Accelerating Materials Genome Ontology Development

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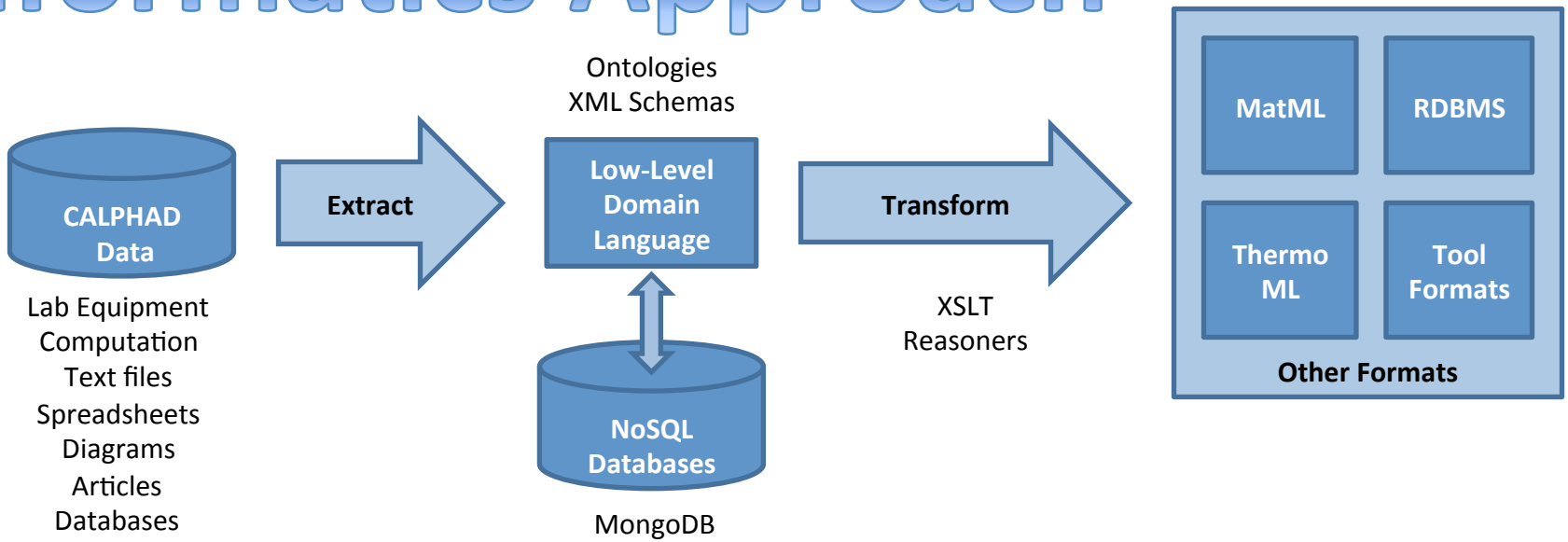
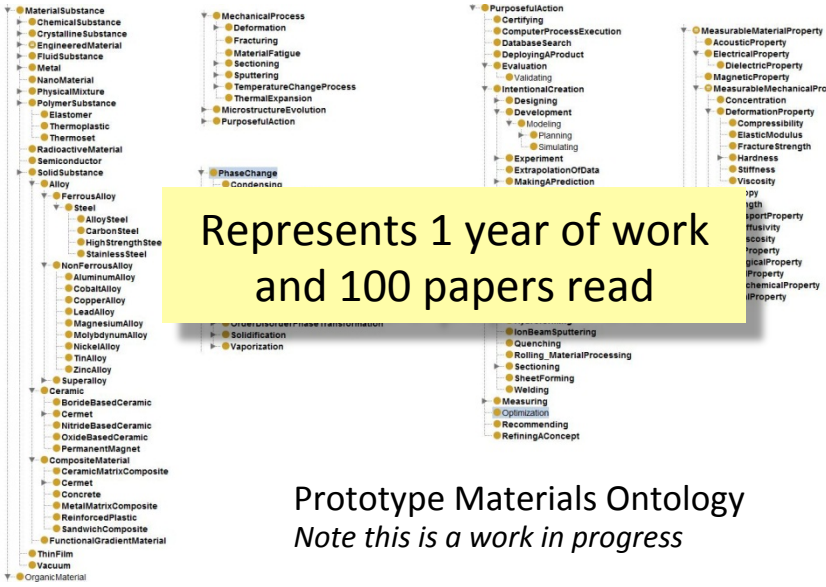
Informatics Approach

