufficient conditions of a class, and support for descriptive rules. The features in OOKB also overlap with the features of logic programming (LP) languages such as

<sup>3</sup> <http://www.projecthalo.com/>

<sup>4</sup> [http://www.aaavideos.org/2012/inquire\\_intelligent\\_textbook/](http://www.aaavideos.org/2012/inquire_intelligent_textbook/)

FDNC [11], *Datalog*<sup>±</sup> [5], and *ASP<sup>fs</sup>* [1] in its support for function symbols. It differs from these previous LP languages as well as from the DL systems in that the functions can be used to specify graph-structured objects which cannot be done in these other languages. The reasoning with OOKBs has been proven to be undecidable [6].

The approach taken in this paper fosters work on multi-paradigm problem solving in the following ways. First, it aims to give a declarative formalization of reasoning tasks that were originally implemented in KM which is a very different paradigm for reasoning as compared to ASP. Second, the conceptual modeling primitives considered here directly overlap with many description logics, thus, providing another example of integration between ASP with DLs.

The primary objective of this paper is to introduce `KB_Bio_101` as a valuable and data set and four queries of practical interest on this KB. These queries have been found extremely useful in the context of *Inquire*. This dataset presents an excellent opportunity for further development of ASP solvers for the following reasons.

- Recent developments in ASP suggest that it could potentially provide an ideal tool for large scale KBs. Yet, most of the KBs described in the literature are fairly small. `KB_Bio_101` provides a real-world ASP program that fits this bill.
- We note that `KB_Bio_101` contains rules with function symbols for which the grounding is infinite. A simple example is a KB consisting of a single class `person`, and a single relation `has-parent`, and a statement of the form “for each `person` there exists an instance of the `has-parent` relation between this person with another individual who is also a `person`”. The skolemized versions of these statements require function symbols. An obvious first challenge that must be addressed is to develop suitable grounding techniques.
- Even though rules in `KB_Bio_101` follow a small number of axiom templates, the size of this KB indicates that this could be a non-trivial task for ASP solvers.
- The `KB_Bio_101` cannot be expressed in commonly available decidable DLs because it contains graph structured descriptions. Efficient reasoning with graph structures is an area of active recent research [15, 16], and since there exists an export of `KB_Bio_101` for DL systems also [7], it provides an ideal usecase to explore the relative effectiveness of DL reasoners vs ASP solvers on a common problem.
- The reasoning tasks of computing differences between two concepts and finding relationships between two individuals are computationally intensive tasks. The implementations of these tasks in *Inquire* rely on graph algorithms and trade completeness for efficiency. These tasks will present a tough challenges to ASP solvers.
- Last but not the least, we believe that the KB could entice the development and/or experimentation with new solvers for extended classes of logic programs (e.g., language with existential quantifiers or function symbols).

In addition to the challenges listed above, it will be possible to define multiple new challenges of increasing difficulty that can be used to motivate further research and development of ASP solvers.

## 2 Background: Logic Programming and OOKB

### 2.1 Logic Programming

A logic program  $\Pi$  is a set of rules of the form

$$c \leftarrow a_1, \dots, a_m, \text{not } a_{m+1}, \dots, \text{not } a_n \quad (1)$$

where  $0 \leq m \leq n$ , each  $a_i$  is a literal of a first order language and  $\text{not } a_j$ ,  $m < j \leq n$ , is called a negation as failure literal (or naf-literal).  $c$  can be a literal or omitted. A rule (program) is non-ground if it contains some variable; otherwise, it is a ground rule (program). When  $n = 0$ , the rule is called a *fact*. When  $c$  is omitted, the rule is a *constraint*. Well-known notions such as substitution, the Herbrand universe  $\mathcal{U}_\Pi$ , and Herbrand base  $\mathcal{B}_\Pi$  of a program  $\Pi$  are defined as usual.

The semantics of a program is defined over ground programs. For a ground rule  $r$  of the form (1), let  $\text{pos}(r) = \{a_1, \dots, a_m\}$  and  $\text{neg}(r) = \{a_{m+1}, \dots, a_n\}$ . A set of ground literals  $X$  is consistent if there exists no atom  $a$  s.t.  $\{a, \neg a\} \subseteq X$ . A ground rule  $r$  is *satisfied* by  $X$  if (i)  $\text{neg}(r) \cap X \neq \emptyset$ ; (ii)  $\text{pos}(r) \setminus X \neq \emptyset$ ; or (iii)  $c \in X$ .

Let  $\Pi$  be a ground program. For a consistent set of ground literals  $S$ , the *reduct* of  $\Pi$  w.r.t.  $S$ , denoted by  $\Pi^S$ , is the program obtained from the set of all rules of  $\Pi$  by deleting (i) each rule that has a naf-literal  $\text{not } a$  in its body with  $a \in S$ , and (ii) all naf-literals in the bodies of the remaining rules.  $S$  is an *answer set* of  $\Pi$  [13] if it satisfies the following conditions: (i) If  $\Pi$  does not contain any naf-literal then  $S$  is the minimal set of ground literals satisfying all rules in  $\Pi$ ; and (ii) If  $\Pi$  contains some naf-literal then  $S$  is an answer set of  $\Pi$  if  $S$  is the answer set of  $\Pi^S$ .

