

Ontology-Based Meta-Inferencing

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Abstract. Project Halo has the long-term objective of developing a *digital Aristotle*, i.e. a knowledge system that is able to answer questions in a particular domain and give explanations for its answers. In this paper we report about the Ontoprise contribution to the Halo Pilot Project, in which various competing ontology engineering methodologies and knowledge system capabilities have been investigated. Concerning the first, we describe how we dealt with engineered a significant set of laws from chemistry that interacted at different levels of generality and in varying orders. With regard to the latter, we report on the ability of our system to produce coherent and concise explanations of its reasoning. The importance of these two aspects can hardly be underestimated in the Semantic Web, as with future growth the interaction of large sets of laws will require dedicated management as well as the ability to let the user explore the trustworthiness of the ontology and the underlying data sources.

Key Words: Query Answering System, Ontology-based inferencing, meta reasoning

1 Introduction

The Halo Pilot Project¹ is the first phase of a projected multi-phase effort by Vulcan Inc.² whose ultimate goal is the creation of a “digital Aristotle”, an expert tutor in a wide variety of subjects. The Halo Pilot was a six-month effort intended to assess the state-of-the-art in question-answering, with an emphasis on deep reasoning. The effort was structured around the challenge of responding to variants of AP Chemistry questions that focused on a portion of the “Advanced Placement test: Chemistry”³.

Our system, OntoNova, answers questions from this AP test. OntoNova justifies its answers in detail-giving, natural-language explanations. The answers have been evaluated by expert graders according to the directives of the Educational Testing Services. Besides Ontoprise, two other contenders, Cycorp Inc.⁴ and SRI International⁵, have built competing systems.

¹ <http://www.projecthalo.com>

² <http://www.vulcan.com>

³ The Advance Placement Program gives students the chance to try college-level work while still in high school. If one gets a “qualifying” grade on the AP Exam, many colleges give credit or advanced placement for these efforts (<http://apcentral.collegeboard.com/program>).

⁴ <http://www.cyc.com>

⁵ <http://www.sri.com>

There are a number of issues that make the Halo Pilot Project as a whole and OntoNova as one of its parts extremely relevant for the Semantic Web:

1. The Halo Pilot constitutes a good match for some of the objectives that the Semantic Web community wants to achieve:
 - a. Exploiting a rich ontology,
 - b. Integrating various sources of knowledge,
 - c. Giving justifications for deduced results.
2. The Halo Pilot Project was a controlled experiment with a cleanly defined setting, independent evaluators, freely available resources and re-produceable results from. Such settings are useful to
 - a. Quantify costs, and
 - b. Quantify adequacy of methods.
3. While the Halo Pilot still produced knowledge bases that appear to be too costly, it also showed that encoding knowledge by experts is “just” one order of magnitude more costly than writing the natural language text itself.

While the description of the overall Halo Pilot Project is currently put together by a joint committee consisting of representatives of Vulcan Inc. and the three teams, we here focus on number 1 (shown in the list above) and in particular on the description of OntoNova and the conclusions we drew from our experiences building it. To do so, we first describe our technical approach to allow for the deduction of answers and justifications. In Chapter 3, we present the architecture of our knowledge base that produced the answers and justifications. Chapter 4 briefly compares the overall results of the project as far as necessary to frame the OntoNova system. We conclude with some lessons learned.

2 Technical Approaches

Our technical approach builds on two main pillars. First (cf. Section 2.1), we build on the OntoBroker® technology that we have developed and that we have continuously improved for over a decade now [1],[4]. A complex ontology with rules, multiple representations of objects, and call-out functionality to particular problem-solving methods has been modeled in F-Logic [8] to allow for inferring answers posed to the system. Second (Section 2.2), the deduction process has been extended and logged in F-Logic according to a particular trace ontology. This result could then be used by a second, but otherwise identical, inference engine in order to reason why a particular result had been achieved.

