# Ontology Engineering, Scientific Method and the Research Agenda

Hans Akkermans[1,2] and Jaap Gordijn[1]

[1] Free University Amsterdam VUA
Business Informatics Department (FEW/BI)
Amsterdam, The Netherlands
gordijn@cs.vu.nl
[2] AKMC Knowledge Management BV
Koedijk, The Netherlands
Hans.Akkermans@akmc.nl

**Abstract.** The call for a "focus on content" in ontology research by Nicola Guarino and Mark Musen in their launching statement of the journal Applied Ontology has quite some implications and ramifications. We reflectively discuss ontology engineering as a scientific discipline, and we put this into the wider perspective of debates in other fields. We claim and argue that ontology is a new scientific method for theory formation. This positioning allows for stronger concepts and techniques for theoretical, empirical and practical validation that in our view are now needed in the field. A prerequisite for this is an emphasis on ontology as a (domain) content oriented concept, rather than as primarily a computer representation notion. We propose that taking domain theories and the associated substantive or content reference of ontologies really seriously as first-class citizens, will actually increase the contribution of ontology engineering to the development of scientific method in general. Next, ontologies should develop from the current static representations of relatively stable domain content into actionable theories-in-use, and a possible way forward is to build in capabilities for dynamic self-organization of ontologies as service-oriented knowledge utilities that can be delivered over the Web.

## 1 Introduction: Focus on Content?

Many believe that ontologies are first of all a computer science (CS) construct. There is some truth in this if one takes as a measure where the main locus and focus is in ontology engineering activities. On the other hand, in other scientific fields there is a significant interest in ontologies for (predominantly non-CS) reasons that relate to the development and growth of the respective domains. Many in computer science, and in knowledge engineering (KE) as well, have however a tendency to see this as 'just another application': something to be happy with because it proves the relevance of ontology engineering, but at the same time as something that is also of lesser (scientific) importance than the core CS issues in ontology such as computer-oriented representation, languages, reasoning techniques, systems development and tools.

In other sciences, we (amusingly?) see a mirror image with regard to CS. The preoccupation in CS with computing and systems-related issues is there often pejoratively

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viewed as ‘just programming’, in other words, as technical engineering that is important and useful to do — but it’s not really (and at the very least, not necessarily) science. This view, commonly found among both natural and social scientists, also extends to ontology engineering.

In this reflective essay we argue that both views, the CS one as well as the non-CS one, are misguided. This has its roots in an inadequate positioning of what ontologies are and can do.

For the CS and KE side, the emphasis on representation and systems aspects is perhaps an understandable attitude, but it is also a self-limiting approach that in the end will not be able to exploit the full potential of the ontology idea. Outside ‘application’ domains are to be taken much more seriously, as *first-class citizens* in CS and KE. In their launching statement of the new journal Applied Ontology, Nicola Guarino and Mark Musen [1] call for a “focus on content” in ontology research. Offen [2] points out that “domain understanding is the key to successful system development”. In this paper we explore some of the consequences for ontology research as a field of scientific endeavour.

For the non-CS side, we argue why and how ontology engineering is contributing to the further development of scientific method in general. The central contribution of this paper is our argument that *ontology is to be seen as a novel and distinct method for scientific theory formation and validation*. But to fully establish this, there are certain specific consequences to be drawn by CS and KE for the ontology research agenda.

## 2 Domain Understanding and the Dual Reference of Ontologies

Ontologies are generally defined as explicit and formal specifications of a shared conceptualization for some domain of interest [3]. The term *shared* refers to an agreement within a community of interest or practice over the description (i.e. conceptualization) of the domain, while *formal* indicates that the representation of this agreement is in some sort of computer-understandable format. Note the rather open notion of a domain conceptualization in the definition: ontology research makes no claim about the nature of the knowledge to be modelled [4].

Thus, as depicted in Figure 1, ontologies have a *dual* reference. They are not only ‘CS’ specs referencing a computational implementation (like conventional information systems (IS) or database models or schemas), but they have an explicit real-world *content or substantive reference* as well [5,6,1,7]. In current CS and KE research the computational reference seems to get more of the attention. However, we believe that the domain content reference is at least equally important, and not just because this is where future massive application of ontologies will be. Offen [2] makes the important general comment that “domain understanding is the key to successful system development”. In our view, this is where the real value of ontologies lies.

