The Neuroscience Information Framework: A Scalable Platform for Information Exploration and Semantic Search Computing

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NEUROSCIENCE INFORMATION FRAMEWORK

NIF is an initiative of the NIH Blueprint consortium of institutes

- What types of resources (data, tools, materials, services) are available to the neuroscience community?
- How many are there?
- What domains do they cover? What domains do they not cover?
- Where are they?
 - Web sites
 - Databases
 - Literature
 - Supplementary material
- Who uses them?
- Who creates them?
- How can we find them?
- How can we make them better in the future?

PDF filesDesk drawers

2013 Summer Institute: Discover Big Data, August 5-9, San Diego, California

http://neuinfo.org

Discovery and utilization of web-based resources for neuroscience

WORK

earch NI

Search No

UCSD, Yale, Cal Tech, George Mason, Washington Uni

Literature Database Federation

Search for All Things Neuroscience

SEARCH TIPS | WHAT IS THIS? (example searches: cerebellum, genetic analysis software, gene:grm1)

- ABOUT

About NIF
People
Publications
Presentations
Brochures
Testimonials
Release Notes 5.1
FAQ
, NIF PRODUCTS
, NIF DATA SHARING
, NIF SYSTEM
, SOCIAL MEDIA

You Tube

Registered with NIF? Place this icon on your site.

Registered NIF

3



NEUROSCIE



Share your data with NIF

Data Sharing Plans | Lab Data Management | Large Data

Click to find out mor



NIF NAVIGATOR



LITERATURE → PubMed (22361958)

NIF DATA FEDERATION \rightarrow

DATA TYPE

Animals (136449) Annotation (17450074) Antibodies (2240902) Atlas (267687512) Biospecimen (253392) Brain Activation Foci (56588) Clinical Trials (274674) Connectivity (50316) Dataset (10397) Disease (3459177) Drugs (3412505) Genes (246030) Grants (2720110) Images (923534) MRI (574809) Microarray (312869038) Models (1414) Multimedia (87247) Pathways (789668) People (377) Phenotype (564493) Plasmids (27649) Registries (6371) Software (1857)

NERVOUS SYSTEM LEVELS Brain Regions (42777)

Cellular Level (59136) Genes (62671895) Molecular Level (693109) Nervous System Function (68672)

NIF REGISTRY (6078) →

A portal for finding and using neuroscience resources

A consistent framework for describing resources

Provides simultaneous search of multiple types of information, organized by category

Supported by an expansive ontology for neuroscience

June10, 2013

Utilizes advanced technologies to search the "hidden web"

NIH Blueprint for Neuroscience Research

A Big, Fat Techno-Philosophical Question

How do we create an information infrastructure that is able to connect a person or a community with the resources they need to accomplish their task at hand?

Resource

- Anything that is tangible and accessible
 - a product, a person, an institution, a piece of data, a connection ...

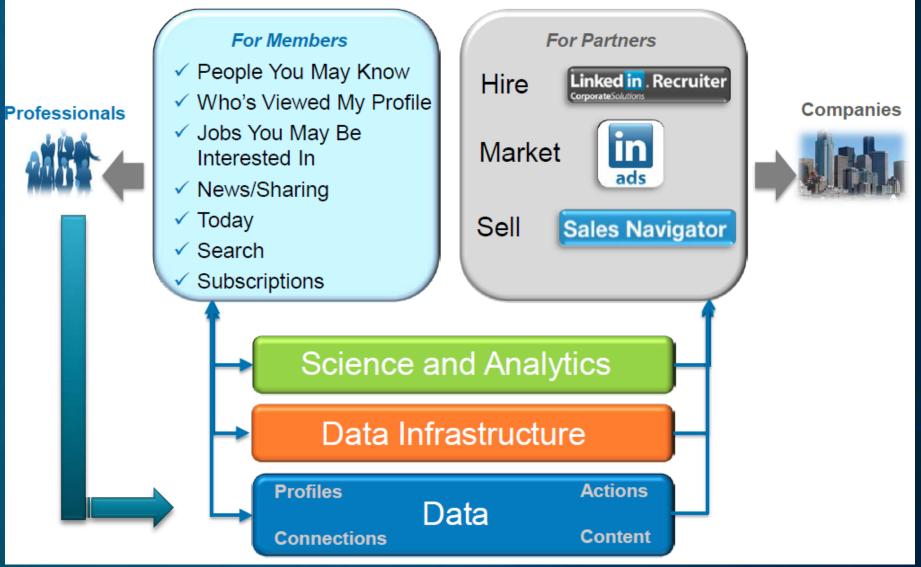
Information Infrastructure

- Enables the entire life cycle of information from acquisition to (potential)archival
- Allows people to find, access, understand and work with information
- A domain-specific example:

Linked in 。

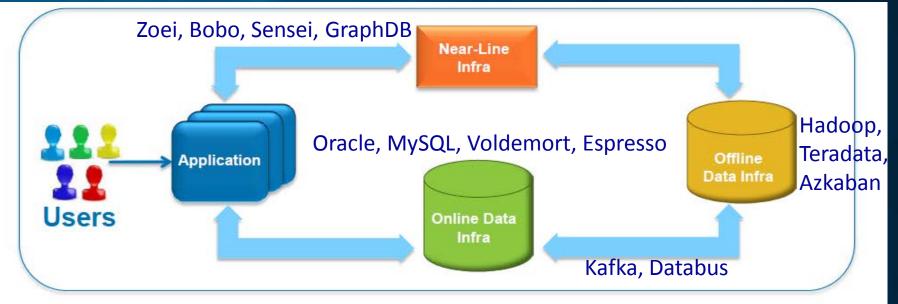
A Digression – Looking at LinkedIn

Credit: Bhaskar Ghosh, LinkedIn



A Digression – Looking at LinkedIn

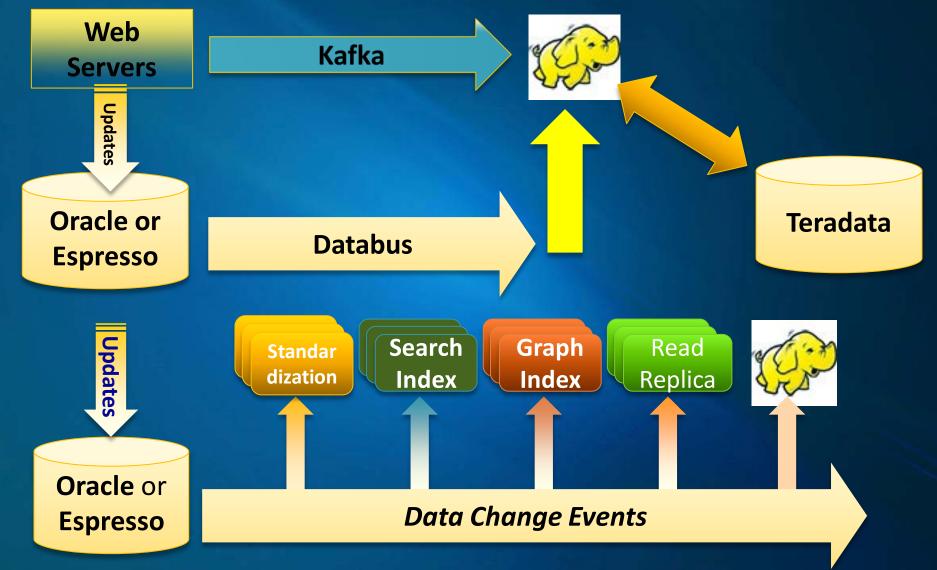
Credit: Bhaskar Ghosh, LinkedIn



Infrastructure	Latency & Freshness Requirements	Products
Online	Activity that should be reflected immediately	 Member Profiles Company Profiles Connections Skills
Near-Line	Activity that should be reflected soon	 Activity Streams Profile Standardization News Messages
Offline	Activity that can be reflected later	 People You May Know Recommendations Connection Strength Next best idea News

A Digression – Looking at LinkedIn

Credit: Hien Luu, Sid Anand, LinkedIn



Resource Finding in Biomedical Sciences



Researcher Activity

✓ Where is data about X?
 ✓ How does Y relate to Z?
 ✓ Accumulate and Analyze
 ✓ Compare X and Y
 ✓ Subscribe to topic T
 ✓ Recommend Resource

- ✓ Funding reports
- ✓ Search and Explore
- ✓ News

Resource Activity

- Resource Promotion
- ✓ Utilization Search
- ✓ Cross-Utilization

Experiential Services

Analysis & Science

Data Infrastructure

Data

And yet, biomedical resource finding is a hard problem

Resource Finding in Biomedical Sciences



Researcher Activity

Where is data about X?
How does Y relate to Z?
Accumulate and Analyze
Compare X and Y
Subscribe to topic T