2.1 Representing the chemistry domain in F-Logic

Conceptual (or Ontology) modeling deals with the question of how to describe in a declarative and abstract way the domain information of an application, its relevant vocabulary, and how to constrain the use of the data, by understanding what can be drawn from it. Corresponding abstract representation languages support the understanding of such descriptions, their rapid development, their maintenance and their reuse.

F-Logic (“F” stands for “Frames”) combines the advantages of a conceptual high-level approach typical for frame-based languages and the expressiveness, the compact syntax, and well-defined semantics from logics. The original features of F-Logic [8] include signatures, object identity, complex objects, methods, classes, inheritance, and rules. Our implementation of F-Logic by OntoBroker [4] introduced extensions and restrictions of the original features to make F-Logic a powerful and efficient language for many respective intended application domains.

Basic concepts of chemistry are represented as concepts in F-Logic and are arranged in an isa-hierarchy:

```
Molecule::Root.
Reaction::Root.
Ion::Molecule.
Anion::Ion.
Cation::Ion.
AlkaliMetalCation::Cation.
AlkalineEarthMetalCation::Cation.
PrecipitationReaction::Reaction.
GaseousReaction::Reaction.
```

Properties of these concepts and relations between these concepts are represented by methods. E.g.:

```
IonicMolecule[
  hasName=>>STRING;
  hasAnion=>>Anion;
  hasCation=>>Cation;
  hasAnionCoefficient=>>NUMBER;
  hasCationCoefficient=>>NUMBER;
  hasFormula=>>STRING].

HomogenousMixture[hasComponent=>>PureSubstance].

Reaction[
  hasReactants=>>Molecule;
  hasReactantnames=>>STRING;
  hasProducts=>>Molecule;
  hasProductnames=>>STRING;
  hasEquation=>>STRING;
  fromMixture=>>Mixture;
  ...
].
```

Complex chemical relationships and axioms are represented by rules:

```
rule burnhydrocarbon: FORALL F,V1,V2,V3
  burned(F):CombustionReaction[hasReactants->>{"O2",F};
    hasProducts->>{"H2O","CO2"}] <-
    burn(F) and hydrocarbon(F).
```

This rule states that if a formula F represents a hydrocarbon and is burned then the reaction is identified as a combustion reaction with the reactants O_2 and F and the products H_2O and CO_2 of the reaction equation .

Within these rules very often the arithmetic built-in functions of OntoBroker have been used:

```
FORALL R,C,C1,M,Re,Pr,L,L1,L2,Z
  R[coefficients->>C;
    hasReactantsList->>L1;hasProductsList->>L2]
  <- reactants(R,Re) and products(R,Pr) and
    and concatlists(Re,Pr,L) and
    matrixbycols(L,M) and lessolve(M,C1)
    wholenumbered(C1,C) .
```

In this rule the reactants and products of a reaction are taken as lists, a matrix for a linear equation system is generated, solved and from the whole-numbered solution vectors, the integer coefficients are generated. Using this approach the problem to balance a chemical equation is solved.

The input for the answering process is either given as ground facts or as constants used in the query. For instance the input “methanol CH_3OH is burned” is given by the F-Logic fact:

```
burn("CH3OH") .
```

Afterwards we can pose a question for the balanced reaction equation

```
FORALL Eq,R <- R:Reaction[hasEquation->Eq] .
```

which results in the following answer:

```
R = burned("CH3OH")
Eq = "2O2 + 3CH3OH -> 4H2O + 2CO2"
```

As a conclusion it turned out that F-Logic is very well suited for capturing the chemical domain. In contrast to the other teams OntoNova provided the most compact encoding of the knowledge base to cover the domain.

OntoBroker provides means for efficient reasoning in F-Logic, performing a mixture of forward and backward chaining based on the dynamic filtering algorithm [7] to compute (the smallest possible) subset of the model for answering the query. During forward chaining, not only single tuples of variable instantiations but sets of such tuples are processed. It is well-known that set-oriented evaluation strategies are much more efficient than tuple-oriented ones. The semantics for a set of F-Logic statements is then defined by a transformation process of F-Logic into normal logic (Horn logic with negation) and the well-founded semantics [6] for the resulting set of facts and rules and axioms in normal logic.