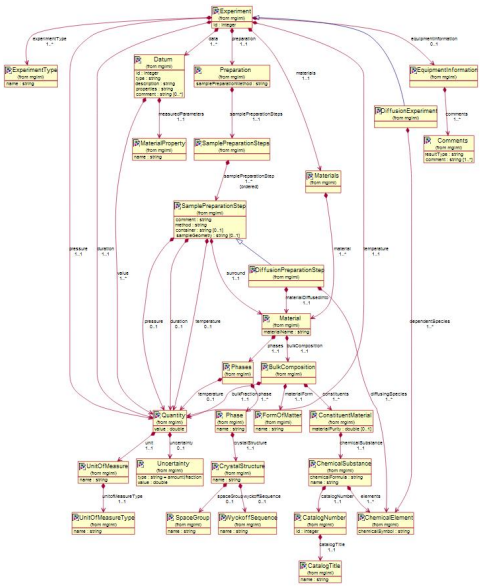




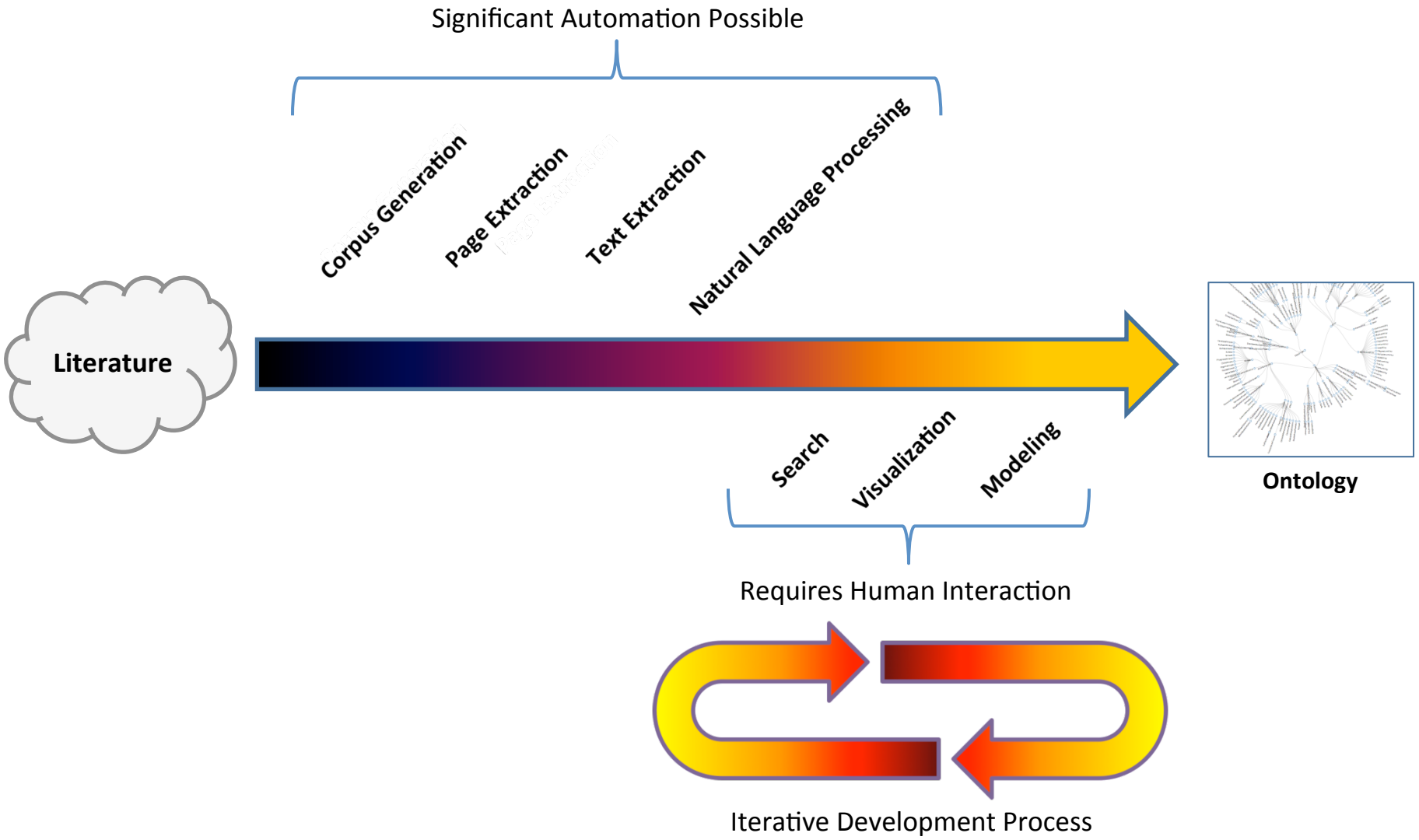
Represents 1 year of work and 100 papers read