- ✓ Recommend Resource
- ✓ Funding reports
- ✓ Search and Explore
- ✓ News

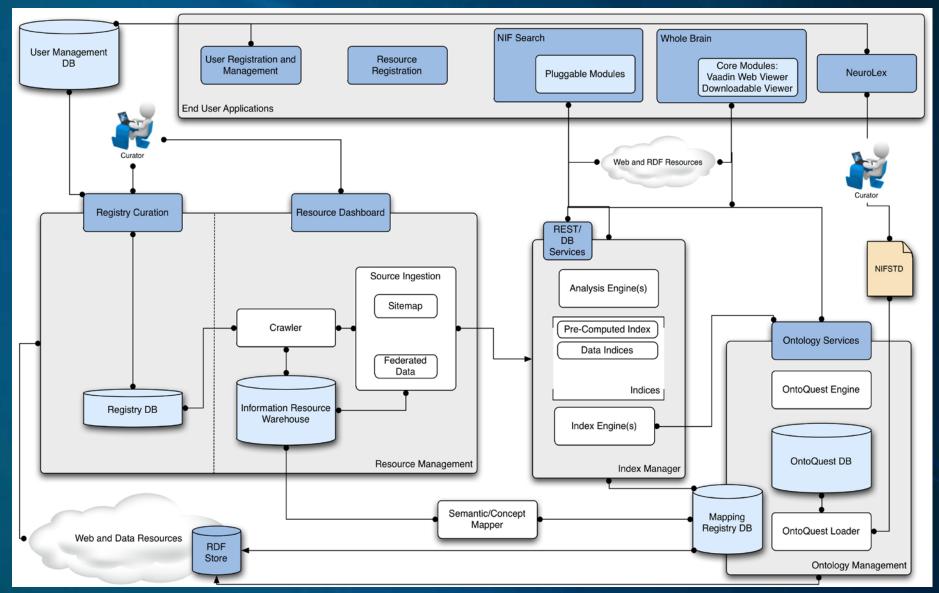
Resource Activity

- Resource Promotion
- ✓ Utilization Search
- ✓ Cross-Utilization

Experiential Services



NIF Architecture



The "Resource Identification" Problem

- Given an infinite number of web accessible resources, which are relevant for Neuroscience?
- Easy Case
 - A resource assigned by a trusted source
- Reasonably Easy Case
 - A resource recommended by a potentially trustable source
- Not-so-easy Case
 - "Mine" for resources from literature/crawler
 - Auto-filter by semantic classification
 - Fully validate by curatorial staff/community 2013 Summer Institute: Discover Big Data, August 5-9, San Diego, California

Semantic Classification

- Is this a potential neuroscience resource?
 - Two-pronged classification problem
 - If it belongs to the class, a reasonable portion of the document term vector will align with a neuroscience vocabulary
 - Necessary but not sufficient
 - The "spread" of the document term vector with respect to a reasonable domain ontology will be limited
 - Pragmatic problems
 - What additional (recognizable) descriptors does the resource have?
 - Is the resource "current"?
 - Are there "other ways" of getting to the content of the site?

Ingestion and Transformation Provenance

- DISCO NIF's Ingestion Manager and Data Tracker
 - "Relationalizes" incoming data when needed
 - Feeds the curators' dashboard for ingestion, update and index management
 - Executes automatic updates per schedule
 - Keeps track of chains of derived views defined by curators
 - Maintains annotations on data and its views
 - Propagates data updates to all derived views through curator notification

The "Information Variety" Problem

The data come

- From too many disparate sources
 - 6000+ neuroscience resources
- In too many different formats and models
 - Relational, XML, RDF, Text, domain-specific, ...
- Having all too diverse semantics
 - "GRM1": a string, a gene, a chromosomal region, a list of interesting SNPs in mice?
- There is a massive data integration problem because only integration of data will lead to insight
 - What possible drugs might be repurposed for human inclusion body myopathy (HIBM)?
 - Data about/from the following to be integrated
 - Organisms, diseases, cross-organism anatomy, phenotypes, genes, proteins, interactions, pathways, genomic variations, pharmaceutical compounds, assays and publications

Hybrid Integration Strategy

- Data integration using schema mappings for similar resources
- Semantics-based integration
 - Using ontologies as the unifying structure
 - Using vocabularies as the connecting substrate

When possible

- Using linked-data graph where applicable
 - Link inference
 - Link prediction

Using machine learning

Term association using active learning with conditional random fields

Integration using Schema Mapping

Commercial solutions exist

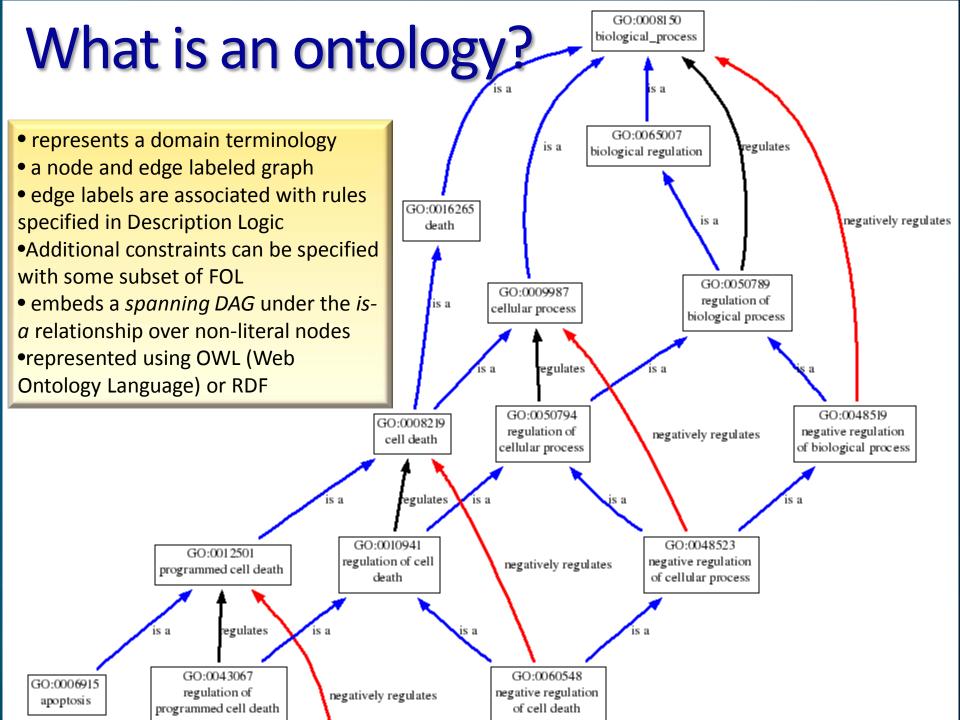
They are not very scalable as number of schemas increase