For a non-ground program  $\Pi$ , a set of literals in  $\mathcal{B}_\Pi$  is an answer set of  $\Pi$  if it is an answer set of  $\text{ground}(\Pi)$  that is the set of all possible ground rules obtained from instantiating variables with terms in  $\mathcal{U}_\Pi$ .  $\Pi$  is *consistent* if it has an answer set.  $\Pi$  *entails* a ground literal  $a$ ,  $\Pi \models a$ , if  $a$  belongs to every answer set of  $\Pi$ . For convenience in notation, we will make use of choice atoms as defined in [20] that can occur in a rule wherever a literal can. Answer sets of logic programs can be computed using answer set solvers (e.g., CLASP [12], **dlv** [8]).

### 2.2 Object-Oriented Knowledge Bases

We will now review the notion of an OOKB [6]. We note that an OOKB could be viewed as a logic program with function symbols and the language of OOKBs contains features that cannot be represented in previous investigated classes of function symbols such as  $\text{FDNC}$  [11], *Datalog*<sup>±</sup> [5], or *ASP*<sup>fs</sup> [1]. In essence, an OOKB is a logic program consisting of the following components:

- *Taxonomic Knowledge*: This group of facts encodes the class hierarchy, the relation hierarchy, individual constants and their class membership. It contains ASP-atoms of the following form:

$$\text{class}(c) \quad (2) \quad \text{relation}(r) \quad (7)$$

$$\text{individual}(i) \quad (3) \quad \text{range}(r, c) \quad (8)$$

$$\text{subclass\_of}(c_1, c_2) \quad (4) \quad \text{domain}(r, c) \quad (9)$$

$$\text{disjoint}(c_1, c_2) \quad (5) \quad \text{subrelation\_of}(r_1, r_2) \quad (10)$$

$$\text{instance\_of}(i, c) \quad (6) \quad \text{compose}(r_1, r_2, r_3) \quad (11)$$

$$\text{inverse}(r_1, r_2) \quad (12)$$

The predicate names are self-explanatory.

- *Descriptive statements*: Relationships between individuals are encoded in OOKB by descriptive statements of the form:

$$\text{value}(r, f(X), g(X)) \leftarrow \text{instance\_of}(X, c) \quad (13)$$

$$\text{value}(r, X, g(X)) \leftarrow \text{instance\_of}(X, c) \quad (14)$$

where  $f$  and  $g$  are unary functions, called *Skolem functions*, such that  $f \neq g$  and  $c$  is a class. Axiom 13 (or 14) describes a relation value of individuals belonging to class  $c$ , encoded by the atom  $\text{value}(r, f(X), g(X))$  (or  $\text{value}(r, X, f(X))$ ). It states that for each individual  $X$  in  $c$ ,  $f(X)$  (or  $X$ ) is related to  $g(X)$  via the relation  $r$ . An example use of axiom 14 is: Every Eukaryotic Cell has part a Nucleus, where *Eukaryotic Cell* and *Nucleus* are individuals from these two classes, and *has part* is a relationship between those individuals. It is required that if  $f$  (or  $g$ ) appears in (13) or (14), then the OOKB also contains the following rule

$$\text{instance\_of}(f(X), c_f) \leftarrow \text{instance\_of}(X, c) \quad \text{or} \quad (15)$$

$$\text{instance\_of}(g(X), c_g) \leftarrow \text{instance\_of}(X, c) \quad (16)$$

which specify the class of which  $f(X)$  (resp.  $g(X)$ ) is a member. For example, if  $f(X)$  represents a nucleus individual, then  $c_f$  will be the class *Nucleus*.

- *Cardinality constraints on relations*: OOKB allows cardinality constraints on relations to be specified by statements of the following form:

$$\text{constraint}(t, f(X), r, d, n) \leftarrow \text{instance\_of}(X, c) \quad (17)$$

where  $r$  is a relation,  $n$  is a non-negative integer,  $d$  and  $c$  are classes, and  $t$  can either be *min*, *max*, or *exact*. This constraint states that for each instance  $X$  of the class  $c$ , the set of values of relation  $r$  restricted on  $f(X)$ —which must occur in a relation value literal  $\text{value}(r, f(X), g(X))$  of  $c$ —has minimal (resp. maximal, exactly)  $n$  values belonging to the class  $d$ . The head of (17) is called a constraint literal of  $c$ .

- *Sufficient conditions*: A *sufficient condition* of a class  $c$  defines sufficient conditions for membership of that class based on the relation values and

constraints applicable to an instance:

$$instance\_of(X, c) \leftarrow Body(\mathbf{X}) \quad (18)$$

where  $Body(\mathbf{X})$  is a conjunction of relation value literals, instance-of literals, constraint-literals of  $c$ , and  $X$  is a variable occurring in the body of the rule.

- *(In)Equality between individual terms:* The rules in this group specify in/equality between terms, which are constructable from Skolem functions and the variable  $X$  ( $t_1$  and  $t_2$ ), and have the following form:

$$eq(t_1, t_2) \leftarrow instance\_of(X, c) \quad (19)$$

$$neq(t_1, t_2) \leftarrow instance\_of(X, c) \quad (20)$$

- *Domain-independent axioms:* An OOKB also contains a set of domain-independent axioms  $\Pi_R$  for inheritance reasoning, reasoning about the relation values of individuals (rules (25)—(27)), in/equality between terms (rules (28)—(40)), and enforcing constraints (rules (42)—(47)).

