

# An Introduction to Semantic Web and Ontologies



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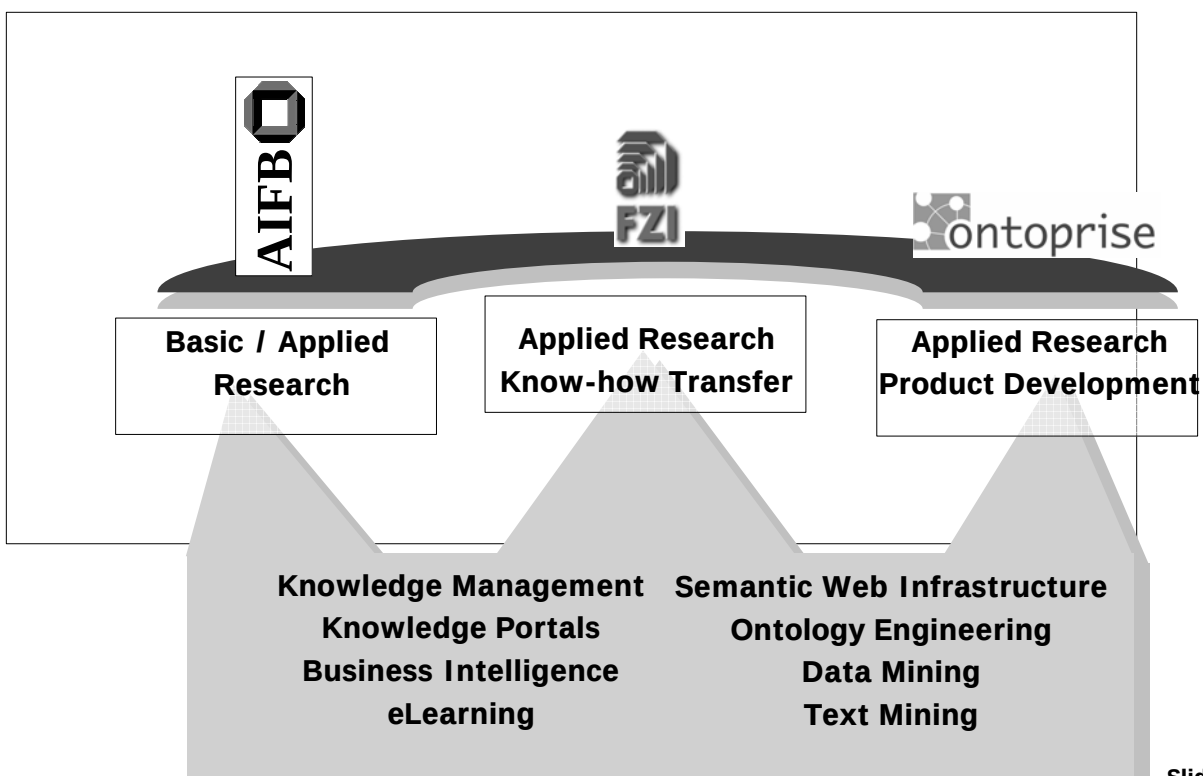
May 10th, 2004

**Dr. York Sure**

Knowledge Management Group  
Institute AIFB  
University of Karlsruhe

## Karlsruhe: Location for Semantic Technologies

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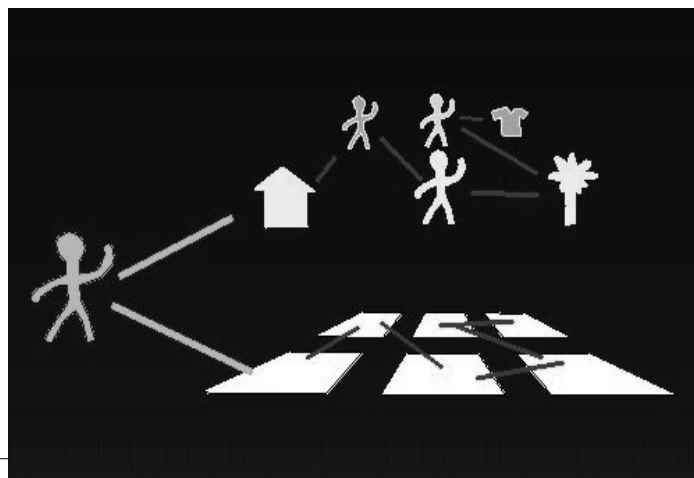
## Agenda

- Semantic Web
- Ontologies
- Modeling Example
- Application Example: Project Halo

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## ... Semantic Web HISTORY

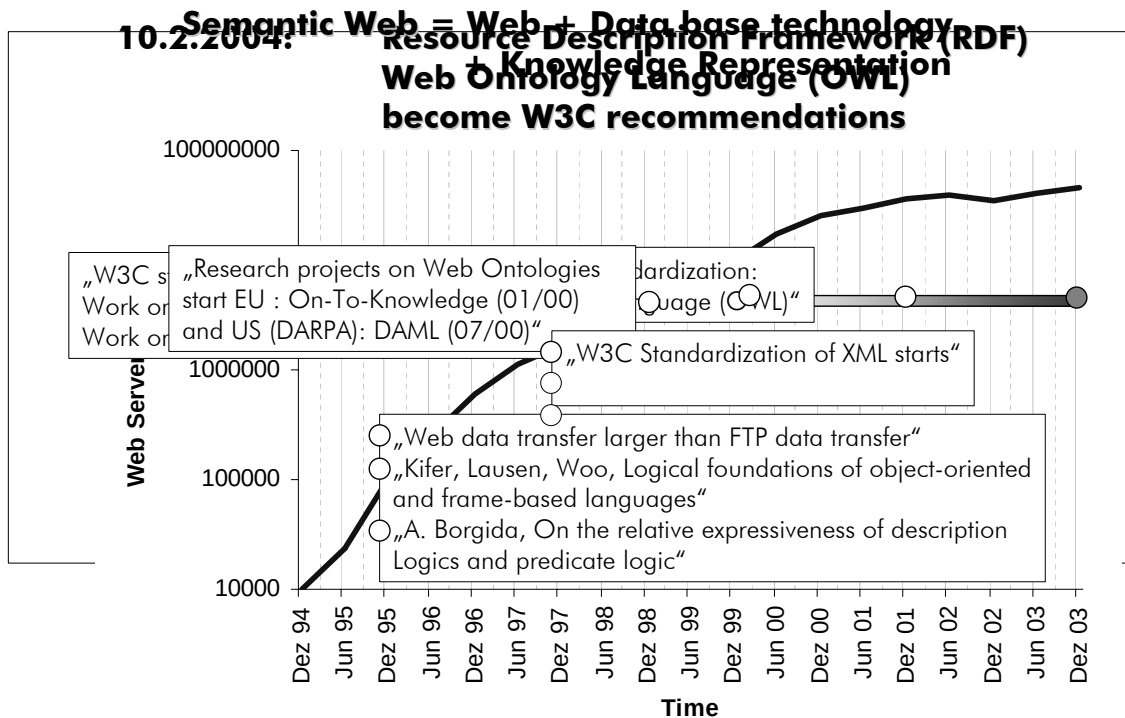
27. May 1994: Sir Tim Berners-Lee: Vision of a Semantic Web  
Closing Key Note, 1. Int. WWW Conference, CERN



Adding semantics to the web involves **two** things: allowing documents which have **information in machine-readable** forms, and allowing **links to be created with relationship values**.

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## ... Semantic Web HISTORY



[ Source: <http://www.zakon.org/robert/internet/timeline/> ]

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## Semantic Web

„The **Semantic Web** is an extension of the current web in which information is given well-defined **meaning**, better enabling computers and people to **work in co-operation**.“

[Berners-Lee et al., 2001]

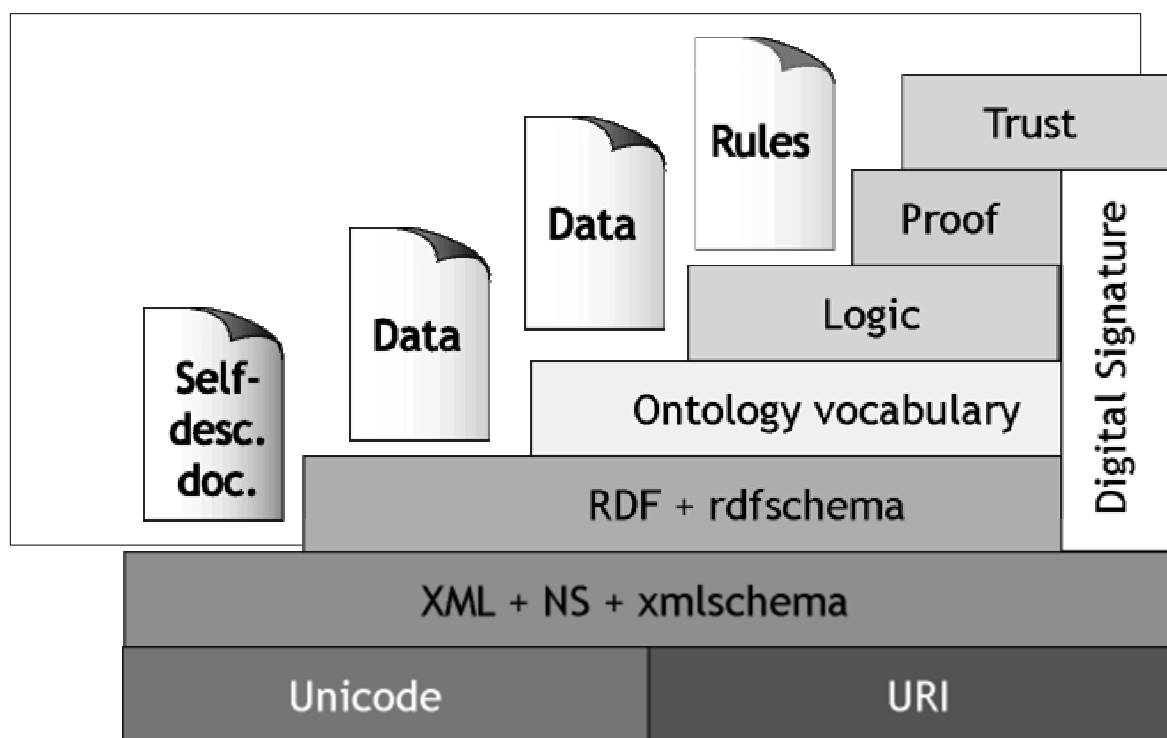


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# Semantic Web Layers (T. Berners-Lee et al.)

