

Scalable Ontology-Based Information Systems

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What is an Ontology?





What is an Ontology?

A model of (some aspect of) the world

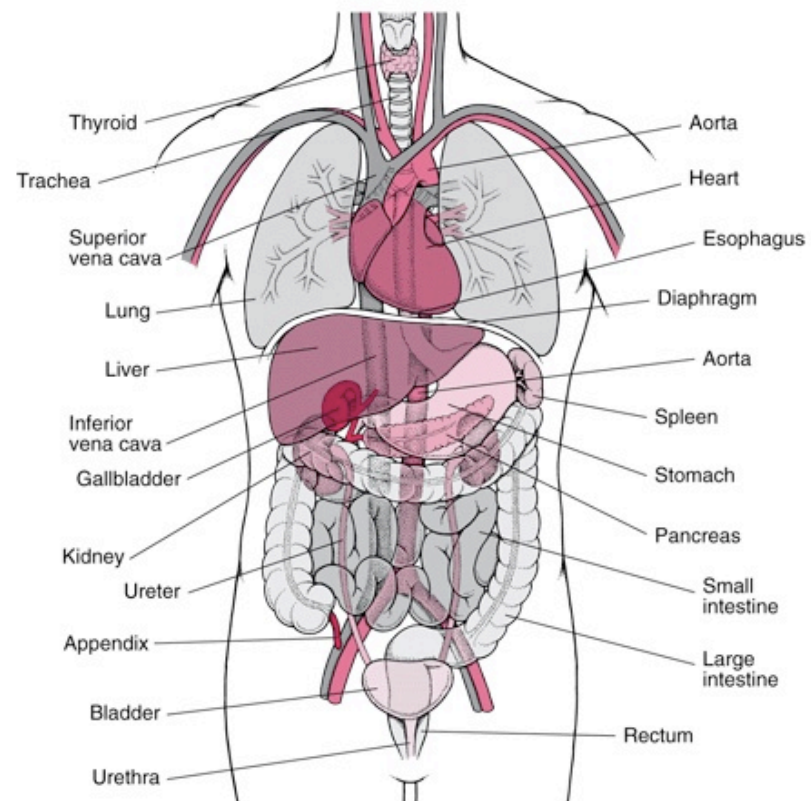




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- Introduces **vocabulary** relevant to domain, e.g.:
 - Anatomy