Prototype Materials Ontology
Note this is a work in progress

Section of XML Schema



Informatics for Ontology Acceleration



Facilitating Materials Ontology Development via NLP and Machine Learning

Starting with a corpus of 5893 PDFs

1 ⇨ 2 ⇨ 3 ⇨ 4

MS&T 2011, 2012

TMS 2009, 2010, 2011, 2012

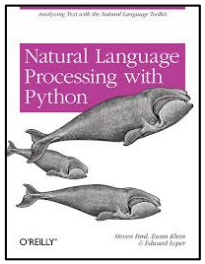
NIST Diffusion Data Center

www.matscitech.org www.tms.org patapsco.nist.gov/diffusion

OCROPUS

thoonk.py

redis



gensim

python

radimrehurek.com/gensim

www.nltk.org

5893 PDFs - 5.8 GB

63K pages

3.8M lines

53GB

3.4M lines extracted

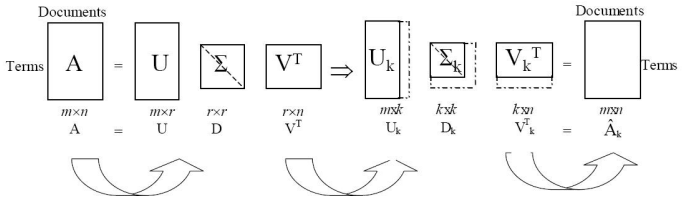
20M tokens

Extract text[1,2]

```
temperatur  66132
materi      53364
process     47990
diffus      45893
result      43681
surfac      33328
```

Identify key stems by frequency[3]

Use Latent Semantic Indexing to group similar concordance entries[4]