We observe that developing this understanding — which is a key practical use of today’s ontology building [4] — is in fact a (real-world domain) conceptualization and theory formation act. The content or substantive reference of ontologies means that ontologies function as ways to build and test what are in fact theories that purport to adequately model an, often empirical, domain or phenomenon. In other words, ontology

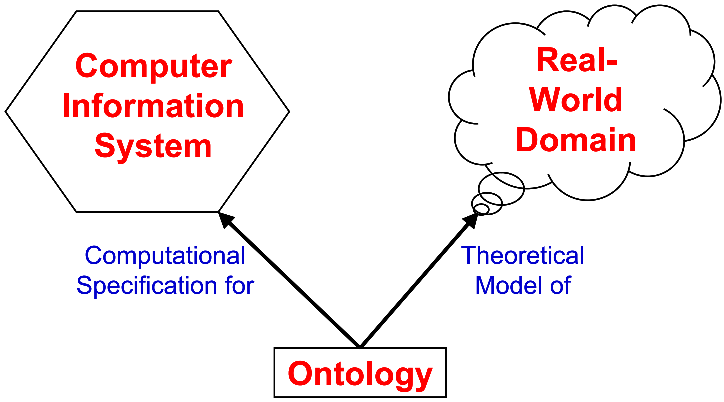


**Fig. 1.** The conceptualization triangle and the dual reference of ontologies

engineering can be viewed and employed as a method for theory formation. And it is one that appears to be useful for a wide variety of domains and disciplines.

## 3 The Conception of Theory in Other Sciences

Many works in the philosophy of science (e.g. [8,9,10,11]) and in scientific research methodology (e.g. [12,13,14,15,16]) emphasize the key importance, and difficulty, of conceptualization and theory formation in scientific research. We believe that the role of ontology as a rigorous instrument for conceptualization and theory formation in this sense is currently often overlooked, within CS and KE as well as outside.

Ontology engineering as a theory formation method is admittedly still at a relatively early stage. It potentially widens the scope and importance of ontology engineering as a scientific method of general interest, but it also comes with additional scientific issues and duties. And first of all, we have to ask the question *what actually counts as a theory* in scientific research.

Already a quick scan of the above-cited literature covering different disciplines, shows that there are very different notions in science what a theory is, ought to be, or looks like. There is sometimes the attitude among researchers that such 'philosophical' issues are external to the scientific debate in a research discipline. Nothing could be further from the truth. Perhaps this inside-the-box thinking is adequate for progress in mainstream normal puzzle-solving science (as Kuhn [8] calls it). In times of change it is different.

For example, in the constitutive era of classical mechanics, scientists such as Newton were not called physicists but (rightly) natural philosophers. Quantum mechanics as formulated by Bohr, Schrödinger, Heisenberg, and others was driven very much by a conceptual and philosophical discussion on foundations. The famous Einstein-Podolski-Rosen 'paradox' debated with Bohr in the 1930's in the Physical Review (not a philosophical journal, by the way) is a case in point [10]; there was not even any technical disagreement about the formalism or the equations or on how to compute things.

The birth of (symbolic) AI as a discipline in the 1950's is another good example (as are the debates concerning the pros and cons of symbolic vs. subsymbolic AI).

And closer to home, the history of Knowledge Engineering itself shows how strongly views concerning the broad conceptual and philosophical foundations of a field are influential in actually shaping it. There is a big difference between the mainstream view on KE during the heydays of expert systems (of, say, the late seventies to mid eighties) to the later conceptual model-based approach (see e.g. [17]) that is closely connected to today's ontology approaches. This becomes clear already by simply glancing over the (about twenty) years of the Proceedings of the present conference, EKAW (or its North-American counterpart KAW, now K-CAP).