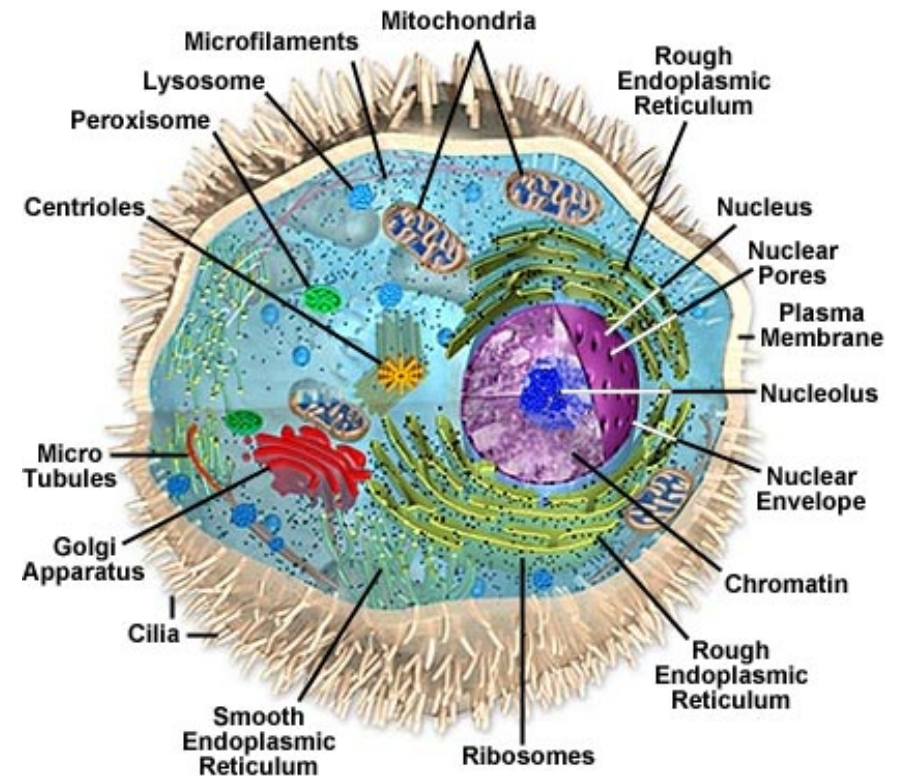




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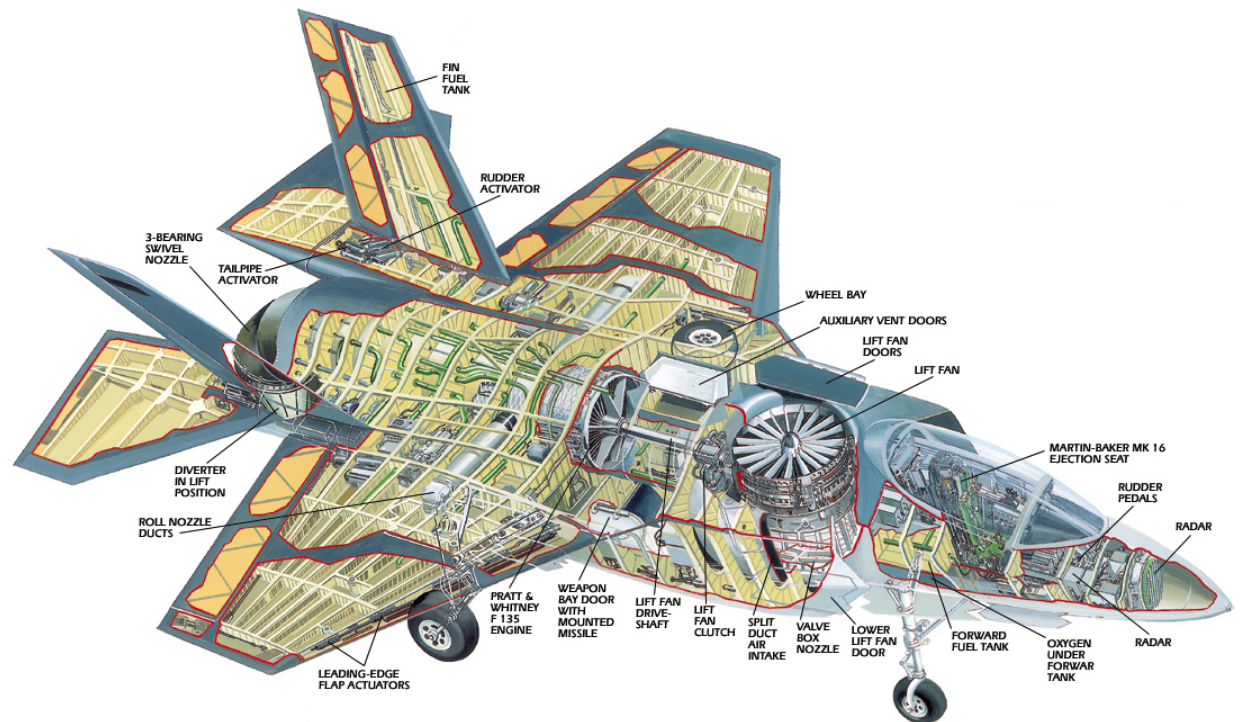




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 - Aerospace



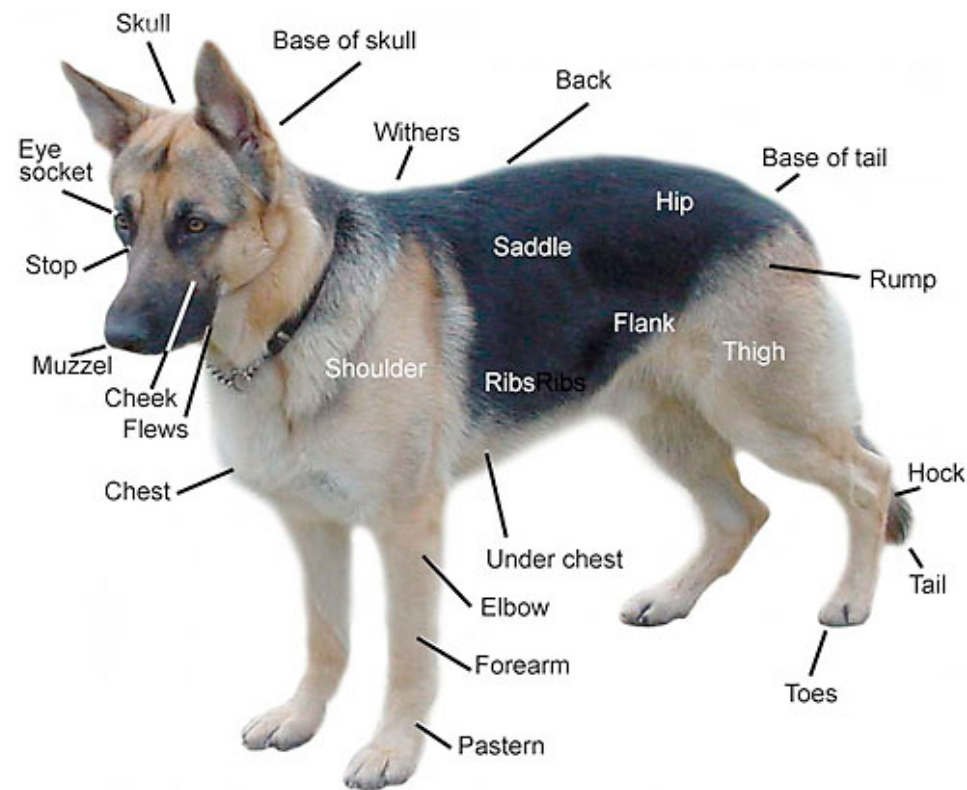


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- Dogs



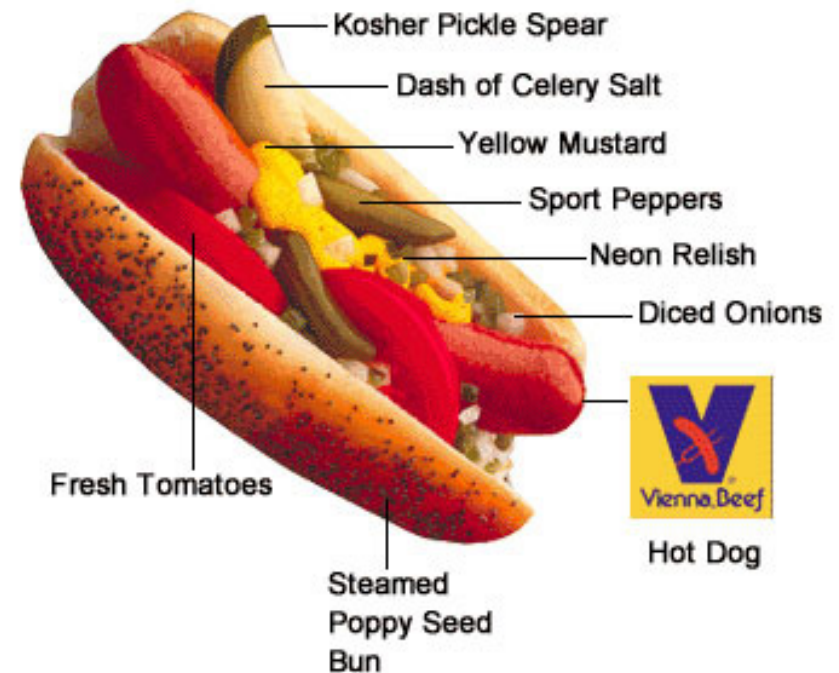


What is an Ontology?

