Acquiring Experience with Ontology and Vocabularies

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About MITRE

- Context of MITRE work:
  - Independent
  - FFRDC
  - No vendor affiliations

Background

- The agency receives a large amount of information through free text documents and images created by external entities.

- The submitted information drives many areas of the agency's work:
  - Enforcement activities
  - Policy development
  - Product approval
  - Public health research

- Regulators and scientists need to:
  - Analyze the submitted documentation
  - Research internal and external documentation related to domain
  - Formulate policies based on document analysis

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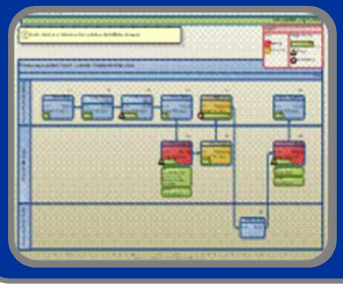
Agency Problem

- Difficult to find relevant documents. Need better ways to support:
  - Naming conventions and data standards
  - Document classifications or taxonomy
  - Document traceability
  - Standard terminology for components described in the documents
- Difficult to query across internal and external information sources: federated search
- Difficult to perform queries using both structured and non-structured information

Take Ways

- This presentation describes work done to:
  - Create an ontology from publicly-available resources
  - Improve search of unstructured data via semantic text mining
  - Enhance data quality by leveraging structured terminologies and data standards

Approach for Applying Ontology and SOA to Improve Federated Search of Documents



1) Define Business Architecture

2) Define Service & Technical Architecture

3) Define Ontology & Vocabularies

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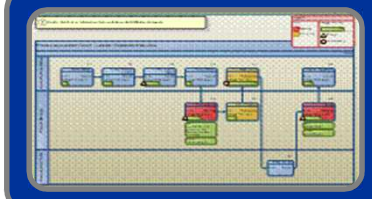

Business Architecture

- **How**
  - **Prioritized relevant business functions as defined by Enterprise Architecture**
  - **Developed business processes**
  - **Used business modeling (BPMN)**
    - **Conducted Workshops with SMEs and key stakeholders**
    - **Leveraged best practices from the field to define business processes**
- **Why**
  - **Align the enterprise business processes to its business vision and strategic goals.**
  - **Identify needed capabilities (what *type of* business services are needed to support ontological search)**
  - **Define roles & responsibilities**
    - **"Who will be responsible for doing what"**
  - **Obtain buy-in**
  - **Disseminate ideas**
  - **Inputs to Requirements**

Service & Technical Architecture

- How
  - Gathered requirements
    - What capabilities are needed?
  - Technology inventory / survey
  - Identified business service blueprint
    - What are the major business & system services?
    - What capabilities they must provide?
  - Mapped business services to business processes
    - What business & system services are need to support the prioritized business processes?
- Why
  - Define an architecture blueprint for business services and technology
  - Identify capabilities gaps
    - What services are currently available?
    - What services are needed?
  - Prioritize procurement process
    - What *type* of COTS can provide the needed capabilities? Such as:
      - ontology engineering tools
      - semantic text mining
      - vocabulary management

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Ontology & Vocabulary

- **How**
  - **Used an approach based on semantic web technology and ontology for:**
    - **Defining data standards**
    - **Creating a conceptual data model**
    - **Addressing federated data integration**
    - **Improving document classification**
    - **Reusing existing ontologies relevant to domain**
- **Why**
  - **Improve search capabilities by scientists**
  - **Define a common vocabulary**
  - **Allow easy integration of structure and unstructured federated data sources**
  - **Allow automatic document classification**
  - **Enhance collaboration among inter- and intra- research groups**