$$subclass\_of(C, B) \leftarrow subclass\_of(C, A), subclass\_of(A, B). \quad (21)$$

$$instance\_of(X, C) \leftarrow instance\_of(X, D), subclass\_of(D, C). \quad (22)$$

$$disjoint(C, D) \leftarrow disjoint(D, C). \quad (23)$$

$$\neg instance\_of(X, C) \leftarrow instance\_of(X, D), disjoint(D, C). \quad (24)$$

$$value(U, X, Z) \leftarrow compose(S, T, U), value(S, X, Y), value(T, Y, Z). \quad (25)$$

$$value(T, X, Y) \leftarrow subrelation\_of(S, T), value(S, X, Y). \quad (26)$$

$$value(T, Y, X) \leftarrow inverse(S, T), value(S, X, Y). \quad (27)$$

$$eq(X, Y) \leftarrow eq(Y, X) \quad (28)$$

$$eq(X, Z) \leftarrow eq(X, Y), eq(Y, Z), X \neq Z \quad (29)$$

$$\leftarrow eq(X, Y), neq(X, Y) \quad (30)$$

$$\{substitute(X, Y)\} \leftarrow eq(X, Y). \quad (31)$$

$$\leftarrow eq(X, Y), \{substitute(X, Z) : eq(X, Z)\}0, \quad (32)$$

$$\{substitute(Y, Z) : eq(Y, Z)\}0. \quad (33)$$

$$\leftarrow substitute(X, Y), substitute(X, Z), \quad (34)$$

$$X \neq Y, X \neq Z, Y \neq Z. \quad (35)$$

$$\leftarrow substitute(X, Y), X \neq Y, neq(X, Y). \quad (36)$$

$$substitute(Y, Z) \leftarrow substitute(X, Z), X \neq Z, eq(X, Y). \quad (37)$$

$$is\_substituted(X) \leftarrow substitute(X, Y), X \neq Y. \quad (38)$$

$$substitute(X, X) \leftarrow term(X), not\ is\_substituted(X). \quad (39)$$

$$term(X) \leftarrow value(S, X, Y). \quad (40)$$

$$term(Y) \leftarrow value(S, X, Y). \quad (41)$$

$$value_e(S, P, Q) \leftarrow value(S, X, Y), substitute(X, P), substitute(Y, Q). \quad (42)$$

$$\leftarrow value(S, X, Y), domain(S, C), not\ instance\_of(X, C). \quad (43)$$

$$\leftarrow value(S, X, Y), range(S, C), not\ instance\_of(Y, C). \quad (44)$$

$$\leftarrow constraint(min, Y, S, D, M), \quad (45)$$

$$\begin{aligned} & \{value_e(S, Y, Z) : instance\_of(Z, D)\} M - 1. \\ \leftarrow & constraint(max, Y, S, D, M), \end{aligned} \tag{45}$$

$$\begin{aligned} & M + 1\{value_e(S, Y, Z) : instance\_of(Z, D)\}. \\ \leftarrow & constraint(exact, Y, S, D, M), \end{aligned} \tag{46}$$

$$\begin{aligned} & \{value_e(S, Y, Z) : instance\_of(Z, D)\} M - 1. \\ \leftarrow & constraint(exact, Y, S, D, M), \end{aligned} \tag{47}$$

$$M + 1\{value_e(S, Y, Z) : instance\_of(Z, D)\}.$$

For a detailed explanation of the above rules, please refer to [6]. An *OO-domain* is a collection of rules of the form (2)—(20). From now on, whenever we refer to an OOKB, we mean the program  $D \cup \Pi_R$ , denoted by  $KB(D)$ , where  $D$  is the OO-domain of the OOKB<sup>5</sup>.

### 2.3 KB\_Bio\_101: An OOKB Usage and Some Key Characteristics

The KB\_Bio\_101 is an instance of OOKB and is available in ASP format<sup>6</sup>. The KB is based on an upper ontology called the Component Library [3]. The biologists used a knowledge authoring system called AURA to represent knowledge from a biology textbook. As an example, in Figure 1, we show an example AURA graph. The white node labeled as `Eukaryotic-Cell` is the root node and represents the universally quantified variable  $X$ , whereas the other nodes shown in gray represent existentials, or the Skolem functions  $f_n(X)$ . The nodes labeled as `has-part` and `is-inside` represent the relation names. The authoring process in

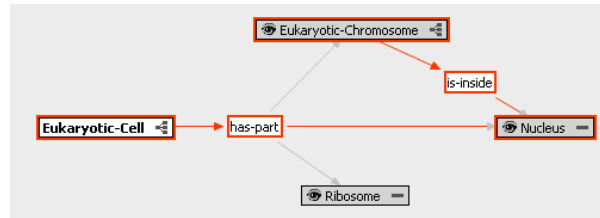


Fig. 1. Example graph for “Eukaryotic-Cell”

AURA can be abstractly characterized as involving three steps: *inherit*, *specialize and extend*. For example, the biologist creates the class `Eukaryotic-Cell` as a subclass of `Cell`. While doing so, the system would first inherit the relation values defined for `Cell` which in this case is a `Chromosome`, and show it in the graphical editor. The biologist then uses a gesture in the editor to specialize the inherited `Chromosome` to a `Eukaryotic-Chromosome`, and then introduces a new `Nucleus` and relates it to the `Eukaryotic-Chromosome`, via an `is-inside` relationship. The

<sup>5</sup> In [6], general OOKBs, that can contain arbitrary logic programming rules, were defined. The discussion in this paper is applicable to general OOKBs as well.

<sup>6</sup> See <http://www.ai.sri.com/~halo/public/exported-kb/biokb.html>

inherited `Chromosome` value for the `has-part` relationship, is thus, specialized to `Eukaryotic-Chromosome` and extended by connecting it to the `Nucleus` by using an `is-inside` relationship.