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- Introduces **vocabulary** relevant to domain, e.g.:

- Anatomy
- Cellular biology
- Aerospace
- Dogs
- Hotdogs
- ...



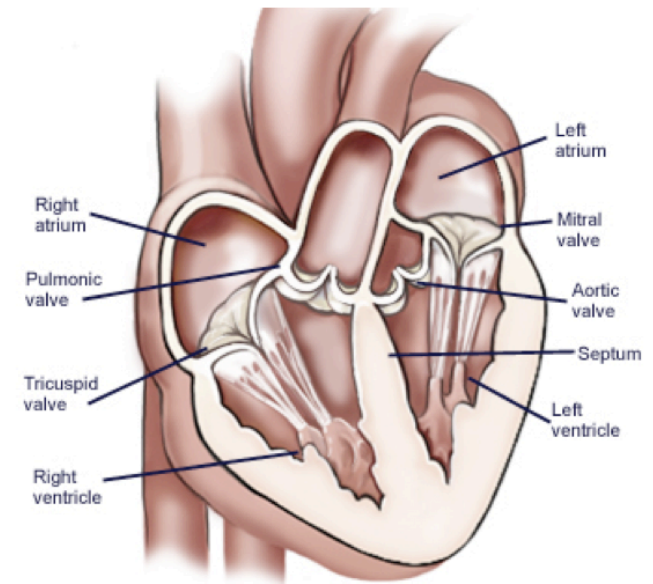


What is an Ontology?

A model of (some aspect of) the world

- Introduces **vocabulary** relevant to domain
- Specifies **meaning** (semantics) of terms

Heart **is** a muscular organ that **is part of** the circulatory system





What is an Ontology?

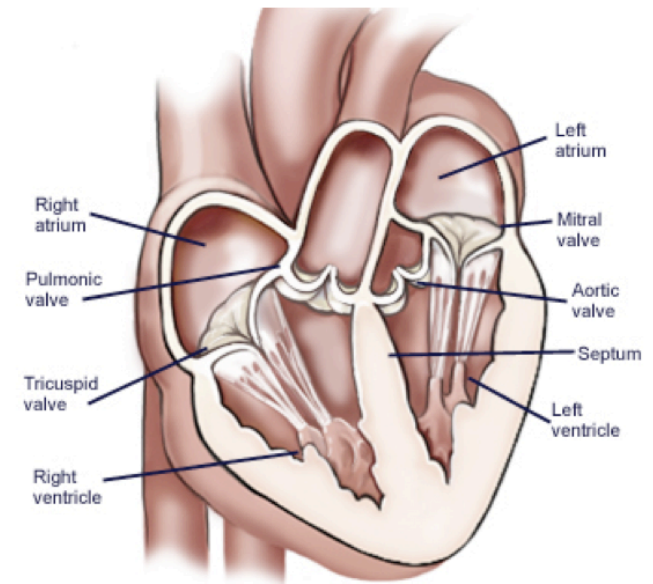
A model of (some aspect of) the world

- Introduces **vocabulary** relevant to domain
- Specifies **meaning** (semantics) of terms

Heart **is** a muscular organ that **is part of** the circulatory system

- **Formalised** using suitable logic

$$\forall x. [\text{Heart}(x) \rightarrow \text{MuscularOrgan}(x) \wedge \exists y. [\text{isPartOf}(x, y) \wedge \text{CirculatorySystem}(y)]]$$





Web Ontology Language OWL (2)

- **W3C** recommendation(s)
- Motivated by **Semantic Web** activity
 - Add meaning to web content by annotating it with terms defined in ontologies
- Supported by **tools and infrastructure**
 - APIs (e.g., OWL API, Thea, OWLink)
 - Development environments (e.g., Protégé, Swoop, TopBraid Composer)
 - Reasoners & Information Systems (e.g., Pellet, Racer, HermiT, Quonto, ...)
- Based on a **Description Logics** (*SHOIN / SROIQ*)





Description Logics (DLs)

- Fragments of **first order logic** designed for KR
- Desirable computational properties
 - **Decidable** (essential)
 - Low complexity (desirable)
- Succinct and **variable free syntax**

$$\forall x. [\text{Heart}(x) \rightarrow \text{MuscularOrgan}(x) \wedge \\ \exists y. [\text{isPartOf}(x, y) \wedge \\ \text{CirculatorySystem}(y)]]$$

$$\text{Heart} \sqsubseteq \text{MuscularOrgan} \sqcap \\ \exists \text{isPartOf}. \text{CirculatorySystem}$$



Description Logics (DLs)

DL **Knowledge Base** (KB) consists of two parts:

- Ontology (aka **TBox**) axioms define terminology (schema)

$\text{Heart} \sqsubseteq \text{MuscularOrgan} \sqcap$
 $\exists \text{isPartOf}.\text{CirculatorySystem}$

$\text{HeartDisease} \equiv \text{Disease} \sqcap$
 $\exists \text{affects}.\text{Heart}$

$\text{VascularDisease} \equiv \text{Disease} \sqcap$
 $\exists \text{affects}.\left(\exists \text{isPartOf}.\text{CirculatorySystem}\right)$