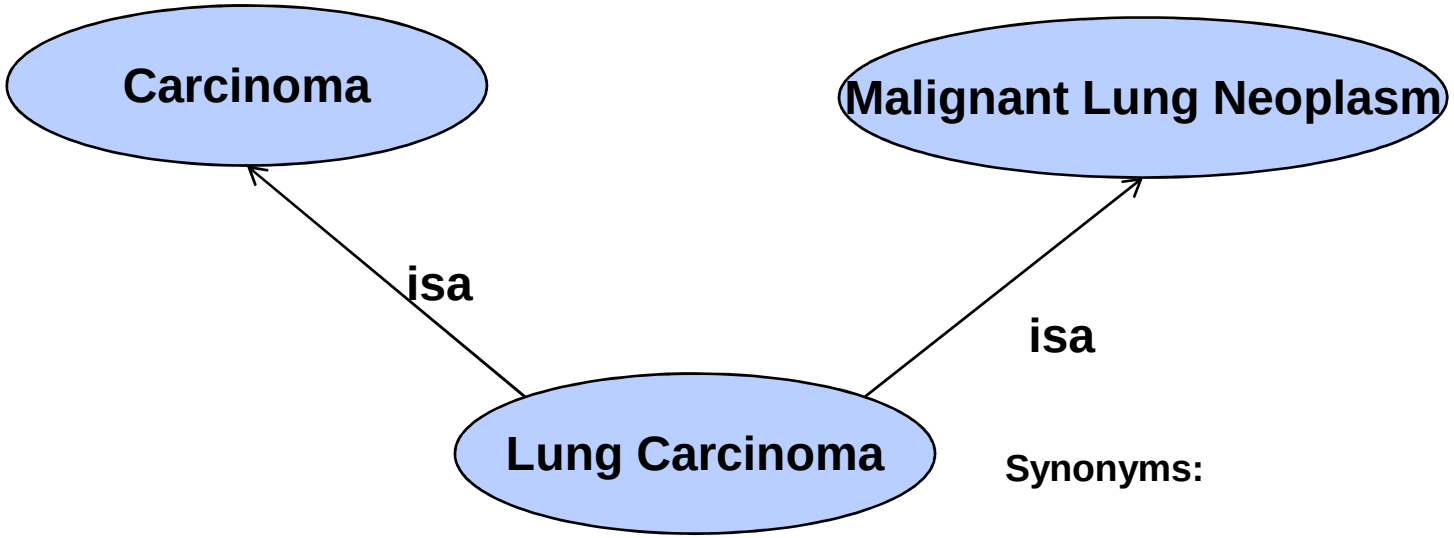
Definitions

- ***What is an Ontology?***
  - An ontology defines the terms used to describe and represent an area of knowledge. It includes computer-usable definitions of concepts in the domain and the relationships among them.
- ***Why should we care?***
  - Ontologies are used by people, databases, and applications that need to share domain information, such as the health care domain

Rationale

- Permit semantic interoperability - standard terminologies ensure the same words and phrases mean the same thing
- Provide consistent way to annotate industry submissions concerning products, ingredients, and constituents
- Enable translation of health-related information received from industry into a structured format that can be analyzed / mined
- Provide structured way to map the domain specific ontology with other relevant ontologies, such as diseases, toxicology, and so on
- Allow the semantic integration of data from different data sources – a semantic data warehouse

