Semantic Web Technologies

Lecture 4: Bottom-up ontology development

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Outline

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Bottom-up

- From *some* seemingly suitable legacy representation to an OWL ontology
  - Database reverse engineering
  - Conceptual model (ER, UML)
  - Frame-based system
  - OBO format
  - Thesauri
  - Formalizing biological models
  - Excel sheets
  - Text mining, machine learning, clustering
  - etc...

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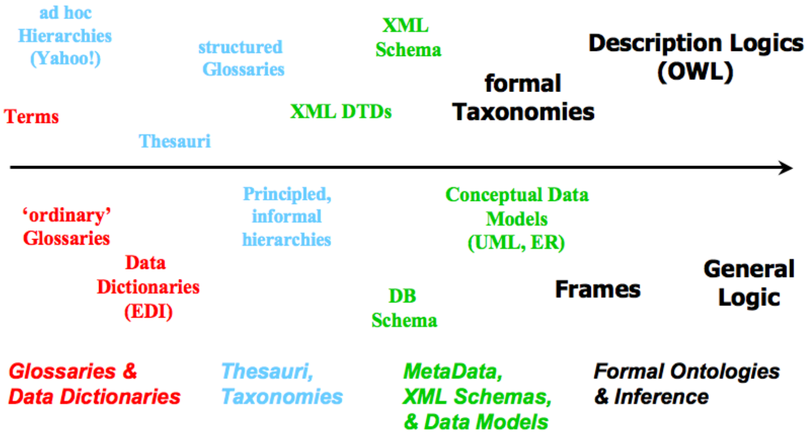
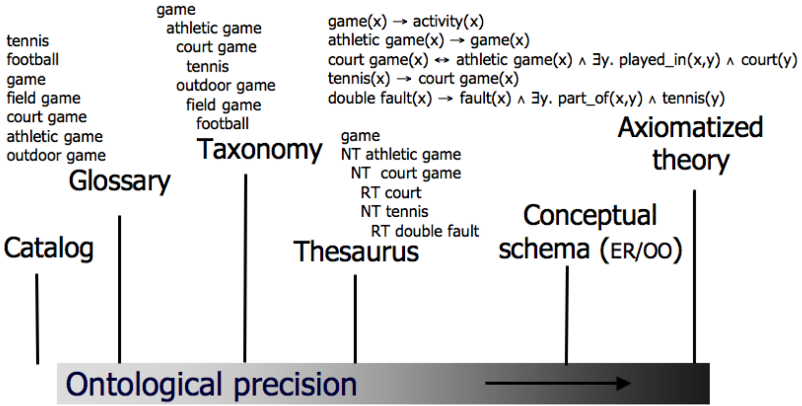
A few languages



Levels of ontological precision



precision: the ability to catch all and only the intended meaning (for a logical theory, to be satisfied by intended models)

(from Gangemi, 2004)

Examples: OBO and Protégé-frames

- OBO in OWL 2 DL
  - OBO is a Directed Acyclic Graph (with is_a, part_of, etc. relationships)
  - with some extras (a.o., date, saved by, remark)
  - and 'work-arounds' (not-necessary and inverse-necessary) and non-mappable things (antisymmetry)
  - There are several OBO-in-OWL mappings, some more comprehensive than others

Examples: OBO and Protégé-frames

- Frames (as in Protégé) into OWL-DL (see Zhang & Bodenreider, 2004), and its problems doing that to the FMA
  - Not a formal transformation
  - Slot values generally correspond to necessary conditions—so they took a first guess to define an anatomical entity as the sum of its parts
  - Global axioms dropped (with an eye on the reasoner)
  - After the conversion of the 39,337 classes and 187 slots from FMA in Protégé (ignoring laterality distinctions), FMAinOWL contains 39,337 classes, 187 properties and 85 individuals
  - Additional optimizations: optimizing domains and subClassOf axioms
  - But still caused Racer to fail to reason over the whole file; restricting properties further obtained results