- Ground facts (aka **ABox**) use the terminology (data)

$\text{John} : \text{Patient} \sqcap$
 $\exists \text{suffersFrom}.\text{HeartDisease}$



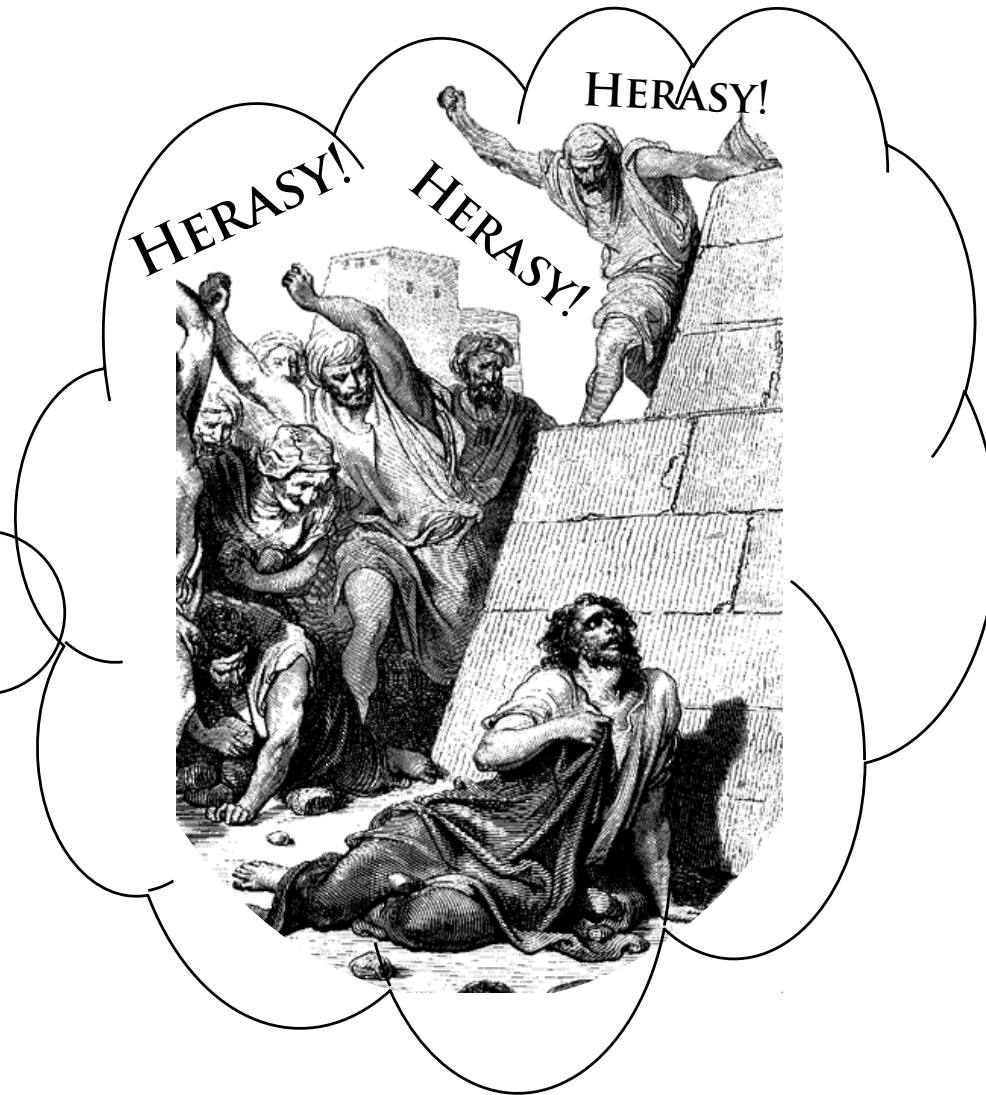


Why Care About Semantics?





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Why Care About Semantics?

Why should I care about semantics?





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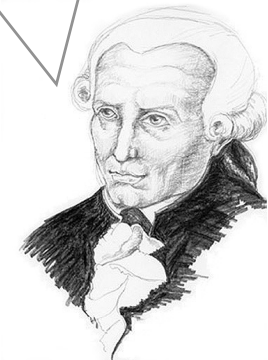




Why Care About Semantics?

Why should I care about semantics?

Well, from a philosophical POV, we need to specify the relationship between statements in the logic and the existential phenomena they describe.



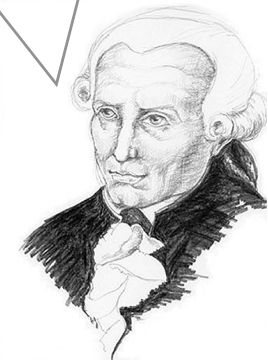


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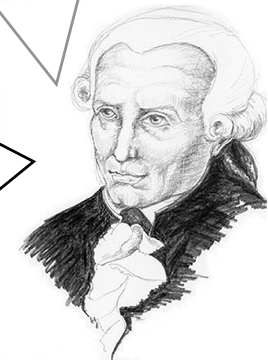
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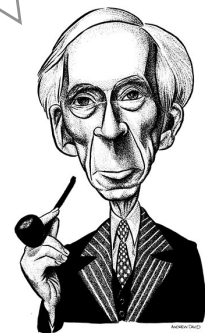
From a practical POV, in order to specify and test ontology-based information systems we need to precisely define their intended behaviour





Why Care About Semantics?

In FOL we define the semantics in terms of models (a model theory). A model is supposed to be an analogue of (part of) the world being modeled. FOL uses a very simple kind of model, in which “objects” in the world (not necessarily physical objects) are modeled as elements of a set, and relationships between objects are modeled as sets of tuples.