Many groups working on it

- Data Tamer an MIT-Intel partnership project on Big Data
 - Matches schema where possible
 - Crowd-sources ambiguous cases
 - Performs entity-consolidation by data clustering
- Our approach
 - Curators use small scale schema mappings using ontology and Google Refine

Know Thy Landscape – Semantic Scouting

- Gather the language of the domain
 - Terms, their variations and term properties
 - "Verbs", relationships, their linguistic variations and their properties
 - Constraints that hold in the domain
- Sources
 - Ontologies
 - Folksonomies
 - image tags, text annotations, ...
 - Literature
 - figure and table captions
 - Data (structured or semi-structured)



Ontology Processing with OntoQuest

- colassi

The exocrine pancreas is composed of acinar enithelial cells and ductal enithelium that m

property name="OBO foundry unique label">exocrine pancreas (zebrafish)</proper

The exocrine pancreas produces and store zymogens of digestive enzymes, such as chym epithelium that manufacture the proteolytic enzymes and bicarbonate required for digestion. [definition

espace">zebrafish anatomy</property property name="database_cross_reference">ZFIN:ZDB-ANAT-050711-6</propert

<id InternalId="264198-1">ZEA_0001249</id> ame>ZFA 0001249</name> <a>label>exocrine pancreas</abel> <url>http://purl.obolibrary.org/obo/ZFA_0001249</url

property name-"has obo nar

property name="id">ZFA:0001249</property>

<property name="id">ZFA:0001249</property></property> property name="database_cross_reference">TAO:0001249</pr

<id InternalId="247995-1">UBERON_0000017</id> <name>UBERON 0000017</name> label>exocrine panereas</label>

url>http://purl.obolibrary.org/obo/UBERON_0000017</url>

<comments>

</r> comments

</other_properties> /class>

comments>

(comment)

dd Internalld="357740-1">HP 0001049</id 0101000 EU

A graph query engine for ontological graphs •

- Accepts OWL, RDFS, RDF ٢
- Ingestors for special cases can be developed ٢
 - MESH XML DTD
- 0 Has a service API

1. Get all human phenotypes property name="database_cross_reference">CALOHA:TS-1241</propert</pre> property name="database_cross_reference">EV:0100093</property http://nif-services-stage.neuinfo.org/ontoquest-lamhdi/concepts/search/HP 2. Find superclasses of "exocrine pancreas" First: http://nif-services-stage.neuinfo.org/ontoquestlamhdi/concepts/term/exocrine+pancreas Then, from the result of the above: http://nif-services-stage.neuinfo.org/ontoquestlamhdi/rel/superclasses/UBERON 0000017 3. Find all direct properties of UBERON 0000017 http://nif-services-stage.neuinfo.org/ontoquest-lamhdi/rel/children/UBERON 0000017 **COMBINED WITH** http://nif-services-stage.neuinfo.org/ontoquest-lamhdi/rel/parents/UBERON 0000017

Computing with OntoQuest

Which skeletal structures in the zebrafish develop from the mesenchyme?

- Return \$x where
 - (\$x (subclassOf)* 'skeletal element') and
 - (\$x develops_from* 'ZFA:mesenchyme')
 - Return \$y where
 - (\$y subclassOf* \$x)
- Query Rewriting
- Return \$x where
 - (\$x develops_from* `mesenchyme') and
 - (\$x has_ontology \$o) (\$x equivalent_to \$z) (\$z has_ontology 'ZFA') and
 - (\$x (subclassOf)* 'skeletal element')