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General considerations

- Let us for a moment ignore the issues of data duplication, violations of integrity constraints, hacks, outdated imports from other databases to fill a boutique database, outdated conceptual data models (if there was one), and what have you
- Some data in the DB—mathematically instances—actually assumed to be concepts/universals/classes
- each tuple is assumed to denote an instance and, by virtue of key definitions, to be unique in that table, but such a tuple has *values* in each cell of the participating columns; however, OWL ABox expects *objects* (impedance mismatch)
- instances-but-actually-concepts-that-should-become-OWL-classes and real-instances-that-should-become-OWL-instances

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- Reuse/reverse engineer the physical DB schema
- Reuse conceptual data model (in ER, EER, UML, ORM, ...)
- But,
  - Assumes there was a fully normalised conceptual data model,
  - Denormalization steps to flatten the database structure, which, if simply reverse engineered, ends up in the ontology as a class with umpteen attributes
  - Minimal (if at all) automated reasoning with it
- Redo the normalization steps to try to get some structure back into the conceptual view of the data?
- Add a section of another ontology to brighten up the 'ontology' into an ontology?
- Establish some mechanism to keep a 'link' between the terms on the ontology and the source in the database?

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Automatic Extraction of Ontologies

- Lina Lubyte/Sergio Tessaris's presentation, moved to the afternoon lab

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Bottom-up overview

Relational databases

- Data analysis
- Automatic Extraction of Ontologies
- Example: manual extraction

Models in biology

- General idea
- Case study

Thesauri

Manual Extraction

- Most database are not neat as assumed in the 'Automatic Extraction of Ontologies' (e.g., denormalised)
- Then what?
  - Reverse engineer the database to a conceptual data model
  - Choose an ontology language for your purpose
- Example: the HGT-DB about horizontal gene transfer (the same holds for the database behind ADOLENA)

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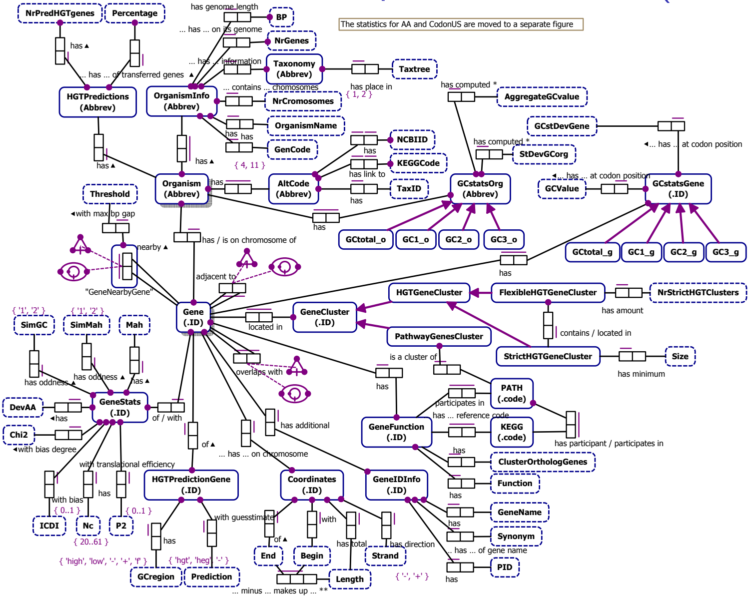
Section of the HGT conceptual data model (in ORM 2)



Manual mapping to $\mathit{DL\text{-}Lite}_{\mathcal{A}}$

- Basic statistics:
  - 38 classes
  - 34 object properties of which 17 functional
  - 55 data properties of which 47 functional
  - 102 subclass axioms
- Subsequently used for Ontology-Based Data Access (more about that in the next block)

Outline

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Overview

- Pure and applied life sciences use many diagrams
- Some diagram hand drawn, but more and more with software
- Come with their own 'icon vocabulary' and many diagrams
- Exploit such informal but structured representation of information to develop automatically (a preliminary version of) a domain ontology
- Formalize the 'icon vocabulary' in a suitable logic language, choose a foundational ontology (taxonomy, relations), categorise the formalised icons accordingly, load each diagram into the ontology, verify with the domain expert