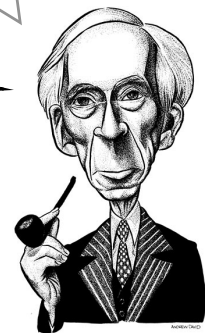


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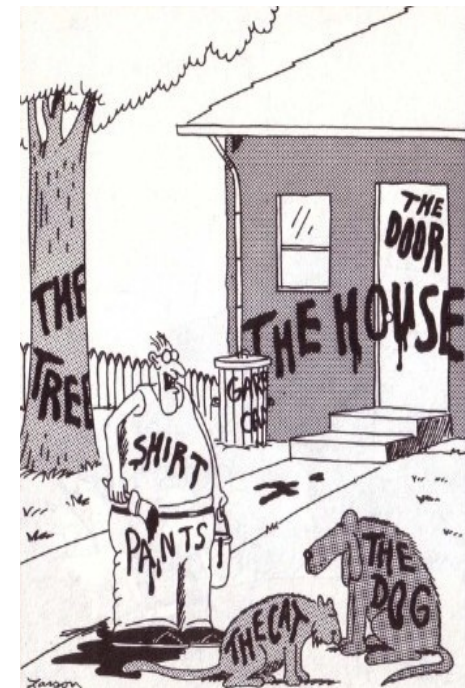
This is exactly the same kind of model as used in a database: objects in the world are modeled as values (elements) and relationships as tables (sets of tuples).





What are Ontologies Good For?

- Coherent **user-centric view** of domain
 - Help identify and resolve disagreements
- Ontology-based **Information Systems**
 - View of data that is independent of logical/physical schema
 - Queries use terms familiar to users
 - Answers reflect schema & data, e.g.:
 - “Patients suffering from Vascular Disease”
 - Query expansion/navigation/refinement
 - Incomplete and semi-structured data
 - Integration of heterogeneous sources



Now... *that* should clear up a few things around here



Healthcare

- UK NHS **£6.2 billion** “Connecting for Health” IT programme
- Key component is **Care Records Service (CRS)**
 - “Live, interactive patient record service accessible 24/7”
 - Patient **data distributed** across local centres in 5 regional clusters, and a national DB
 - Detailed **records** held by local service providers
 - Diverse **applications** support radiology, pharmacy, etc
 - **Summaries** sent to national database
 - **SNOMED-CT** ontology provides common **vocabulary** for data
 - Clinical data uses terms drawn from ontology





SNOMED-CT

- It's **BIG** – over **400,000** concepts
- Language used is **EL** profile of **OWL 2**
- **Multiple hierarchies** and **rich definitions**





CliniClue 2006: SNOMED CT(International 0801int[Release]) [Registered user: phendler@hotmail.com]

File Edit Subsets Restrict Language Layout Tools Help

Concept Id 154283005 **TB - Pulmonary tuberculosis**

DescriptionId 1784750013 clinical finding

Words - any order

Find pulmonary tuber

- P pulmonary tuberculosis
- S TB - Pulmonary tuberculosis**
- P pulmonary tuberosa sclerosis
- S PTB - Pulmonary tuberculosis
- S inactive pulmonary tuberculosis

caused by Mycobacterium tuberculosis complex

Hierarchy Subtype hierarchy

- C 205237003 pneumonitis
- C 56717001 tuberculosis
- C 84353005 pulmonary disease due to Mycobacteria
 - 154283005 **pulmonary tuberculosis**
 - C 428897002 inactive tuberculosis of lung
 - C 186175002 infiltrative lung tuberculosis
 - C 186188004 isolated tracheal or bronchial tuberculosis
 - C 77688003 isolated tracheal tuberculosis
 - C 80602006 nodular tuberculosis of lung
 - C 186192006 respiratory tuberculosis, bacteriologically and histologically confirmed
 - C 186202007 respiratory tuberculosis, not confirmed bacteriologically
 - C 186177005 tuberculosis of lung with cavitation
 - C 81554001 tuberculosis of lung with involvement of bronchus
 - C 186204008 tuberculosis of lung, bacteriologically and histologically confirmed
 - C 186194007 tuberculosis of lung, confirmed by culture only
 - C 186193001 tuberculosis of lung, confirmed by sputum microscopy
 - C 186195008 tuberculosis of lung, confirmed histologically
 - C 23022004 tuberculous bronchiectasis
 - C 90117007 tuberculous fibrosis of lung

found in lung structure

pulmonary tuberculosis - Definition
Concept Status: **Current**

- Descriptions
 - F pulmonary tuberculosis (disorder)
 - P pulmonary tuberculosis
 - S PTB - Pulmonary tuberculosis
 - S TB - Pulmonary tuberculosis
- Definition: Fully defined by ...
- is a
 - D pneumonitis
 - D inflammatory disorder of lower respiratory tract
 - D disorder of lung
 - D inflammation of specific body organs
 - D tuberculosis
 - D pulmonary disease due to Mycobacteria
 - D infectious disease of lung
 - D bacterial lower respiratory infection
 - D mycobacteriosis
- causative agent
 - D Mycobacterium tuberculosis complex
- Group
 - associated morphology
 - finding site
 - D lung structure
- Qualifiers
 - severity
 - p severities
 - episodicity
 - p episodicities
 - clinical course
 - p courses
- Codes
 - Original SnomedId : R-F46B3

Pulmonary Tuberculosis

kind of pneumonitis

kind of tuberculosis

kind of Pulmonary disease due to Mycobacteria



SNOMED-CT

- Over **400,000 concepts**
- Language used is **EL fragment of OWL 2**
- **Multiple hierarchies** and **rich definitions**
- Supports, e.g., retrieving details of **all patients having pulmonary TB**





