Towards a Semantic Web

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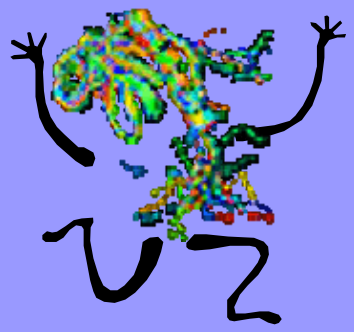
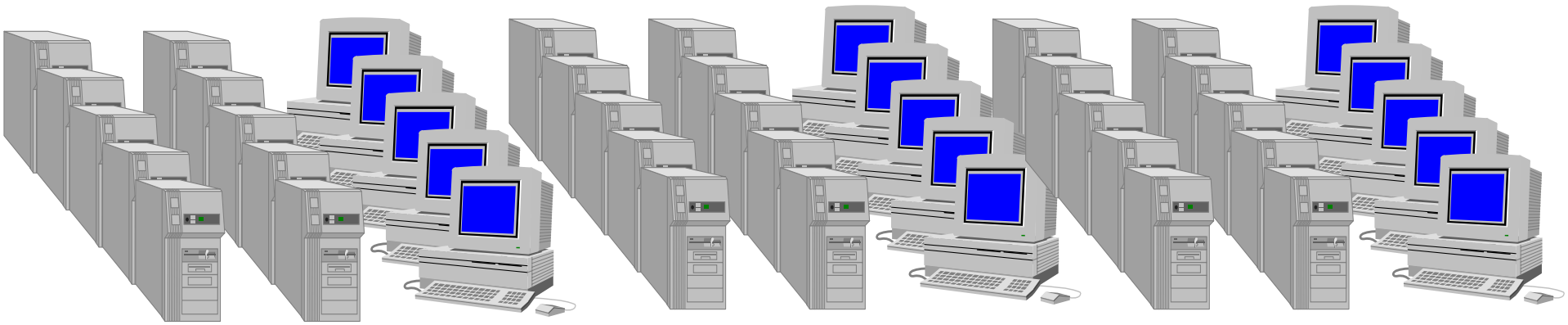
Linköpings universitet

GET THAT PROTEIN!