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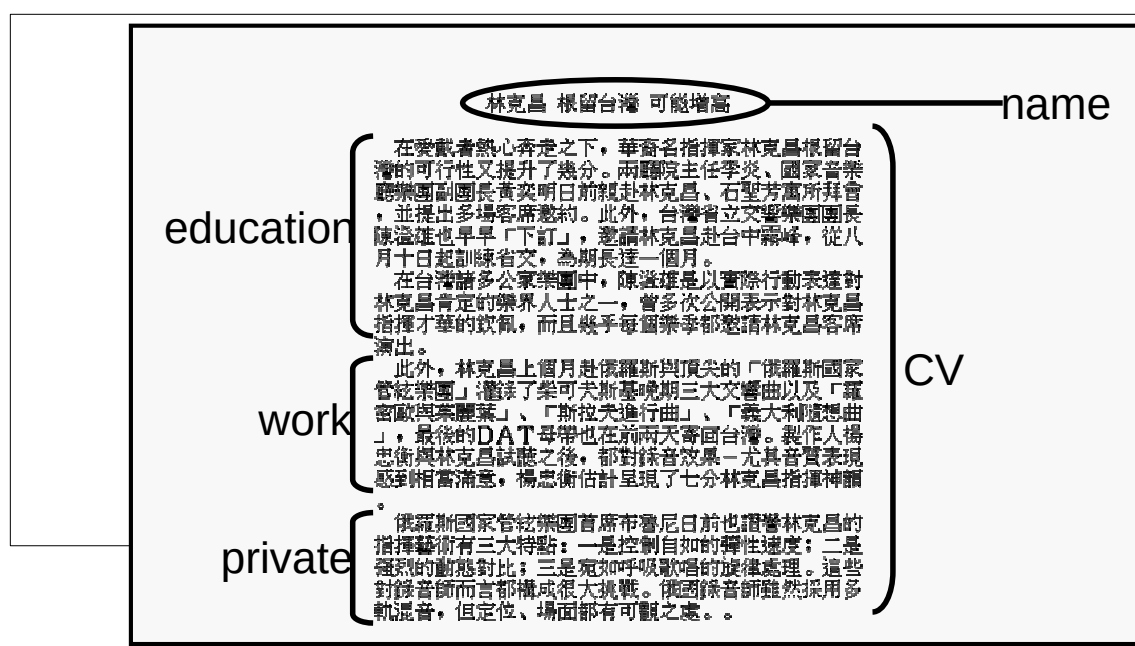
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## Machine accessible meaning

*(What it's like to be a machine)*

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## XML:

User definable and domain specific markup

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### HTML:

```
<H1>Knowledge Management</H1>
  <UL>
    <LI>Teacher: Rudi Studer
    <LI>Students: Master
  </UL>
```

### XML:

```
<course>
  <title>Knowledge Management</title>
  <teacher>Rudi Studer</teacher>
  <students>Master</students>
</course>
```

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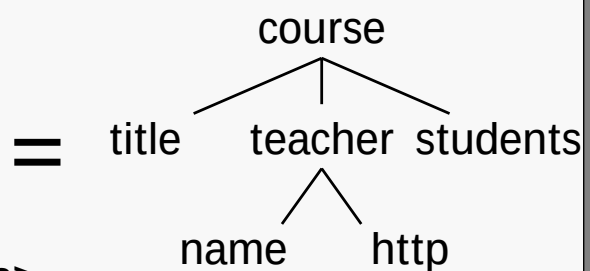
## XML: Document = labelled tree

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- node = label + attr/values + contents

```
<course date="...">
  <title>...</title>
  <teacher>...</teacher>
    <name>...</name>
    <http>...</http>
  <students>...</students>
</course>
```



- DTD: simple grammars to describe legal trees

- So:

**why not use XML to represent ontologies?**

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# XML: limitations for semantic markup

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XML *per se* makes no commitment on:

- ❶ Domain specific ontological **vocabulary**
- ❷ Ontological **modelling primitives**

⇒ requires pre-arranged agreement on ❶ & ❷

Only feasible for closed collaboration

- agents in a small & stable community
- pages on a small & stable intranet

**.. not for sharable Web-resources**



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## XML ≠ machine accessible meaning

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<εδυχατιον>

<ωορκ>

<πριωατε>

林克昌 根留台灣 可能增高

在愛戴者熱心奔走之下，華裔指揮家林克昌根留台灣的可行性又提升了幾分。兩廳院主任李炎、國家音樂廳樂團副團長黃奕明日前親赴林克昌、石聖芳寓所拜會，並提出多場客席邀約。此外，台灣省立交響樂團團長陳澄雄也早早「下訂」，邀請林克昌赴台中霧峰，從八月十日起訓練省交，為期長達一個月。

在台灣諸多公家樂團中，陳澄雄是以實際行動表達對林克昌肯定的樂界人士之一，曾多次公開表示對林克昌指揮才華的欽佩，而且幾乎每個樂季都邀請林克昌客席演出。

此外，林克昌上個月赴俄羅斯與頂尖的「俄羅斯國家管絃樂團」灌錄了柴可夫斯基晚期三大交響曲以及「羅曼歐與朱麗葉」、「斯拉夫進行曲」、「義大利隨想曲」，最後的DAT母帶也在前兩天寄回台灣。製作人楊忠衛與林克昌試聽之後，都對錄音效果—尤其音質表現感到相當滿意，楊忠衛估計呈現了七分林克昌指揮神韻。

俄羅斯國家管絃樂團首席布魯尼日前也讚譽林克昌的指揮藝術有三大特點：一是控制自如的彈性速度；二是強烈的動感對比；三是宛如呼吸歌唱的旋律處理。這些對錄音師而言都構成很大挑戰。俄國錄音師雖然採用多軌混音，但定位、場面都有可觀之處。

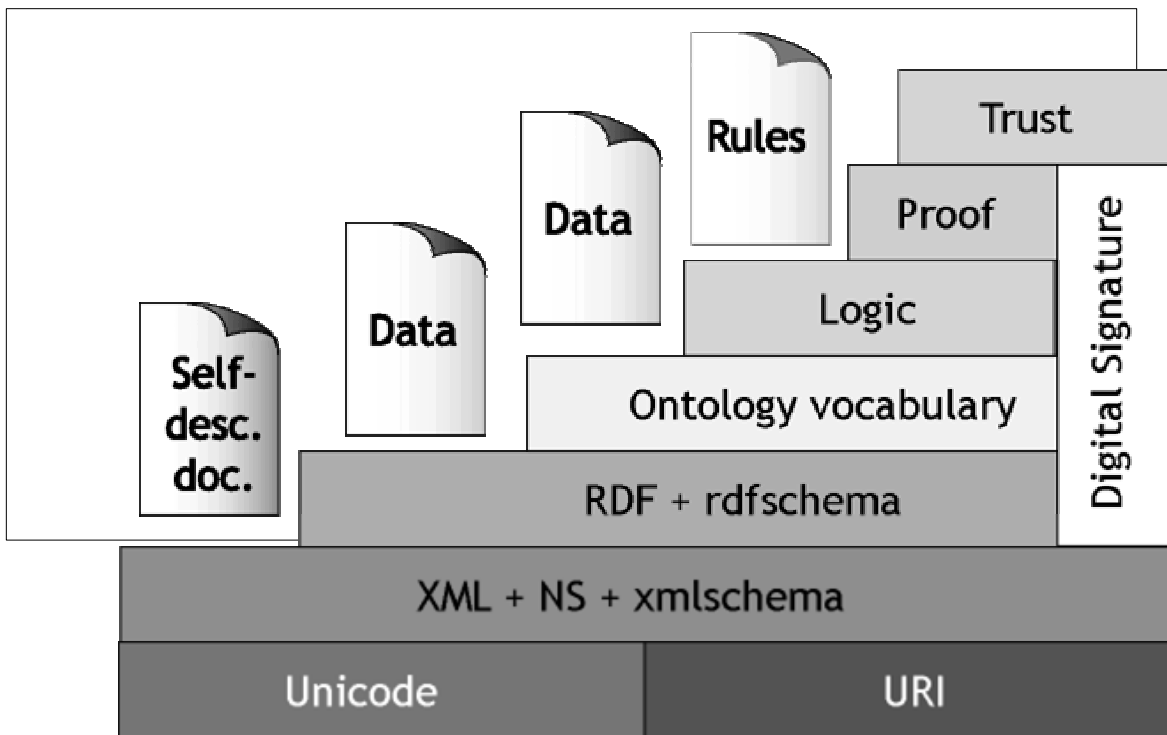
< ναμε >

< Xς >

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# The semantic pyramid again

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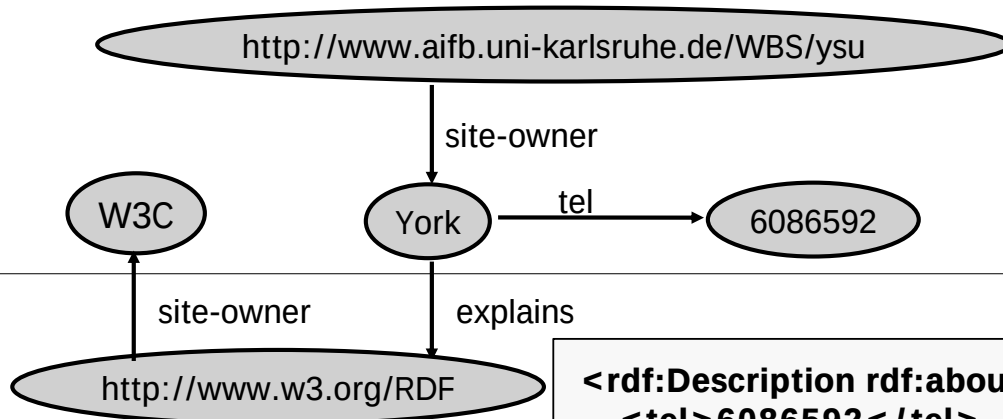
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## RDF for semantic annotation

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- RDF provides metadata about Web resources
- **Object -> Attribute-> Value** triples
- It has an **XML syntax**
- Chained triples form a **graph**



```
<rdf:Description rdf:about="#York">
  <tel>6086592</tel>
</rdf:Description>
```

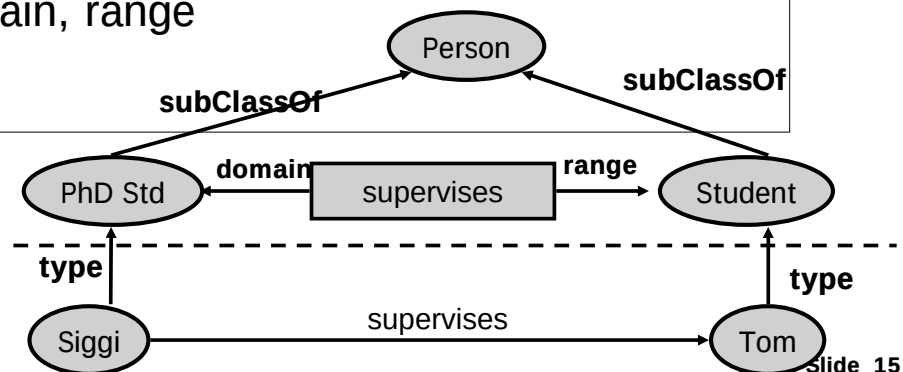
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# What does RDF Schema add?