	<pre>- <relationship> - <subject id="SomeValuesFrom Restriction" internalid="118064-3"> something [exists]"develops from" "future cardiac ventricle" </subject> <property id="RO_0002202" internalid="4558-15">RO_0002202</property> <object id="UBERON_0010226" internalid="590274-1">future cardiac ventricle</object> </relationship> - <relationship> - <relationship> <subject id="ZFA_0009351" internalid="591402-1">thromboblast</subject> RO_0002202</relationship></relationship></pre>
"develops from"	<pre><pre><pre><pre><pre><pre><pre>cobject InternalId="591954-1" id="ZFA_0009022">megakaryocyte erythroid progenitor cell </pre></pre></pre></pre></pre></pre></pre>
http://nif-services-	- <relationship></relationship>
	<subject id="UBERON_0004764" internalid="585974-1">intramembranous bone tissue</subject> <property id="RO_0002202" internalid="4558-15">RO_0002202</property>
stage.neuinfo.org/ontoquest-	<object id="UBERON_0003104" internalid="583746-1">mesenchyme</object>
lamhdi/rel/edge-relation/id/RO_0002202	- <relationship></relationship>
	- <subject id="SomeValuesFrom Restriction" internalid="114818-3"> something [exists]"develops from" "early telencephalic vesicle"</subject>
	 <property id="RO 0002202" internalid="4558-15">RO 0002202</property>
	<object id="UBERON_0009676" internalid="585190-1">early telencephalic vesicle</object>
	 - <relationship></relationship>
	<subject id="UBERON_0000080" internalid="584423-1">mesonephros</subject> <property id="RO_0002202" internalid="4558-15">RO_0002202</property>
	<object id="UBERON_0002120" internalid="588719-1">pronephros</object>
"equivalenceClass" http://nif-services-stage.neuinfo.org/ontoquest- lamhdi/rel/children/term/skeletal%20element?lev el=1	<pre> <relationship> <subject id="ZFA_0005494" internalid="777193-1">skeletal element</subject> <subject id="equivalentClass" internalid="5360-15">equivalent</subject> <subject id="UBERON_0004765" internalid="585975-1">skeletal element</subject> </relationship> </pre>
	<relationship></relationship>
	<subject <="" internalid="778440-1" th=""></subject>
Subclasses of "skeletal element" (incl. its	id="ZFA_0001635">intramembranous
equivalenceClasses) in ZFA	bone <property <="" internalid="5389-15" th=""></property>
http://nif-services-stage.neuinfo.org/ontoquest-	id=" <i>subClassOf</i> ">subClassOf <object< th=""></object<>
lamhdi/rel/subclasses/term/skeletal%20element?level=3	InternalId="777874-1" id="ZFA_0001514">bone
	 element

The Entity Recognition Problem

Tagging of Antibody Records using a machine learning technique with Conditional Random Fields

A first-order linear-chain CRF

$$p_{\Lambda}(\mathbf{y}|\mathbf{x}) = \frac{1}{\mathsf{Z}(\mathbf{x})} \exp(\sum_{t=1}^{\mathsf{T}} \sum_{k=1}^{\mathsf{K}} \lambda_k \mathbf{f}_k(\mathbf{y}_{t-1}, \mathbf{y}_t, \mathbf{x}, \mathbf{t}))$$

Expression|0:{NN,NPC} of|0:{IN}

belonging to any NE by 0.

where

- glutamate|B-PROTEIN:{NN,NPC}
 glutamate|B-PROTEIN:{NN,NPC}
 carboxypeptidase|I-PROTEIN:{VBP} II|I-PROTEIN:{NNP,NPC}
- x input data. in | 0: {IN} human | 0: {JJ} brain | 0: {NN, NPC} . | 0: {.}
- f_k(y_{t-1}, y_t, x, output(IOB la
 An example sentence labeled via extended IOB format. The prefix B denotes the beginning on a named entity.

 λ_k weight of t maximum like

Z(x) normaliz

t index to the

 IOB format is extended to include additional information, namely, part-of-speech tags and noun phrase membership.