Accordingly, different seemingly 'philosophical' views on the foundations of a field do have important practical consequences for research as it is actually organized, carried out, and reviewed (and so, accepted or rejected), cf. [18,19]. Elsewhere, we have discussed at some length various scientific disciplines and research approaches that turn out to have fundamentally different views on what a theory is and how it can or should be evaluated [20].

As pointed out there, theory in the natural sciences appears to be basically equated with formal math and its associated machinery. The logic-oriented research approaches in CS and KE are clearly heavily influenced by this image of science in what a theory is. However, another important element in natural science theorizing is the underlying assumption that the scientific method is first of all about uncovering the (abstract) fundamental 'first' principles as the (axiomatic) basis for universal theories and laws. This is not really the same as formal mathematical representation of theory (witness for example the mentioned Einstein-Bohr debate). It is first of all a matter of conceptualization that precedes the formal representation. Einstein is said to have the habit to start lectures with extensive fundamental conceptual discussions and only after some time to move to the formal equations: "Nun wollen wir *x*-en" — Now we will write down the *x*'s, the formal symbolism. An example of ontology research in this area attempting to combine formal math with conceptual modelling is the PHYSSYS ontology of [21] for physical systems modelling and simulation (Figure 2).

The social sciences provide yet other images of science that are relevant to ontology research (cf. Peter Mika's viewpoint article [22]). A major distinction here is that between the 'quantitative' and 'qualitative' schools of methodological thought (for extensive overviews, good sources are Robson [13] and Bryman [15]). Characteristic for the quantitative school is the reductionist approach from complex conceptual frameworks and concepts ('constructs') to *variables* as its theoretical languange and its preference for statistical methods for testing. Cohen's work on Empirical Methods for Artificial Intelligence [23] is in fact to a significant extent a translation of the school thought and empirical testing methodology of quantitative social research to AI and CS. Information Systems research as published in journals such as the MIS Quarterly, an important forum for much business school related research on IT, is also strongly influenced by this quantitative school. The prototypical form that theory assumes here is that of a small directed graph with variables as nodes; the edges represent the putative relationships between the variables and so supply the hypotheses to be tested.


**Fig. 2.** The PHYSSYS ontology has for example been used in the computer-aided design of this car. Constable Rob Piper shows the new electric patrol car of the Kidderminster police, England. Courtesy photograph: Associated Press Photo/David Jones.

The qualitative school in social research also has an empirical focus [24] but emphasizes that (unlike the natural sciences) it is not so much the outside and context-free view of the researcher/observer that is important in explaining the world, but the context-inclusive interpretation and meaning that people themselves attach to their social world. Works in KE close to the 'interpretive' or 'social constructivist' approach to science are for example the volumes Knowledge Acquisition as Modeling edited by Ken Ford and Jeffrey Bradshaw [25], and Expertise in Context edited by Feltovich et al. [26]. Characteristic for the qualitative and interpretive approach are methods such as interview, focus group, observation, ethnography, action research, case study — empirical research methods widely used in Information Systems research and practice (e.g. [27]) and, to a lesser extent, also employed in ontology research [6,5,28]. Theory in the qualitative school of thought is typically in the form of an extensive conceptual framework and argument put forward in an essay-like style, although there are attempts toward more formal approaches (cf. [24]; a specific example is grounded theory — which interestingly has similarities with good old bottom-up knowledge elicitation). In Knowledge Management theory, a good example is [29], but we also find it in AI (e.g. [30]; by the way, it also applies to the present paper). With respect to this style of theorizing, ontology methods and representations can add significant clarity and rigour, as we will argue below.

In sum, we believe it is important to investigate the underlying but often tacit assumptions made in researching, publishing and reviewing in the (theoretical as well as applied) ontology field. The content/substantive reference of ontologies implies that ontology engineering is an inherently multidisciplinary approach to theory formation. Therefore, it has to deal with very different conceptions and styles of scientific research and of what the form and nature of a scientifically acceptable theory is. This impacts for example the representation of ontologies: it is unlikely that with RDF and OWL as Web standards we have reached the end of representation (and even less so, of reasoning methodology), given the indicated highly diverse forms of scientific theorizing.

