
MULTILEVEL ONTOLOGIES FOR DOMAINS WITH COMPLICATED STRUCTURES¹

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Abstract: The article defines the class of domains with complicated structures, gives the definition of multilevel ontologies and determines the method for developing such ontologies.

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Introduction

At present there are the following ontology application categories: Knowledge management systems, Controlled vocabulary, Web site or document organization and navigation support, Browsing support, Search support (semantic search), Generalization or specialization of search, Sense "disambiguation" support, Consistency checking (use of restrictions), Auto-completion, Interoperability support (information/process integration), Support validation and verification testing, Configuration support, Support for structured, comparative, and customized search [Denny, 2002], [Gavrilova, 2006], [Zagorulko et al, 2006], [Ontos Miner], [<http://www.alphaworks.ibm.com/contentnr/semanticsfaqs>]. The goal of research into ontologies is to create explicit, formal catalogues of knowledge that can be used by intelligent systems (see <http://www.aaai.org/AITopics/html/ontol.html>). The following definitions of an ontology are used:

- An ontology defines the terms used to describe and represent an area of knowledge. Ontologies are used by people, databases, and applications that need to share domain information (a domain is merely a specific subject area or area of knowledge, such as petroleum, medicine, tool manufacturing, real estate, automobile repair, financial management, etc.). Ontologies include computer-usable definitions of basic concepts in the domain and the relationships among them. They encode knowledge in a domain and also knowledge that spans domains. In this way, they make that knowledge reusable. (see <http://www.w3.org/TR/webont-req/>).

- An ontology comprises a formal explicit description of concepts (often called classes) in a domain of discourse, properties (sometimes called slots) of each concept describing various features and attributes of the concept, and restrictions on properties (sometimes called facets). An ontology together with a set of individual instances of classes constitutes a knowledge base. In reality, there is a fine line between where the ontology ends and the knowledge base begins, and a fine line between a class and an instance. Classes are the focus of most ontologies. Classes describe concepts in the domain. (see <http://www.alphaworks.ibm.com/contentnr/semanticsfaqs>).

At present there are various ontology-design methodologies [Cristani & Cuel, 2005], [Denny, 2002], [Gavrilova, 2006], [Jones, et al], [Corcho et al, 2003] for the above applications. Many methodologies include defining classes in the ontology, arranging the classes in a taxonomic (subclass–superclass) hierarchy, defining slots and describing set of values for these slots, filling in the values for slots for instances [Noy, 2001]. Different ontologies

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(see, for example, <http://musing.deri.at/ontologies/v0.3/> and <http://www.daml.org/ontologies/>) designed to be used in program systems of the above classes were developed using these methodologies.

However the specified tasks are only a subset of applied tasks for the automated solutions of which intelligent systems are required, and a number of domains have characteristics that are not taken into consideration by the existing ontology-design methodologies. The aim of this article is describing the class of such domains, structure of their ontologies, and method of developing their ontologies.

Domain class definition

Domains with complicated structures have the following characteristics:

- they have sections that are described in different but resembling notion systems [Kleshchev & Artemjeva, 2005a];
- the sections have subsections that are described in different but resembling notion systems;
- any subsection can have subsections with the above characteristic.

Sections (and subsections) of domains with complicated structures are also domains with their own kinds of activity and sets of applied tasks; some applied tasks from different sections may be similar. Notions of ontologies and knowledge of different sections can be used to solve applied tasks in domains with complicated structures.

Medicine is an example of a domain with complicated structure [Kleshchev et al, 2005a]. The examples of sections of this domain are therapeutics, surgery and others. The ontology terms of each section are names of diseases studied in this section and names of signs the values of which are used to diagnose diseases. Each section has its own sets of names of diseases and signs.

Chemistry is another example of a domain with complicated structure. The examples of its sections are physical chemistry, organic chemistry and analytical chemistry. Physical chemistry deals with the physicochemical processes [Artemieva, Tsvetnikov, 2002]. These processes are described in terms of characteristics of matters and reactions that take part in the processes. Organic chemistry adds terms relating to structural properties of matters [Artemieva et al, 2005, 2006]. Analytical chemistry studies processes of influence on matters with various kinds of radiation [Artemieva, Miroshnichenko, 2005]. Chemical thermodynamics and chemical kinetics are examples of sections of physical chemistry; sections of analytical chemistry depend on analysis techniques (for example, X-ray fluorescence analysis). Another example of a domain with complicated structure is the domain of program transformations. The processes of changing programs as a result of applying different transformations are studied in this domain [Artemieva et al., 2002]. The examples of the sections are transformations of structural programs and transformations of parallel programs. The transformations are described in terms of properties of languages of these programs.