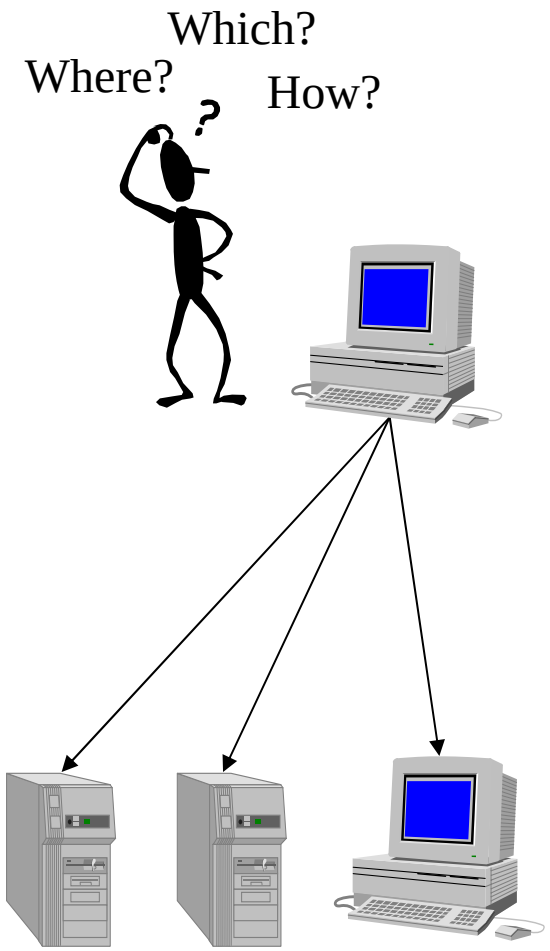




Locating relevant information

Vision: Web services

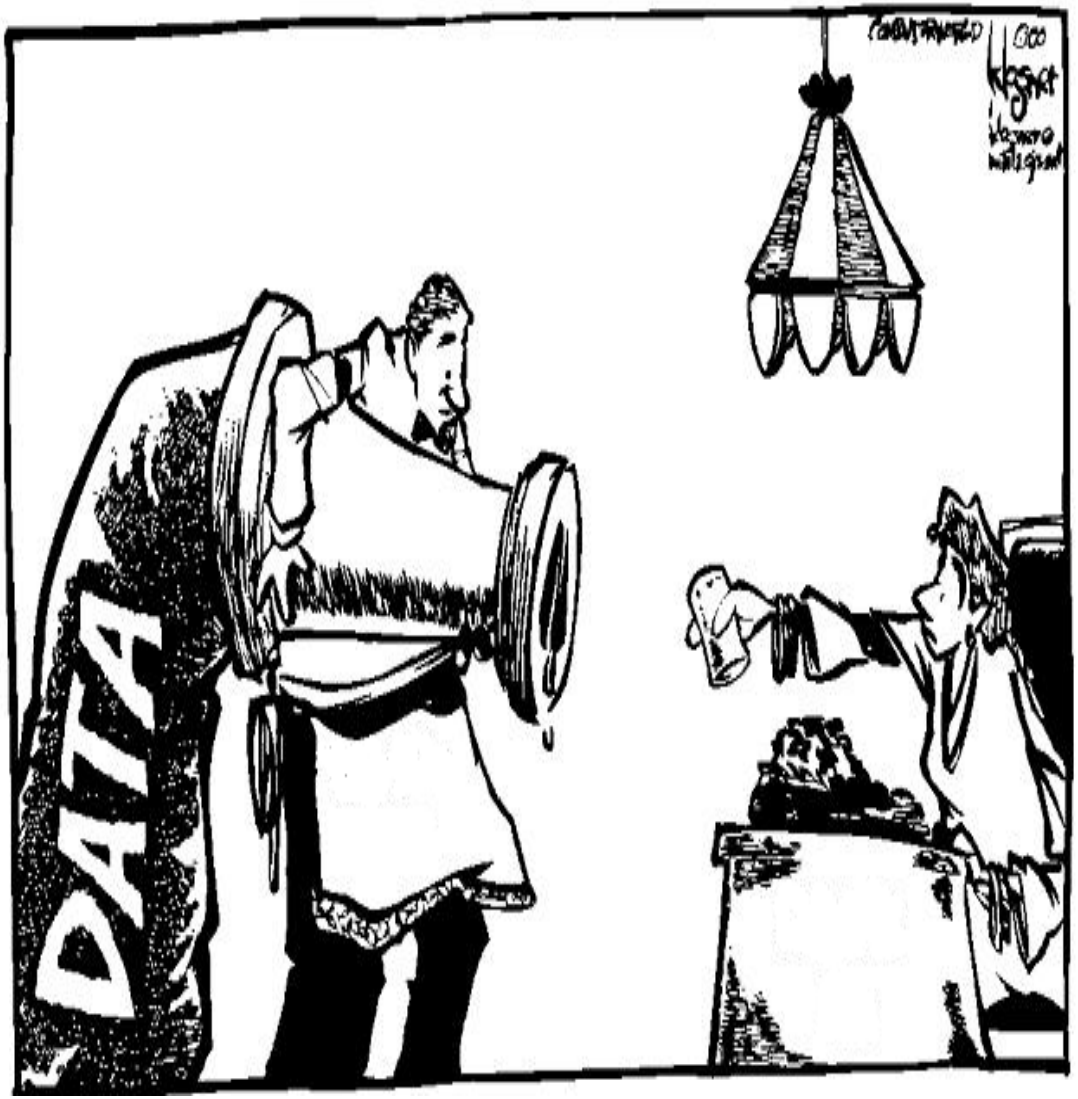
- Databases and tools (service providers) announce their service capabilities
- Users request services which may be based on task descriptions
- Service matchers find relevant services (composition) based on user needs and user preferences, negotiate service delivery, and deliver results to user



Retrieving relevant information

Vision:

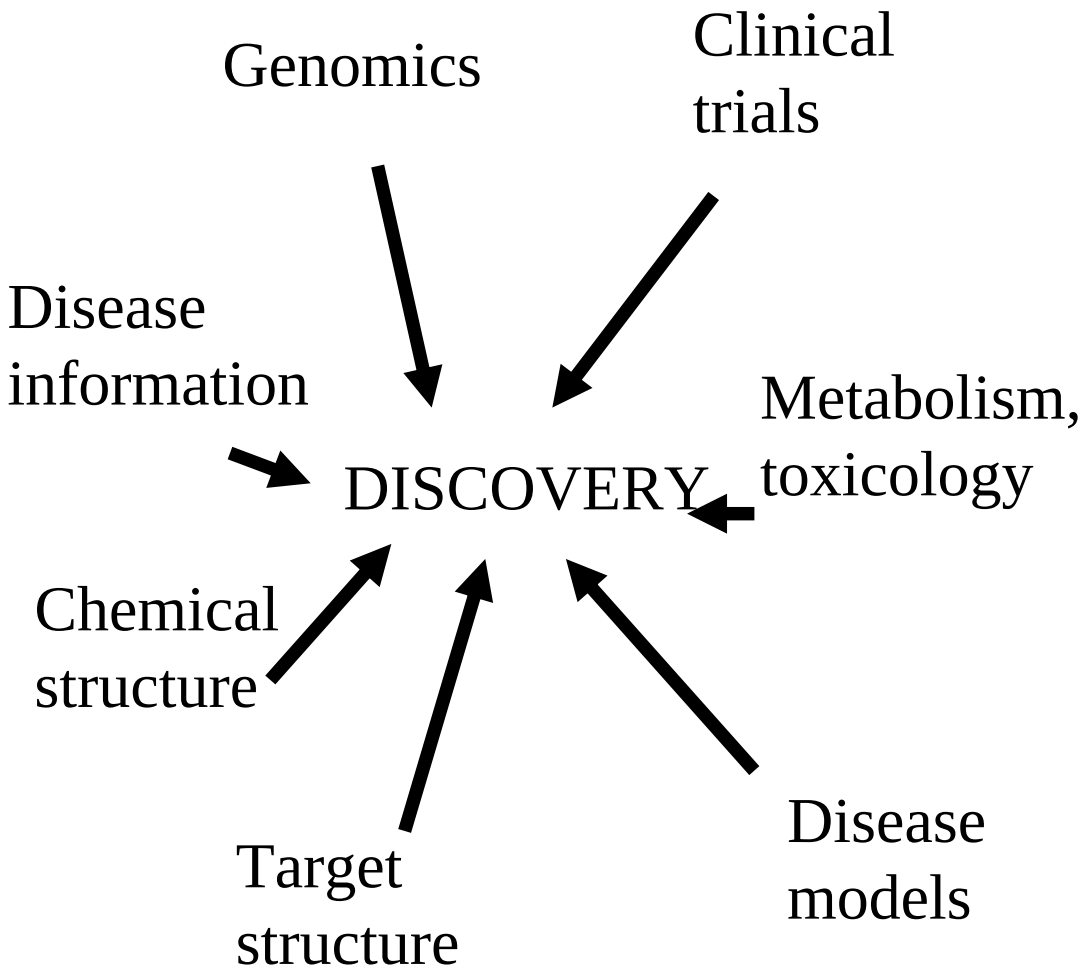
Based on the meaning of the query:
- only relevant information is retrieved
- all relevant information is retrieved



Integrating information

Vision:

Integrate data sources that are heterogeneous in content, data quality, data models, access methods, terminology



Today: syntactic Web

- A library of documents (web pages) interconnected by links
- A common portal to applications accessible through web pages, and presenting their results as web pages

A place where computers do the presentation (easy) and people do the linking and interpreting (hard).