## 4 Ontology as Scientific Method for Theory Formation

The content reference of ontologies is the primary entry that makes ontologies interesting and useful for experts outside the CS domain. Ontologies as substantive theories offer ways to model phenomena of interest, and in particular model theories that are cast in the form of a conceptual framework (common in social sciences, as discussed above) in a much more rigorous fashion. In addition, and this is where the second, computational reference of ontologies comes in, they offer ways for testing such models by means of simulation, calculation, or other computational means. But even more importantly, ontology engineering — as an advanced branch of conceptual modelling — is providing richer and more flexible ways for conceptualization and theory formation than currently in use in many domains and scientific disciplines.

Scientific theory generally seems to assume two extreme forms: either formal-mathematical (as typically encountered in the 'exact' natural sciences), or informal in natural language and essayistic (common in social sciences and the humanities). In contrast, IS-style conceptual modelling and particularly ontology engineering have over the years developed novel methods for conceptualization that are more formal and rigorous than theories in natural language, thus allowing for stronger, computational and other forms of validation for example by CASE and simulation tools.

At the same time, the graphical and diagram representations developed and employed in conceptual modelling and ontology engineering make the associated theories much more understandable and accessible to experts and practitioners in other domains compared to formal math and logic. Conceptual and ontological analysis, graphical

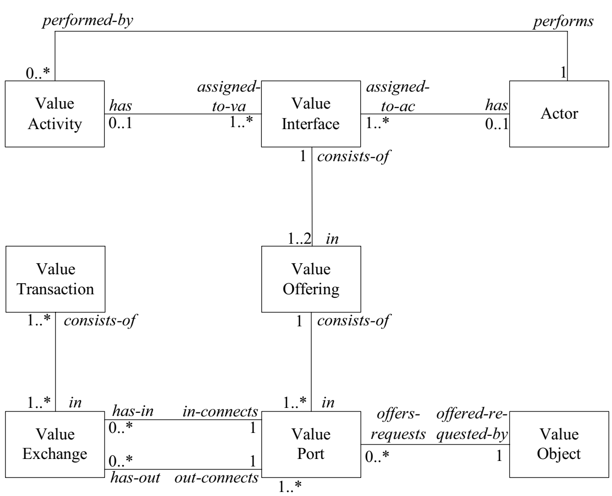


**Fig. 3.** The $e^3$*value* ontology for networked business models

diagramming methods, and their combination with formal computational reasoning techniques have over the years been elaborated into a fine art at a level of sophistication not found elsewhere.

A practical example that demonstrates several of the above points is the $e^3$*value* ontology for networked business modelling (Figure 3; [31,6,5,28]). As a theory, it effectively formalizes existing concepts from business research literature about which there is a good deal of consensus [31]. A formal ontology goes however much further: it includes rules and constraints (many of them present but rather implicit in the domain literature) which with it is possible to reason, and so to find out what the inferential consequences of a theory are. It is here that the computational paradigm shows its value with regard to other disciplines. In the present example, it makes it possible to design and reason about the potential of new business model ideas (including net present value and cashflow analyses in a business network). Given the complexity of such reasoning methods that surpasses the possibilities of manual analysis, computational tooling is necessary and important.