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Example of a PathwayAssist diagram

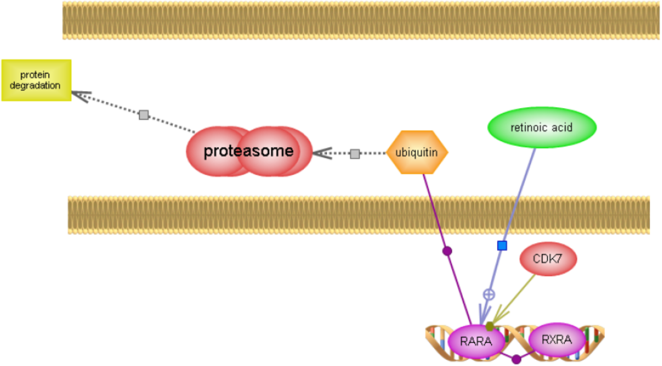
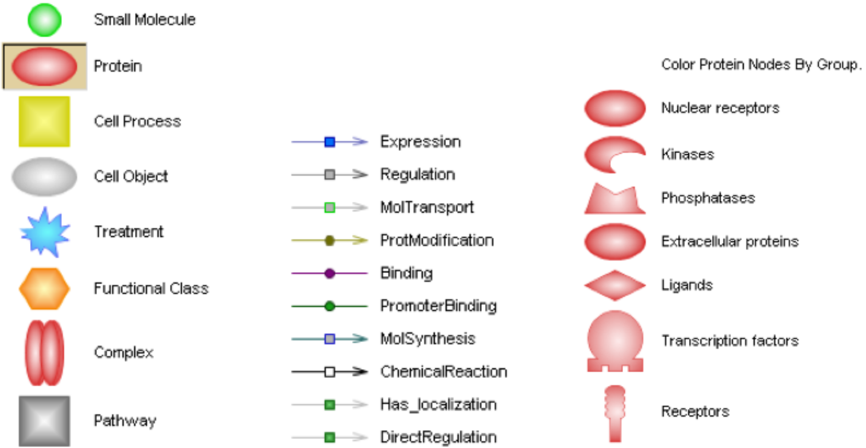


Figure: **Node** description: red: proteins, green: small molecules, orange: functional classes, yellow: cell processes, violet: nuclear receptors. **Link** description: grey dotted: regulation, violet solid: binding, yellow-green solid: protein modification, blue solid: expression.

Kindly provided by Kristina Hettne

PathwayAssist vocabulary



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Motivation

- Experiment in 2005 (Keet, 2005), but progress made in ecology (Madin et al, 2008; MTSR'09 proceedings)
- Extensive use of modelling in ecology, but not much shared (depending on sub-discipline)
- Models used with independent software tools (DB and other applications)
- 'Legacy code' (procedural), moving toward more OO, and ontologies
- Requirement for (re re-)analysis to upgrade legacy SW), develop new SW to meet increasing, complexities and rising demands.
- **use the opportunity to create a more durable, yet computationally usable, shared, agreed upon representation of the knowledge about reality**