Semantic Web

W3C: Facilities to put machine-understandable data on the Web are becoming a high priority for many communities. The Web can reach its full potential only if it becomes a place where data can be shared and processed by automated tools as well as by people. For the Web to scale, tomorrow's programs must be able to share and process data even when these programs have been designed totally independently. The Semantic Web is a vision: the idea of having data on the web defined and linked in a way that it can be used by machines not just for display purposes, but for automation, integration and reuse of data across various applications.

What is the problem?

- Date: June 13–15, 2005
- Location: Linköping University, Sweden
- Sponsors: IEEE Computer Society, Concurrent Engineering Research Center (CERC) at West Virginia University (USA), Linköping University (Sweden)

14th IEEE International Workshops on Enabling Technologies: Infrastructures for Collaborative Enterprises (WETICE–2005).

Home
Agenda
List of Workshops
Call For Papers
Call For Proposals
Dates/Deadlines

Latest Announcements

Advance Registration Closed.
On–Site Registration Only.

Visa Letters

Paper Submission deadline to individual workshops: Closed

All Announcements...

WETICE–2005 will be held at Linköping University, Sweden
Date: June 13–15, 2005
Sponsors: IEEE Computer Society, Concurrent Engineering Research Center at West Virginia University, Linköping University,

Home

Welcome to WETICE–2005

Paper submission to individual workshops: Closed

Advance Registration Closed. On–Site Registration Only. **Registration Fees**

Visa Letters

Hotels in Linköping (English)

Hotels in Linköping (Swedish, source www.linkoping.se)

How to get to Linköping and Conference Venue **Maps (English & Swedish)**

Train Schedule **Plenary Talks**

Special issue of International Journal – Multiagent and Grid Systems
Selected papers from WETICE 2005 will be published in the journal (editors: Ramana Reddy, Sumitra Reddy).

WETICE is an annual, international forum for state–of–the–art research in enabling technologies for collaboration.

WETICE–2005 will consist of a number of workshops on different topics related to collaboration technology. The ongoing workshops are listed **here**. In addition to the ongoing workshops, there will be new workshops. Please see the **Call for Proposals** for the topics.

What sets WETICE apart from larger conferences is that the workshops are kept small enough to

Example based on example on slides by P. Patel-Schneider

What information can we see…

Date: 13-15 June, 2005

Location: Linköping

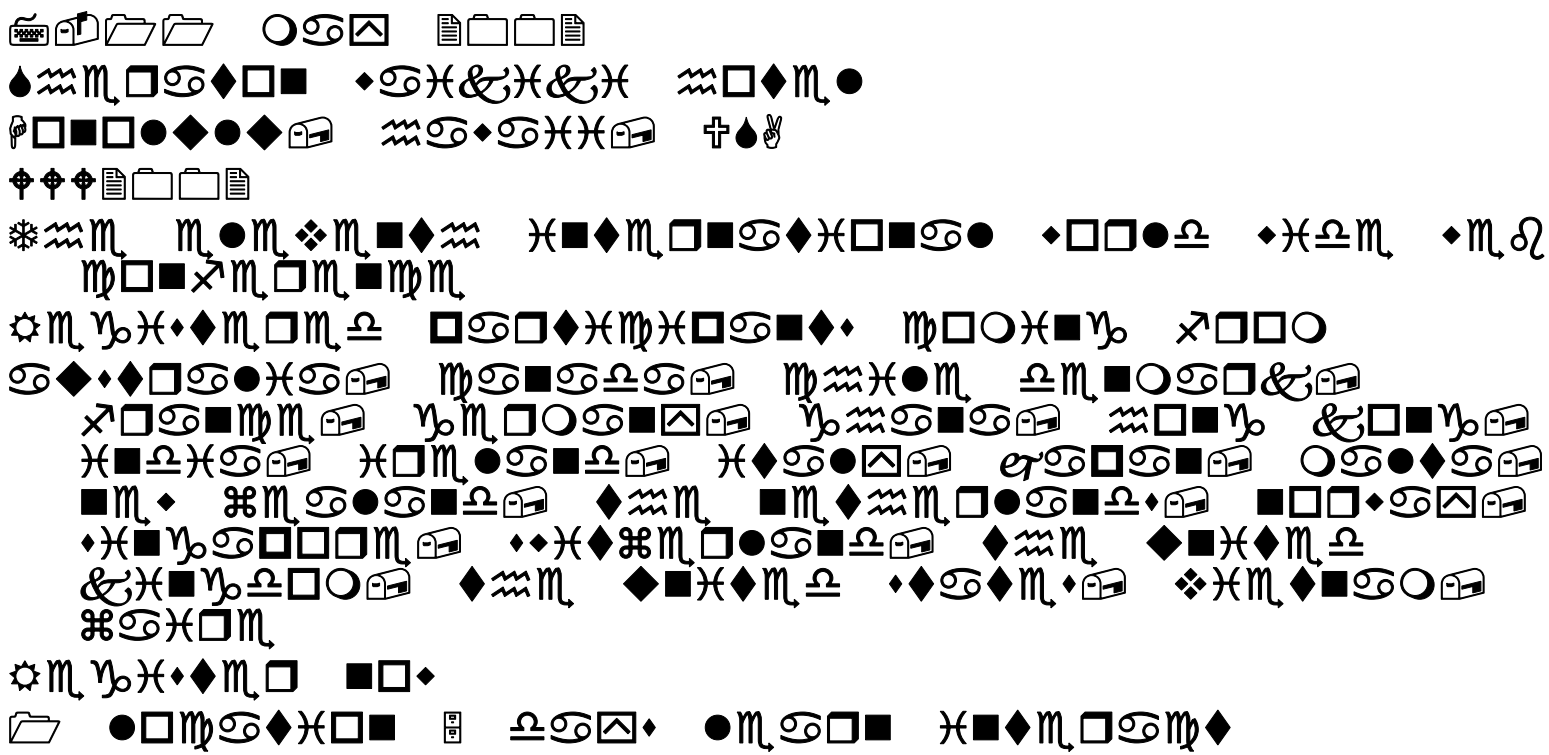
Sponsors: IEEE, CERC, LiU

14th IEEE International Workshops on Enabling Technologies: Infrastructures for Collaborating Enterprises (WETICE-2005)