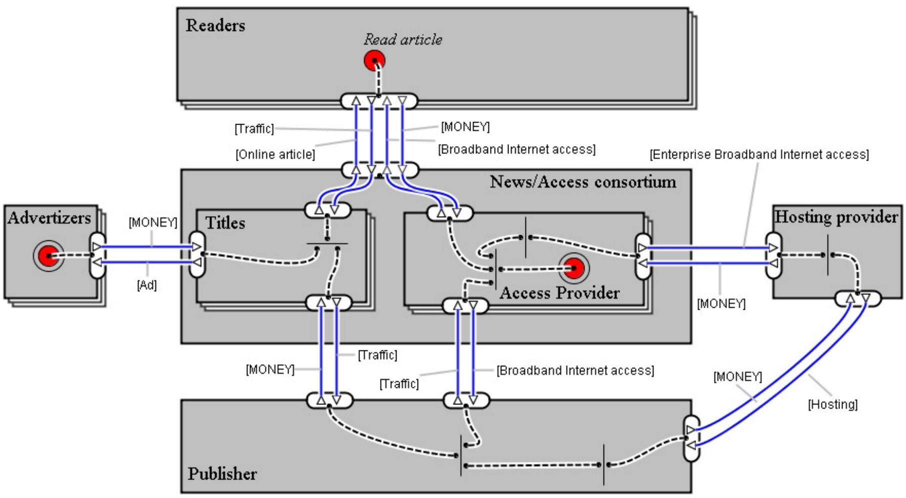


**Fig. 4.** Visual representation of an $e^3$*value* business model for a news media e-service

However, tooling should be ideally such that it hides the complexity 'under the hood' as far as possible, in order to facilitate work with users and practioners. Figure 4 shows an example of the graphical diagram representation of an ontology instance. The associated $e^3$*value* tool for networked business modelling (www.e3value.com) employs internally the formal ontology, but enables the user to develop the application ontology in an almost fully graphical way. The RDF(S) representation of the application ontology is not constructed by the user or ontology developer, but is automatically generated by the tool.

In summary, looking at ontologies from their content reference point of view suggests that ontology engineering can be usefully interpreted as a scientific method for conceptualization and theory formation, and one that brings several novel contributions.

## 5 Reuse: Ontologies as Middle-Range Theories

Conceiving the content/domain reference of ontologies as ‘the application view’ is quite natural for CS researchers, but overly limiting. Domain experts, on their turn, often see it equally simply the other way around: the CS work as the application side (or even worse: as ‘just programming’).

Ontologies as theories — that are to be sharable and reusable — go significantly beyond the application view. Already in ontology research quite long ago (e.g. [32,21]), distinctions have been made in different types of ontologies that have different levels of generality, and therefore of reusability. A simplified picture distinguishes three different levels of generality:

1. At the top level, with maximum genericity, we have the upper ontologies that formalize highly generic (‘universal’) concepts concerning, say, mereology, taxonomy, space, time, etc. (see for example IEEE Upper Ontology work at http://suo.ieee.org/SUO/SUMO/, or some ontology engineering patterns of the W3C Semantic Web Best Practices & Deployment Working Group, http://www.w3.org/2001/sw/BestPractices/Overview.html).
2. At the bottom level, we have the application ontologies that are key in driving specific applications and tasks, but in terms of their generality tend to trade reusability for practical usability.
3. In-between we have what we call middle-range ontologies: they concern a domain, are less universal than the top-level ontologies, but generic and reusable across many different applications. The $e^3$*value* ontology is an example of an ontology as such a middle-range theory.

What in CS and KE are called application domains are in fact themselves broad areas where ontologies can be (made) sharable and reusable beyond a specific application context. Here, ontologies have the capability to express what in social science research are called “middle-range theories” (hence our terminology): theories that have a much wider applicability than the situations, contexts, or cases from which they actually originate.

For an interesting methodological discussion how to develop middle-range theories in scientific research, we refer to the book of one of the grand old men of sociology, Howard Becker [12]). One practical recommendation he gives to come to middle-range theories and hypotheses, is to describe case-study conclusions without being allowed to mention the specific case itself anywhere. This forces one to come up with and consider more generally valid formulations. It is also good advice for knowledge acquisition in ontology development.

## 6 Ontology Evaluation and Validation

Scientific theories are supposed to be empirically and/or pragmatically valid in their domain of reference. In terms of the dual reference of Figure 1, ontologies are to be both computationally and epistemologically adequate.

CS tends to focus on methods for the former, and indeed here it has a lot of added value for scientists and practitioners in other domains: it is usually impossible to foresee all consequences that a theory has manually, or to get a grip on all possible paths that motivating domain scenarios might follow. Computational implementation and test of ontologies is thus necessary and useful, but its strength is in forms of consistency and validity that are internal to the theory that is tested. It is restricted to what in philosophical terms is called a coherence conception of truth, and this is what logic-based and computational evaluation does for us.