Examples of tasks solved in domains with complicated structures are diagnosing, designing, planning, etc. One needs terms required for defining characteristics of a patient (object of diagnosis) which are input data of the task, intermediate data or the result of the task and not for defining characteristics of a disease (that are stored in knowledge bases) to specify a medical diagnosis task. Terms that describe characteristics of substances used in experiments, reactions, chemical process conditions [Artemieva, Reshtanenko, 2006] and not known characteristics of substances and reactions that are traditionally stored in chemistry databases are necessary for specifying a task of planning a chemical experiment.

Some problems arise when intelligent systems for domains with complicated structures are designed. The first problem is integration of knowledge from various sections and subsections within the framework of one knowledge base. A means of such integration is ontology that must take into account that notion systems (ontologies of sections and subsections) used in different sections and subsections differ. The second problem is

a way of integration of notion systems (ontologies). A means of such integration can be ontology of higher level of generality.

Defining level of generality of ontologies

Ontologies are used to verbally represent information. Verbal representation of information is a mapping of a finite set of terms into a set of possible values of terms. Verbal representation of information has level 0.

Ontology with the system of knowledge that specifies a particular set of verbal representations of information has level 1. At level 1 ontology terms has no values. Setting values to ontology terms make the verbal representation of the particular information have level 0.

Ontology without knowledge system has level 2. When different knowledge are added, different specifications of verbal representations of information are received.

Ontology in terms of which ontology of level i can be specified has level $i + 1$. All ontologies of levels more than 2 are metaontologies.

In every hierarchy the language of specification of ontologies has level that is 1 more than the highest level in the hierarchy (and in this hierarchy there are no ontologies of higher levels).

Let us explain the difference between level 1 and level 2. Ontology defines a set of terms used to verbally represent information, a set of possible values of each term, and relations between terms (ontological constraints). Ontology is the result of agreement among people that use the same information in their professional activity; therefore ontology is obviously the result of agreement among these people on what verbal representations in the domain have meaning. We will call a set of all verbal representations of information that have meaning conceptualization. Knowledge imposes additional constraints on a set of verbal representations and picks a subset out of conceptualization. Thus, level 2 specifies conceptualization, level 1 specifies its subset, where knowledge defines characteristics of this subset.

Ontology of the next level specifies a larger set of verbal representations of information as compared with ontology of the previous level. Transition from level i to level $i-1$ restricts this set and defines its subset. Transition from ontology of level $i-1$ to ontology of level i is considering ontology of level $i-1$ as verbalized information.

Let us consider domains as examples of verbalized information. Knowledge is represented verbally if it is specified as an array of pairs consisting of a term and its value. Terms included into the ontology of knowledge is used to verbally represent knowledge [Kleshchev & Artemjeva, 2006]. If verbalized information is a base of knowledge of a domain, then its representation has level 0. If this is a case, level 1 is ontology of knowledge consisting of definitions of terms with their sets of values and knowledge consistency constraints as well. Level 2 specifies sets of ontologies of knowledge.

Let us consider the example when information is the description of a state of affairs of the domain [Kleshchev & Artemjeva, 2006]. In respect of physical chemistry level 0 represents the information of a certain physicochemical process that took place at a certain period of time and under certain external conditions. To describe the process one may use the terms with the following values: "process steps", "chemical substances at each process step", "chemical reactions at each process step", etc. The terms used for describing level 0 for the domain form the ontology of reality. Level 1 specifies the reality model of the given domain and describes all possible chemical processes the information about which can be represented in terms of the ontology; the representation of the information about each chemical process is not inconsistent with the ontological constraints and domain knowledge. The domain knowledge describes laws for going of chemical reactions, formation laws of substance from chemical elements, etc. Level 2 specifies the conceptualization of reality that is an idea about reality that the domain specialist has. This level defines concepts for this reality description.