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- Defines **vocabulary** for RDF
- Organizes this vocabulary in a **typed hierarchy**
  - Class, subClassOf, type
  - Property, subPropertyOf
  - domain, range



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## RDF Schema syntax in XML

```
<rdf:Description ID="MotorVehicle">
  <rdf:type resource="http://www.w3.org/...#Class"/>
  <rdfs:subClassOf rdf:resource="http://www.w3.org/...#Resource"/>
</rdf:Description>

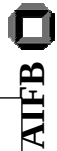
<rdf:Description ID="Truck">
  <rdf:type resource="http://www.w3.org/...#Class"/>
  <rdfs:subClassOf rdf:resource="#MotorVehicle"/>
</rdf:Description>

<rdf:Description ID="registeredTo">
  <rdf:type resource="http://www.w3.org/...#Property"/>
  <rdfs:domain rdf:resource="#MotorVehicle"/>
  <rdfs:range rdf:resource="#Person"/>
</rdf:Description>

<rdf:Description ID="ownedBy">
  <rdf:type resource="http://www.w3.org/...#Property"/>
  <rdfs:subPropertyOf rdf:resource="#registeredTo"/>
</rdf:Description>
```

# Conclusions about RDF(S)

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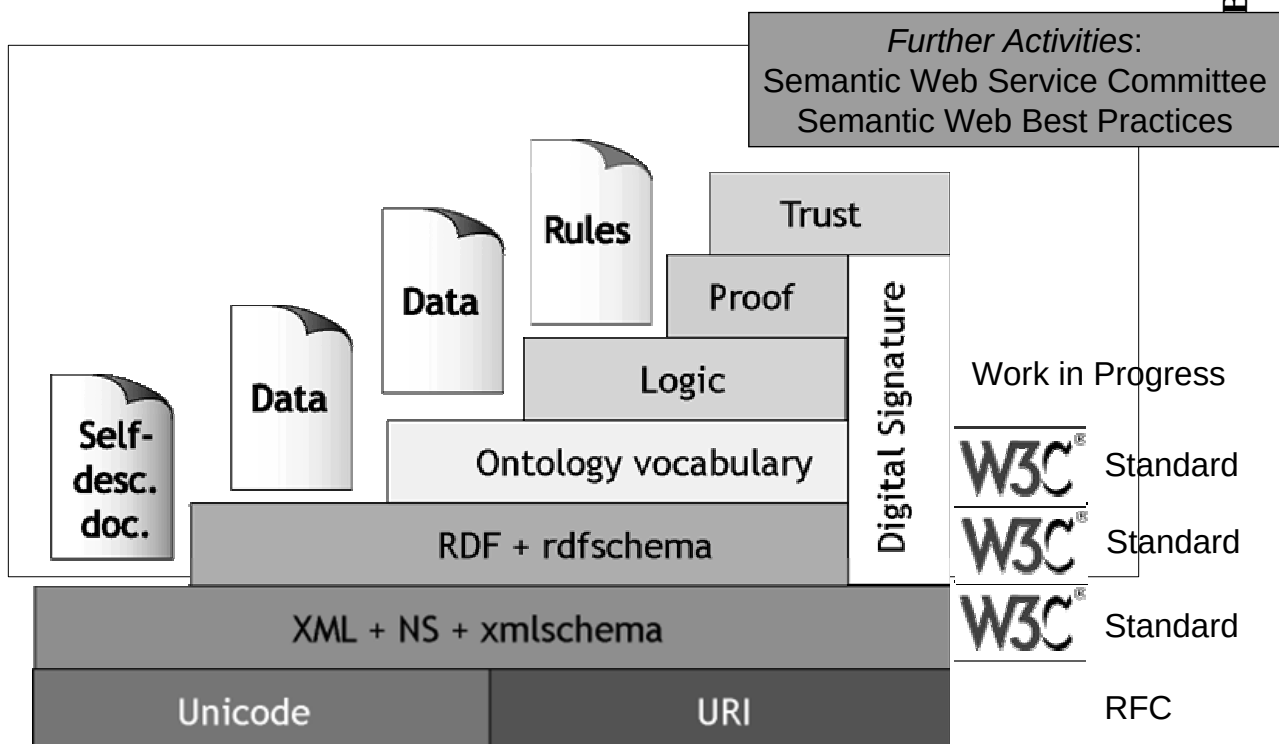


- Next step up from plain XML:
  - (small) **ontological commitment** to modeling primitives
  - possible to define **vocabulary**
- However:
  - **no** precisely described meaning
  - **no** inference model

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## Last but not least ...

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## Ontologies

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## Origin and History

- Ontology in Philosophy

a philosophical discipline, branch of philosophy that deals with the nature and the organisation of reality

- Science of Being (Aristotle, Metaphysics, IV, 1)

- Tries to answer the questions:

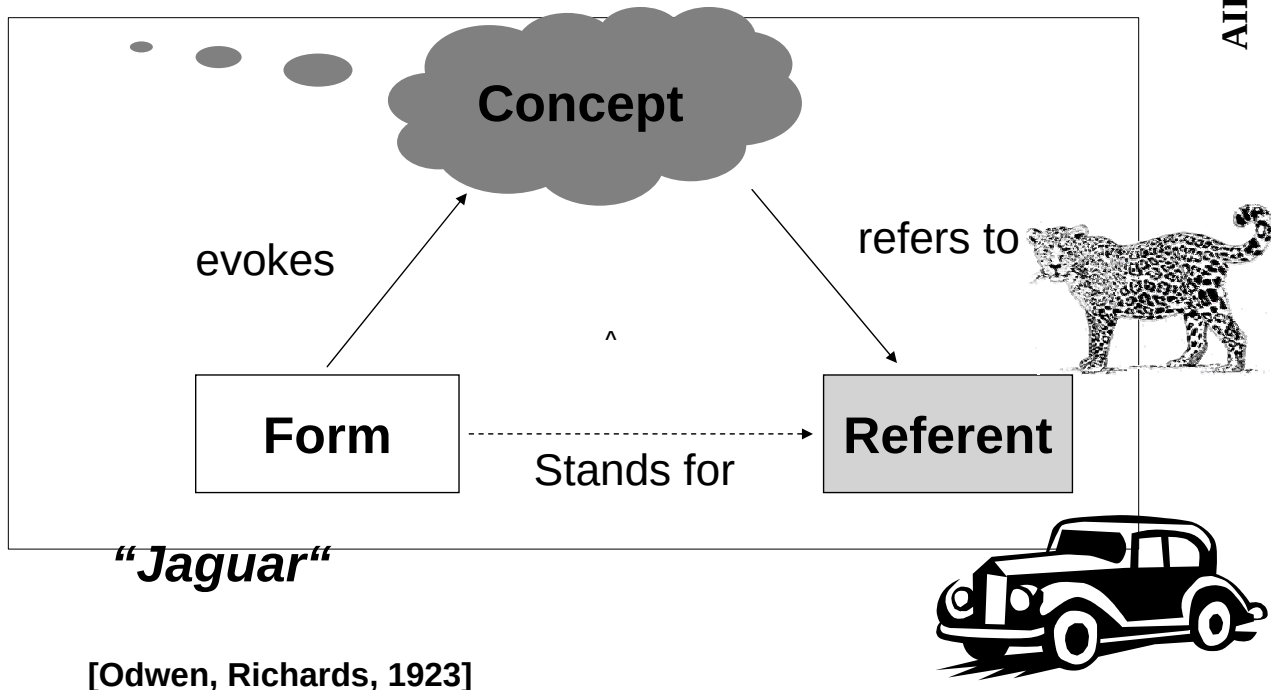
*What characterizes being?*

*Eventually, what is being?*

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# Ontologies in Linguistics

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[Odwen, Richards, 1923]

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# Ontologies in Computer Science

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„An ontology is an explicit specification of a conceptualization.“ [Gruber, 93]  
„An ontology is a shared understanding of some domain of interest.“ [Uschold, Gruninger, 96]

- Ontology refers to an engineering artifact:
  - It is constituted by a specific vocabulary used to describe a certain reality, plus
  - a set of explicit assumptions regarding the intended meaning of the vocabulary.
- Thus, ontologies describe a formal specification of a certain domain:
  - Shared understanding of a domain of interest
  - Formal and machine executable model of a domain of interest

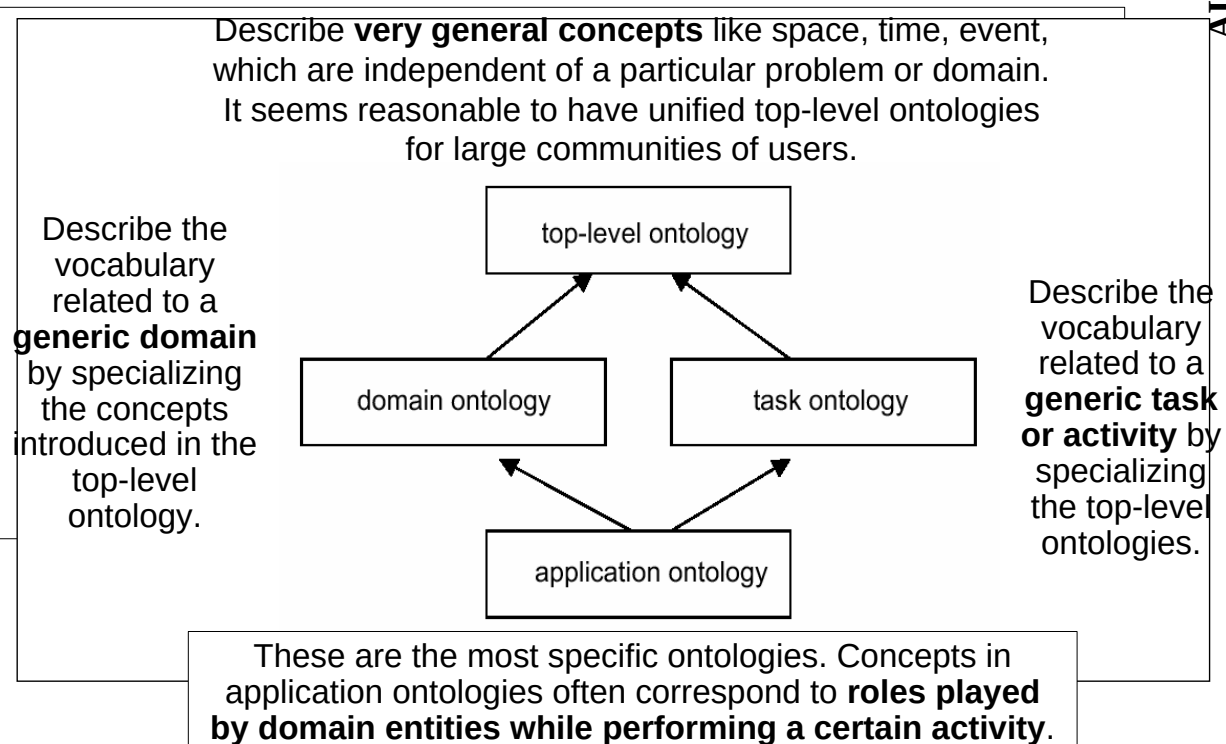
# Why develop an ontology?