The statistics about the size of the exported OOKB are summarized in Table 1. In total `KB_Bio_101` has more than 300,000 non-ground rules. It contains 746 individuals which are members of classes which represent constants of measurements, colors, shapes, quantity, priority, etc. The KB does not contain individuals of biology classes such as `cell`, `ribosome`, etc. For computing properties of an individual or comparing individuals, the input needs to introduce the individuals.

classes	6430	<i>domain</i> constraints	449
individuals	746	<i>range</i> constraints	447
relations	455	<i>inverse</i> relation statements	442
<i>subclass_of</i> statements	6993	<i>compose</i> statements	431
<i>subrelation_of</i> statements	297	qualified number constraints	936
<i>instance_of</i> statements	714	sufficient conditions	198
<i>disjoint-ness</i> statements	18616	descriptive rules	6430
avg. number of Skolem functions in each descriptive rule	24	equality statements	108755

**Table 1.** Statistics on `KB_Bio_101`

### 3 Queries in OOKBs

We will now describe the queries given an OOKB, say  $KB(D)$ . These queries play a central role in the educational application `Inquire` [17] which employs the knowledge encoded in `KB_Bio_101`. These queries were developed by extensive analysis of the questions from an exam, the questions at the back of the book, and the questions that are educationally useful [4, 18].

We divide these queries into four groups. The first type of queries which includes the first two queries asks about facts and relationships. The second type of queries asks about the taxonomic information. These first two question types are usually referred to as the *wh*-questions. The third type is about the differences and similarities between individuals from different classes. This type of query has been traditionally studied as an example of analogical reasoning [10]. The fourth type of queries that includes the last two questions query for relationships between concepts and are unique to our work.

- what is a `eukaryotic cell`?
- what process provides raw materials for the `citric acic cycle` during *cellular respiration*?
- is `oocyte` a subclass of a `eukaryotic cell`?
- describe the differences and similarities between `mitochondrions` and `chloroplasts`
- What is the relationship between a `mitochondrion` and a `chloroplast`

- in the absence of oxygen, yeast cells can obtain energy by *which process?*

Let  $Z$  be a set of literals of  $KB(D)$ ,  $r$  be a relation, and  $i$  be an individual from a class  $c$ .  $\mathcal{T}(i)$  denotes the set of terms constructable from Skolem functions and the individual  $i$ . We characterize the set of pairs in the relation  $r$  w.r.t.  $Z$  in  $KB(D)$  by the set  $V(r, i, c, Z) = \{(r, x, y) \mid \text{value}(r, x, y) \in Z, x, y \in \mathcal{T}(i)\}$  if  $\text{instance\_of}(i, c) \in Z$ ; otherwise,  $V(r, i, c, Z) = \emptyset$ .

**Definition 1 (Value set of an individual).** Let  $KB(D)$  be an OOKB. For an answer set  $M$  of  $KB(D)$ , the value set of an individual  $i$  at a class  $c$  w.r.t.  $M$ ,  $\Sigma(i, c, M)$ , is defined by  $\Sigma(i, c, M) = \bigcup_{\text{relation}(r) \in M} V(i, c, r, M)$ .

Observe that the rules (29)—(41) indicate that  $KB(D)$  can have multiple answer sets. Nevertheless, the structure of  $KB(D)$  allows us to prove the following important property of answer sets of  $KB(D)$ .

**Proposition 1.** Let  $KB(D)$  be an OOKB. For every two answer sets  $M_1$  and  $M_2$  of  $KB(D)$ , every literal in  $M_1 \setminus M_2$  has one of the following forms: (i)  $\text{substitute}(x, y)$ ; (ii)  $\text{is\_substituted}(x, y)$ ; or (iii)  $\text{value}_e(r, x, y)$ .

The above proposition indicates that  $\Sigma(i, c, M_1) = \Sigma(i, c, M_2)$  for arbitrary individual  $i$  and class  $c$  and answer sets  $M_1$  and  $M_2$  of  $KB(D)$ . The relationship between atoms of the form  $\text{value}(r, x, y)$  and  $\text{value}_e(r, x, y)$  is as follows.

**Proposition 2.** Let  $KB(D)$  be an OOKB,  $i$  an individual, and  $c$  a class. For every answer sets  $M$  of  $KB(D)$ , we have that  $\text{value}_e(r, x, y) \in M$  iff there exists  $x', y'$  such that (i)  $M$  contains the following atoms  $\text{eq}(x', x)$ ,  $\text{eq}(y', y)$ ,  $\text{substitute}(x', x)$ , and  $\text{substitute}(y', y)$ ; and (ii)  $(r, x', y') \in \Sigma(i, c, M)$ .

The significance of these two propositions is that cautious reasoning about values of individuals at classes can be accomplished by computing *one* answer set of  $KB(D)$ . As we will see, the majority of queries is related to this type of reasoning. We next describe, for each query  $Q$ , an input program  $I(Q)$  and a set  $R(Q)$  of rules for computing the answer of  $Q$ . Throughout the section,  $KB$  denotes an arbitrary but fixed OOKB  $KB(D)$  and  $KB(Q) = KB(D) \cup I(Q) \cup R(Q)$ .