Welcome to WETICE-2005

…

What information can a machine see…



Use XML markup with “meaningful” tags

<date> 13-15 June 2005 </date>

<location> Linköping </location>

<sponsors>IEEE, CERC, LiU </sponsors>

<name> 14th IEEE International Workshops on Enabling Technologies: Infrastructures for Collaborating Enterprises (WETICE-2005) </name>

<welcome> Welcome to WETICE-2005 </welcome>

Machine sees …

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But what about …

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<sponsors>IEEE, CERC, LiU </sponsors>

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<introduction> Welcome to WETICE-2005 </introduction>

Machine sees …

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Adding “Semantics” – first approach

External agreement on meaning of annotations

- Agree on the meaning of a set of annotation tags
- Problems with this approach:
  - Inflexible
  - Limited number of things can be expressed

Adding “Semantics” – second approach

Use on-line ontologies to specify meaning of annotations

- Ontologies provide a vocabulary of terms
- New terms can be formed by combining existing ones
- Meaning (semantics) of such terms is formally specified

Scientific American, May 2001:

THE SEMANTIC WEB

A new form of Web content
that is meaningful to computers
will unleash a revolution of new abilities

by
TIM BERNERS-LEE,
JAMES HENDLER and
ORA LASSILA

- First step towards the vision:
  adding semantic annotation to web resources

Semantic annotations based on ontologies

- Locating information
  - Web service descriptions use ontologies
  - Users use ontologies when formulating requests
  - Service matchers find services based on meaning
- Retrieving relevant information
  - Reduce non-relevant information (precision)
  - Find more relevant information (recall)
- Integrating information
  - Relating similar entities in different databases

Ontologies

Ontologies

- Definition
- Use
- Components
- Knowledge representation

Ontologies

"*Ontologies define the basic terms and relations comprising the vocabulary of a topic area, as well as the rules for combining terms and relations to define extensions to the vocabulary.*"

(Neches, Fikes, Finin, Gruber, Senator, Swartout, 1991)

Definitions

- Ontology as specification of a conceptualization
- Ontology as philosophical discipline
- Ontology as informal conceptual system
- Ontology as formal semantic account
- Ontology as representation of conceptual system via a logical theory
- Ontology as the vocabulary used by a logical theory
- Ontology as a meta-level specification of a logical theory

(Guarino, Giaretta)

Definitions

- An ontology is an explicit specification of a conceptualization (Gruber)
- An ontology is a hierarchically structured set of terms for describing a domain that can be used as a skeletal foundation for a knowledge base. (Swartout, Patil, Knight, Russ)
- An ontology provides the means for describing explicitly the conceptualization behind the knowledge represented in a knowledge base. (Bernaras, Lasergoiti, Correra)
- An ontology is a formal, explicit specification of a shared conceptualization (Studer, Benjamins, Fensel)

Example

GENE ONTOLOGY (GO)

immune response
- **i-** acute-phase response
- **i-** anaphylaxis
- **i-** antigen presentation
- **i-** antigen processing
- **i-** cellular defense response
- **i-** cytokine metabolism
  - **i-** cytokine biosynthesis synonym cytokine production
    - …
  - **p-** regulation of cytokine biosynthesis
    - …

…
- **i-** B-cell activation
  - **i-** B-cell differentiation
  - **i-** B-cell proliferation
- **i-** cellular defense response

…
- **i-** T-cell activation
  - **i-** activation of natural killer cell activity
    - …

Example Ontologies

- Knowledge representation ontology: frame ontology
- Top level ontologies: TLO, Cyc
- Linguistic ontologies: GUM, WordNet
- Engineering ontologies: EngMath, PhysSys
- Domain ontologies: CHEMICALS, Gene Ontology, Open Biomedical Ontologies

Ontologies used …

- for communication between people and organizations
- for enabling knowledge reuse and sharing
- as basis for interoperability between systems
- as repository of information
- as query model for information sources

Key technology for the Semantic Web

Biomedical Ontologies - efforts

OBO – Open Biomedical Ontologies
http://www.obofoundry.org/
(over 50 ontologies)

” The mission of OBO is to support community members who are developing and publishing ontologies in the biomedical domain. It is our vision that a core of these ontologies will be fully interoperable, by virtue of a common design philosophy and implementation, thereby enabling scientists and their instruments to communicate with minimum ambiguity. In this way the data generated in the course of biomedical research will form a single, consistent, cumulatively expanding, and algorithmically tractable whole. This core will be known as the "OBO Foundry". .”

OBO Foundry

1. open and available
2. common shared syntax
3. unique identifier space
4. procedures for identifying distinct successive versions
5. clearly specified and clearly delineated content
6. textual definitions for all terms
7. use relations from OBO Relation Ontology
8. well documented
9. plurality of independent users
10. developed collaboratively with other OBO Foundry members

Biomedical Ontologies - efforts

National Center for Biomedical Ontology
http://bioontology.org/index.html

Funded by National Institutes of Health

”The goal of the Center is to support biomedical researchers in their knowledge-intensive work, by providing online tools and a Web portal enabling them to access, review, and integrate disparate ontological resources in all aspects of biomedical investigation and clinical practice. A major focus of our work involves the use of biomedical ontologies to aid in the management and analysis of data derived from complex experiments.”