An Example: Deceases

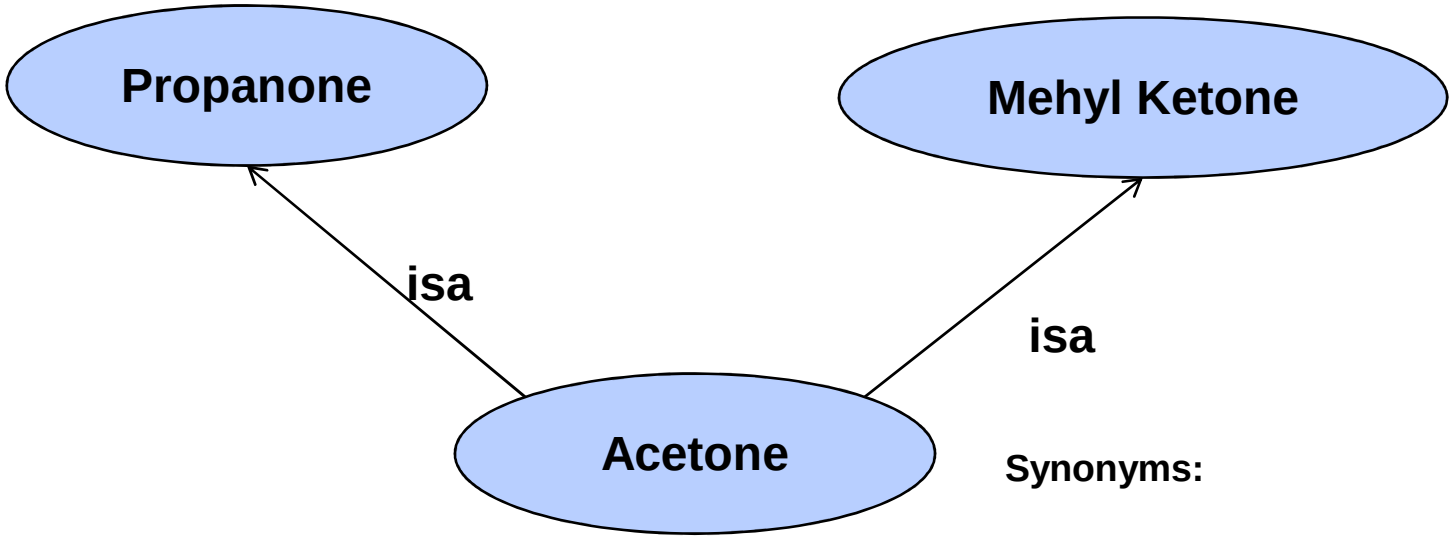


Synonyms:

- **Cancer of Lung**
- **Lung Cancer**
- **Cancer of the Lung**
- **Carcinoma of the Lung**

Disclaimer: this is not the actual ontology created by the agency

An Example: Chemical Substances

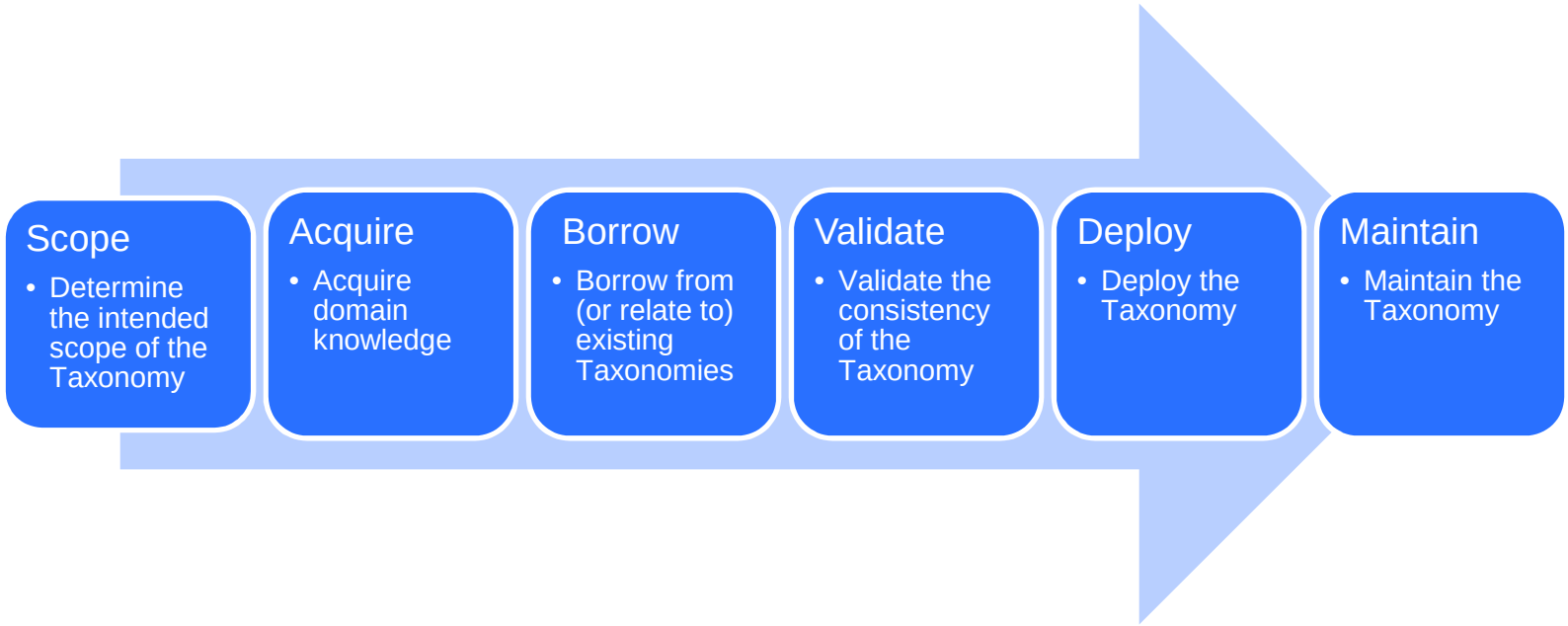


Synonyms:

- **Dimethyl ketone**
- **2-Propanone**
- **C3H6O**
- **dimethylcetone**

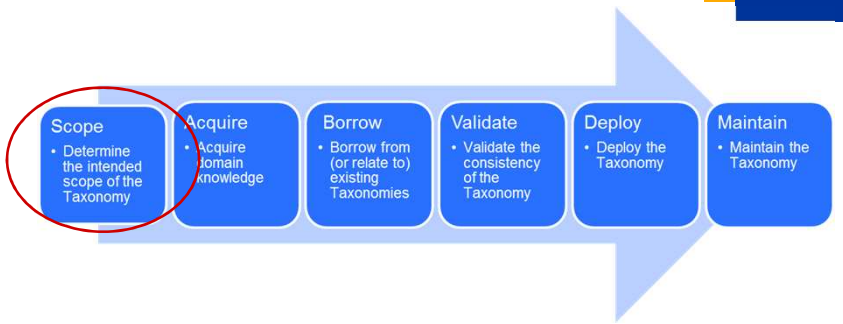
Disclaimer: this is not the actual ontology created by the agency

High Level View of the Ontology Development Cycle



Baclawski K, Niu T. Ontologies for bioinformatics. Cambridge: MIT Press; 2006.

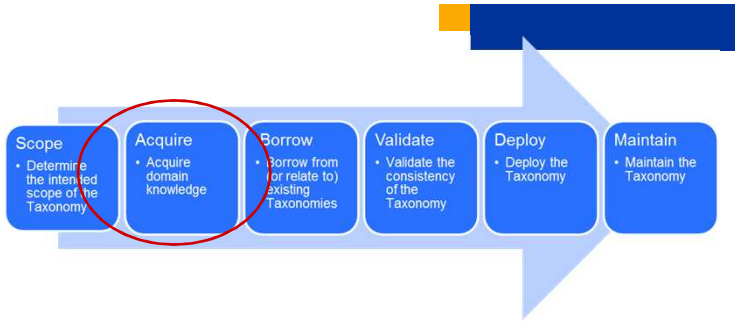
Scope



A bio-medical domain with a strong interrelationship with other domains

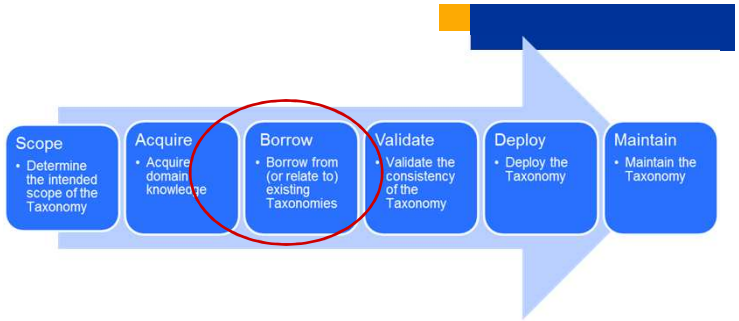
- **Medical**
- **Chemical**
- **Diseases**
- **Toxicology**
- **Legal entities**
- **Standard organizations**

Acquire Domain Knowledge



- Leverage SME from different domains:
  - Chemical
  - Medical
  - Toxicology
  - Manufacture
  - Public Health
- Utilize public domain publications
  - Specialized publications
  - Well known web sites maintained by non profit organizations
  - Standards
- Reuse existing efforts
  - National Cancer Institute (NCI)
  - National Library of Medicine