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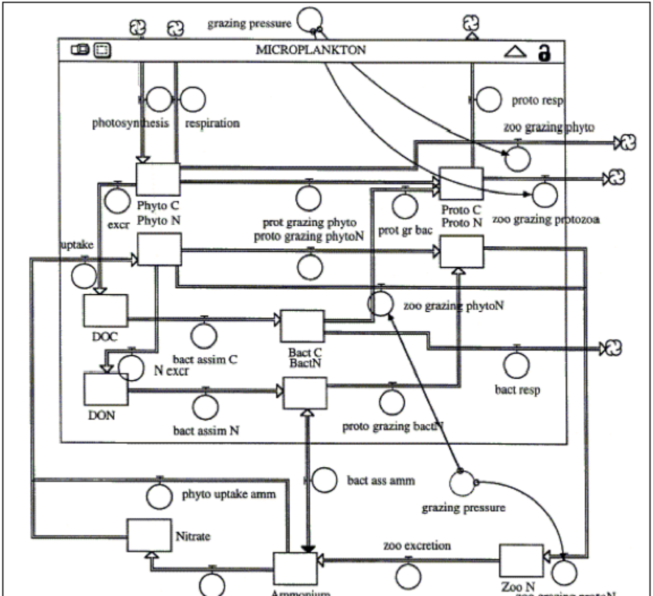
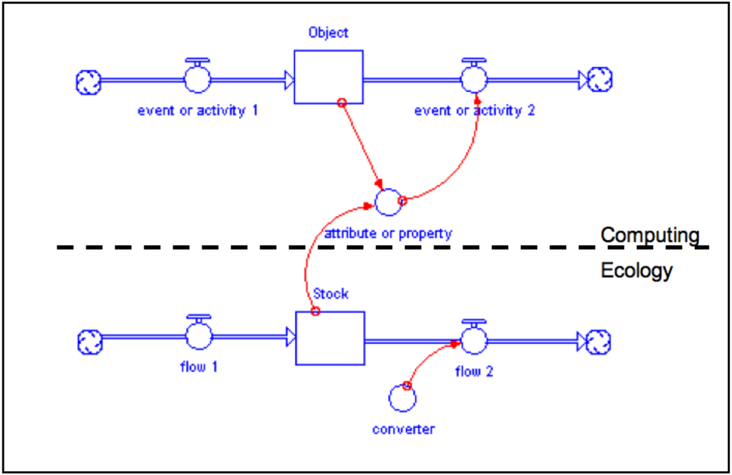
Example: the Microbial Loop [Tett&Wilson04]



Key aspects in the ecological model: Flow, Stock, Converter, Action Connector



Informal 'Translation'

- A `Stock` correspond to a noun (particular or universal)
- `Flow` to verb
- `Converter` to attribute related to Flow or Stock
- `Action Connector` relates the former
- Object is candidate for an *Endurant*
- Event_or_activity for a method or *Perdurant*
- Converter maps to *Attribute_or_property*
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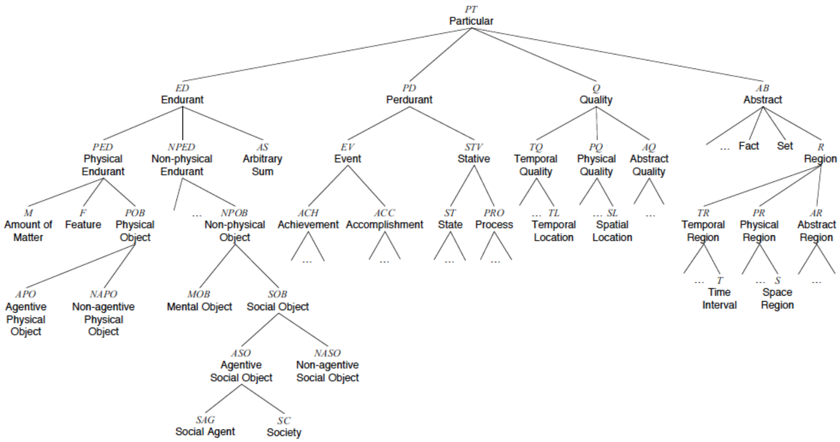
'Translation' w.r.t. DOLCE categories

- Basic mapping to DOLCE categories:
    - $\forall x((Stock(x) \leftrightarrow Entity(x)) \rightarrow ED(x))$
    - $\forall x((Flow(x) \leftrightarrow Entity(x)) \rightarrow PD(x))$
    - $\forall x((Converter(x) \leftrightarrow Entity(x)) \rightarrow (Q(x) \vee ST(x)))$
    - $\forall x(ActionConnector(x, y) \rightarrow Relationship(x, y))$

DOLCE categories



ML to Microbial Loop domain ontology

- Aim: to test translations with a real STELLA model
- ML's initial mapping to ontological categories contain 38 STELLA elements: 11 Stock/ED, 21 Flow/PD, 2 Converters/ST, 4 Action Connectors/Relationships
- The MicrobialLoop ontology has 59 classes and 10 properties
- Increase due to including DOLCE categories and implicit knowledge of ML that is explicit in MicrobialLoop