http://liqiangguo.wordpress.com/2011/06/09/latent-semantic-analysis/

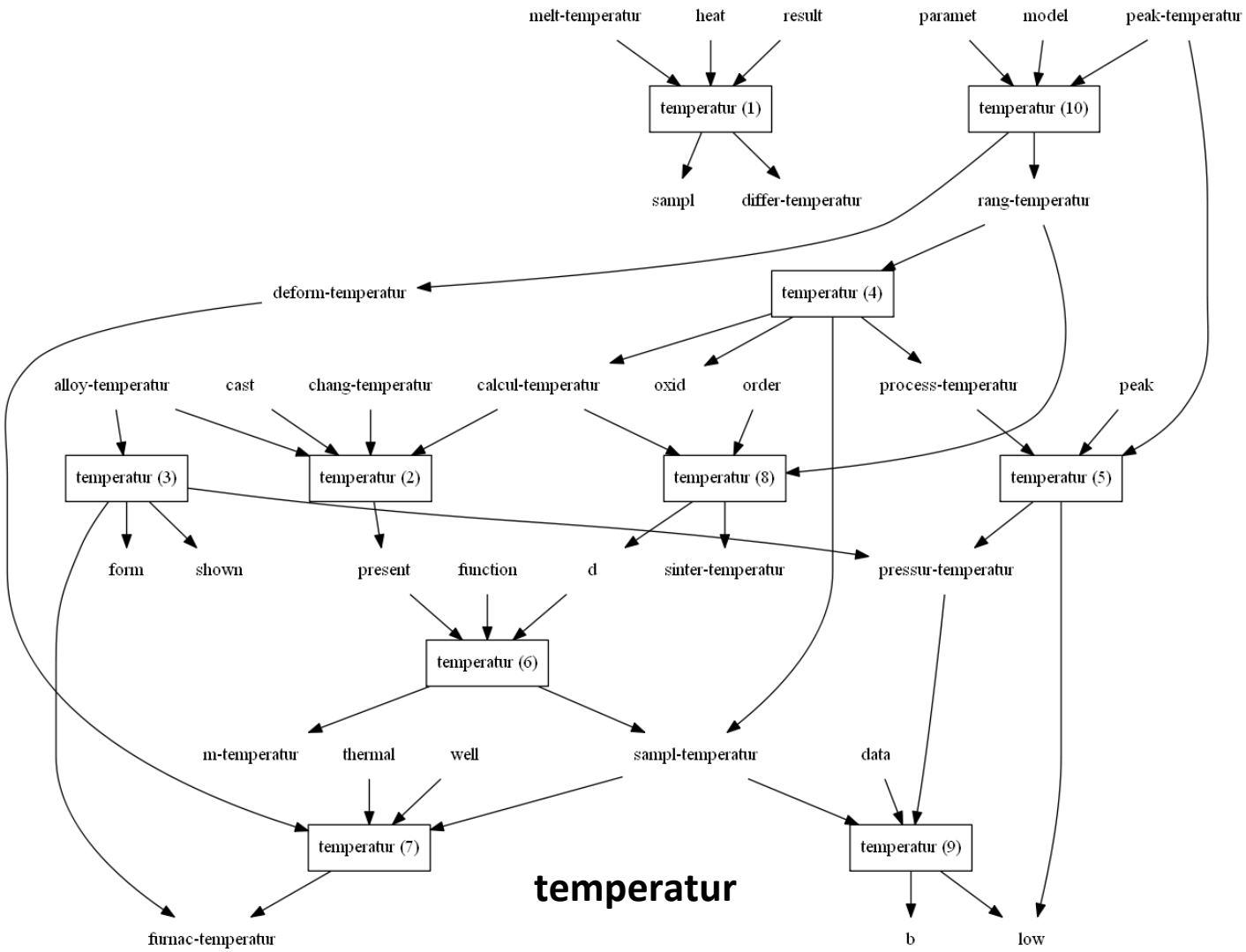
Generate concordances for key stems[3]

```
tivity method. Lattice diffusion coefficients and grain boundary diffusion coe
nts and grain boundary diffusion coefficients were measured. Plots of the data
r all the alloys , the diffusion coefficients at tempe- ratures 1150 'C and hi
, were only accepted. From these coefficients , the parameters of temperature
 those alloys the self-diffusion coefficients of which were also determined at
ting intercrystallite diffu sion coefficients , the following rel ation coeffi
 place. Values of bulk diTfusion coefficients at temperatures below 1j50 ' C w
```