Regarding X-ray fluorescence analysis, a section of analytical chemistry, level 0 represents the information about a certain physical process that took place at a certain period of time and under certain external conditions. To describe the process one may use the terms with the following values: “analytes”, “sample qualitative composition”, “percentage of an analyte in a sample” [Artemieva, Miroshnichenko, 2005]. The domain knowledge describes laws of physical processes during high-frequency electromagnetic radiation directed at a sample, values of characteristic radiation of analytes, etc.

The domain knowledge defines characteristics of its reality as sets of states of affairs that can take place in it. If the domain knowledge can be verbally represented, then the ontology of level 2 contains sets of terms for their representation. This ontology is a pair of two ontologies (reality and knowledge) and relations between them (additional ontological constraints). If the domain knowledge cannot be verbally represented (e.g. physics), then the ontology of level 2 coincides with the ontology of reality. In this case, the ontology of level 3 specifies a set of ontologies of reality.

There are domains where only part of knowledge is verbally represented. In this case, the ontology of knowledge contains terms that can represent this knowledge. This is characteristic of physical chemistry: knowledge about various properties of chemical elements (atomic weight, atomic number, etc.), physicochemical characteristics of substances (density, formula, etc.), reaction properties (e.g. catalyst) and so on is verbally represented in it. Laws of physical processes cannot be represented verbally.

Properties of multilevel ontologies for domains with complicated structures and method of their development

For the domain with complicated structure the level with the maximum number n is ontology of the domain. The level contains the terms with the help of which the ontology of the next level is determined. The transition to the next level means specifying ontology terms and ontological constraints of the next level [Artemieva, 2006]. If all the domain knowledge and ontological constraints of all the levels can be represented verbally, then the ontology of level n defines properties of all sets of terms of all ontologies of lower levels. The simplified ontology of medical diagnosis has this property [Kleshchev & Artemieva, 2005b].

The ontology of level $n-1$ consists of modules. Each module defines the ontology of a certain section of the domain. The ontology of level $n-2$ also consists of modules. Each module defines the ontology of a subsection. All the ontologies of level lower than n are modular. The domain knowledge base is also modular.

Let us describe the method for developing the multilevel ontology of the domain.

The development starts with defining verbalized information about the domain reality and terms for its verbal representation. The domain expert participate in this work. The knowledge engineer and the expert make a list of terms used for representing the reality, record meanings of terms and values, principles of representing states of affairs with their help. A set of all possible meanings is defined for each term (denotation of the term). Ontological constraints specifying constraints for a set of meanings of terms are formed (domain state of affairs consistency constraints).

A set of applied tasks of the professional activity is analyzed in order to define what information about the reality is to be verbally represented. Terms used for specifying input data and their results and terms used for representing values of intermediate data are defined. Ontological constraints specifying relations between all these terms are also defined. A set of tasks of the professional activity unambiguously defines the domain. Thus, the ontology of the reality contains terms that are used in applied tasks to specify input data and results of solutions, intermediate data, and relations between terms of the three groups. Then, the knowledge system, probably defining the reality of the domain more accurately, is to be designed.

Developing the ontology of level 2 starts with answering the question whether the domain knowledge can be represented verbally. If the answer is in the negative (i.e. the knowledge cannot be represented verbally), the knowledge system is developed in the same form as the system of ontological constraints (in terms of the ontology of the reality). If the answer is in the affirmative (i.e. the knowledge can be represented verbally), a list of terms for representing the domain knowledge is made with the help of an expert, definitions of these terms are developed, knowledge consistency constraints and interrelations between the reality and the knowledge are formulated. This list of terms for representing the domain knowledge and the set of knowledge consistency constraints form the ontology of the knowledge of this domain. If only a part of the knowledge can be represented verbally, a list of terms for representing only this part is made. The system of knowledge consists of two components: a set of assertions in terms of the ontology of the reality and mapping of a set of terms for representing knowledge into a set of values. The ontology of the reality, the domain knowledge ontology, and interrelations between the reality and the knowledge form the ontology of level 2 for the domain.

The ontology of level 3 (and all following levels) can be developed if the ontologies of level 2 (and all the previous levels) of several sections of the domain are developed since this ontology specifies a set of ontologies of level 2. This step starts with answering whether the ontologies of level 2 can be represented verbally. If the answer is in the negative, developing stops. If the answer is in the affirmative, a list of terms for its representing is made, definitions of these terms are developed, consistency constraints for the ontology of level 2 are formulated. The task of this level and the following ones is searching for "regularities" in the ontology of the previous level, grouping terms with some similar properties into one set, formulating the term properties of these sets and relations between them.