QOMCriteria - Microsoft Internet Explorer

Query Model

Save CQML | VCG/HCM Metadata | Run | Clear

Criteria Link | Export | Help

Query Details

Query Name:
Query Desc:
INI: EDG Clinical (Diagnosis)
Load CQML:

Property Based Query

Icd-9 Code	Value	300000	300010
<input type="text"/>			
<input type="text"/>			
<input type="text"/>			
<input type="text"/>			

Add more rows +

Hierarchical Based Query

SCTID	<input type="text"/>
SCTID	<input type="text"/>
SCTID	<input type="text"/>

Add more rows +

Subsumption Based Query

Add concept with +

Is A: +

Role: +

Results

1 Total Results = 15

Exclude	CSM ID	item 2	item 1	item 11	item 40	item 2000
<input type="checkbox"/>	105302	TB LUNG, BRONCHIECTASIS	26224	12126224	011.50A	011.50
<input type="checkbox"/>	105303	TB LUNG, FIBROSIS	26225	12126225	011.40A	011.40
<input type="checkbox"/>	105825	TB LUNG, CAVITARY	26747	12126747	011.20A	011.20
<input type="checkbox"/>	124660	TB LUNG, CULTURE DIAGNOSIS	27295	12127295	011.94A	011.94
<input type="checkbox"/>	127809	MYCOBACTERIAL PNEUMONIA, NON TB	28774	12128774	500725	500725
<input type="checkbox"/>	132112	TUBERCULOSIS (TB), PULMONARY, ACTIVE.	31139	12131139	011.90D	011.90
<input type="checkbox"/>	171105	PULMONARY MYCOBACTERIAL AVIUM	37507	12137507	031.0D	031.0
<input type="checkbox"/>	184096	TB LUNG, CONFIRMED HISTOLOGICALLY	39390	12139390	011.95A	011.95
<input type="checkbox"/>	189147	TB OF LUNG, INFILTRATIVE	39861	12139861	011.00A	011.00
<input type="checkbox"/>	189149	TB PNEUMONIA	39863	12139863	011.60A	011.60





SNOMED-CT

- Over **400,000 concepts**
- Language used is **EL fragment of OWL 2**
- **Multiple hierarchies** and **rich definitions**
- Supports, e.g., retrieving details of **all patients having pulmonary TB**
 - information used e.g., to improve Quality of Care, for Reporting, in epidemiological research, in Decision Support, ...
- **Building and maintenance** is a huge task
 - supported by reasoning tools, e.g., to enrich hierarchies





What About Scalability?

- Only **useful in practice** if we can deal with large ontologies and/or large data sets
- Unfortunately, many ontology languages are highly intractable
 - Satisfiability for OWL 2 ontologies is **2NEXPTIME-complete**
- Problem addressed in practice by
 - Algorithms that work well in **typical cases**
 - Highly **optimised implementations**
 - Use of tractable fragments (aka **profiles**)





Tableau Reasoning Algorithms





Tableau Reasoning Algorithms

Standard technique based on (hyper-) **tableau**

- Reasoning tasks reducible to (un)**satisfiability**
 - E.g., $\text{KB} \models \text{HeartDisease} \sqsubseteq \text{VascularDisease}$ iff
 $\text{KB} \cup \{x:(\text{HeartDisease} \sqcap \neg \text{VascularDisease})\}$ is *not* satisfiable





Tableau Reasoning Algorithms

Standard technique based on (hyper-) **tableau**

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 $\text{KB} \cup \{x:(\text{HeartDisease} \sqcap \neg \text{VascularDisease})\}$ is *not* satisfiable
- Algorithm tries to construct (an abstraction of) a model in which some individual (x) is an instance of **HeartDisease** and not an instance of **VascularDisease**
 - such a model is a counter-example for postulated subsumption





Highly Optimised Implementations

- Lazy unfolding
- Simplification and rewriting,
e.g., $A \sqcap B \sqsubseteq C \longrightarrow A \sqsubseteq C \sqcup \neg B$
- HyperTableau (reduces non-determinism)
- Fast semi-decision procedures
- Search optimisations
- Reuse of previous computations
- Heuristics

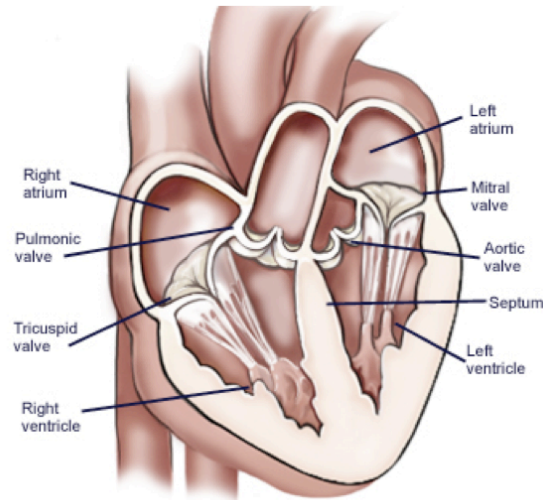
**Not computationally optimal,
but effective with many realistic ontologies**





Scalability Issues

- Problems with very **large and/or cyclical ontologies**



LeftSide $\sqsubseteq \exists$ hasComponent.AorticValve
LeftSide $\sqsubseteq \exists$ hasComponent.MitralValve
AorticValve $\sqsubseteq \exists$ hasConnection.LeftVentricle
MitralValve $\sqsubseteq \exists$ hasConnection.LeftVentricle
LeftVentricle $\sqsubseteq \exists$ isDivisionOf.LeftSide

- Ontologies may define 10s/100s of thousands of terms
 - can lead to construction of *very* large models
 - requires many (worst case n^2) tests to construct taxonomy