Reuse: Ontologies Being Investigated

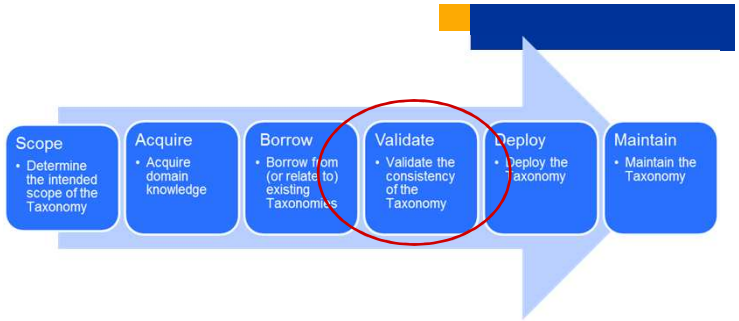


- Chemical Entities of Biological Interest ~ freely available dictionary of molecular entities focused on 'small' chemical compounds.
- National Cancer Institute (NCI) Thesaurus ~ widely recognized standard for biomedical coding and reference, used by a broad variety of public and private partners both nationally and internationally.
- SNOMED CT (Systematized Nomenclature of Medicine--Clinical Terms).
- And so on

Do not re-invent the wheel:

- Import existing ontologies
- Map created concepts to these ontologies

Validation



Method	Notes
Gold Standard	Compare to a gold standard. *In our case, there is no gold standard, but it is possible to develop metrics of quality (such as term coverage, lack of ambiguity) that can be applied to candidate taxonomies.*
Task Based	This approach involves testing the candidate taxonomies against a specific task (such as identifying all variations on a specific chemical component) and assessing the results.
Data or Corpus Driven	*This method compares the fit of a terminology to texts in a domain. In our case, this involves testing how many concepts in the terminology were found in a set of industry documents and evaluating how useful the terminology was in navigating through the documents.*
Manual Assessment Against A Set Of Pre-Defined Criteria	This would involve manual inspection of the terminology and development of specific related criteria, such as the number of synonyms that were correctly identified. *In our case, this validation was not yet done.*

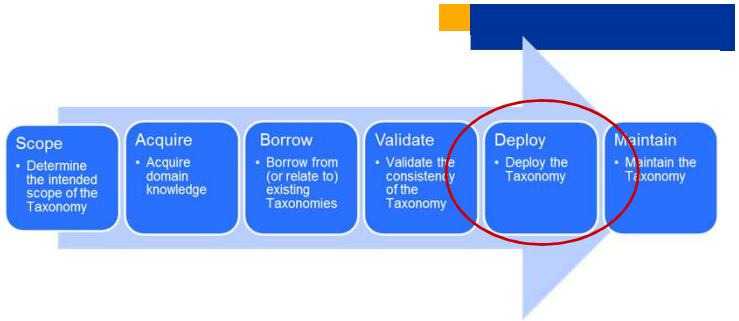
G MAIGA, DDEMBE WILLIAMS, "A Flexible Approach for User Evaluation of Biomedical Ontologies."

Int'l Journal of Computing and ICT Research, Vol. 2, No. 2, December 2008

Corpus Driven Validation: an example

Concept	Preferred Name	NIST	CAS#
CHEBI_15347	acetone	Yes	67-64-1
CHEBI_15366	acetic acid	Yes	64-19-7
CHEBI_22698	benzaldehydes		
CHEBI_31457	decanal	Yes	112-31-2
CHEBI_29309	methyl	Yes	2229-07-4
CHEBI_29805	glycolate		
CHEBI_35701	ester		
CHEBI_18346	vanillin	Yes	121-33-5
CHEBI_22695	base		
CHEBI_25627	octadecadienoic acid		
CHEBI_27542	methyl oleate		
CHEBI_32368	undecanoic acid	Yes	112-37-8
CHEBI_32544	nicotinate		
CHEBI_35209	label		
CHEBI_35366	fatty acid		
CHEBI_42504	pentadecanoic acid	Yes	1002-84-2
CHEBI_48408	ethyl vanillin	Yes	121-32-4