### 3.1 Subsumption Between Classes ( $Q_1$ )

Subsumption requires us to compute whether a class  $c_1$  is subsumed by a class  $c_2$ , i.e., whether for each answer set  $M$  of  $KB(Q_1)$ , we have for each  $\text{instance\_of}(x, c_1) \in M$  also  $\text{instance\_of}(x, c_2) \in M$ . We can answer this question by introducing a fresh constant  $i$  in the OOKB and set  $I(Q_1) = \{\text{instance\_of}(i, c_1)\}$ .  $R(Q_1)$  consists of a rule:

$$\text{subclass\_of}(c_1, c_2) \leftarrow \text{instance\_of}(i, c_2) \quad (48)$$

Indeed, we then have that a class  $c_1$  is subsumed by  $c_2$  iff for each answer set  $M$  of  $KB(Q_1)$ ,  $\text{subclass\_of}(c_1, c_2) \in M$ . Proposition 1 can be extended to  $KB(Q_1)$  and thus we only need to compute one answer set of  $KB(Q_1)$ . Note that this shows how, as in description logics, subsumption can be reduced to entailment in the OOKB framework. We can show that



**Proposition 3.** *If  $KB(Q_1)$  has an answer set  $M$  and  $subclass\_of(c_1, c_2) \in M$  then  $c_1$  is subsumed by  $c_2$ .*

We note that computing answer sets of  $KB(Q_1)$  is not a simple task (see [6]). In particular, the problem for `KB_Bio_101` is quite challenging due to its size and the potential infiniteness of the grounding program of  $KB(Q_1)$ .

One can define many more taxonomic queries than what we have considered here. Some examples of such queries are as follows. Given a class  $C$ , compute all its super classes or subclasses? Given a class, return only most specific superclass? Given two classes, return their nearest common superclass?

Some of the taxonomic queries can require a higher order representation. For example, given two classes, compute a class description that is their union or intersection. Such queries are straightforward in a DL system, and are examples of capabilities that are challenging for the current ASP systems.

### 3.2 Description of an Individual ( $Q_2$ )

Queries about the description of an individual ask for a description of an individual of a class  $c$ , represented by a fresh constant  $i$  in the language of  $KB(D)$ . This query can be represented by the program  $I(Q_2) = \{get\_value(i, c).instance\_of(i, c).\}$  where  $get\_value(i, c)$  encodes the query of “inquiring about values of  $i$  at the class  $c$ .” We will now discuss the answer to this query. Intuitively, a complete description of  $i$  should contain the following information:

- $C(c) = \{d \mid KB(D) \models subclass\_of(c, d)\}$ , the classes from which  $i$  inherits its relation values; and
- its relation values, i.e., the triples in  $\Sigma(i, c, M)$  where  $M$  is a given answer set of  $R(Q_2)$ .

Computing a complete description of  $i$  could be achieved by the following rules:

$$out\_member\_of(Y) \leftarrow get\_value(I, C), instance\_of(I, C), instance\_of(I, Y). \quad (49)$$

$$out\_value(R, X, Y) \leftarrow get\_value(I, C), value(R, X, Y), relation(R), \quad (50)$$

$$term\_of(X, I), term\_of(Y, I).$$

where  $term\_of(X, I)$  defines a term ( $X$ ) that is constructable from Skolem functions and an individual ( $I$ ),  $out\_member\_of(d)$  indicates that  $i$  is an instance of the class  $d$  (i.e.,  $d \in C(c)$ ), and  $out\_value(r, x, y)$  says that  $KB(D) \models value(r, x, y)$ . This answer is correct but may contain *too much* information for users of an OOKB who have knowledge about the class hierarchy. This is because the above description could also include values that  $i$  can inherit from the superclasses of  $c$ . This can be seen in the next example.

*Example 1.* Let us consider the class `Eukaryotic cell`. The description of this class contains 88 statements of the form (13)–(14) that involve 167 classes and 150 equality specifications. A first-level answer<sup>7</sup> computed using (49)–(50)

<sup>7</sup> Current solvers can only approximate the answer due to the infiniteness of the grounding program. We computed the answer by limiting the maximum nesting level for complex terms of the term to be 1 (e.g., the option `maxnesting` in `dlv`).

contains 9 atoms of the form *out\_member\_of(x)* which indicate that a **eukaryotic cell** is also a **cell**, a **living entity**, a **physical object**, etc. In addition, there are 643 atoms of the form *out\_value(r, x, y)* which contains inverse, composition, sub-relation, and the relation value defined in statements of the form (13)–(14) and those that are obtained by the rules (25)–(27).

The example highlights two challenges in computing the description of an individual. First, since the grounding of the KB is infinite, it raises the question of what counts as an adequate grounding that returns a sufficient description of an individuals? Second, for practical query answering applications that use KB\_Bio\_101, one must post-process the results to deciding which subset of the answers should be presented to the user. It should be noted that because of the infiniteness of the grounded KB, current ASP solvers can be used to approximate the answers, by setting depth bounds. Whether this will result in acceptable performance, both in terms of the quality of the answers and the efficiency, is a topic open for future research.

### 3.3 Comparing between Classes ( $Q_3$ )

A comparison query takes the general form of “What are the differences/similarities between  $c_1$  and  $c_2$ ?” (e.g., “what are the differences between *chromosome* and *ribosome*?”). More specific versions of the query may ask for specific kinds of differences, e.g., structural differences.