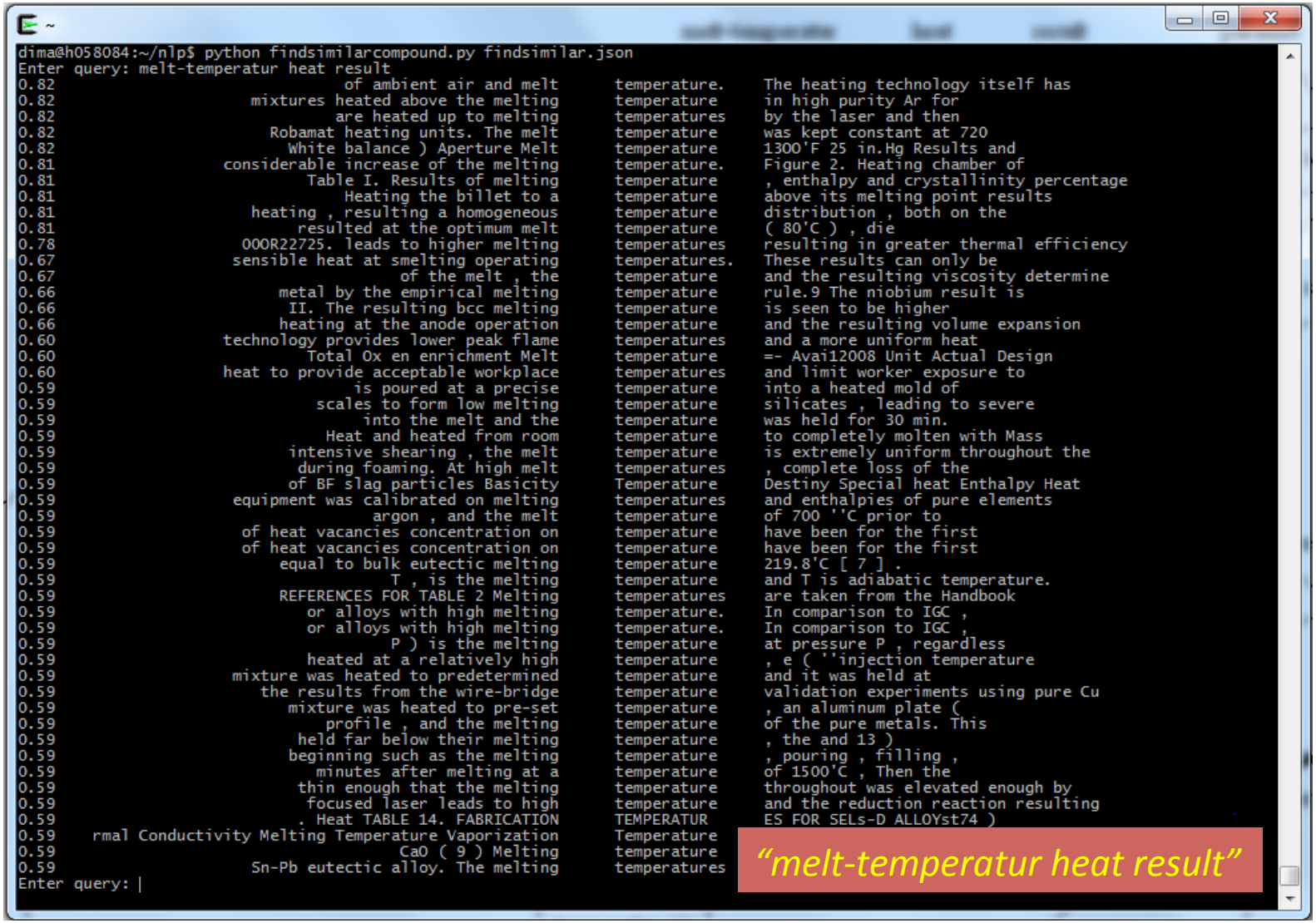
Cosine Distances Between Stems

	temperatur	diffusi	diffusion	equilib	equilibr	equilibria	equilibrium	entropi	enthalpi	energi	crystal	compos	composi	composit	thermo	thermodi	thermodynam	pressur	densit	densiti	liquid	solution	defect	gradient
temperatur	**1.00**	0.83	0.95	-0.04	0.99	-0.11	-0.18	0.01	0.01	-0.09	-0.06	0.18	0.44	-0.11	0.08	-0.06	0.02	0.06	-0.12	-0.10	-0.04	0.45	-0.12	0.50
diffusi	0.83	**1.00**	0.85	0.06	0.81	0.00	-0.14	0.20	0.19	0.37	-0.13	0.19	0.51	-0.11	0.18	-0.03	0.02	0.02	-0.16	-0.14	0.15	0.47	0.03	0.46
diffusion	0.95	0.85	**1.00**	0.26	0.96	0.18	-0.09	0.09	0.09	-0.03	-0.04	0.38	0.66	-0.14	0.33	0.16	0.21	0.19	-0.21	-0.16	-0.05	0.42	-0.02	0.45
equilib	-0.04	0.06	0.26	**1.00**	0.05	0.94	0.51	0.12	0.12	-0.10	-0.03	0.54	0.77	-0.01	0.88	0.85	0.71	0.47	-0.16	-0.11	0.07	0.02	0.18	0.09
equilibr	0.99	0.81	0.96	0.05	**1.00**	-0.04	-0.09	-0.03	-0.03	-0.11	-0.04	0.22	0.50	-0.11	0.15	0.02	0.09	0.11	-0.14	-0.13	-0.04	0.43	-0.11	0.54
equilibria	-0.11	0.00	0.18	0.94	-0.04	**1.00**	0.33	0.11	0.12	-0.07	0.01	0.53	0.72	0.04	0.93	0.91	0.81	0.18	-0.16	-0.09	0.04	0.07	0.11	-0.14
equilibrium	-0.18	-0.14	-0.09	0.51	-0.09	0.33	**1.00**	0.01	-0.02	-0.12	-0.04	-0.01	0.40	0.02	0.39	0.48	0.36	0.43	0.03	-0.11	0.08	-0.28	0.25	0.62