Biomedical Ontologies - efforts

- Gene Ontology Consortium (GO): molecular function, biological process, cellular component
- Standards and Ontologies for Functional Genomics (SOFG): meeting and website
- Proteomics Standards Initiative
- Plant Ontology consortium

Biomedical Ontologies - efforts

- International Health Terminology Standards Development Organisation

  http://www.ihtsdo.org

SNOMED CT (**S**ystematized **No**menclature of **Med**icine-**C**linical **T**erms)

Ontologies in biomedical research

- many biomedical ontologies

  e.g. GO, OBO, SNOMED-CT

- practical use of biomedical ontologies

  e.g. databases annotated with GO

GENE ONTOLOGY (GO)

immune response
- **i-** acute-phase response
- **i-** anaphylaxis
- **i-** antigen presentation
- **i-** antigen processing
- **i-** cellular defense response
- **i-** cytokine metabolism
  - **i-** cytokine biosynthesis
    - synonym cytokine production
    - …
  - p- regulation of cytokine biosynthesis
  - …
- …
- **i-** B-cell activation
  - **i-** B-cell differentiation
  - **i-** B-cell proliferation
- **i-** cellular defense response
- …
- **i-** T-cell activation
  - **i-** activation of natural killer cell activity
  - …

Components

- concepts

  - represent a set or class of entities in a domain

    immune response

  - organized in taxonomies
    (hierarchies based on e.g. *is-a* or *is-part-of*)

    immune response is-a *defense response*

- instances

  - often not represented in an ontology
    (instantiated ontology)

Components

- relations

  R: C1 x C2 x … x Cn

  Protein hasName ProteinName

  Chromosone hasSubcellularLocation Nucleus

Components

- axioms

  ‘facts that are always true’

The origin of a protein is always of the type ‘gene coding origin type’

Each protein has at least one source.

A helix can never be a sheet and vice versa.

Different kinds of ontologies

- Controlled vocabularies

  Concepts
- Taxonomies

  Concepts, is-a
- Thesauri

  Concepts, predefined relations
- Data models (e.g. EER, UML)

  Concepts, relations, axioms
- Logics

  Concepts, relations, axioms

Taxonomy - GeneOntology

id: GO:0003674 name: molecular_function

def: “Elemental activities, such as catalysis or binding, describing the actions of a gene product at the molecular level. A given gene product may exhibit one or more molecular functions.”

id: GO:0015643 name: binding

def: “The selective, often stoichiometric, interaction of a molecule with one or more specific sites on another molecule.”

is-a: GO:0003674 ! molecular_function

id: GO:0008289 name: lipid binding

is_a: GO:0015643 ! binding

id: GO:0016209 name: antioxidant activity

def: “Inhibition of the reactions brought about by dioxygen (O2) or peroxides. Usually the antioxidant is effective because it can itself be more easily oxidized than the substance protected.”

is_a: GO:0003674 ! molecular_function

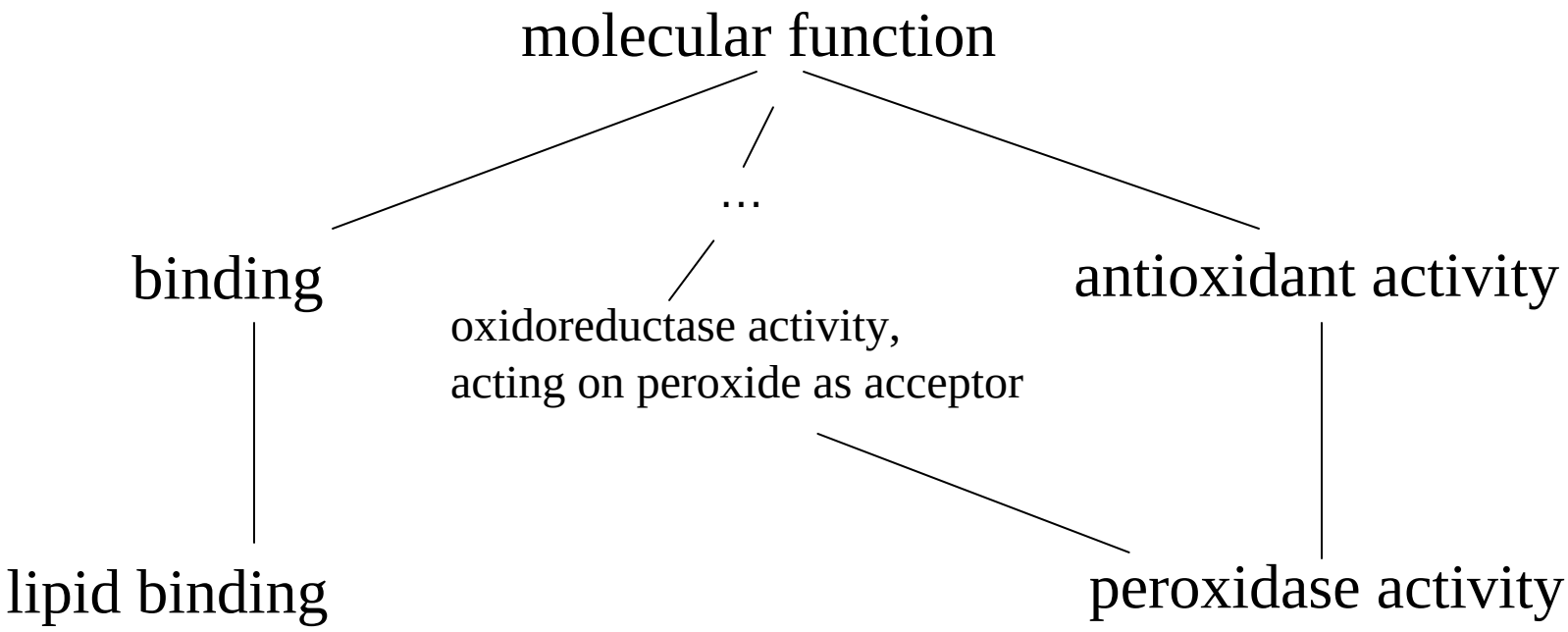
id: GO:0004601 name: peroxidase activity

def: "Catalysis of the reaction: donor + H2O2 = oxidized donor + 2 H2O."