2.2 Answer Justification

There are many reasons that users and applications in the Semantic Web need to understand the provenance of the information they get back from applications. One major motivating factor is trust. Trust and reuse of retrieval and deduction processes is facilitated when explanations are available. Ultimately, if users and/or applications are expected to trust, use and reuse application results, potentially in combination with other information or other application results, users and agents may need to understand where the derived and source information came from at varying degrees of

detail. This information, sometimes called provenance, may be viewed as meta-information about given information. Provenance information may include source name, date and author(s) of last update, authoritativeness of the source, degree of belief, degree of completeness, etc.

Even more, additional types of information may be required if users need to understand the meaning of terms or implications of query answers. If applications make deductions or otherwise manipulate information, users may need to understand how deductions were made and what manipulations were done. Information concerning derived or manipulated information may include term or phrase meaning, term inter-relationships (ontological relations including subclass, super-class, part-of, etc.), the source of derived information, reasoner description and others. In [9] an overview about requirements for answer explanation components may be found.

Recognition of the importance of explanation components for reasoning systems existed in a number of fields for many years. For example, expert systems researchers understood the need for systems that understood their reasoning processes and could generate explanations in a language understandable to its users [SHORT76]. A more detailed description about requirements and the necessity of answer explanation components can be found in [10], literature on explanations for expert systems [12], theorem proving explanations [5] or [3].

2.2.1 Approach

Our approach for answer justification is based on meta-inferencing. While processing a query the inference engine is producing a log-file of the proof tree for any given answer. This proof tree itself is represented in F-Logic. It contains the instantiated rules that were successfully applied to derive an answer. This file acts as input for a second inference run, where answers are produced, that are explaining the proof tree in natural language and by that, how the answer to the original query was inferred.

We shortly will illustrate this approach with a sample question. The question asks for the K_a value if *mole* and *pH* of a substance is given

Encoded question:

```
<- exists Ka MPhKa(0.2,3.0,Ka).
```

An extract from the log-file of the proof tree:

```
a15106:Instantiation[ofRule->>kavalueMPhKa;
  dependsOnInstantiation->>{a15092};
  instantiatedVars->>{i(M,0.2),i(PH,3.0),
                    i(Ka,4.99E-6),i(H,0.0010),i(HH,1.0E-6)}].
a15092:Instantiation[ofRule->>phvaluepH;
  instantiatedVars->>{i(H,0.0010),i(Ph,3.0),i(R,-3.0)}].
```

The first statement means the rule *kavalueMPhKa* had been applied at the point in time logged here. Then, the variables *M* had been instantiated by 0.2, *PH* by 3.0, *Ka* by 4.99E-6, *H* by 0.0010 and *HH* by 1.0E-6 respectively.

Rules which are important for justifying results were named like “kavalueMPhKa” or “phvaluepH”. For these rules certain explanation rules are formulated which will be

applied in the second, meta-inference run. Frequently the named rules corresponded to important chemistry laws, which would also be found in the text book, while less important rules were typically required for technical reasons, e.g. in order to translate between two alternative representations of the same content, but were not important for the human to understand the solution proposed by the system.

For the first named rule of the proof tree, the corresponding explanation-rule is:

```
FORALL I, M1, PH1, Ka1, H1, HH1, EX1, Ka1R
explain(EX1, I) <-
  I:Instantiation[ofRule->>kavalueMPhKa;
  instantiatedVars->>{i(M, M1), i(PH, PH1),
  i(Ka, Ka1), i(H, H1), i(HH, HH1)}]and
  dround(Ka1, 2, Ka1R) and EX1 is
  ("The equation for calculating the acid-dissociation
  constant Ka for monoprotic acids is <b>Ka=[H+] [A-]
  ]/[HA]</b>. For monoprotic acids the concentrations for
  hydrogen [H+] and for the anion [A-] are the same:
  <b>[H+]=[A-]</b>. Thus, we get <b>Ka= "+H1+" * "+H1+" /
  "+M1+" = "+Ka1R+" </b>for a solution concentration
  <b>[HA] = "+M1+" M</b>.").
```