- To make domain assumptions explicit
  - Easier to change domain assumptions
  - Easier to understand and update legacy data
- To separate domain knowledge from operational knowledge
  - Re-use domain and operational knowledge separately
- A community reference for applications
- To share a consistent understanding of what information means

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## Types of Ontologies

[Guarino, 98]



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# Ontologies and their Relatives (I)

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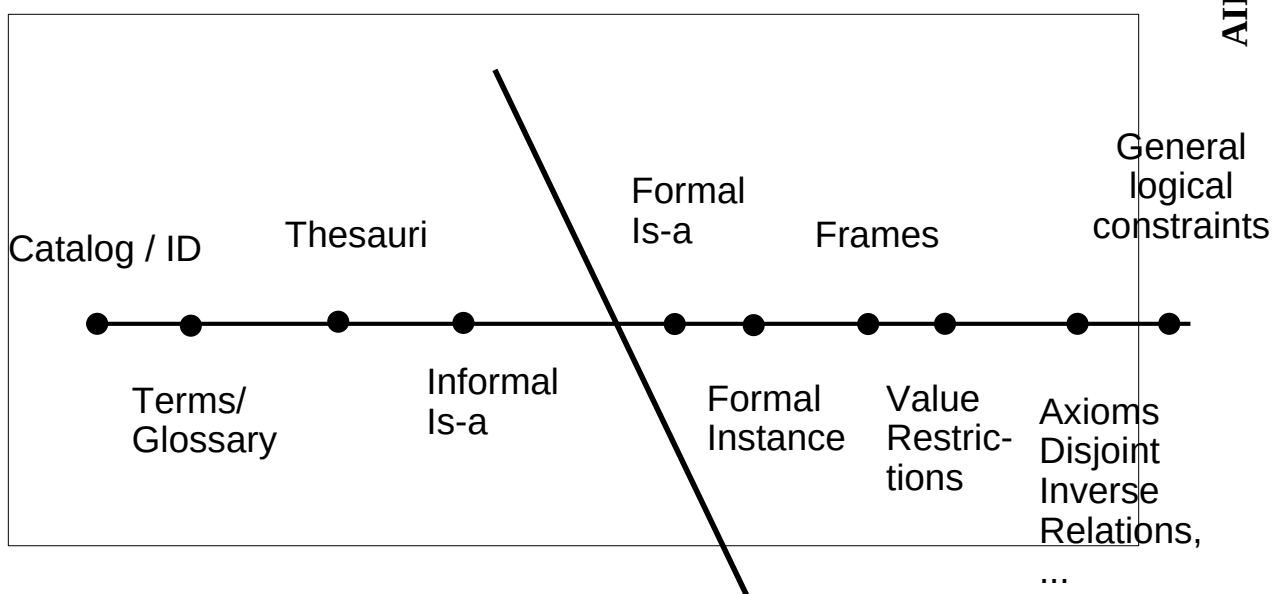


- There are many relatives around:
  - **Controlled vocabularies, thesauri and classification systems available in the WWW**, see <http://www.lub.lu.se/metadata/subject-help.html>  
Classification Systems (e.g. UNSPSC, Library Science, etc.)  
Thesauri (e.g. Art & Architecture, Agrovoc, etc.)
  - **Lexical Semantic Nets**  
WordNet, see <http://www.cogsci.princeton.edu/~wn/>  
EuroWordNet, see <http://www.hum.uva.nl/~ewn/>
  - **Topic Maps**, <http://www.topicmaps.org> (e.g. used within knowledge management applications)
- In general it is difficult to find the border line!

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# Ontologies and their Relatives (II)

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# Ontologies - Some Examples

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- **General purpose ontologies:**

- WordNet / EuroWordNet, <http://www.cogsci.princeton.edu/~wn>
- The Upper Cyc Ontology, <http://www.cyc.com/cyc-2-1/index.html>
- IEEE Standard Upper Ontology, <http://suo.ieee.org/>

- **Domain and application-specific ontologies:**

- RDF Site Summary RSS, <http://groups.yahoo.com/group/rss-dev/files/schema.rdf>
- UMLS, <http://www.nlm.nih.gov/research/umls/>
- RETSINA Calendaring Agent, <http://ilrt.org/discovery/2001/06/schemas/ical-full/hybrid.rdf>
- AIFB Web Page Ontology, <http://ontobroker.semanticweb.org/ontos/aifb.html>
- Web-KB Ontology, <http://www-2.cs.cmu.edu/afs/cs.cmu.edu/project/theo-11/www/wwkb/>
- Dublin Core, <http://dublincore.org/>

- **Meta-Ontologies**

- Semantic Translation, <http://www.ecimf.org/contrib/onto/ST/index.html>
- Evolution Ontology, <http://kaon.semanticweb.org/examples/Evolution.rdfs>

- **Ontologies in a wider sense**

- Agrovoc, <http://www.fao.org/agrovoc/>
- Art and Architecture, <http://www.getty.edu/research/tools/vocabulary/aat/>
- UNSPSC, <http://eccma.org/unspsc/>
- DTD standardizations, e.g. HR-XML, <http://www.hr-xml.org/>

- **DAML.org library with all kinds of different ontologies!**

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## Wordnet (<http://www.cogsci.princeton.edu/~wn>)

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- **WordNet contains**

- 118.000 word forms
- 90.000 word meanings

- **WordNet categorizes word into syntactic categories**

- (N, noun)
- (V, verb)
- (Adj, adjective) und
- (Adv, adverb).

- **WordNet additional contains lexical-semantic relations between word meanings**

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# Lexical-semantic relations

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| Lexical - semantic relations | syntactic categories | examples                                              |
|------------------------------|----------------------|-------------------------------------------------------|
| Synonymy                     | N, V, Adj, Adv       | jolly, merry                                          |
| Antonymy                     | Adj, Adv, (N, V)     | fast, slow<br>friendly, unfriendly                    |
| Hyperonymy                   | N                    | animal, living being<br>mammal, animal<br>dog, mammal |
| Meronymy                     | N                    | flour, cake<br>tyre, car                              |
|                              |                      |                                                       |

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## WordNet

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- Lexical semantic relations in WordNet mainly correspond to their counterparts of object-oriented representation formalisms
  - hyperonym / hyponym is analog to *is-a*-relation
  - meronym / holonym corresponds to *has-part* / *part-of*-relations
    - important: *part-of* expresses different lexical semantic relations, e.g.:
      - component-of: *handle - cup*
      - element-of: *ship - fleet*
  - WordNet* allows floating transition between linguistic information and conceptual structures

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## news item IS A KIND OF ...

1 sense of news item

Sense 1

**news item** -- (an item in a newspaper)

=> **item, point** -- (a distinct part that can be specified separately in a group of things that could be enumerated on a list; "he noticed an item in the New York Times"; "she had several items on her shopping list"; "the main point on the agenda was taken up first")

=> **part, portion, component part, component** -- (something determined in relation to something that includes it; "he wanted to feel a part of something bigger than himself"; "I read a portion of the manuscript"; "the smaller component is hard to reach")

=> **relation** -- (an abstraction belonging to or characteristic of two entities or parts together)

=> **abstraction** -- (a general concept formed by extracting common features from specific examples)

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## Problems with WordNet

- In WordNet: clear that news\_item **is-a** item
- Maybe acceptable that news\_item **is-a** part
- But what of news\_item **is-a** relation !?
  - depends on *context, role played...*
- But: "role" and "context" knowledge is missing
- Also: some lexicographer's bias is present

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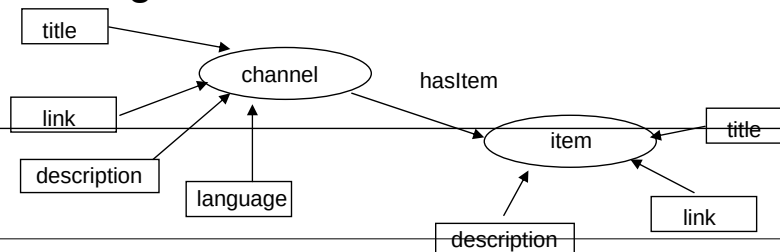
# RSS (RDF Site Summary)

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- RDF Site Summary (RSS) is a lightweight multipurpose extensible metadata description and syndication format.
- RSS is an XML application, conforms to the W3C's RDF Specification and is extensible via XML-namespace and/or RDF based modularization.
- The underlying ontology is extremely simple, mainly consisting of:

**RSS**



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# UMLS (Unified Medical Language System) (I)

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- provided by the National Library of Medicine (NLM), a database of medical terminology
- terms from several medical databases (MEDLINE, SNOMED International, Read Codes, etc.) are unified so that different terms are identified as the same medical concept
- Access at <http://umlsks.nlm.nih.gov/>
- Documentation available at <http://www.nlm.nih.gov/research/umls/UMLSDOC.HTML>

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## UMLS Knowledge Sources:

- Metathesaurus provides the concordance of medical concepts:
  - 730.000 concepts
  - 1.5 million concept names in different source vocabularies
- SPECIALIST Lexicon provides word synonyms, derivations, lexical variants, and grammatical forms of words used in MetaThesaurus terms
  - 130,000 entries
- Semantic Network codifies the relationships (e.g. causality, "is a", etc.) among medical terms.
  - 134 semantic types, 54 relationships.

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## AIFB Web Page

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- The AIFB Internet and Intranet is based on an institute ontology



- The ontology is describing people, events, education, etc.
- Important aspect of the ontology is a topic hierarchy modeled on the instance level
- <http://www.aifb.uni-karlsruhe.de/WBS>

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- The Dublin Core Metadata Initiative is an open forum engaged in the development of interoperable online metadata standards that support a broad range of purposes and business models
- Ontology includes elements like
  - TITLE
  - CREATOR
  - SUBJECT
  - DESCRIPTION
  - PUBLISHER
  - CONTRIBUTORS
  - DATE

Simple set of elements that people can agree on!

see <http://dublincore.org/>

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## Ontologies in a wider sense (I)

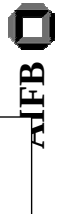
- AGROVOC: Agricultural Vocabulary

The screenshot shows the AGROVOC web application interface. At the top, there is a search bar with the text "Enter the word you are looking for:" and a search button. Below the search bar, there are radio buttons for selecting the language: English (selected), Portuguese, French, and Spanish. The search results are displayed in a table with columns for "TermStatus" and "Descriptor". The results include "FLOODED RICE", "RICE", "UPLAND RICE", "african rice", "hungry rice", "japanese rice bean", "jungle rice", "kaon rice", and "rice beans". The "FLOODED RICE" entry is highlighted, and its details are shown in a separate box on the right, including its status as a "Descriptor", its language as "English", and its scope as "FLOODED RICE".

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# Ontologies in a wider sense (II)

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## ■ AAT: Art & Architecture Thesaurus

### AAT Term Information

Descriptor: **Renaissance**

Term ID: 21140

Hierarchy: **Styles and Periods** [FL]

Scope note - Refers to the intellectual movement, style, and culture that originated in Italy in the late 14th century, spread throughout Europe, and culminated in the 16th century. Style is characterized by a deliberate reference to the art, architecture, literature, and ideals of Classical Rome and Greece.

### Styles and Periods Hierarchy

- ☐  ...<European styles and periods>
- ☐  .....<Renaissance-Baroque styles and periods>
- ☐ .....  Renaissance
- ☐ ..... Early Renaissance
- ☐ ..... High Renaissance
- ☐ ..... Late Renaissance

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# Ontologies in a wider sense (III)

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## ■ UNSPSC: Product Classification

| Seg  | Title                                                                                 |
|------|---------------------------------------------------------------------------------------|
| [10] | -[23.00.00.00.00] Industrial Manufacturing and Processing Machinery and Accessories   |
| [11] | -family-[23.10.00.00.00] Raw materials processing machinery                           |
| [12] | -class-[23.10.15.00.00] Machinery for working wood and stone and ceramic and the like |
| [13] | -commodity-[23.10.15.01.00] Coping machines                                           |
| [14] | -commodity-[23.10.15.02.00] Drilling machines                                         |
| [15] | -commodity-[23.10.15.03.00] Broaching machines                                        |
| [20] | -commodity-[23.10.15.04.00] Bending machines                                          |
| [21] | -commodity-[23.10.15.05.00] Boring machines                                           |
| [22] | -commodity-[23.10.15.06.00] Grinding machines                                         |

- A comprehensive list is provided at
  - <http://www.lub.lu.se/metadata/subject-help.html>
- Thesauri act as a good starting point for developing an ontology!