is_a: GO:0016209 ! antioxidant activity

is_a: GO:0016684 ! oxidoreductase activity, acting on peroxide as acceptor

Taxonomy - GeneOntology



Thesaurus

- graph
- fixed set of relations

  (synonym, narrower term, broader term, similar)

Thesaurus - WordNet

thesaurus, synonym finder
=> wordbook
=> reference book, reference, reference work, book of facts
=> book
=> publication
=> print media
=> medium
=> means
=> instrumentality, instrumentation
=> artifact, artefact
=> object, inanimate object, physical object
=> entity
=> work, piece of work
=> product, production
=> creation
=> artifact, artefact
=> object, inanimate object, physical object
=> entity

OO Data models

- EER

  entity types, attributes, relationships,

  cardinality constraints, taxonomy

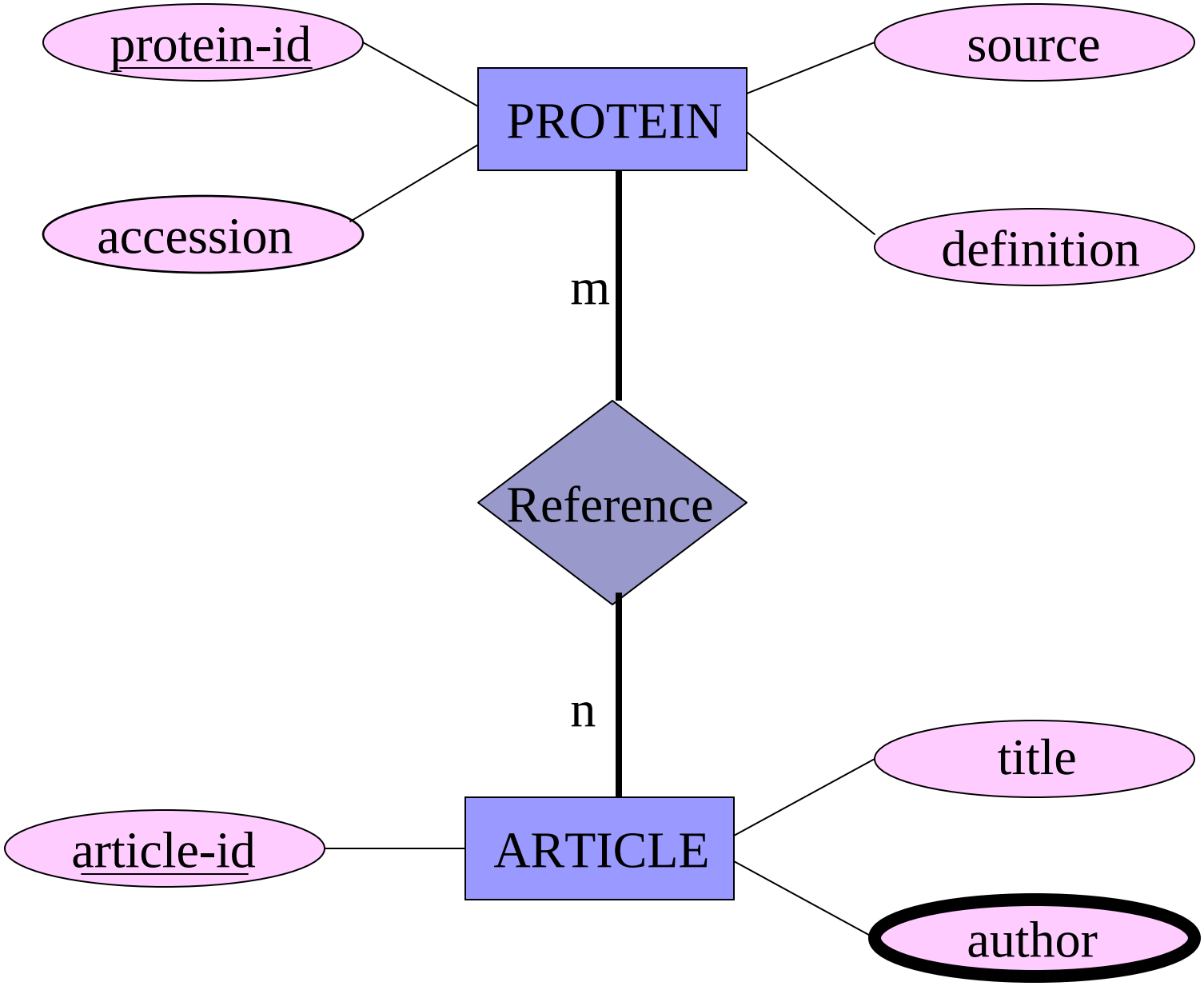
- UML

  classes, attributes, associations,

  cardinality constraints, taxonomy, operations

- Taxonomy/inheritance – semantics?
- Intuitive, lots of tools, widely used.