An explanation-rule is specified by its reference to the rule (*kavalueMPhKa*), by accessing the instantiations of the variables of the answer producing rule, e.g. *M1* accesses the instantiation of variable *M*, and a text referring to these variables which is presented in the explanation.

These explanation rules are applied to the proof tree of our example and produce the following justification output:

- The equation for calculating the acid-dissociation constant K_a for monoprotic acids is $K_a = \frac{[H^+][A^-]}{[HA]}$. For monoprotic acids the concentrations for hydrogen $[H^+]$ and for the anion $[A^-]$ are the same: $[H^+] = [A^-]$. Thus, we get $K_a = 0.0010 * 0.0010 / 0.2 = 5.0E-6$ for a solution concentration $[HA] = 0.2$ M.
 - The equation for calculating the pH-value is $ph = -\log[H^+]$. Thus we get pH-value $ph = 3$, H^+ concentration $[H^+] = 0.0010$.

2.2.2 Advantages of the Approach

This two-step process for creating explanations allows for applying the full power of inferencing to generate explanations. For OntoNova, we have developed an entire knowledge base for this purpose. Thus, one may (i) integrate additional knowledge, (ii) reduce redundancies of explanations, (iii) abstract from fine-grained explanations, and (iv) provide personalized explanations.

(i), when the proof tree does not contain enough information in itself, additional information will be needed to create comprehensible explanations. In our context, e.g., the proof tree contains the formulae of the different substances. However, in the explanations the names of the formulae are often necessary to produce understandable

justifications. The generation of names from formulae then requires additional information not found within the proof tree.

(ii), in knowledge bases different paths often lead to the same result. For instance, the acidity order of two substances may be determined by the pH-values that may be computed from the amount of substances in aqueous solutions – or they may be given by qualitative criteria like the number of oxygen elements in the formulae of the substances. Both criteria lead to the same ordering. As a consequence, there are two different explanation paths for the same result. An explanation rule may rank these two explanation paths and ignore one of them when formulating the justification. Thus, redundancies in generated explanation may be reduced.

(iii), often it is necessary to come to different abstractions of explanations. E.g. for the purpose of debugging the knowledge base, a very fine-grained explanation level is necessary, while for an expert a low-grained explanation level is sufficient. The single inference steps and thus the proof tree, which is a representation of these single inference steps, provide the finest resolution of explanations. Additional rules may summarize these steps and may thus produce higher abstracted explanations. E.g. in our domain such rules may summarize the three different steps of a reaction like the (a) decomposition of the substances into their ionic compounds, (b) the composition of an insoluble substance out of these compounds and (c) the precipitation of the resulting substance from the solution as a precipitation reaction.

(iv), the three means (i)-(iii) just mentioned may all be used for generating specialized explanations for different contexts and for generating personalized explanations. Domain experts need other explanations than freshmen or novices and different types of explanations have to be given in different functional situations and contexts like science, research or in AP exam, respectively.

3. Encoding

3.1 Encoding of the KB

For testing purposes in the dry run Vulcan Inc. provided 50 syllabus questions for each team. The encoding of the corpus (80 pages from [2]) has been done in three different phases. During the first phase the knowledge within the corpus has been encoded into the ontology and into rules, without considering the 50 syllabus questions. This knowledge has been tested with some 40 exercises of [2]. For each of these exercises an encoded file and an output file by pair have been created. These pairs have been used for automatically testing the knowledge base.