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## Ontologies in a wider sense (IV)

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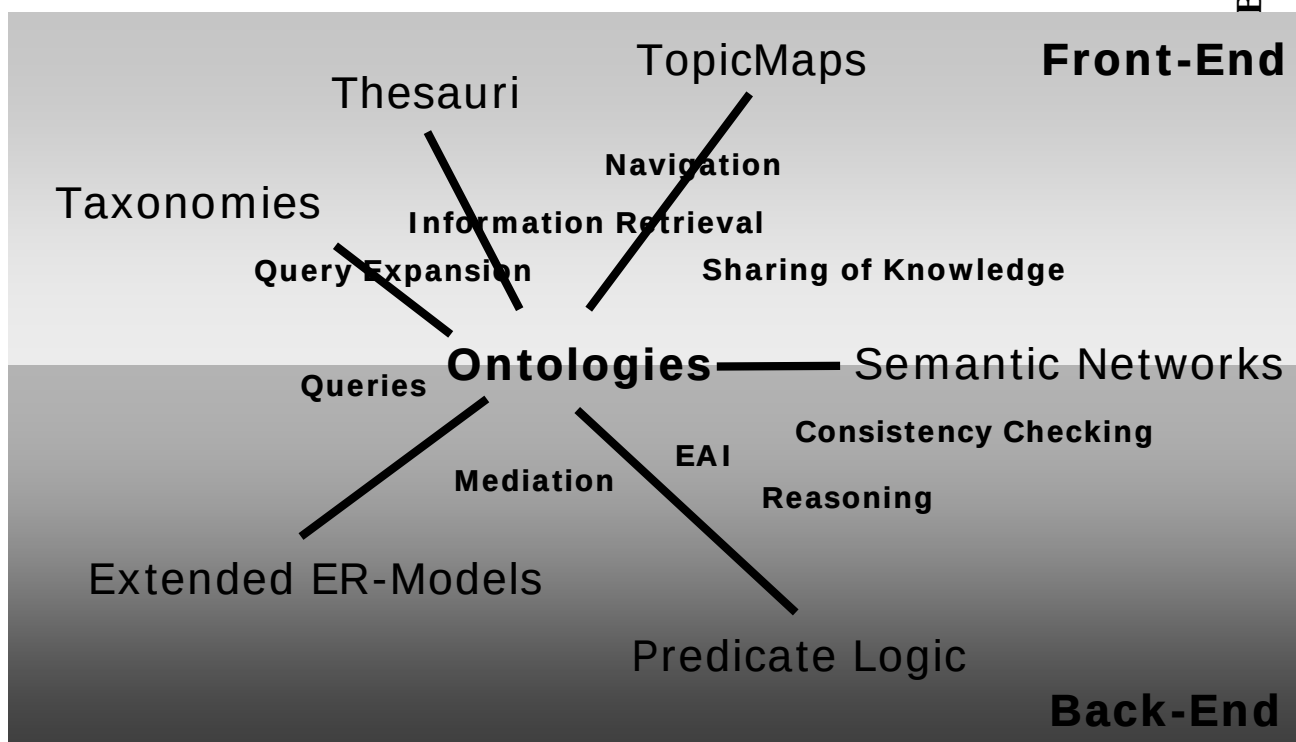


- There are many standardization initiatives, currently mainly focusing on the XML level, using DTDs and XML-Schema as underlying representation mechanisms
- Examples are:
  - <http://www.dmtf.org> develops Ontologies for the Telecommunication Industry
  - <http://www.bpmi.org> develops a Process Ontology for Representing Business Processes
  - <http://www.papinet.org> develops global transaction standards for the paper supply chain.
  - <http://www.hr-xml.org> is dedicated to the development and promotion of standardized XML vocabularies for human resources (HR).

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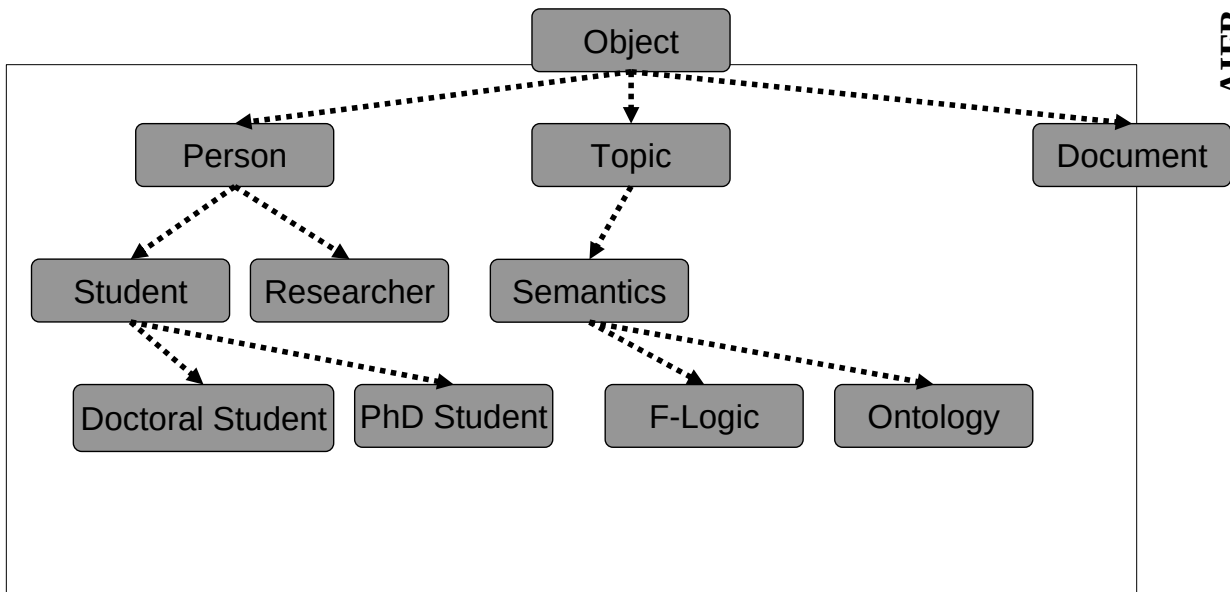
## Ontologies and their Relatives (con'd)

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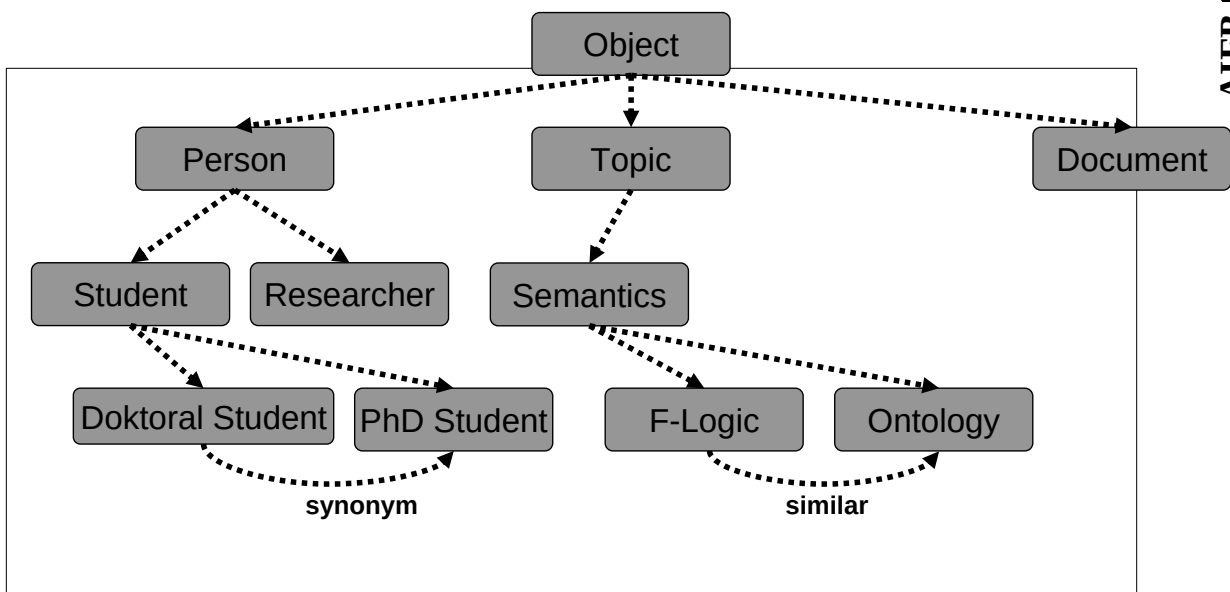
# Taxonomy



**Taxonomy := Segementation, classification and ordering of elements into a classification system according to their relationships between each other**

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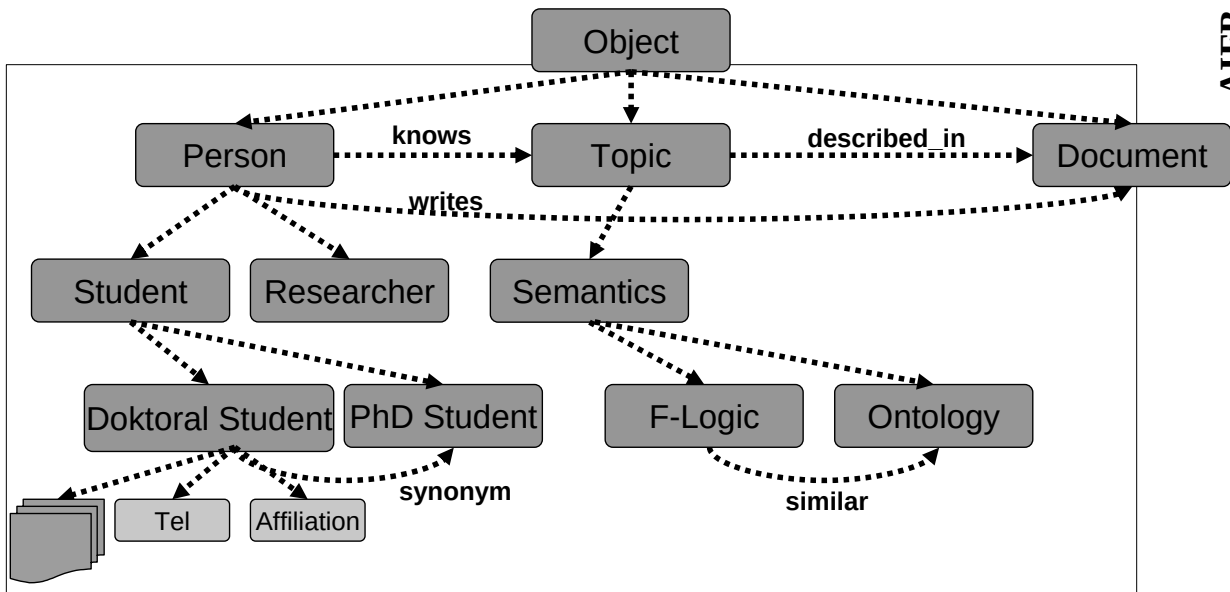
# Thesaurus



- Terminology for specific domain
- Graph with primitives, 2 fixed relationships (similar, synonym)
- originate from bibliography