• The rest of terms in the NE are denoted by the prefix I and terms not

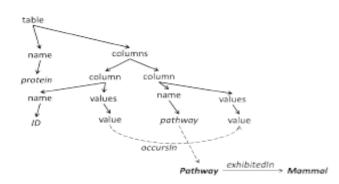
The Learning Tool and Minimal Models

000	Named Entity Annotator Tool				
File Tools	Help				
C 🛍 🛸	Named Entities Extracted Records				
antibody 🗧					
Sentences	Named Entity Annotator Tool				
Next , the sections were incubated	Is Named Entities Extracted Records	Help			
Antibodies -LRB- anti-ERK , anti-p	Named Enuties Extratieu Records				
Anti-BrdU antibody was obtained fi Single cells were cultured in DMEM-	ody Filter Sentence contains Full Set NE Stats				
For immunofluorescence double lat	65				
, meet this is a set of the the the	he sections were incubated with 1:50 anti-D2 receptor mouse monocional IgG -LRB- D2DR , Santa Cruz Biotechnology -RRB- and 1:1000 anti-SHT1A receptor rabbit polyco	c			
Anti-Record Anti-R	ies -LRB- anti-ERK, anti-p-ERK, anti-JNK, anti-p-JNK, anti-p38, anti-p-p38, anti-β actin and anti-cleaved caspase 3 -RRB- were obtained from Cell Signaling. IU antibody was obtained from Sigma, anti-TuJ antibody was from Covance, anti-S100 antibody was from Dako, and anti- MBP was from Novus Biologicals. OPG and RAN	N			
	ells were cultured in DMEM-high glucose and F12 -LRB- mixed 1:1 -RRB- supplemented with N2 and B27 -LRB- Invitrogen -RRB- , EGF -LRB- 20 ng\/mL ; Chemicon -RRB iunofluorescence double labeling -LRB- n = 3 -RRB- , brain sections -LRB- – 2.56 to – 3.30 caudal to the bregma , i.e. levels 1 and 2 -RRB- were first incubated in BS fol				
	1000000000000000000000000000000000000				
The second primer pairs for any	ishing with PBS three times for 5 min , the sections were reacted with Alexa Fluor 488-conjugated anti-rabbit IgG antibody -LRB- 1:500 , invitrogen , Carlsbad , CA -RRB- a tions were incubated with primary antibodies -LRB- RANTES Antibody -LRB- RF478 , 1:10 dilution , R&D SYSTEMS , Minneapolis , MN -RRB- , NeuN -LRB- MAB377 , 1:50 (
For immunodetection of TRPC3 pro	owing primers -LRB- Sigma-Aldrich , Japan -RRB- were used : mouse RANTES -LRB- forward , 5 ' - ATATGCCTCGGACACCC-3 ' ; reverse , 5 ' - TGACAAAGACGACTG	(C			
	The primary antibodies used in this study were purchased from Cell Signaling Technology -LRB- CST, Boston, MA -RRBLRB- total Akt -LRB- # 4691, 1:1000 dilution -RRB-, p Gene-specific primer pairs for amplification of TRPC1, TRPC3, TRPM2, HO-1 and GAPDH were designed using Primer Express ® v2.0 -LRB- Applied Biosystems, Foster City, C				
	For immunodetection of TRPC3 protein, nitrocellulose membranes -LRB- Perkin-Elmer, Woodbridge, ON -RRB- were blocked with 0.5 % egg white albumin -LRB- 1 h, room tem; For immunodetection of TRPM2, membranes were blocked with 5 % milk\/1 % bovine serum albumin -LRB- 1 h, RT -RRB-, then incubated with 1:500 anti-TRPM2 antibody -LRB				
After rinsing in PBS for 5 min , the sec For β -					
antibody -LRB- 1:500 , Wake , Osaka Monock					
The foll	owing cell-type specific markers were used : rabbit polyclonal anti-Olig2 -LRB- Cat #AB 9610 , 1:400 , Millipore , Temecula , CA -RRB- , rabbit polyclonal anti-doublecorti	ie 🛛			
Sections	were stained with rat anti-BrdU antibodies -LRB- Cat #MCA 2060T, 1:500, AbD Serotec, Raleigh, NC -RRB- or mouse monoclonal anti-PCNA -LRB- Cat #sc -25280, 1	1			
L	·				
Antib	ady 1	÷			
-Antibo	dy Frame				
source_organism target antibody close	y polycional antibody -LRB- 1:500 , Wako , Osaka -RRB- for microglia				
vendor	Wako				
Overlapping Entities source	organism rabbit				
After rinsing in PBS for 5 min , the sec antibody - LRB- 1:500 , Wako , Osaka	organism				
clonality	y polyclonal				
catnum					
target	anti-Iba l				
/Users/bozyurt/elsevier10_idx_ie.xml /Users/boz	yurt/elsevier10_idx_ie.xml				

The Mapping Problem – Connecting Data to the Ontology

🖳 🖲 Thing

- --- Oncept
- 🗝 🖲 Entity
- InterConceptRelationship
- 🗝 🛑 InterEntityRelationship
- instanceOfConcept
- referencesConcept
 - isAboutConcept
 - denotesConcept
 - mentionsConcept
- isEquivalentToConcept
 - isEquivalentToSomeInstanceOfConcept
 - isEquivalentToSomeSubclassOfConcept
- referencesEntity
 - isCompositionalPartOfEntity
 - isDescriptorOfEntity
 - 🔻 🛑 isGroupNameOfEntity
 - isClassificationBasedGroupingOfEnity
 - isIdentifierOfEntity
 - isNameOfEntity
 - isPropertyOfEntity
 - isRelationshipOfEntity
- referencesInterConceptRelationship
 - isAboutInterConceptRelationship
 - isEquivalentToInterConceptRelationship
 - isEquivalentToSomeSubpropertyOfInterConceptRelationship
- referencesInterEntityRelationship
 - isCompositionalPartOfRelationship
 - isDescriptorOfRelationship
 - isIdentifierOfRelationship
 - 🗝 🛑 isNameOfRelationship
 - isPropertyOfRelationship



A high-level statement

- The ontology O is a graph of concepts and inter-concept relationships
- The data is a semistructured object S with groupings
- A mapping structure is a graph of mapping edges from S to O + intra-source map edges + intra-ontology map edges