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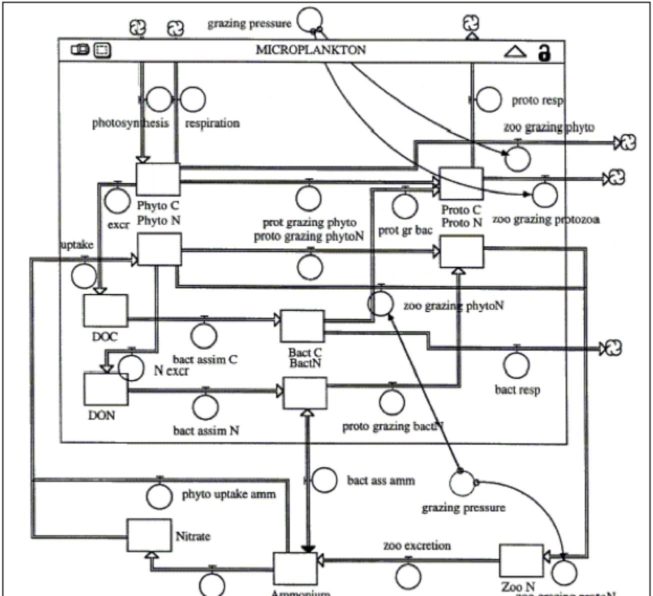
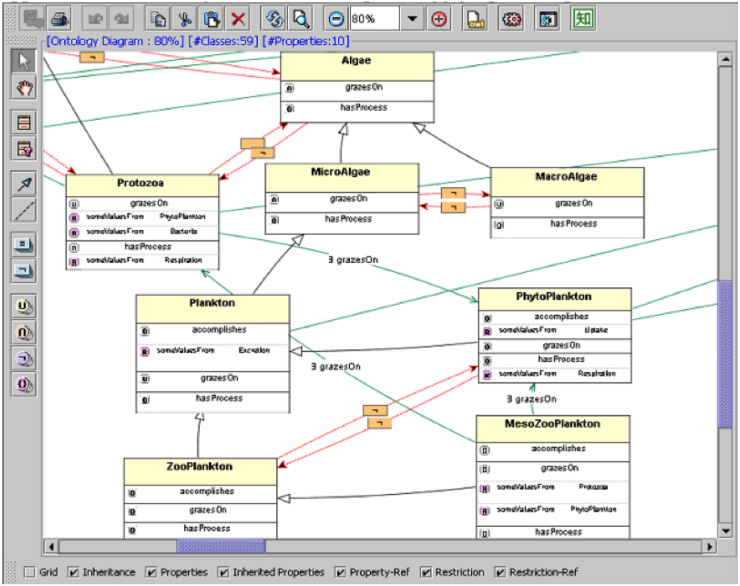


Section of more refined mapping to DOCLE categories

Phyto C	**NAPO**	**Phyto C = phytoplankton organic carbon. Phytoplankton is an APO, but 'phyto C' is *part* of the APO: only the organic carbon of the phytoplankton, not the organism as an active agent as such**
Phyto N	NAPO	Phyto N = phytoplankton nitrogen
DOC	NAPO	DOC = detrital organic carbon. Detritus is an ED with no unity, thus an amount of matter (M), but here, like with the organisms, there is focus on only a *part* of the NAPO
Nitrate	NAPO	Dissolved nitrate. Molecules are non agentive physical objects.
Flow		
Photosynthesis	PRO	To phytoplankton N
Respiration	PRO	From phytoplankton N
Prot gr bac	**PRO**	**Protozoa that are grazing on the Bacterial C**
Converter		
Grazing pressure	**ST**	**Acts on a PRO affecting the process of grazing; 'grazing pressure' is there (might reach zero), hence a ST.**
Action connector		
"1"	Yes	Acts on the mesozooplankton grazing on the protozoa, and acts on the mesozooplankton grazing on the phytoplankton: relation *hasGrazingPressure*