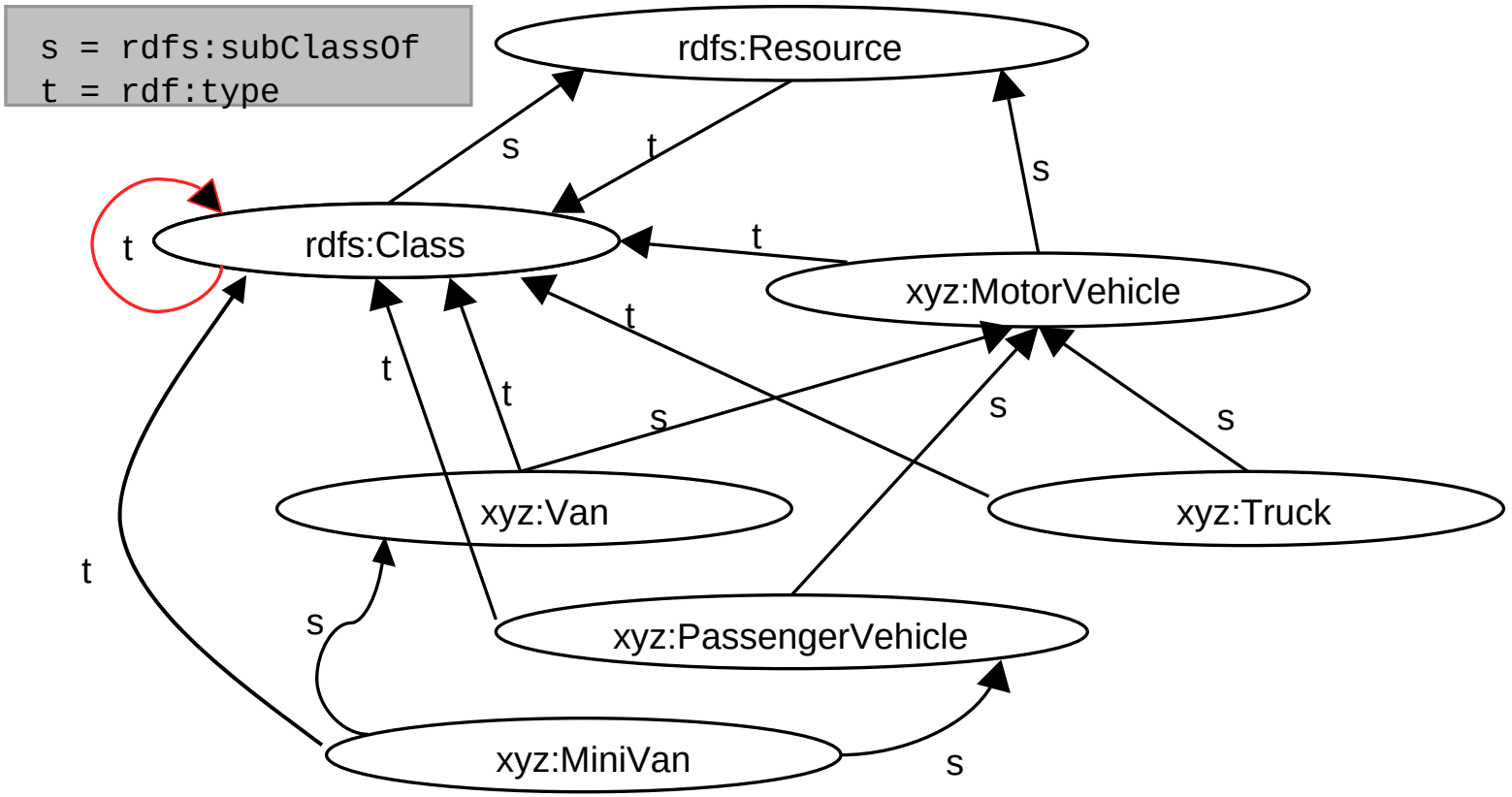
Entity-relationship



RDF + RDF Schema

- Basic construct: sentence: *Subject Predicate Object*
  - Encoded in XML
  - Can be seen as ground atomic formula
  - Represented as graph
- RDF Schema
- Editors, query tools exist

RDF Schema - example



Logics

- Formal languages
- Syntax, semantics, inference mechanisms

Logics

Reasoning services used in

- Ontology design

  Check concept satisfiability, ontology satisfiability and (unexpected) implied relationships

- Ontology aligning and merging

  Assert inter-ontology relationships.

  Reasoner computes integrated concept hierarchy/consistency.

- Ontology deployment

  Determine if a set of facts are consistent w. r. t. ontology.

  Determine if individuals are instances of ontology concepts.

  Query inclusion.

  Classification-based querying.

Description Logics

- A family of KR formalisms tailored for expressing knowledge about concepts and concept hierarchies
- Based on FOPL, supported by automatic reasoning systems
- Basic building blocks: concepts (concepts), roles (binary relations), individuals (instances)
- Language constructs can be used to define new concepts and roles (axioms).
  - Intersection, union, negation, quantification, …
- Knowledge base is Tbox + Abox
  - Tbox: concept level - axioms: equality and subsumption (is-a)
  - Abox: instance level - axioms: membership, relations
- Reasoning services
  - Satisfiability of concept, Subsumption/Equivalence/Disjointness between concepts, Classification, Instantiation, Retrieval

Description Logics

Intersection

Signal-transducer-activity $\cap$ binding

Negation

$\neg$ Helix

Quantifiers

$\exists$ hasOrigin.Mitochondrion

$\forall$ hasOrigin.Gene-coding-origin-type

DAML+OIL / OWL

- DAML+ OIL almost equivalent to SHIQ
- DAML+ OIL supports the full range of XML Schema data types

- OWL updated DAML+OIL

DAML+OIL Class Constructors

Constructor	DL Syntax	Example
intersectionOf	$C_1 \sqcap \ldots \sqcap C_n$	Human $\sqcap$ Male
unionOf	$C_1 \sqcup \ldots \sqcup C_n$	Doctor $\sqcup$ Lawyer
complementOf	$\neg C$	$\neg$Male
oneOf	$\{x_1 \ldots x_n\}$	{john, mary}
toClass	$\forall P.C$	$\forall$hasChild.Doctor
hasClass	$\exists P.C$	$\exists$hasChild.Lawyer
hasValue	$\exists P.\{x\}$	$\exists$citizenOf.{USA}
minCardinalityQ	$\geqslant n P.C$	$\geqslant$2hasChild.Lawyer
maxCardinalityQ	$\leqslant n P.C$	$\leqslant$1hasChild.Male
cardinalityQ	$=n\, P.C$	$=1$ hasParent.Female