Let us consider a fragment of the ontology of level 4 for chemistry represented by an applied logic language to exemplify the usage of a top-level ontology in the domain [Kleshchev & Artemjeva, 2005b].

1. sort Types of objects: $\{N \setminus \emptyset$

Term "Types of objects" means non-empty set of names of object types of the domain.

2. (Type: Types of objects) sort Type: $\{(R \cup I \cup N \cup L)$

Each type of objects is a set of objects; each object can be named, represented with a number, can be logical value.

3. sort Types of object components: Types of objects $\rightarrow \{ \}$ Types of objects

Term "Types of object components" means the function that maps object type on non-empty set of names of object types. If Types of object components(t)=t' and t'={t₁,t₂} then objects from the set t₁ or the set t₂ that can be components of objects with type t.

4. Set of objects $\equiv \{(Type: Types of objects) j(Type)\}$

This auxiliary term means a set of objects of all types.

5. Own properties of objects $\equiv (\lambda(Type: Types of objects) (\lambda(Area of possible values: \{(Value sets \cup \{Value corteges)\}) (j(Type) \rightarrow Area of possible values))$

Term "Own properties of objects" means the function the argument of which is object type and the result of which is a set of functions. The argument of each function is a set of values or a set of corteges; the result is a set of functions. If Own properties of objects(t) = f1 and f1(m)=f2 then an argument of the function f2 is an object with type t and the result is an element of the set m.

6. Properties of components of given types $\equiv (\lambda(Type1: Types of objects) (Type2: Types of object components (Type1)) (\lambda(Area of possible values: \{(Value sets \cup \{Value corteges\}) (Object that has type 1 \rightarrow j(Type1),$

Object that has type 2 \rightarrow Object components(Type1, Type2)(Object that has type 1) \rightarrow Area of possible values))

Term "Properties of components of given types" means the function the arguments of which are two object types - t1 and t2, and the result is a set of functions the argument of each one is m set of values or corteges of values, and the result is a set of functions the arguments of each one is object of t1 type and object of t2 type which is a component of object of type t1, and the result is m set element.

7. sort Number of process steps: $I[0, \infty)$

Term "Number of process steps" means a number of steps included in a physicochemical process.

8. sort Types of process objects: $\{ \text{Types of objects} \setminus \emptyset$

Term "Types of process objects" means a set of object types that are considered as components of a physicochemical process.

9. Process components $\equiv (\lambda(\text{Type: Type of process objects}) (I[1, \text{Number of process steps}] \rightarrow \{ \{v: \text{Set of objects} \mid \text{Object type}(v) = \text{Type} \} \setminus \emptyset$)

Term "Process components" means a function the argument of which is t object type, and the result is a set of functions the argument of each one is the number of a process step, and the result is a set of components of a process – non-empty subset of objects of type t.

10. Properties of process components $\equiv (\lambda(\text{Type: Types of process objects}) (\lambda(\text{Область возможных значений: } \{ \{ \text{Value sets} \cup \{ \text{Value corteges} \} \}) (\text{Step number} \rightarrow I[1, \text{Number of process steps}], \text{Process component} \rightarrow \text{Process components}(\text{Type})(\text{Step number})) \rightarrow \text{Area of possible values}))$

Term "Properties of process components" means the function the argument of which is t object type, and the result is the function the argument of which is m set of values or corteges of values, and the result is the function the arguments of which are the number of a process step and a component of this step (object of type t), and the result is m set element.

Let us now consider the example of using the ontology of level 4 when defining the ontology of level 3 for X-ray fluorescence analysis [Artemieva, Miroshnichenko, 2005]. First, let us define the values of the parameters of ontology of level 4 (a set of terms of ontology of level 3).

1. Types of objects $\equiv \{ \text{Shells of chemical element atoms, Radiation transition of orbital electrons, Chemical elements} \}$

The ontology defines the objects of the given types. This set specifies types of objects that are studied in the section of the domain.