Scalability Issues

- Problems with **large data sets** (ABoxes)
 - Main reasoning problem is (conjunctive) query answering, e.g., retrieve all patients suffering from vascular disease:
 $Q(x) \leftarrow \text{Patient}(x) \wedge \text{suffersFrom}(x, y) \wedge \text{VascularDisease}(y)$
 - Decidability still open for OWL, although minor restrictions (on cycles in non-distinguished variables) restore decidability
 - Query answering reduced to standard decision problem, e.g., by checking for each individual x if $\text{KB} \models Q(x)$
 - Model construction starts with *all* ground facts (data)
- Typical applications may use data sets with **10s/100s of millions** of individuals (or more)





OWL 2 Profiles

- OWL recommendation now updated to **OWL 2**
- OWL 2 defines several **profiles** – fragments with desirable computational properties
 - **OWL 2 EL** targeted at very large ontologies
 - **OWL 2 QL** targeted at very large data sets





OWL 2 EL

- A (near maximal) fragment of OWL 2 such that
 - Satisfiability checking is in PTime (**PTime-Complete**)
 - Data complexity of query answering also PTime-Complete
- Based on \mathcal{EL} family of description logics
- Can exploit **saturation** based reasoning techniques
 - Computes classification in “one pass”
 - Computationally optimal
 - Can be extended to Horn fragment of OWL DL



Saturation-based Technique (basics)

- Normalise ontology axioms to standard form:

$$A \sqsubseteq B \quad A \sqcap B \sqsubseteq C \quad A \sqsubseteq \exists R.B \quad \exists R.B \sqsubseteq C$$

- Saturate using inference rules:

$$\frac{A \sqsubseteq B \quad B \sqsubseteq C}{A \sqsubseteq C}$$

$$\frac{A \sqsubseteq B \quad A \sqsubseteq C \quad B \sqcap C \sqsubseteq D}{A \sqsubseteq D}$$

$$\frac{A \sqsubseteq \exists R.B \quad B \sqsubseteq C \quad \exists R.C \sqsubseteq D}{A \sqsubseteq D}$$

- Extension to Horn fragment requires (many) more rules



Saturation-based Technique (basics)

Example:

OrganTransplant \equiv Transplant $\sqcap \exists$ site.Organ

HeartTransplant \equiv Transplant $\sqcap \exists$ site.Heart

Heart \sqsubseteq Organ





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OrganTransplant \sqsubseteq Transplant

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OrganTransplant \equiv Transplant \sqcap \exists site.Organ

HeartTransplant \equiv Transplant \sqcap \exists site.Heart

Heart \sqsubseteq Organ

OrganTransplant \sqsubseteq Transplant

OrganTransplant \sqsubseteq \exists site.Organ

\exists site.Organ \sqsubseteq SO

Transplant \sqcap SO \sqsubseteq OrganTransplant





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OrganTransplant \equiv Transplant $\sqcap \exists \text{site}.Organ$

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$$\frac{A \sqsubseteq \exists R.B \quad B \sqsubseteq C \quad \exists R.C \sqsubseteq D}{A \sqsubseteq D}$$

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$\text{OrganTransplant} \sqsubseteq \text{Transplant}$
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 $\text{HeartTransplant} \sqsubseteq \text{Transplant}$
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$\text{OrganTransplant} \sqsubseteq \text{Transplant}$
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 \exists site.Heart \sqsubseteq SH
Transplant \sqcap SH \sqsubseteq HeartTransplant
Heart \sqsubseteq Organ

HeartTransplant \sqsubseteq SO
HeartTransplant \sqsubseteq OrganTransplant





Saturation-based Technique

Performance with large bio-medical ontologies:

	GO	NCI	Galen v.0	Galen v.7	SNOMED
Concepts:	20465	27652	2748	23136	389472
FACT++	15.24	6.05	465.35	—	650.37
HERMIT	199.52	169.47	45.72	—	—
PELLET	72.02	26.47	—	—	—
CEL	1.84	5.76	—	—	1185.70
CB	1.17	3.57	0.32	9.58	49.44
Speed-Up:	1.57X	1.61X	143X	∞	13.15X



OWL 2 QL

- A (near maximal) fragment of OWL 2 such that
 - Data complexity of conjunctive query answering in **AC⁰**, i.e., query answering is *first order reducible*
- Based on **DL-Lite** family of description logics
- Can exploit **query rewriting** based reasoning technique
 - Computationally optimal
 - Data storage and query evaluation can be delegated to standard RDBMS
 - Can be extended to more expressive languages (beyond AC⁰) by delegating query answering to a Datalog engine



Query Rewriting Technique (basics)

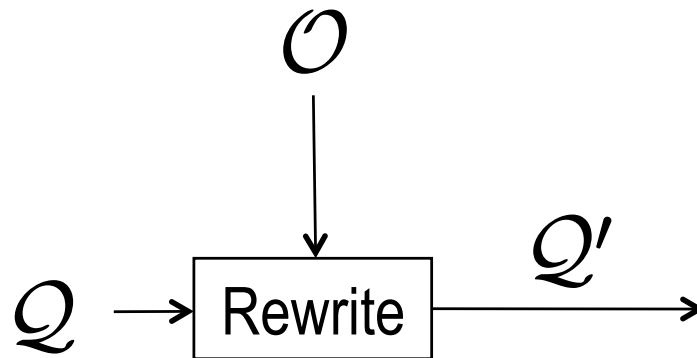
- Given ontology \mathcal{O} and query Q , use \mathcal{O} to rewrite Q as Q' such that, for any set of ground facts \mathcal{A} :
 - $\text{ans}(Q, \mathcal{O}, \mathcal{A}) = \text{ans}(Q', \emptyset, \mathcal{A})$