The query can be represented and answered by (i) introducing two new constants  $i_1$  and  $i_2$  which are instances of  $c_1$  and  $c_2$ , respectively; and (ii) identifying the differences and similarities presented in the descriptions of  $i_1$  and  $i_2$ . We therefore encode  $I(Q_3)$  using the following program:

$$\textit{instance\_of}(i_1, c_1). \quad \textit{instance\_of}(i_2, c_2). \quad \textit{comparison}(i_1, c_1, i_2, c_2). \quad (51)$$

Let us first discuss the features that can be used in comparing individuals of two classes. Individuals from two classes can be distinguished from each other using different dimensions, either by their superclass relationship or by the relations defined for each class. More specifically, they can be differentiated from each other by the generalitation and/or specialitation between classes; or the properties of instances belonging to them. We will refer to these two dimensions as *class-dimension* and *instance-dimension*, respectively. We therefore define the following notions, given an answer set  $M$  of  $KB(Q_3)$ :

- *The set of similar classes between  $c_1$  and  $c_2$* : is the intersection between the set of superclasses of  $c_1$  and of  $c_2$   $U(c_1, c_2) = C(c_1) \cap C(c_2)$ .
- *The set of different classes between  $c_1$  and  $c_2$* : is the set difference between the set of superclasses of  $c_1$  and of  $c_2$   $D(c_1, c_2) = (C(c_1) \setminus C(c_2)) \cup (C(c_2) \setminus C(c_1))$ .

where  $C(c)$  denotes the set of superclasses of  $c$ .

We next discuss the question of what should be considered as a similar and/or different property between individuals of two different classes. Our formalization is motivated from the typical answers to this type of question such as an answer “a chromosome has a part as protein but a ribosome does not” to the query

“what is the different between a chromosome and a ribosome?” This answer indicates that for each chromosome  $x$  there exists a part of  $x$ , say  $f(x)$ , which is a protein, i.e.,  $value(has\_part, x, f(x))$  and  $instance\_of(f(x), protein)$  hold; furthermore, no part of a ribosome, say  $y$ , is a protein, i.e., there exists no  $g$  such that  $value(has\_part, y, g(y))$  and  $instance\_of(g(y), protein)$  hold.

For a set of literals  $M$  of  $KB(Q_3)$  and a class  $c$  with  $instance\_of(i, c) \in M$ , let  $T(i, c)$  be the set of triples  $(r, p, q)$  such that  $(r, x, y) \in \Sigma(i, c, M)$ ,  $instance\_of(x, p) \in M$ , and  $instance\_of(y, q) \in M$ .  $p$  ( $q$ ) is called the domain (range) of  $r$  if  $(r, p, q) \in T(i, c)$ . We define

- *The set of similar relations between  $c_1$  and  $c_2$* : is the set  $R^s(c_1, c_2)$  of relations  $s$  such that (i)  $c_1$  and  $c_2$  are domain of  $s$ ; (ii)  $c_1$  and  $c_2$  are range of  $s$ ; or (iii) there exist  $(p, q)$  such that  $(s, p, q) \in T(i_1, c_1) \cap T(i_2, c_2)$ .
- *The set of different relations between  $c_1$  and  $c_2$* : is the set  $R^d(c_1, c_2)$  of relations  $s$  such that (i)  $c_1$  is and  $c_2$  is not a domain of  $s$  or vice versa; (ii)  $c_1$  is and  $c_2$  is not a range of  $s$  vice versa; or (iii) there exist  $(p, q)$  such that  $(s, p, q) \in (T(i_1, c_1) \setminus T(i_2, c_2)) \cup (T(i_2, c_2) \setminus T(i_1, c_1))$ .

An answer to  $\mathbf{Q}_3$  must contain information from  $U(c_1, c_2)$ ,  $D(c_1, c_2)$ ,  $R^s(c_1, c_2)$ , and  $R^d(c_1, c_2)$ . Computing  $U(c_1, c_2)$  and  $D(c_1, c_2)$  rely on the rules for determining the most specific classes among a group of classes which can easily be implemented using the naf-operator.

We now describe the set of rules  $R(Q_3)$ , dividing it into different groups. First, the set of rules for computing  $U(c_1, c_2)$  is as follows:

$$shared(C, P, Q) \leftarrow comparison(X, P, Y, Q), subclass\_of(P, C), subclass\_of(Q, C). \quad (52)$$

The rule identifies the classes that are superclass of both  $c_1$  and  $c_2$ . We can show that  $KB(Q_3) \models shared(c, c_1, c_2)$  iff  $c \in U(c_1, c_2)$ .

The next set of rules is for computing  $D(c_1, c_2)$ .

$$dist(C, P, Q) \leftarrow comparison(X, P, Y, Q), subclass\_of(P, C), not subclass\_of(Q, C). \quad (53)$$

$$dist(C, P, Q) \leftarrow comparison(X, P, Y, Q), not subclass\_of(P, C), subclass\_of(Q, C). \quad (54)$$

The two rules identify the classes that are superclass of  $c_1$  but not  $c_2$  and vice versa. Again, we can show that  $KB(Q_3) \models dist(c, c_1, c_2)$  iff  $c \in D(c_1, c_2)$ .

For computing  $R^s(c_1, c_2)$  and  $R^d(c_1, c_2)$ , we need to compute the sets  $T(i_1, c_1)$  and  $T(i_2, c_2)$ . For this purpose, we define two predicates  $t_1$  and  $t_2$  such that for every answer set  $M$  of  $KB(Q_3)$ ,  $t_k(s, p, q) \in M$  iff  $(s, p, q) \in T(i_k, c_k)$  for  $k = 1, 2$ . Before we present the rules, let us denote a predicate  $msc\_of$ , called the *most specific class of an individual*, by the following rules.

$$not\_msc\_of(X, P) \leftarrow subclass\_of(Q, P), instance\_of(X, P), instance\_of(X, Q). \quad (55)$$

$$msc\_of(X, P) \leftarrow instance\_of(X, P), not not\_msc\_of(X, P). \quad (56)$$