If however we take the content reference aspect of ontologies seriously, a much stronger emphasis on empirical ontology validation is called for. Ontologies are good only insofar as they are empirically valid from the domain theory point of view. This requires more and different validation activities than just computer-oriented ones. This is a KE theme recurring in the work of Tim Menzies, e.g. [33], and it is also the thrust of Cohen's [23] call to AI. We believe that these authors make a point that is very valid in current ontology research. Richer and stronger notions of validation, in particular external validity, are in need of more emphasis in the ontology research field.

How can ontology evaluation and validation be practically done? In our view, there are several different approaches that may be employed in parallel. Not only there are, as discussed above, several different conceptions of theory, there are also multiple notions of validity that are applicable. In other sciences (notably social research), the various notions of validity have been discussed in quite some more depth than is the case in CS, and many corresponding suitable scientific methods for evaluation and validation have been developed. However, mainstream ontology research tends to employ an (overly) limited repertoire of available scientific methods for testing its claims.

As we have argued elsewhere [20], validation of claims to knowledge assumes in science the form of a *rational communicative argument* that must be defended and made credible. In scientific work, available empirical data and theory are systematically brought together such that knowledge claims follow in a step-by-step and transparent process of rational reasoning. Ontologies, as they represent knowledge structures that are reusable and community-sharable, should satisfy general criteria of validity concerning rational communicative argument.

The general structure and rules of argument have been investigated in past years in philosophy [34], communication theory [35], and critical thinking and informal logic [36]. A simple model of the general layout of arguments due to Toulmin [34] is depicted in Figure 5.

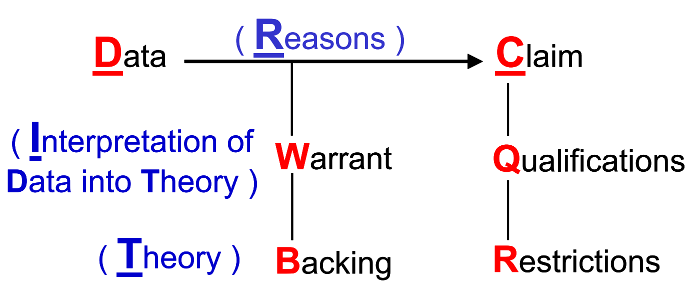


**Fig. 5.** The structure of argument

This model suggests a checklist of criteria and questions [20] that is also practically useful to review the adequacy of the computational and especially content references of ontologies:

1. *Descriptive validity* $\boldsymbol{D}$: do the supplied empirical (domain) data provide a truthful description of the situation or problem that is considered?
2. *Theoretical validity* $\boldsymbol{T}$: are the employed theories or conceptual frameworks explicated and shown to be appropriate for the (domain) purpose?
3. *Interpretive validity* $\boldsymbol{I}$: is the way in which all available data are mapped onto or interpreted in the employed theories or frameworks clear and adequate?
4. *Reasoning validity* $\boldsymbol{R}$: are all steps in the reasoning sound and, in addition, consistent and coherent with other knowledge that we possess?
5. *Internal validity* $\boldsymbol{C}_{int}$: are the claims made acceptable 'beyond reasonable doubt' *within* the situation or context (or sample) considered in the study?
6. *External validity* $\boldsymbol{C}_{ext}$: are any generalization claims that go *beyond* the studied situation sufficiently credible?

These different questions as to validity require different kinds of test methods [20,18,19]. In CS and KE, methods for logico-mathematical demonstration ('proof') are well developed: if a theory is sufficiently rigorously specified, certain desired properties may be strictly mathematically or logically derived. This is seen in formal ontology, from description logics to OntoClean.

A further step, one that is also well developed, is computational simulation and analysis: the computer has made it possible to run very high numbers of scenarios and explore a large parameter space. This approach to validation might be viewed as the computational extension of the thought experiment (a very ancient technique, famous as a result of the Einstein-Bohr debate on the interpretation of quantum mechanics — in today's terms very much a discussion on ontologies). In ontological analysis, the direct analogy with thought experiments are walkthrough methods that employ mental or paper simulations of simple application scenarios; they are in our experience a quite effective method at an early stage of development. A main caveat here is that in the end the motivating scenarios selected for computational evaluation should not be toy examples, but be sufficiently real-world like and cover a good part of the design space, in order to be convincing in terms of validation of claims. There is some room for improvement here in current CS and KE research.