- XMLS **datatypes** as well as classes
- Arbitrarily complex **nesting** of constructors
  - E.g., Person $\sqcap \forall$hasChild.(Doctor $\sqcup \exists$hasChild.Doctor)

DAML+OIL Axioms

Axiom	DL Syntax	Example
subClassOf	$C_1 \sqsubseteq C_2$	Human $\sqsubseteq$ Animal $\sqcap$ Biped
sameClassAs	$C_1 \equiv C_2$	Man $\equiv$ Human $\sqcap$ Male
subPropertyOf	$P_1 \sqsubseteq P_2$	hasDaughter $\sqsubseteq$ hasChild
samePropertyAs	$P_1 \equiv P_2$	cost $\equiv$ price
sameIndividualAs	$\{x_1\} \equiv \{x_2\}$	{President_Bush} $\equiv$ {G_W_Bush}
disjointWith	$C_1 \sqsubseteq \neg C_2$	Male $\sqsubseteq \neg$Female
differentIndividualFrom	$\{x_1\} \sqsubseteq \neg\{x_2\}$	{john} $\sqsubseteq \neg${peter}
inverseOf	$P_1 \equiv P_2^-$	hasChild $\equiv$ hasParent$^-$
transitiveProperty	$P^+ \sqsubseteq P$	ancestor$^+ \sqsubseteq$ ancestor
uniqueProperty	$\top \sqsubseteq \leqslant 1P$	$\top \sqsubseteq \leqslant 1$hasMother
unambiguousProperty	$\top \sqsubseteq \leqslant 1P^-$	$\top \sqsubseteq \leqslant 1$isMotherOf$^-$

☞ Axioms (mostly) **reducible to subClass/PropertyOf**

OWL

- OWL-Lite, OWL-DL, OWL-Full: increasing expressivity
- A legal OWL-Lite ontology is a legal OWL-DL ontology is a legal OWL-Full ontology
- OWL-DL: expressive description logic, decidable
- XML-based
- RDF-based (OWL-Full is extension of RDF, OWL-Lite and OWL-DL are extensions of a restriction of RDF)

OWL-Lite

- **Class**, subClassOf, equivalentClass
- intersectionOf (only named classes and restrictions)
- **Property**, subPropertyOf, equivalentProperty
- domain, range (global restrictions)
- inverseOf, TransitiveProperty (*), SymmetricProperty, FunctionalProperty, InverseFunctionalProperty
- allValuesFrom, someValuesFrom (local restrictions)
- minCardinality, maxCardinality (only 0/1)
- **Individual**, sameAs, differentFrom, AllDifferent

(*) restricted

OWL-DL

- **Type separation (**class cannot also be individual or property, property cannot be also class or individual), Separation between DatatypeProperties and ObjectProperties
- **Class –complex classes**, subClassOf, equivalentClass, *disjointWith*
- intersectionOf, *unionOf*, *complementOf*
- **Property**, subPropertyOf, equivalentProperty
- domain, range (global restrictions)
- inverseOf, TransitiveProperty (*), SymmetricProperty, FunctionalProperty, InverseFunctionalProperty
- allValuesFrom, someValuesFrom (local restrictions), *oneOf*, *hasValue*
- minCardinality, maxCardinality
- **Individual**, sameAs, differentFrom, AllDifferent

(*) restricted

Defining ontologies is not so easy ...

The Celestial Emporium of Benevolent Knowledge, Borges

"On those remote pages it is written that animals are divided into:

a. those that belong to the Emperor

b. embalmed ones

c. those that are trained

d. suckling pigs

e. mermaids

f. fabulous ones

g. stray dogs

h. those that are included in this classification

i. those that tremble as if they were mad

j. innumerable ones

k. those drawn with a very fine camel's hair brush

l. others

m. those that have just broken a flower vase

n. those that resemble flies from a distance"

Slide from talk by C. Goble

Defining ontologies is not so easy ...

Dyirbal classification of objects in the universe

- Bayi: men, kangaroos, possums, bats, most snakes, most fishes, some birds, most insects, the moon, storms, rainbows, boomerangs, some spears, etc.
- Balan: women, anything connected with water or fire, bandicoots, dogs, platypus, echidna, some snakes, some fishes, most birds, fireflies, scorpions, crickets, the stars, shields, some spears, some trees, etc.
- Balam: all edible fruit and the plants that bear them, tubers, ferns, honey, cigarettes, wine, cake.
- Bala: parts of the body, meat, bees, wind, yamsticks, some spears, most trees, grass, mud, stones, noises, language, etc.

Slide from talk by C. Goble

Ontology tools

- Ontology development tools
- Ontology merge and alignment tools
- Ontology evaluation tools
- Ontology-based annotation tools
- Ontology storage and querying tools
- Ontology learning tools

Further reading

Starting points for further studies

Further reading ontologies

- KnowledgeWeb (http://knowledgeweb.semanticweb.org/) and its predecessor OntoWeb (http://ontoweb.aifb.uni-karlsruhe.de/)
- Lambrix, Tan, Jakoniene, Strömbäck, Biological Ontologies, chapter 4 in Baker, Cheung, (eds), *Semantic Web: Revolutionizing Knowledge Discovery in the Life Sciences*, 85-99, Springer, 2007. ISBN: 978-0-387-48436-5.

(general about ontologies)

- Lambrix, Towards a Semantic Web for Bioinformatics using Ontology-based Annotation, *Proceedings of the 14th IEEE International Workshops on Enabling Technologies: Infrastructures for Collaborative Enterprises*, 3-7, 2005. Invited talk.

(ontologies for semantic web)

- OWL, http://www.w3.org/TR/owl-features/ , http://www.w3.org/2004/OWL/