Table: protein(ID, symbol, name, pathway)**Mapping:**

pathway mapsTo ontoID(Pathway). (exhibitedIn(ontoID(Pathway), ontoID(mammal)) AND occursIn(value(ID), value(pathway)))

over Big Data<mark>, August 5-9, San Diego, Calitornia</mark>

The Concept Mapping Tool

2013 Summer Institute: Dis

		Concept	Map Tool						
Browse Add Import									
	View Definition (SQL)			c	heck View & Upo	date Columns			
Basic Information View Definition Mappings Display	<pre>select distinct replace(b.e_uid,':','') as e_uid, replace(replace (b.resource_name, '_', resource_name, b.abbrev, b.availability, b.comment, replace(replace(b.definition, ' ',' b.definingcitation as url, lower(replace(replace(replace(replace (replace(replace(replace(replace(replace (replace(replace(replace(replace(replace (replace(replace(replace(replace(replace ',' from b.has_role),')',''),'0',''),'9',''),'' (nlx_res_',''),'nlx_inv_',''),'_,'')</pre>	Columns Facet Name Modify Column Information Description Basic Information Description Name: species Facet Name: Organism Data Type: VARCHAR Weight: 10		ame Data type					
	<pre>replace(b.is_part_of, 'Resource:','') b.keyword, b.created_date as date_created, b.last_update_date as date_updated, case when b.pmid_is null then '' else nif_pmid_display, O Vocabulary View</pre>	Delimiter: Indexable?: Facet?: Is Key?: Exportable?:	 Yes Yes 	○ No ○ No ④ No ○ No		Add S	emantic Mappin	9	
		Column Mapping	gs						
Source Browser Table/View Ba	rowser 🕷 View Editor 🕷	Add New Delete	Modify						
		Concept Id	Concept Name	On	tology	Rule	Last Upda	Update Time	
		birnlex_2	Organism	NIF			anita	Thu Feb 21 16	
				Save	e Ca	ancel			

Querying the Mapping Structure

What are the top 10 genes you have most information about?

- Which sources have information about "genes"?
 - Find the ontology term for gene \rightarrow CHEBI_23367
 - Call <u>http://cm.neuinfo.org:8080/cm_services/column/mapping/ontoterm?ontologyTermId=CHEBI_23367</u>
 - For each table and column thus found, call http://cm.neuinfo.org:8080/cm_services/column/valuefreqs?s 1&columnName=transgenic_line
 - Now group and rank merge
 - in parallel if needed
 - Get top 10

<results method="getColumnValueFrequencies"> <value freq="209"/> <value freq="4">Etv1-CreERT2</value> <value freq="4">Grik4-Cre</value> <value freq="3">Syt6-Cre</value> <value freq="3">Rbp4-Cre</value> <value freq="3">Nr5a1-Cre</value> <value freq="3">Gal-Cre</value> <value freq="2">Slc6a4-CreERT2</value> <value freq="2">Pmch-Cre</value> <value freq="2">Lepr-IRES-Cre</value> <value freq="2">Ntsr1-Cre</value> <value freq="1">Pomc-Cre (ST)</value> <value freq="1">Oxt-IRES-Cre</value> <value freg="1">Erbb4-2A-CreERT2</value> <value freq="1">Scnn1a-Tg3-Cre</value> </results>

<result source="nif-0000-00096" table="nif-0000-00096-1" column="Gene_/Protein_Name"/>
<result source="nif_0000-34000" table="nif_0000-34000-1" column="gene_symbol"/>
<result source="nif-0000-7730" table="nif-0000-07300-1" column="allele_name"/>
<result source="nif-0000-7730" table="nif-0000-0730-1" column="dB_TARGET"/>
<result source="nif-0000-07310" table="nif-0000-0730-1" column="dB_TARGET"/>
<result source="nif-0000-03213" table="nif-0000-03213-1" column="dB_TARGET"/>
<result source="nif-0000-03213" table="nif-0000-03213-1" column="dB_TARGET"/>

table="nif-0000-23326-1" column="allele type"/> table="nif-0000-02683-1" column="chemicalname"/> table="nif-0000-08127-1" column="gene_symbol"/> ble="nlx 152726-1" column="model receptors"/> le="nlx_98194-1" column="ensembl_gene_symbol"/> ble="nlx 149225-1" column="reverse primer"/> ble="nlx 149225-1" column="encoding protein product"/> ble="nlx 152726-1" column="model neurotransmitters"/> ble="nlx 149225-1" column="rna polymerase"/> le="nlx 23971-1" column="ensembl gene symbol"/> table="nif-0000-02683-2" column="chemicalid"/> table="nif-0000-34000-1" column="allele_symbol3"/> table="nif-0000-00517-1" column="geneset_name"/> table="nif-0000-20925-1" column="symbol"/> table="nif-0000-20925-1" column="cas"/> table="nif-0000-34000-1" column="marker symbol"/> ble="nlx_146253-1" column="transgenic_line"/> " table="nif-0000-20925-1" column="chebi"/> ble="nlx 149225-1" column="gene"/>