These rules state that the class  $p$  is the most specific class of an individual  $x$  if  $x$  is a member of  $p$  and  $x$  is not an instance of any subclass  $q$  of  $p$ . This will allow us to define the set  $T(i_1, c_1)$  and  $T(i_2, c_2)$  as follows.

$$3\{t_1(R, P, Q), \leftarrow comparison(X_1, C_1, Y_1, C_2), value(R, X, Y), \quad (57)$$

$$\begin{aligned}
& q.d(R, P), \quad term\_of(Y, X_1), term\_of(X, X_1), \\
& q.r(R, Q) \} \quad msc\_of(X, P), msc\_of(Y, Q). \\
3\{t_2(R, P, Q), \leftarrow comparison(X_1, C_1, Y_1, C_2), value(R, X, Y), \quad (58)
\end{aligned}$$

$$\begin{aligned}
& q.d(R, P), \quad term\_of(X, Y_1), term\_of(Y, Y_1), \\
& q.r(R, Q) \} \quad msc\_of(X, P), msc\_of(Y, Q). \quad (59)
\end{aligned}$$

The following rules identify relations that are similar between  $c_1$  and  $c_2$ :

$$shared\_property(R) \leftarrow comparison(X_1, C_1, Y_1, C_2), t_1(R, C_1, Q_1), t_2(R, C_2, Q_2). \quad (60)$$

$$shared\_property(S) \leftarrow comparison(X_1, C_1, Y_1, C_2), t_1(R, P_1, C_1), t_2(R, P_2, C_2). \quad (61)$$

$$shared\_property(S) \leftarrow comparison(X_1, C_1, Y_1, C_2), t_1(R, P, Q), t_2(R, P, Q). \quad (62)$$

The rules say that individuals  $i_1$  and  $i_2$  from class  $c_1$  and  $c_2$  respectively share a relation  $r$ . The first rule says that  $i_k$  ( $k = 1, 2$ ) is a source in the relation  $r$  (i.e., there exists some  $t_k$  such that  $(r, i_k, t_k) \in \Sigma(i_k, c_k, M)$ ); The second rule says that  $i_k$  is a destination in the relation  $r$  (i.e., the first rule: there exists some  $t_k$  such that  $(r, t_k, i_k) \in \Sigma(i_k, c_k, M)$ ). The third rule says that there exist some pair  $t_k^1, t_k^2$  such that  $t_k^1$  and  $t_k^2$  are instances of the same class and  $(r, t_k^1, t_k^2) \in \Sigma(i_k, c_k, M)$ .

The set of rules for computing  $R^d(c_1, c_2)$  is similar to the above set of rules. It is omitted here for space reason.

The key challenge in computing the differences/similarities between classes in KB\_Bio\_101 are the same as for  $Q_2$ . First, since the grounded program is infinite, one has to determine what is an adequate description that should be used for the purposes of comparison. Second, even though the computation will return all differences and similarities, the users are frequently interested in knowing about salient differences. The current AURA system uses a complex set of heuristics to post process the results to group and rank the results to draw out the salience. The description of such heuristics is outside the scope of the present paper.

### 3.4 Relationship between Individuals ( $Q_4$ )

A relationship query takes the general form of ‘‘What is the relationship between individual  $i_1$  and individual  $i_2$ ?’’, e.g., ‘‘what is the relationship between a **biomembrane** and a **carbohydrate**?’’. Since this type of query refers to a path between two individuals, it can involve significant search in the KB making it especially suitable for solution by ASP solvers. In more specific forms of this query, the choice of relationships can be limited to a specific subset of relationships in the KB. For example, ‘‘What is the structural or functional relationship between individual  $i_1$  and individual  $i_2$ ?’’ We can formulate this query as follows. Given a set of literals  $M$  of an OOKB and a set of relations  $S$ , a sequence of classes alternated with relation  $\omega = (c_1, s_1, c_2, s_2, \dots, s_{n-1}, c_n)$  is called a *path between  $q_1$  and  $q_n$*  with restrictive relations  $S$  in  $M$  if there exists  $instance\_of(t, c_1) \in M$  and Skolem functions  $f_1 = id, f_2, \dots, f_{n-1}$  such that  $value(s_i, f_i(t), f_{i+1}(t)) \in M$  for  $i = 1, \dots, n - 1$  and  $instance\_of(f_i(t), c_i) \in M$  for  $i \geq 2$  and  $s_i \in S$  for

$1 \leq i < n$ . A query of type  $\mathbf{Q}_4$  asks for a path between  $c_1$  and  $c_2$  with restrictive relations in  $S$  and is encoded by the program  $I(Q_4)$ :

$instance\_of(i_1, c_1). \quad instance\_of(i_2, c_2). \quad p\_relation(c_1, c_2). \quad include(r). \quad (r \in S)$

The answer to the query should indicate paths between  $c_1$  and  $c_2$  with restrictive relations in  $S$ . Observe that an answer can be generated by (i) selecting some atoms of the form  $value(s, x, y)$  such that  $s \in S$ ; and (ii) checking whether these atoms create a path from  $c_1$  to  $c_2$ . We next present the set of rules  $R(Q_4)$ , dividing them into two groups that implement the steps (i) and (ii) as follows.