entropi	0.01	0.20	0.09	0.12	-0.03	0.11	0.01	**1.00**	1.00	-0.07	-0.06	0.06	0.39	-0.04	0.09	-0.08	-0.16	0.05	0.06	0.02	-0.07	-0.02	0.75	0.02
enthalpi	0.01	0.19	0.09	0.12	-0.03	0.12	-0.02	1.00	**1.00**	-0.10	-0.06	0.06	0.39	-0.04	0.09	-0.07	-0.15	0.00	0.05	0.02	-0.04	0.01	0.72	-0.02
energi	-0.09	0.37	-0.03	-0.10	-0.11	-0.07	-0.12	-0.07	-0.10	**1.00**	-0.04	0.03	-0.09	-0.05	0.03	-0.08	-0.04	-0.07	-0.06	-0.05	-0.02	-0.10	0.00	0.01
crystal	-0.06	-0.13	-0.04	-0.03	-0.04	0.01	-0.04	-0.06	-0.06	-0.04	**1.00**	0.71	0.15	-0.05	0.00	-0.05	-0.04	-0.06	-0.04	-0.03	-0.03	0.04	0.50	0.05
compos	0.18	0.19	0.38	0.54	0.22	0.53	-0.01	0.06	0.06	0.03	0.71	**1.00**	0.62	-0.05	0.49	0.33	0.25	0.33	-0.22	-0.11	-0.01	0.16	0.46	0.06
composi	0.44	0.51	0.66	0.77	0.50	0.72	0.40	0.39	0.39	-0.09	0.15	0.62	**1.00**	-0.01	0.79	0.64	0.55	0.29	-0.21	-0.21	0.01	0.19	0.43	0.41
composit	-0.11	-0.11	-0.14	-0.01	-0.11	0.04	0.02	-0.04	-0.04	-0.05	-0.05	-0.05	-0.01	**1.00**	0.18	0.15	-0.11	-0.05	0.00	-0.03	-0.07	-0.17	0.00	0.18
thermo	0.08	0.18	0.33	0.88	0.15	0.93	0.39	0.09	0.09	0.03	0.00	0.49	0.79	0.18	**1.00**	0.95	0.86	0.12	-0.07	-0.04	-0.13	0.05	0.14	0.10