more mappings at http://www.meteck.org/supplDILS.html

Section in ezOWL



The serialized version of the ontology (section)

```
- <owl:Class rdf:ID="Protozoa">
    <owl:disjointWith rdf:resource="#Algae" />
    <owl:disjointWith rdf:resource="#Bacteria" />
  - <rdfs:subClassOf>
    - <owl:Restriction>
        <owl:onProperty rdf:resource="#hasProcess" />
        <owl:someValuesFrom rdf:resource="#Respiration" />
      </owl:Restriction>
    </rdfs:subClassOf>
  - <rdfs:subClassOf>
    - <owl:Restriction>
      - <owl:onProperty>
          <owl:ObjectProperty rdf:about="#grazesOn" />
        </owl:onProperty>
        <owl:someValuesFrom rdf:resource="#PhytoPlankton" />
      </owl:Restriction>
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  </owl:Class>
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Discussion

- Formalising ecological natural, functional and integrative concepts
  - aids comparison of scientific theories
  - makes the implicit explicit, and more expressive than other modelling practices, therefore useful:
    - points to ambiguous sections,
    - part of/extra tool for doing science,
    - importance ontology maintenance, comparisons
- Modular, backbone or all-encompassing ontology/ies
- With the mappings, a quicker bottom-up development of ecological ontologies

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To summarize

- Taxonomies insufficiently expressive compared to existing ecological modelling techniques
- Perspective of flow in ecological models cannot be represented adequately in a taxonomy
- More comprehensive semantics of formal ontologies
- Formalised mapping between STELLA and ontology elements facilitates bottom-up ontology development and has excellent potential for semi-automated ontology development
- STELLA as intermediate representation, widely used by ecologists and is translatable to a representation usable for ontologists

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Bottom-up overview

Relational databases
- Data analysis
- Automatic Extraction of Ontologies
- Example: manual extraction

Models in biology
- General idea
- Case study

Thesauri

Overview

- Thesauri galore in medicine, education, agriculture, ...
- Core notions of **BT** broader term, **NT** narrower term, and **RT** related term (and auxiliary ones UF/USE)
- E.g. the Educational Resources Information Center thesaurus:

```
reading ability
  BT ability
  RT reading
  RT perception
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- E.g. AGROVOC of the FAO:

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- *How to go from this to an ontology?*

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  RT perception
```

- E.g. AGROVOC of the FAO:

```
milk
  NT cow milk
  NT milk fat
```

- *How to go from this to an ontology?*

Problems

- Lexicalisation of a conceptualisation
- Low ontological precision
- BT/NT is not the same as *is_a*, RT can be any type of relation: overloaded with (ambiguous) subject domain semantics
- Those relationships are used inconsistently
- Lacks basic categories alike those in DOLCE and BFO (ED, PD, SDC, etc.)

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A rules-as-you-go approach

- A possible re-engineering procedure:
  - Define the ontology structure (top-level hierarchy/backbone)
  - Fill in values from one or more legacy Knowledge Organisation System to the extent possible (such as: which object properties?)
  - Edit manually using an ontology editor:
    - make existing information more precise
    - add new information
    - automation of discovered patterns (rules-as-you-go)

see (Soergel et al, 2004)

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    - automation of discovered patterns (rules-as-you-go); e.g.
      - observation: *cow* NT *cow milk* should become *cow <hasComponent> cow milk*
      – pattern: *animal <hasComponent> milk* (or, more generally *animal <hasComponent> body part*)
      — derive automatically: *goat* NT *goat milk* should become *goat <hasComponent> goat milk*
      other pattern examples, e.g., *plant <growsIn> soil type* and *geographical entity <spatiallyIncludedIn> geographical entity*

see (Soergel et al, 2004)

Summary

Bottom-up overview

Relational databases

- Data analysis
- Automatic Extraction of Ontologies
- Example: manual extraction

Models in biology

- General idea
- Case study

Thesauri