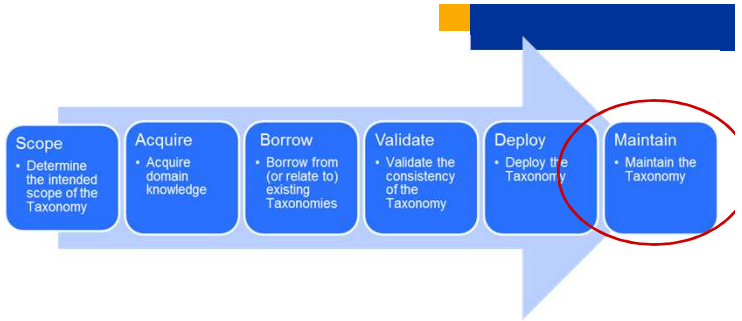
Deploy



- **Several alternatives**
  - **Internal**
    - **Only for inter agency systems , users, and authorized partners**
    - **Normative**
  - **External**
    - **Available to external communities of interest**
      - **Open Source ontology?**
      - **National Center for Biomedical Ontology?**
      - **NCI EVS (Enterprise Vocabulary Services (EVS)?**
    - **Guidance and reference**
  - **A combination of both**

Alternatives being evaluated

Maintain

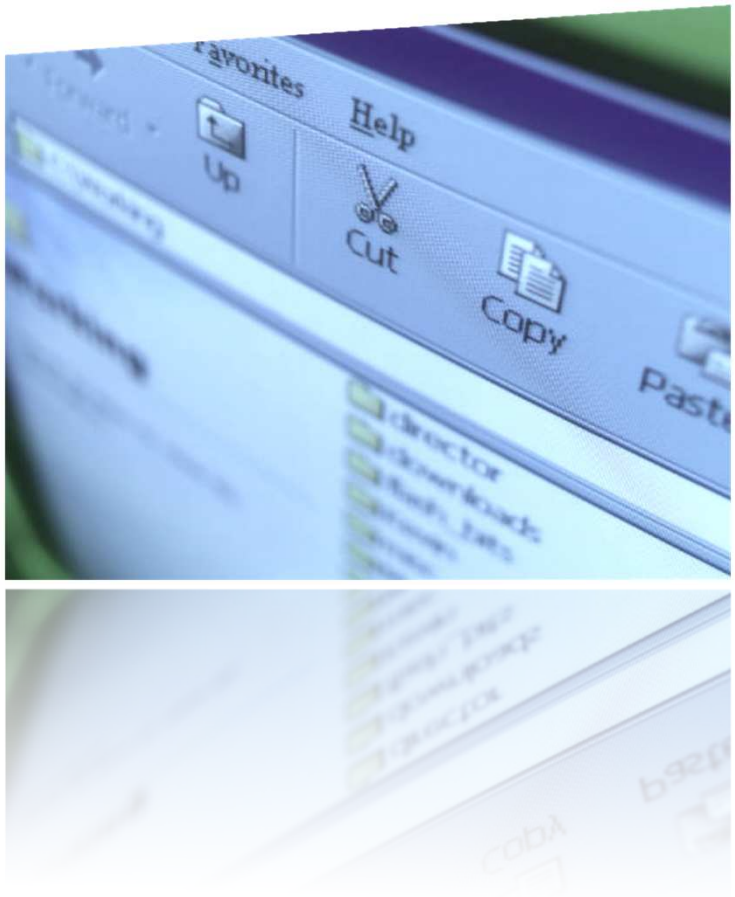


- Create a taxonomy management group
  - Unified team composed of key stakeholders
  - Data standard group

- Leverage collaborative development tools, such as Collaborative Protégé, supporting:
  - Discussion threads
  - Proposing and voting
  - Annotating ontology components
  - Support for user, groups, and access policies
  - Version and release control

Tools

- Ontology Engineering Tool
  - Protégé
  - TopBraid
- Semantic Text Mining
  - ODIE
  - NCBO Annotator
  - Open Calais
  - SmartLogic
- Ontology repository
  - Virtuoso
  - AllegroGraph



Market research is in progress:
This list is not exhaustive

Conclusion

- Semantic Web technology and products can be used integrate heterogeneous data sources in an architecture where semantics plays a pivotal role with metadata exchanges and ontology-based searches

- Semantic Text Mining tools allow analysts to:
  - execute queries which combine structured data with unstructured data
  - navigate unstructured data in a structured way

- Ontologies, taxonomies, and vocabularies can improve the productivity of those who need to review and evaluate large amount of documentation from different information sources