In the next phase the syllabus questions have been tested with a covering of around 30% of these questions. During this phase the knowledge base has been refined until coverage of around 70% of these questions has been reached. Additionally, in parallel during this phase, the explanation rules have been encoded. In the so-called dry run itself, the encoded syllabus questions have been sent to Vulcan to test the installed systems. The remaining time to the challenge run has been used to refine the encoding of the knowledge base and the explanation rules. During the entire process, the library

of test cases has been extended and used for automatic testing purposes. This ensured stability of the knowledge base against changes.

3.2 Question Encoding

The syllabus contained two major types of questions: multiple choice questions and detailed answer questions.

3.2.1 Multiple Choice

An example for a multiple choice question is the following:

Which of the following compounds will produce a gas when HCl is added to the solid compound? HCl is a strong acid producing a yellow-green colored gas above the acid solution.

- a. Ba(OH)₂ (s)
- b. CaCO₃ (s)
- c. CuSO₄ (s)
- d. Na₃PO₄ (s)
- e. NaCl (s)

For the multiple choice section, two different encoding schemas have been used. The first schema encoded the multiple choice questions where our knowledge base could conclude the correct answer. E.g.:

```
//input facts
m1:Mixture[hasComponents->>{"HCl", "Ba(OH)2"}].
m5:Mixture[hasComponents->>{"HCl", "NaCl"}].
// encoding of the options
answer("A") <- exists P P:GaseousReaction[fromMixture->>m1].
answer("E") <- exists P P:GaseousReaction[fromMixture->>m5].
// query for the correct option
FORALL X <- answer(X).
```

The second schema encoded multiple choice questions where all but one of the options could be excluded by the knowledge base:

```
// all options
possibleanswer("A").
...
possibleanswer("E").
// encoding wrong options
FORALL X wronganswer("A") <- checkequation(ra,X).
...
FORALL X wronganswer("E") <- checkequation(re,X).
// exclude wrong options
FORALL Answer <-
    possibleanswer(Answer) and not wronganswer(Answer).
```

3.2.2 Detailed Answer Questions

The detailed answer questions, for which an exact answer like the pH-value had to be delivered, have been encoded as direct queries to the knowledge base. E.g.:

```
// give the pH-value of the buffer solution
FORALL Ph <- ml:BufferSolution[hasPHValue->>Ph].
```

4 Conclusion

From the development of OntoNova we gained a range of insights valuable for traditional knowledge systems – as well as for the Semantic Web.

1. F-Logic appeared as a representation language which is very well suited to be used in complex, rule-intensive domains. One obviously required addition to this language could be a package construct which divides the knowledge base into different parts. Our addition of namespace constructs is one step into F-Logic towards this objective (cf. [11]).
2. Our inference engine OntoBroker has performed very well in answer and justification generation.
3. We also noticed that we have to improve our knowledge modeling environment by a better support for rule editing and rule debugging.
4. Another insight was that at the end of the knowledge base modeling domain, experts should be able to extend and modify the knowledge base on their own. For that purpose, a two-step process will be necessary. First the basic building blocks (like basic representation of formulas, basic chemical operations etc.) must be developed by a knowledge engineer in a general development environment like OntoEdit. In a second step such an environment must be specialized for a tool which comprises the special view of the domain expert and gives him the elementary building blocks as modeling primitives.

Concerning the evaluation results, Ontoprise finished second according to the scores in answer generation and justification, respectively. This result seems very formidable, because we used just two person-years instead of the four person years consumed by the other two teams, and by that showed up with half the costs for encoding. Compared to other teams, our encodings are very compact and do not require specific hardware resources to be processed (experiments were performed on a standard current version of a Linux machine).

The processing performance of OntoNova has been faster than its competitors by factors between 5 and 30, depending on the systems used to perform the challenge run. The challenge run could have been done in some three to four minutes using a special twin-server that would have done answer generation and justification in parallel instead of sequentially. Additionally, we could have applied several optimization strategies to improve performance, so that there is much more potential for improvement matters – and will be needed for the Semantic Web to scale in size, scope and trust – by the advancement of OntoNova in the Halo Pilot Project.

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