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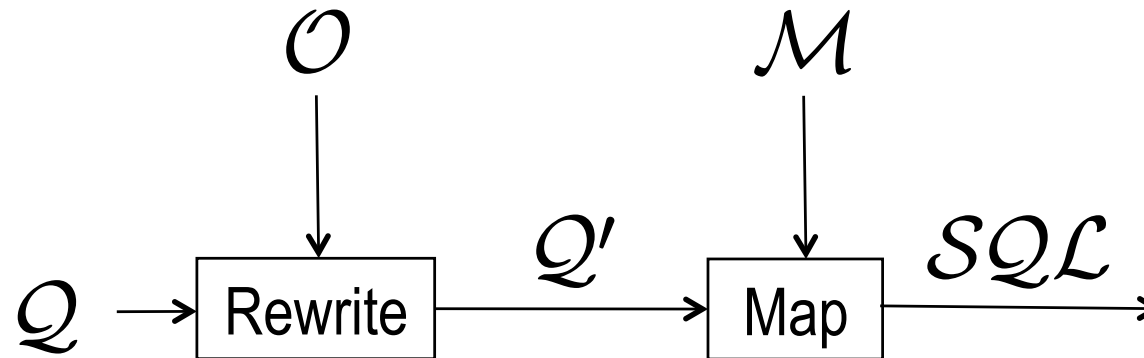
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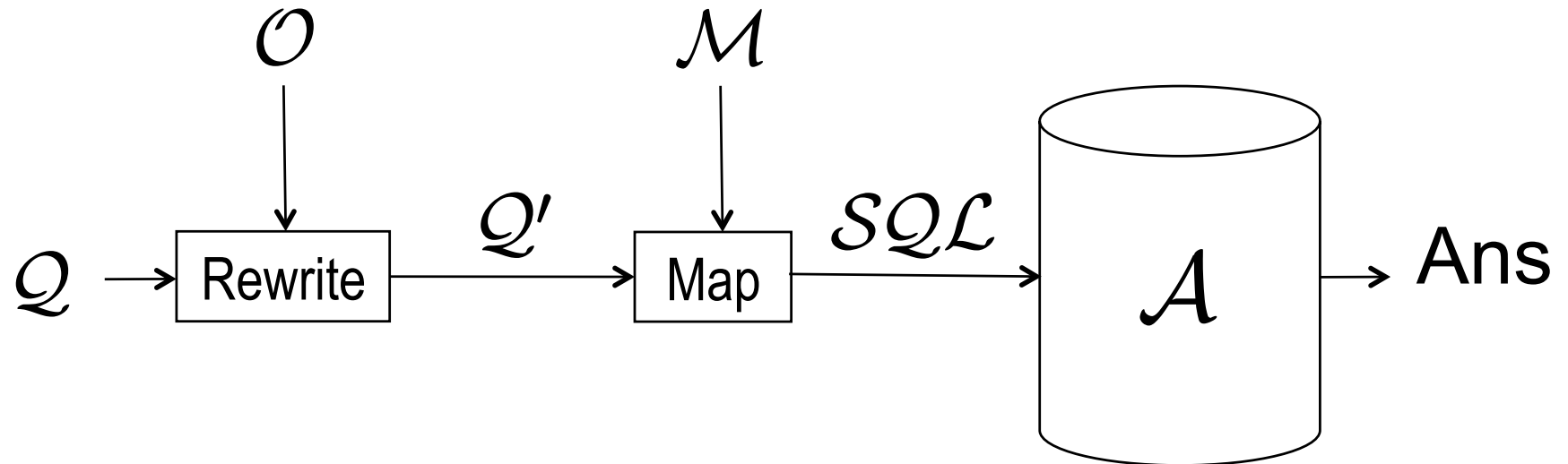
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 - $\text{ans}(Q, \mathcal{O}, \mathcal{A}) = \text{ans}(Q', \emptyset, \mathcal{A})$
- Resolution based query rewriting
 - **Clausify** ontology axioms
 - **Saturate** (clausified) ontology and query using resolution
 - **Prune** redundant query clauses



Query Rewriting Technique (basics)

- Example:

Doctor \sqsubseteq \exists treats.Patient

Consultant \sqsubseteq Doctor

$$Q(x) \leftarrow \text{treats}(x, y) \wedge \text{Patient}(y)$$





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- For DL-Lite, result is a union of conjunctive queries



Query Rewriting Technique (basics)

- Data can be stored/left in **RDBMS**
- Relationship between ontology and DB defined by **mappings**, e.g.:

Doctor \mapsto SELECT Name FROM Doctor

Patient \mapsto SELECT Name FROM Patient

treats \mapsto SELECT DName, PName FROM Treats

- UCQ translated into **SQL query**:

```
SELECT Name FROM Doctor UNION
```

```
SELECT DName FROM Treats, Patient WHERE PName=Name
```



Some Research Challenges

- Extend saturation-based techniques to non-Horn fragments
 - SNOMED users want negation and/or disjunction
 - Non infectious Pneumonia
 - Infectious or Malignant disorder of lung
 - Burn injury of face neck or scalp
- Extend reasoning support
 - Modularity
 - Explanation
 - ...





Some (more) Research Challenges

- Open questions w.r.t. query rewriting
 - FO rewritability (AC^0) only for very weak ontology languages
 - Even for AC^0 languages, queries can get very large (order $(|\mathcal{O}| \cdot |\mathcal{Q}|)^{|\mathcal{Q}|}$), and existing RDBMSs may behave poorly
 - Larger fragments require (at least) Datalog engines and/or extension to technique (e.g., partial materialisation)
- Integrating DL/DB research
 - Ontologies -v- dependencies
 - Open world -v- closed world





Thanks To

- Boris Motik
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- Rob Shearer





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