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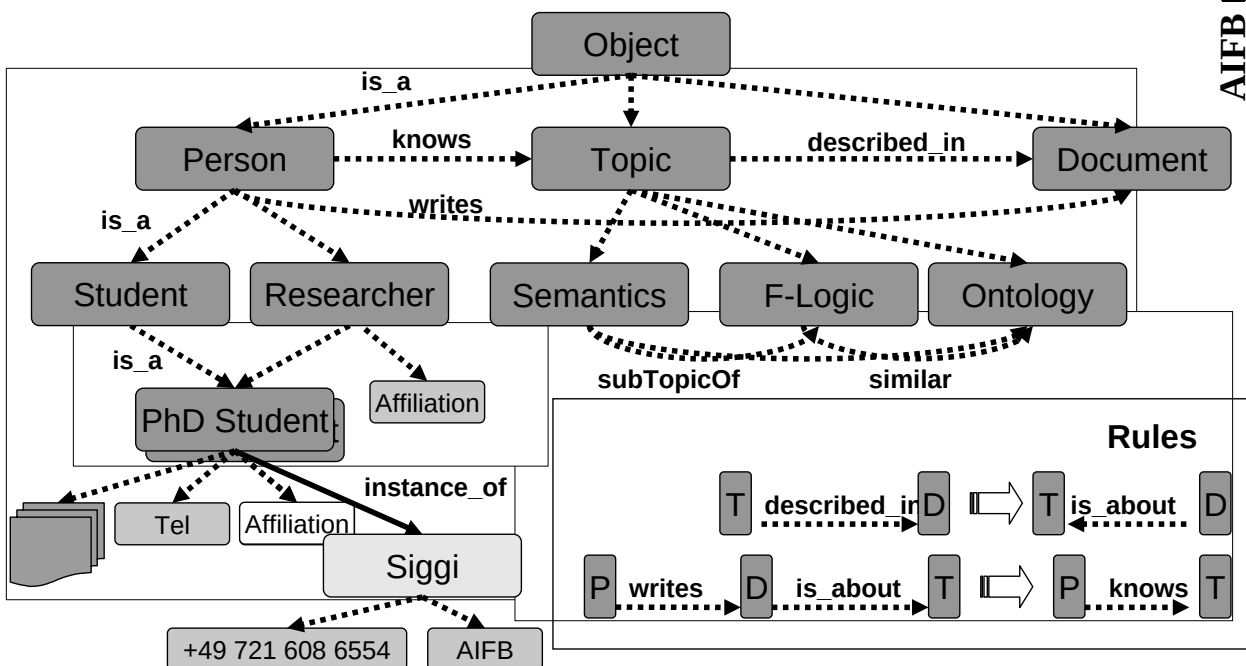
# Topic Map



- Topics (nodes), relationships and occurrences (to documents)
- ISO-Standard
- typically for navigation- and visualisation

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## Ontology (in our sense)

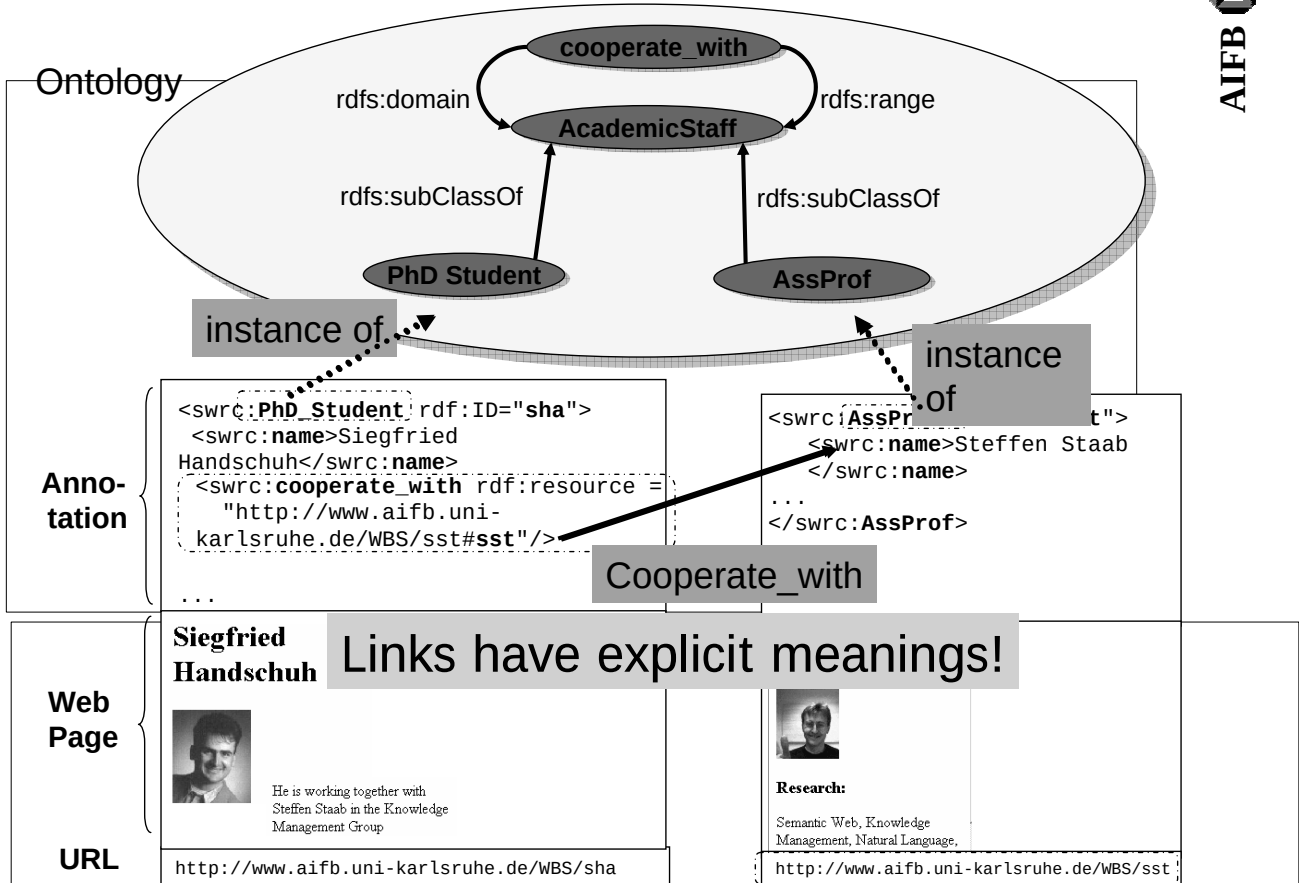


- Representation Language: Predicate Logic (F-Logic)
- Standards: RDF(S); OWL

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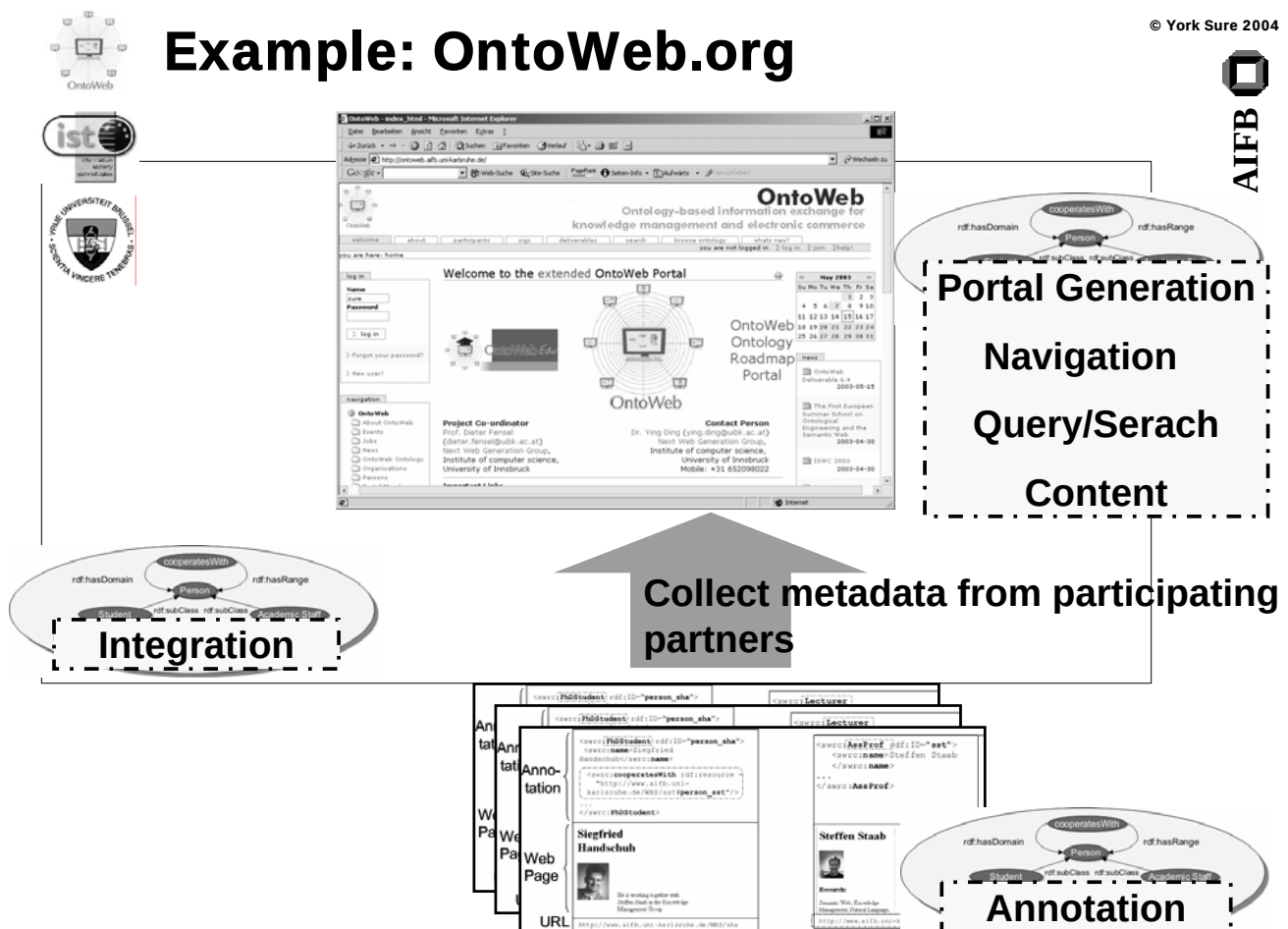
# Ontology & Annotation