2. Types of object components $\equiv (\lambda(\text{Type: } \{ \text{Shells of chemical element atoms, Radiation transition of orbital electrons, Chemical elements} \}) (\text{Type} = \text{Chemical elements} \Rightarrow \text{Radiation transition of orbital electrons}), (\text{Type} \neq \text{Chemical elements} \Rightarrow \emptyset)$

Energy levels and radiation transition of orbital electrons are defined for chemical elements; energy levels are defined for shells. Objects of other types do not have components.

3. Types of process objects $\equiv \{ \text{Chemical elements, Radiant energies} \}$

Types of chemical process objects are chemical elements and radiant energies.

Now let us define examples of ontological constraints that are part of ontology of level 3.

1. Shells of chemical element atoms $\subset \{ \mathbb{N} \setminus \emptyset$

Shells of chemical element atoms is name of set. This set consists of designation for shells.

2. Chemical elements $\subset \{N \setminus \emptyset$

Chemical elements is name of set. This set consists of designation of elements.

3. Radiation transition of orbital electrons $\subset \{N \setminus \emptyset$

Radiation transition of orbital electrons is name of set. This set consists of designation of transitions.

Then let us define examples of terms that are part of ontology of level 3 that mean names of functions.

1. Own properties of shells \equiv Own properties of objects (Shells of chemical element atoms)

Term "Own properties of shells" means the function the argument of which is a set of values or set of corteges of values m , and the result is the function the argument of which is shell, and the result is an element of m set.

2. Own properties of radiation transitions \equiv Own properties of objects (Radiation transition of orbital electrons)

Term "Own properties of radiation transitions" means the function the argument of which is a set of values or set of corteges of values m , and the result is the function the argument of which is radiation transition, and the result is an element of m set.

3. Properties of radiation transition of orbital electrons of elements \equiv Properties of components of the given types (Chemical elements, Radiation transition of orbital electrons).

Term "Properties of radiation transition of orbital electrons of elements" means the function the argument of which is a set of values or set of corteges of values m , and the result is the function the arguments of which are chemical element and its radiation transition, and the result is an element of m set.

4. Properties of elements of a sample \equiv Properties of process components (Chemical elements)

Term "Properties of elements of a sample" means the function the argument of which is a set of values or set of corteges of values m , and the result is the function the arguments of which are the number of a process step and chemical element of this step, and the result is an element of m set.

Finally let us define examples of terms that are part of ontology of level 2.

1. sort Binding energy of electrons on an energy level for an element: Properties of energy levels for an element $(R(0, \infty))$

Binding energy of electrons on an energy level for an element is a function the first argument of which belongs to the set with name Chemical elements, and the second argument of which belongs to the set with name Energy level. The result of the function belongs to the set of real number.

2. sort Characteristic radiation frequency: Properties of radiation transition of orbital electrons of elements $(R(0, \infty))$

Characteristic radiation frequency is a function the first argument of which belongs to the set with name Chemical elements, and the second argument of which belongs to the set with name Radiation transition of orbital electrons. The result of the function belongs to the set of real number.

3. sort Wave-length of characteristic radiation: Properties of radiation transition of orbital electrons of elements $(R(0, \infty))$

Wave-length of characteristic radiation is a function the first argument of which belongs to the set with name Chemical elements, and the second argument of which belongs to the set with name Radiation transition of orbital electrons. The result of the function belongs to the set of real number.

4. sort Energy of characteristic radiation: Properties of radiation transition of orbital electrons of elements $(R(0, \infty))$

Energy of characteristic radiation is a function the first argument of which belongs to the set with name Chemical elements, and the second argument of which belongs to the set with name Radiation transition of orbital electrons. The result of the function belongs to the set of real number.

Conclusion

Top-level (or upper-level) ontologies are described in many papers. Such ontologies define terms used for highly abstract notions that studied by philosophy. They are aimed at defining all meanings of these terms.

However in domains of professional activity considered in this paper it is assumed that meanings of domain ontology terms are fixed. Terms of ontology of higher level of generality defined in the article specify properties of sets of these terms and have fixed meanings themselves.

The method of development of multilevel ontologies was used to create multilevel ontology of chemistry [Artemieva et al, 2005, 2006], [Artemieva, Miroshnichenko, 2005], [Artemieva, Tsvetnikov, 2002], and multilevel ontology of domain "Optimization of sequential programs" [Artemieva et al, 2002].

Properties of an intelligent system based on multilevel ontology were described in the article [Artemieva, Reshtanenko, 2006].

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