$$p\_segment(R, E, C, F, D) \leftarrow include(R), value(R, E, F), instance\_of(E, C), \quad (63)$$

$$instance\_of(F, D).$$

$$\{seg(S, E, C, F, D)\} \leftarrow p\_segment(S, E, C, F, D). \quad (64)$$

$$\leftarrow p\_relation(C_1, C_2), \{seg(-, -, C_1, -, -)\}0. \quad (65)$$

$$\leftarrow p\_relation(C_1, C_2), 2\{seg(-, -, C_1, -, -)\}. \quad (66)$$

$$\leftarrow p\_relation(C_1, C_2), \{seg(-, -, -, -, C_2)\}0. \quad (67)$$

$$\leftarrow p\_relation(C_1, C_2), 2\{seg(-, -, -, -, C_2)\}. \quad (68)$$

The first rule defines possible segments of the path. The second rule, a choice rule, picks some arbitrary segments to create the path. A segment is represented by the atom  $seg(s, e, c, e', c')$  that encodes a relation  $s$  between  $e$  (an instance of class  $c$ ) and  $e'$  (an instance of class  $c'$ ). The rest of the rules eliminate combinations that do not create a path from  $c_1$  to  $c_2$ . For example, the first two constraints make sure that there must be exactly one segment starting from  $c_1$ ; the next two ensure that there must be exactly one segment that ends at  $c_2$ . The next four constraints make sure that the segments create a path.

$$\leftarrow p\_relation(C_1, C_2), seg(S, E, C, E_1, D), D \neq C_2, \{seg(-, E_1, D, -, -)\}0. \quad (69)$$

$$\leftarrow p\_relation(C_1, C_2), seg(S, E, C, E_1, D), D \neq C_2, 2\{seg(-, E_1, D, -, -)\}. \quad (70)$$

$$\leftarrow p\_relation(C_1, C_2), seg(S, E, C, E_1, D), D \neq C_2, C \neq C_1, \{seg(-, -, -, E, C)\}0. \quad (71)$$

$$\leftarrow p\_relation(C_1, C_2), seg(S, E, C, E_1, D), D \neq C_2, C \neq C_1, 2\{seg(-, -, -, E, C)\}. \quad (72)$$

Even if one could define a suitable finite grounding of  $KB\_Bio\_101$ , computing  $KB(\mathbf{Q}_4)$  can be exponential in the worst case. The implementation of this query in AURA relies on a set of heuristics and depth-bound incomplete reasoning. E.g., one heuristic involves first performing the search on the subclass relationships. The existing implementation is unsatisfactory as it misses out important relationships. In an ideal implementation, one would first compute all candidate paths, and then rank them based on user provided criteria. Computing all such paths especially at the runtime has been infeasible in AURA so far. We hope that ASP could provide a solution for an efficient path computation.

## 4 Discussion

We observe that there was no use of default negation in the axioms (2)-(20) that specify OOKB. The default negation is used in the domain independent axioms,

for example, in axiom (38) and in axioms (53)-(54). In principle, default negation could be used in axioms (13) or axiom (14), but in our practical experience in developing KB\_Bio\_101 such usage has not been necessary. That is primarily because while formalizing the textbook knowledge, one typically requires classical negation. It is only for query answering that the usage of negation becomes critical. If one generalizes OOKB to other domains, it may well be necessary to use default negation in the domain specification axioms (2)-(20), but we have not considered such usage in our work so far. Since default negation is necessary to specify query answering for OOKB, ASP provides a compelling paradigm for declarative specification of such reasoning.

Let us also consider comparison between using ASP vs DLs for OOKB queries presented here. There are two key features of OOKBs that are not directly expressible in description logics: graph-structured objects and (in)equality statements. Using axioms (13) and (14), it is possible to define a graph structure. It is well known that graph structured descriptions usually lead to undecidability in reasoning [16]. In(equality) statements as in axiom (19) and (20), allow us to relate skolem functions that have been introduced as part of two different class descriptions. Such modeling paradigm is not supported by DLs. Of course, the reasoning with OOKBs in full generality is undecidable, and it is an open question whether there exist decidable fragments of OOKB for which the reasoning is decidable [6].

Another important difference between a DL and ASP is in handling of constraints. To illustrate this difference, consider a KB that has a statement: every person has exactly two parents, and further individuals  $p_1$ ,  $p_2$ ,  $p_3$  and  $p_4$ , such that  $p_2$ ,  $p_3$  and  $p_4$  are the parents of  $p_1$ . With axioms (43)-(47), such a KB will be inconsistent. In contrast, most DL system will infer that either  $p_2$  must be equal to  $p_3$ , or  $p_3$  must be equal to  $p_4$ , or  $p_4$  must be equal to  $p_2$ . The semantics of constraints in AURA conform to the semantics captured in axioms (43)-(47). Our work on formalizing the OOKB queries in ASP has been only theoretical, and an experimental evaluation is open for future work. Some example answers of the queries considered in Section 3 which are produced by the Inquire system can be seen at [17].

## 5 Conclusions

We described the contents of an OOKB knowledge base, and formulated ASP programs for answering four classes of practically interesting queries. We also presented a practical OOKB, KB\_Bio\_101, whose size and necessary features make the computation of the answers to these queries almost impossible using contemporary ASP solvers. The specific challenges include developing suitable grounding strategies and dealing with potential undecidability in reasoning with an OOKB. Given the large overlap in features supported by OOKB and DLs, the KB\_Bio\_101 also presents a unique dataset which could be used to explore relative tradeoffs in reasoning efficiency across these two different paradigms. Being a concrete OOKB, KB\_Bio\_101 presents a real challenge for the development

of ASP-solvers. This also calls for the development of novel query answering methods with huge programs in ASP. We welcome engaging with both the ASP and DL research communities so that KB\_Bio\_101 could be used as a driver for advancing the state of the art in efficient and scalable reasoning.

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