These methods can establish the validity of the computational reference of ontologies. In terms of the above validity checklist, they establish reasoning validity and, but only partially, help answer other validity questions such as theoretical and internal validity. To validate the substantive content reference of ontologies, however, other notions of validity are more prominent, in particular descriptive and external validity, and they require other methods for their evaluation. It is here that CS and KE can learn quite a lot from other disciplines that have put major efforts into the development and refinement of experimental methods (in the lab, but for our purposes especially in the field) as well as of empirical methods for practice/experience-oriented field studies [13,15,14,16,24,37,12].

An essential issue for ontology evaluation and validation that needs to be more explicitly considered in research is the aspect of *context*. Ontologies are usable because they function successfully in specific domain, task, and/or application contexts that exist in the field. Ontologies are reusable only if we succeed in solving the (external validity) question to what extent they work satisfactorily across different contexts (compare also [22]). This issue is behind our above-discussed idea of ontologies as middle-range theories.

Our position here is that approaches to ontology evaluation and validation need to be (field) context inclusive, in ways that are in clear contrast with the orthodox context-free scientific ideals of empirical confirmationist/falsificationist research (often associated with writers such as Popper). These issues have been discussed extensively in social research, especially in the context of case study methodology [37] and action research [13,27], but they are too much ignored in CS and KE. Avoiding to deal with context is minimally a very (and in our view too) high price to pay for scientific research in ontologies, an important point that was already made in older KE work [25,26] but needs to be reiterated. Focus on content entails dealing with context.

## 7 No Ontology Without Methodology

The call for a "focus on content" in ontology research by Nicola Guarino and Mark Musen [1] in their launching statement of the journal Applied Ontology has quite some implications and ramifications. In particular, we have argued that:

- Ontology engineering offers a potential contribution to scientific method in general, as a fundamental approach to conceptualization and theory formation with new techniques valuable to many (non-CS) domains and disciplines.
- This however requires that the content or substantive reference of ontologies is taken to heart by ontology engineers in addition to the common CS issues.
- This goes against the not uncommon attitude that outside domains represent application research (that academically speaking has a lower rank than fundamental research).
- Especially, this requires that issues and methods of empirical and practical validation of theories — as much further developed in other scientific disciplines — become more prominent and adopted in ontology engineering.

Taking application domain theories and the associated content reference of ontologies really seriously as first-class citizens in our research will actually increase the contribution of ontology engineering to the development of scientific method in general.

A further step on the research agenda to be taken in our view is that ontologies should develop from the current static representations of relatively stable domain content into actionable theories-in-use (as opposed to 'espoused theories'; these are concepts stemming from organizational learning [38,39,40]). We believe it is a fair characterization of the state of the art to say that ontologies are still quite generally perceived as *static* representations and metadata annotations of knowledge.

However, ontologies have *to do* something for people: they are to provide actionable knowledge, and this involves system *dynamics*. Ontologies can therefore not (or no longer) be specified 'as such'. In addition, the specific forms and methods of reasoning they employ or presuppose is to become an inherent part of the specification.

An observation resulting from the mentioned context-relatedness of ontologies is that in practice there are many different methods that make them do useful work. This is already true if we limit ourselves to the formal logic-based approaches that go with different deduction engines. It is even more true if we consider reasoning machineries needed for Semantic Web Services. And the scope of dynamic methods is even broader if we consider ontologies as part of rational communicative argument (cf. Figure 5) constructed and shared within a community of practice, a perspective common in ontology-based Knowledge Management. In other words: no ontology without methodology.

Beyond this, a further way forward for the research agenda would be to start to employ the computational paradigm for the dynamic feedback loops in Knowledge Engineering and Knowledge Management themselves. Given the significant amounts of knowledge available on the Web, plus a broad repertory of dynamic reasoning methods available, it seems well possible to build in capabilities for *self-organization* of systems and services, in which ontologies act as service-oriented knowledge utilities that can be delivered over the Web. There are currently several useful hooks from ongoing research, although they are still in an early stage of technical development, content and detail. So that is a story to be told elsewhere, another time.

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