thermodi	-0.06	-0.03	0.16	0.85	0.02	0.91	0.48	-0.08	-0.07	-0.08	-0.05	0.33	0.64	0.15	0.95	**1.00**	0.94	0.05	-0.02	-0.01	-0.11	0.00	-0.03	0.03
thermodynam	0.02	0.02	0.21	0.71	0.09	0.81	0.36	-0.16	-0.15	-0.04	-0.04	0.25	0.55	-0.11	0.86	0.94	**1.00**	-0.14	0.03	0.04	-0.15	0.09	-0.15	-0.08
pressur	0.06	0.02	0.19	0.47	0.11	0.18	0.43	0.05	0.00	-0.07	-0.06	0.33	0.29	-0.05	0.12	0.05	-0.14	**1.00**	-0.15	-0.12	-0.06	-0.27	0.26	0.42
densit	-0.12	-0.16	-0.21	-0.16	-0.14	-0.16	0.03	0.06	0.05	-0.06	-0.04	-0.22	-0.21	0.00	-0.07	-0.02	0.03	-0.15	**1.00**	0.97	0.00	0.40	0.15	0.03
densiti	-0.10	-0.14	-0.16	-0.11	-0.13	-0.09	-0.11	0.02	0.02	-0.05	-0.03	-0.11	-0.21	-0.03	-0.04	-0.01	0.04	-0.12	0.97	**1.00**	0.01	0.48	0.10	-0.10
liquid	-0.04	0.15	-0.05	0.07	-0.04	0.04	0.08	-0.07	-0.04	-0.02	-0.03	-0.01	0.01	-0.07	-0.13	-0.11	-0.15	-0.06	0.00	0.01	**1.00**	0.63	-0.16	0.02
solution	0.45	0.47	0.42	0.02	0.43	0.07	-0.28	-0.02	0.01	-0.10	0.04	0.16	0.19	-0.17	0.05	0.00	0.09	-0.27	0.40	0.48	0.63	**1.00**	-0.14	0.00
defect	-0.12	0.03	-0.02	0.18	-0.11	0.11	0.25	0.75	0.72	0.00	0.50	0.46	0.43	0.00	0.14	-0.03	-0.15	0.26	0.15	0.10	-0.16	-0.14	**1.00**	0.26
gradient	0.50	0.46	0.45	0.09	0.54	-0.14	0.62	0.02	-0.02	0.01	0.05	0.06	0.41	0.18	0.10	0.03	-0.08	0.42	0.03	-0.10	0.02	0.00	0.26	**1.00**