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## Example: OntoWeb.org

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## Modeling Example

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## Technologies

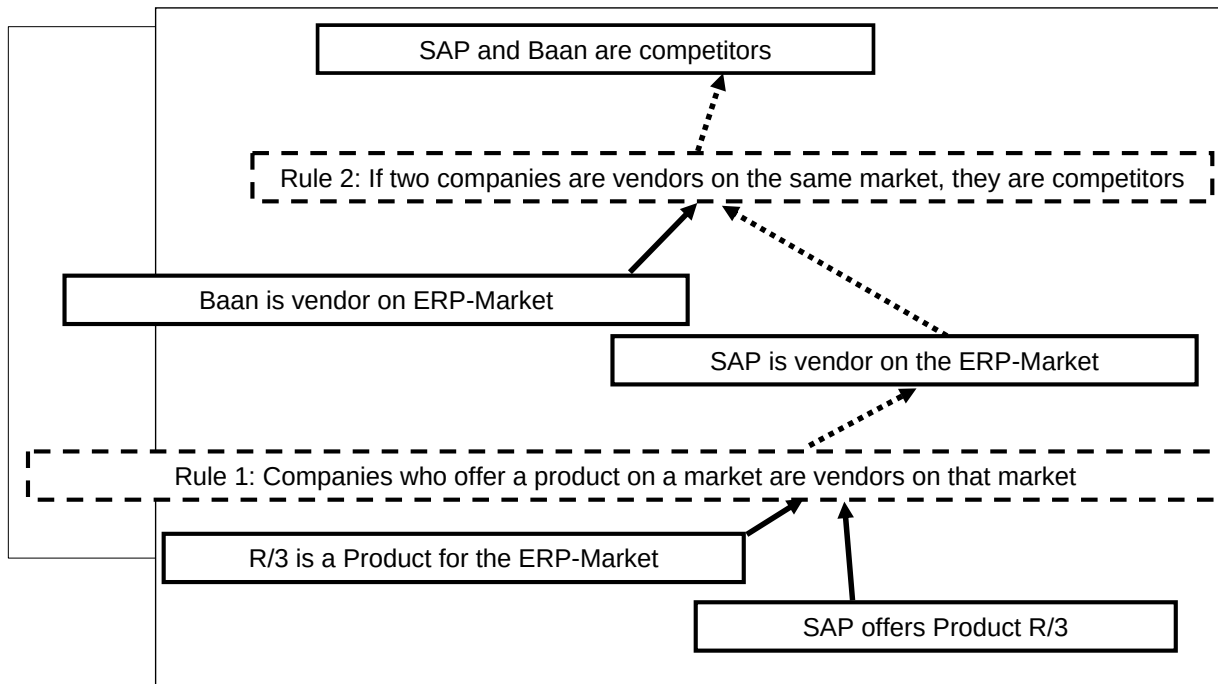
- Ontology Editors
  - OImodeler/KAON
  - OntoEdit
  - Protégé 2000
  - WebODE
  - ...
  - XML.com survey lists over 50 “ontology editors”!  
[http://www.xml.com/2002/11/06/Ontology\\_Editor\\_Survey.html](http://www.xml.com/2002/11/06/Ontology_Editor_Survey.html)
- Inference Engines
  - DL-based: FaCT, Racer, ...
  - LP-based: Ontobroker, XSB, ...
- Recent state-of-the-art overviews and further information:
  - [www.ontoweb.org](http://www.ontoweb.org) (deliverables 1.x)
  - [www.semanticweb.org](http://www.semanticweb.org)

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# Example

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## Application Example: Project Halo

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# Project Halo

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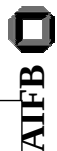


- Funded by Vulcan Inc. Seattle
- See <http://www.projecthalo.com>
- Task:
  - development of a query answering system containing the knowledge about 50 pages of chemistry book
- Evaluation:
  - sequestration of system
  - 100 novel questions (AP exam)
  - encoding of the questions
  - chemistry professors graded results
- Participants: SRI, Cyc Corp, Ontoprise

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# OntoNova and Semantic Web

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- Similar objectives
  - Exploiting **rich ontology**
  - Integration of **various sources** of knowledge
  - Giving **justifications** for deduced results
- Controlled experiment with
  - cleanly defined setting,
  - independent evaluators,
  - **freely available resources** and
  - re-producible results.
- Quantify **costs** and **adequacy** of methods

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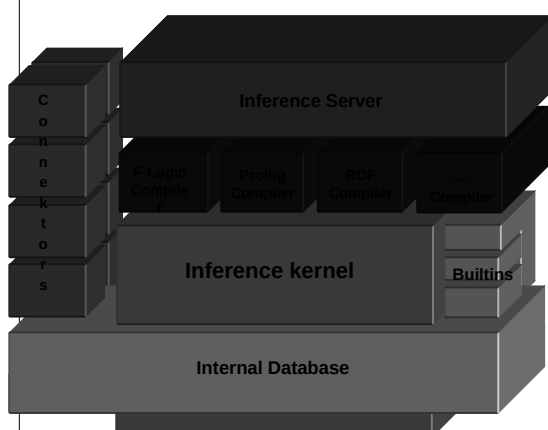
- Technology: Inference Engine **Ontobroker**
- Modelling of complex ontology (in F-Logic)
  - Rules
  - Multiple representations of objects
  - Call-out functionalities to particular problem-solving methods
  - **Stored in 1st Inference Engine to allow for query answering**
- Extension of deduction process
  - Logging into separate „trace-ontology“ (also in F-Logic)
  - Modelling of answer justifications
  - **Stored in 2nd Inference Engine to allow for meta-reasoning and answer justification**

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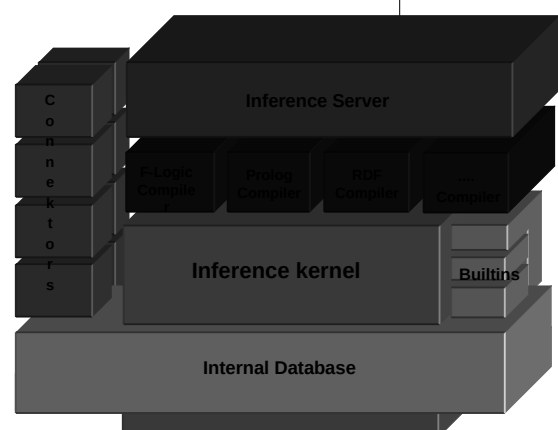
## Meta-Reasoning & Answer Justification

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FORALL R,P <- R:PrecipitationReaction[precipitate->>P]



knowledge base



explanation knowledge base

**Answer = A**

Pbl is not soluble since it is not found in table 4.2. Therefore it precipitates out of the solution

```
a20157:ins:lanlation[onRule=>>230; dependsOnins:lanlation=>>@a20154; ins:lanlationVars=>>{(Answer,"A")}.
a20154:ins:lanlation[onRule=>>225; dependsOnins:lanlation=>>@a17476;a17560; ins:lanlationVars=>>{(R,precip("PbI2","NaF"))J(P,"PbI2")}.
a17476:ins:lanlation[onRule=>>precipitation:action; dependsOnins:lanlation=>>@a17162;a17460; ins:lanlationVars=>>{(F1,"PbI2")J(F2,"NaF")J(X,"NaF")J(Mun1)J(K1,"Pb")J(C K1,2.0)J(A1,"F")J(C A1,1.0)}.
a17560:ins:lanlation[onRule=>>precipitation:action; ins:lanlationVars=>>{(F1,"PbI2")J(F2,"NaF")J(X,"NaF")J(Mun1)J(K1,"Pb")J(C K1,2.0)J(A1,"F")J(C A1,1.0)}.
a17162:ins:lanlation[onRule=>>ins:oktable; dependsOnins:lanlation=>>@a16749;a16553; ins:lanlationVars=>>{(Mun1)J(K1,"Pb")J(C K1,2.0)J(A2,"F")J(C A2,1.0)}.
a16749:ins:lanlation[onRule=>>45; ins:lanlationVars=>>{(Mun1)J(F,"Pb")J(C K,2.0)J(K,"Lead(II")}.
a16553:ins:lanlation[onRule=>>43; dependsOnins:lanlation=>>@a16180; ins:lanlationVars=>>{(Mun1)J(A,F,"F")J(C A,1.0)J(KF,"NaF")J(C K,1.0)J(F,"NaF")J(M1,SodiumIodide)J(K,Sodium)J(A,Iodide)}.
a16180:ins:lanlation[onRule=>>250; ins:lanlationVars=>>{(X,SodiumIodide)}.
a17460:ins:lanlation[onRule=>>47; ins:lanlationVars=>>{(Mun1)J(F,"NaF")J(K1,"Pb")J(C K1,2.0)J(A2,"F")J(C A2,1.0)J(C A1,1.0)J(X,callout)}.
```

# Advantages of Meta-Reasoning for Explanations

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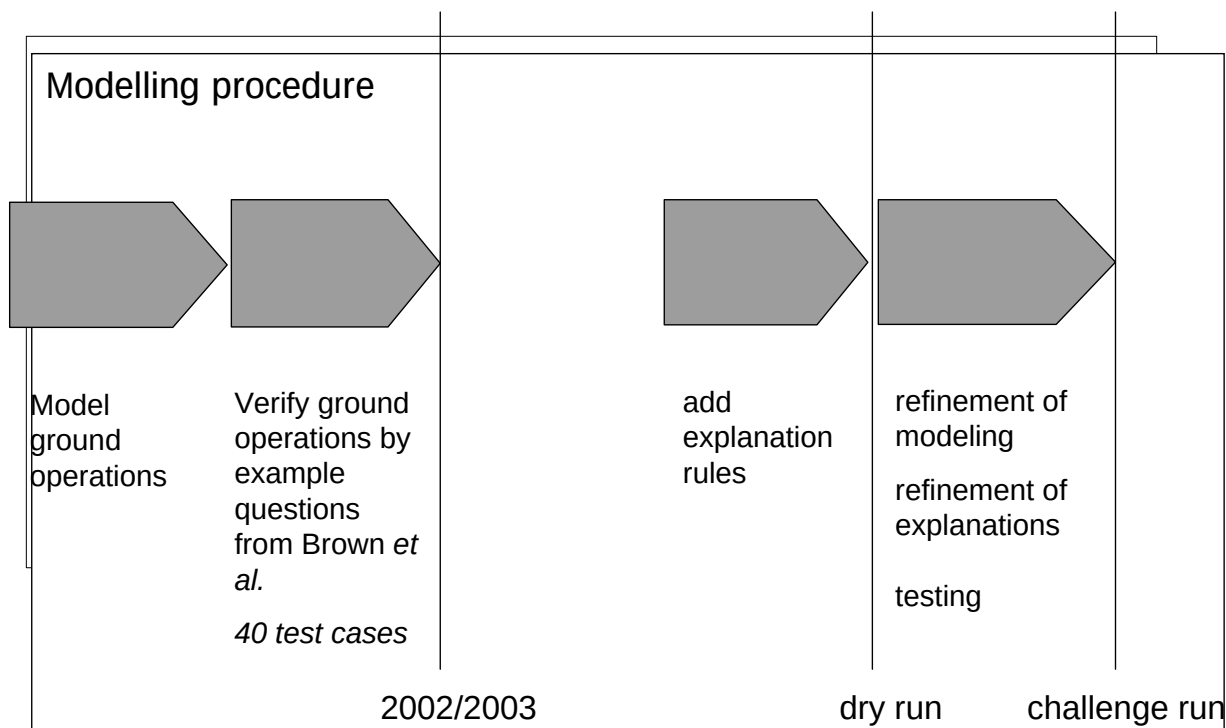


- Use the full power of inferencing to generate explanations
- Develop separate (reusable) knowledge base
  - Facilitates integration of new knowledge
  - Reduce redundancies
  - Different explanations abstractions can be created on the fly
  - Personalized explanations can be created on the fly

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## Encoding

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# Question encoding

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A 0.3M solution of acetic acid has a pH of 2.63.  
The ionization constant of this acid is

- a)  $1.8 \times 10^{-5}$
- b)  $7.0 \times 10^{-4}$
- c)  $1.1 \times 10^{-6}$
- d)  $7.8 \times 10^{-3}$
- e)  $1.9 \times 10^{-6}$

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## Question encoding – multiple choice strategy (I)

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```
m1:Mixture[hasComponents->>{"HCl","Ba(OH)2"}].
m2:Mixture[hasComponents->>{"HCl","CaCO3"}].
m3:Mixture[hasComponents->>{"HCl","CuSO4"}].
m4:Mixture[hasComponents->>{"HCl","Na3PO4"}].
m5:Mixture[hasComponents->>{"HCl","NaCl"}].
```

**Input facts**