Topic Models



LSI-based Query



Semantic Medline (SM)

1. What is it?

1. SM is a semantic layer on top of PubMed
2. SM supports semantic applications of semantic search, semantic visualization, and automatic summarization

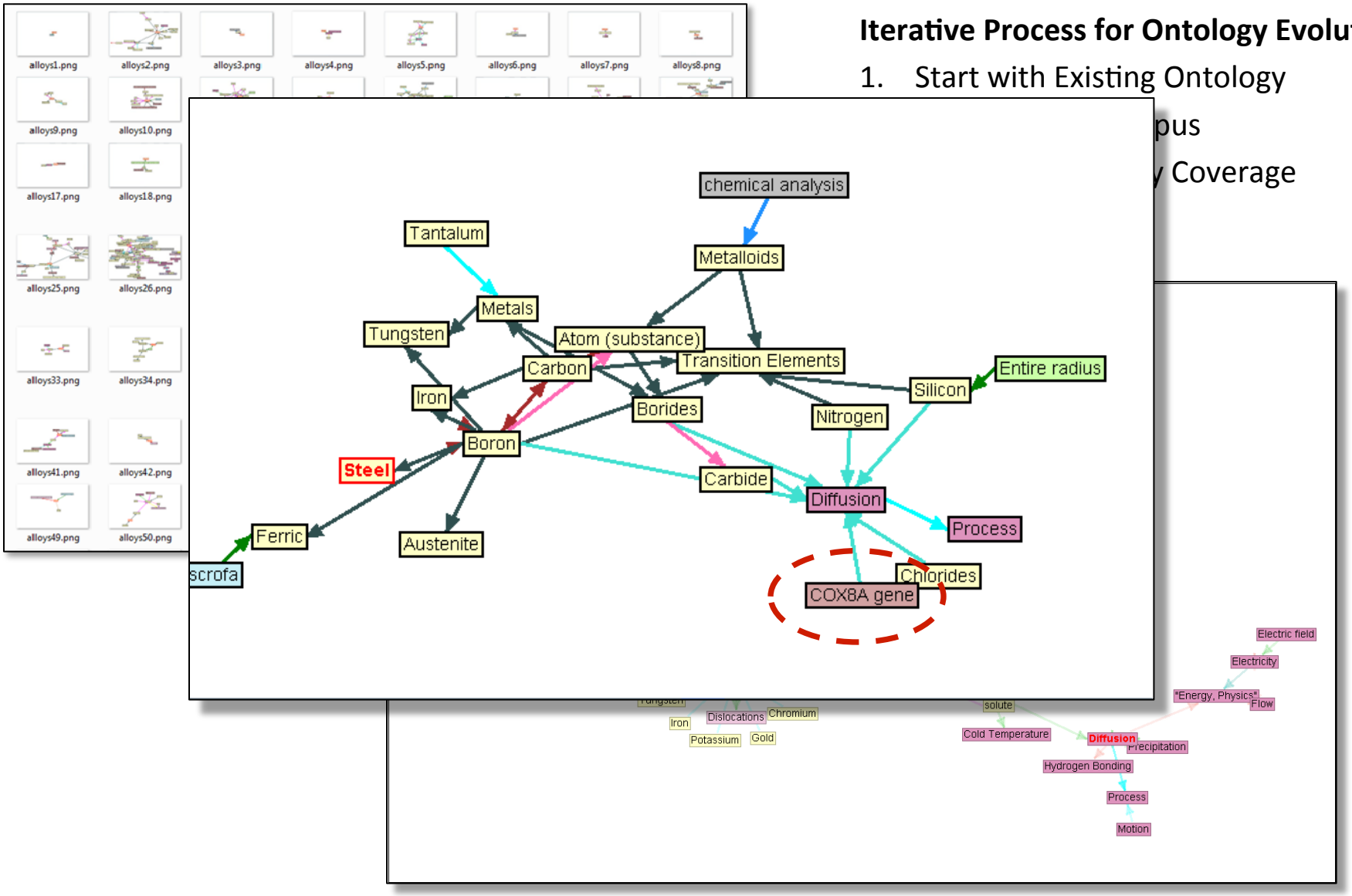
2. Collaborators: NIH/NLM

3. How does it work?

1. Supported by DB of corpus-based semantic information
2. Uses search to access semantic-info which supports semantic application operations

4. GOAL: *Retarget* SM from **biomedical** domain to **MS** domain.

Ab Initio Ontology – Semantic Medline



Iterative Process for Ontology Evolution

1. Start with Existing Ontology

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Coverage

Ontology Acceleration - Recap