```
answer("A") <- exists P P:GaseousReaction[fromMixture->>m1].
answer("B") <- exists P P:GaseousReaction[fromMixture->>m2].
answer("C") <- exists P P:GaseousReaction[fromMixture->>m3].
answer("D") <- exists P P:GaseousReaction[fromMixture->>m4].
answer("E") <- exists P P:GaseousReaction[fromMixture->>m5].
```

**Definition of alternatives**

**FORALL X <- answer(X).**

**Strategy I: ask for alternative**

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## Question encoding – multiple choice strategy (II)

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```
possibleanswer("A").  
possibleanswer("B").  
possibleanswer("C").  
possibleanswer("D").  
possibleanswer("E").
```

**All possible  
answers**

```
FORALL X wronganswer("A") <- checkequation(ra,X).  
FORALL X wronganswer("B") <- checkequation(rb,X).  
FORALL X wronganswer("C") <- checkequation(rc,X).  
FORALL X wronganswer("D") <- checkequation(rd,X).  
FORALL X wronganswer("E") <- checkequation(re,X).
```

**Definition of  
wrong  
alternatives**

```
FORALL Answer <- possibleanswer(Answer) and not wronganswer(Answer).
```

**Strategy II: exclude wrong alternatives**

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## Question encoding – Detailed Answer Section

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MC48

1.0 L of a buffer formed by mixing 0.25 moles of ammonia solution with 0.25 moles of ammonium nitrate has a pH of  
(For ammonia,  $K_b = 1.8 \times 10^{-5}$ )

```
FORALL X,Y  
m1:BufferSolution[hasComponents->>X;hasMole->>c(X,0.25);  
hasVolume->>c(X,1.0)] and Y[hasKb->>1.8E-5]  
    <- Y[hasName->>"Ammonia";hasFormula->>X].
```

```
FORALL X,Y  
m1:BufferSolution[hasComponents->>X;hasMole->>c(X,0.25);  
hasVolume->>c(X,1.0)]  
    <- Y[hasName->>"ammonium nitrate";hasFormula->>X].
```

```
FORALL Ph <- m1[hasPHValue->>Ph].
```

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# Basic Chemical Operations

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Classify compound as ionic (aequous.flo, utils.flo)

Balance chemical equation (balancing.flo)

Determine solubility (acidbase.flo)

Determine equilibrium expression

Rank strength of metal ions as lewis acids

.....

.....

.....

Determine acid/base conjugate

Determine strengths of acids/bases

Determine products of reaction and type of reaction

Calculate PH (ph.flo)

Determine position of equilibrium

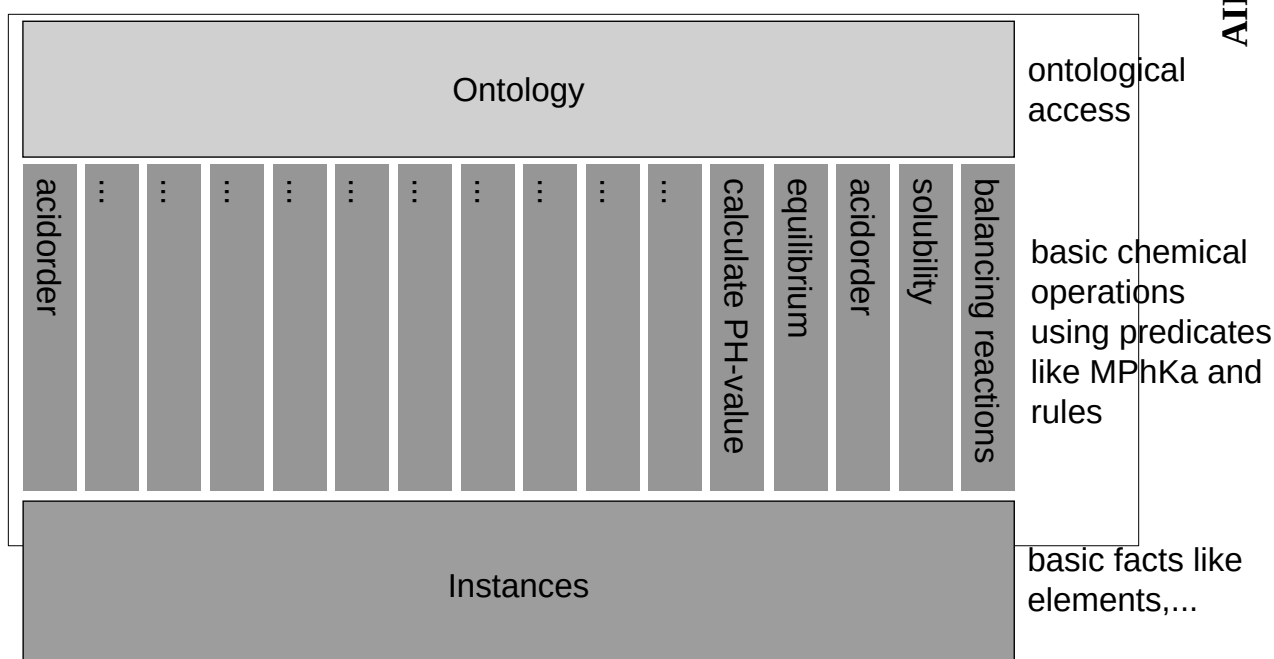
Describing substances

Naming

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# Architecture of KB

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# Example for KB Architecture

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## Strong Acid – Strong Base Titration (ch. 17.3, p. 671)

FORALL Acid,Base,AcidQuantity,AcidMole,BaseQuantity,BaseMole,  
PH,OHMole,HMole,Volume,HAAfterReaction,HConc,PH,A,B

**strongacidstrongbasetitration**(Acid,AcidQuantity,AcidMole, Base,BaseQuantity,BaseMole,PH)  
<-

A:StrongAcid[hasFormula->>Acid] and B:WeakBase[hasFormula->>Base] and  
multiply(BaseQuantity,BaseMole,OHMole) and  
multiply(AcidQuantity,AcidMole,HMole) and  
greater(HMole,OHMole) and  
add(AcidQuantity,BaseQuantity,Volume) and  
add(HAAfterReaction,OHMole,HMole) and  
multiply(HConc,Volume,HAAfterReaction) and  
pH(HConc,PH).

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# Example for KB Architecture

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## define Wrapper

FORALL M,PH,F1,F2,Q1,Q2,M1,M2

M:Mixture[hasPHvalue->>PH] <-

M:Mixture[hasComponent->>{F1,F2}; hasQuantity->>c(F1,Q1);  
hasQuantity->>c(F2,Q2); hasMole->> c(F1,M1); hasMole->> c(F2,M2)]

and **strongacidstrongbasetitration** (F1,Q1,M1,F2,Q2,PH).

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# Summary KB Architecture

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AIFB

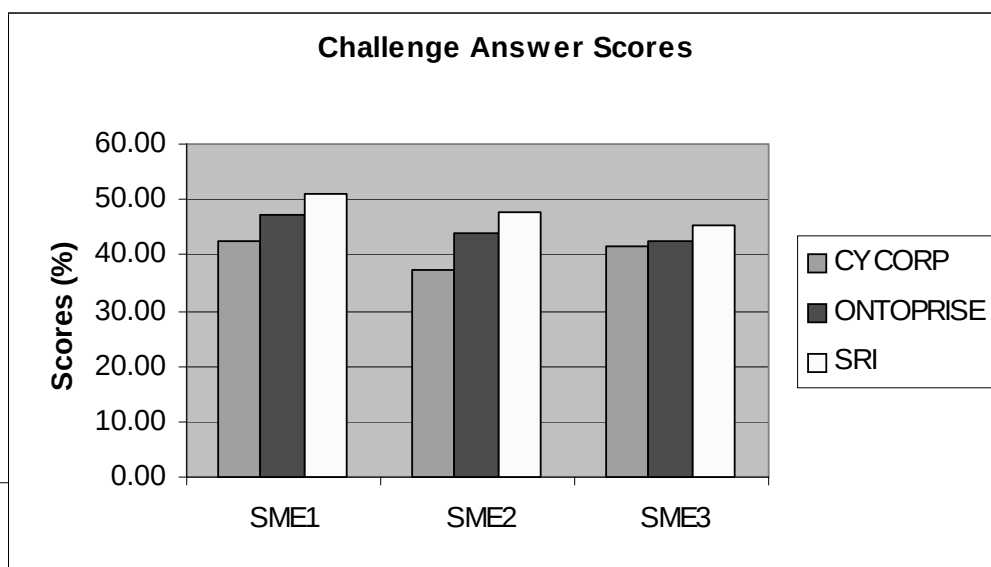
- Chemical operations:
  - independent knowledge chunks
  - collaborative development of KB
  - reduce complexity
  - reduce testing effort
- Wrapper: ontological access
  - eases access
  - closer to NL

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## Results

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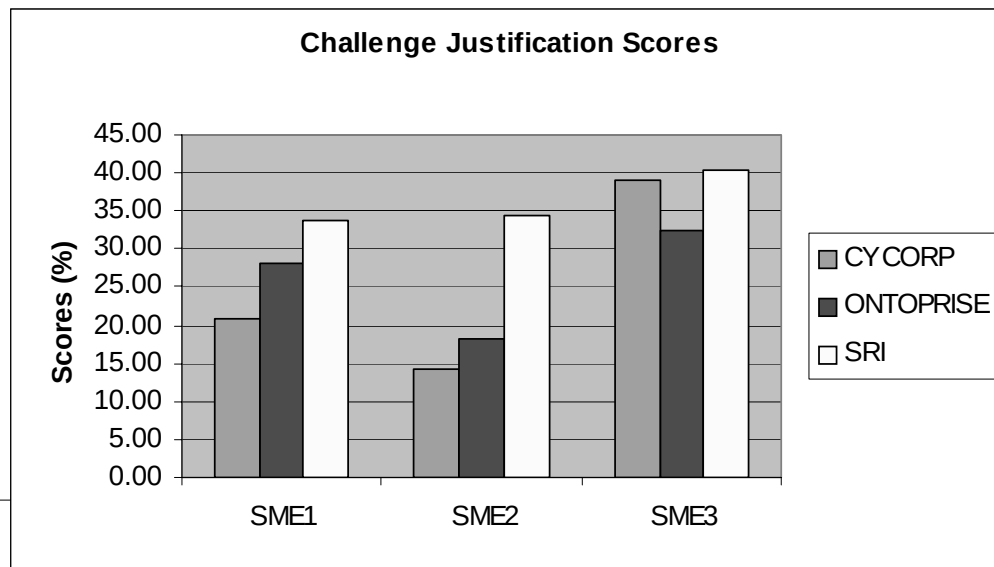
AIFB



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# Results

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# Performance

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| Team End-To-End Challenge Run Times |             |            |
|-------------------------------------|-------------|------------|
| Team                                | Sequestered | Improved   |
| Cycorp                              | > 12 hours  | > 27 hours |
| SRI                                 | 5 hours     | 38 minutes |
| Ontoprise                           | 2 hours     | 9 minutes  |

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# Summary

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- Similar results of teams
- High and scalable performance for Ontobroker
- only 2 MY used

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**The End.**

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## Let's see what you have learned today!

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- Q: What are the Semantic Web layers?
- Q: Why should you use ontologies?
- Q: ... homework 😊

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<http://www.aifb.uni-karlsruhe.de/WBS>  
<http://www.fzi.de/WIM>  
<http://www.ontoprise.de>

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# Thank You.

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