3

Search: The Keyword Query Interface

NIF Home	IF Home myNIF Neurolex Search Recommend a Resource Login Register Tutorial Help									
N	ĪF		e.g., cerebellum, "pulvinar nu DCAMPUS gene						Å	٩
Data () Literature Registry Funding (0	Displaying WormBase	237,666,448 results <u>WormBase: WormF</u> WormBase provides an Information on WormBa	atomical and genetic inform	nation of C. elegans and rel	ated research nematodes.	•	Search Options	Semantic Expansi ammon's horn, ammo hippocampus proper,	n horn,
Web (∝ Hide se Data Tj Animals	NIF Home myNIF	Neurole:	x Search Reco search for (e.g., cerebellum Hippocampu						Login	Register Tutorial
Antibod Atlas (1 Cell line Datase	Data () AutDB (2271) Literature () Registry ()		AutDB:Anim AutDB provides informat More Information on Aut Displaying results 1 - 20	ion on animal models used DB	in autism research.			Source Opti	Semantic	Expansion [+]
Drugs (Genes	Funding () Web (∞)				Gene Name	Aliases S	Phenotype Profile 🔍 🖨	Experimental S	Reference For States	Reference For S
Images Interact Nervou	Hide search filters Animal Model [+] Gene Symbol [–]		UBE3A_1_KO_HM	Ube3a	ubiquitin protein ligase E3A	Hpve6a; KIAA4216; mKIAA4216; 4732496B02; 5830462N02Rik; A130086L21Rik; Ube3a	Neurophysiology: Description: Decreased chloride inhibitory currents in cornu ammonis 1 (CA1) pyramidal ne[more]	Intracellulr recordings after hippocampal cannulation and drug infusion	PMID:19430469, 20211139, 20696245, 21974935, 21974935, 22381732, 9808466, 9808466, 9808466, 9808466	PMID:11543639, 16575182, 16754645, 18846633, 19404257, 19430469, 21624971, 8988171
	mecp2 (264) fmr1 (140) disc1 (122) ube3a (89) gabrb3 (78)		NRP2_4_KO_HT	Nrp2	neuropilin 2	RP23-149A5.1, 1110048P06Rik, Np-2, Np2, Npn-2, Npn2	Neurophysiology: Description: Increased excitation as inferred by population spike amplitude in field CA1 [more]	I/O analysis	PMID:10707970, 10707970, 18657176, 18657176, 18657177	PMID:10707971, 17259176, 17329436, 17427189, 17443771, 9288754
	nf1 (78) foxp2 (69) oxtr (67) shank3 (65)		NTNG1_1_KO_HM	Ntng1	Netrin G1	laminet 1; laminet-1; netrin-G1	Molecular profile: Description: Decreased Ngl-1 immunoreactivity in hippocampus, layer I of the parietal c[more]	Immunohistochmical analysis	PMID:17785411	PMID:14595443, 15870826, 16980967, 17785411, 17973922, 18384956
	reln (52)	-	FMR1 1 KO HM	Fmr1	Iragile X mental	FMRP; Fmr-1; Fmr1	Molecular profile:		PMID:16055059,	PMID:11773805,

SKEYQL – extending a Keyword QL

	Feature	Description	Example
Jery	Boolean search	in addition to search with explicit AND, OR,	The query +(neuron protein)
		NOT, a query can specify terms to be in-	-gene searches for documents
		cluded (with a +) and terms to be excluded	neuron and protein and not with
			gene
	Fielded search	A search can be issued against stpecific fields	The query title:gaba searches for
		of a document	"gaba" only in the title of the doxu-
			ment
	(Extended) Dismax search	User queries are phrases without Boolean	The query international
		connectives; where matches are performed	knockout mouse with minimal
		across multiple fields of a document, and in	match = 2 and query slop = 1 will
		the case of multiple matches of a term in dif-	penalize the matching text "the
		ferent fields, the max score is used. The query	international conference on genetic
		also allows parameters like the minimal num-	mouse design was a knockout
		ber of terms that must be matched, and "query	success".
		slop factor" that determines the importance of	
		the proximity between query terms.	
	phrase weights	A query phrase can be given additional mul-	
		tiplicative weight	

- FIND:(image video) hippocampus
- anatomy:hippocampus component:"plasma membrane"
- anatomy::organism:human

Lucene Qu

- anatomy:hippocampus[::organism:human]
- RELATED:(Tenascin rabbit) RELATED::measuredBy:("cell signaling" cytometry)

Semantic Rewriting of SKEYQL

Queries

- FIND:(image video) hippocampus
 - Find the ontological class of the query term "hippocampus"
 - Ans: anatomical_entity
 - Does "hippocampus" have a non-empty has_part tree underneath?
 - Every node in the ontology keeps an approximate statistics of descendant counts across various edge labels
 - Rewrite query to:
 - FIND: (image video) has_part*(synonyms(hippocampus))
 - Issue:
 - A cell is a part of any brain region.
 - Should the expansion include the cells of hippocampus?
 - No, because "cell" is a different module of the ontology whose top-level is "cell".
 - Partonomic expansion stays within module of the ontology
 - Final rewrite:
 - FIND: (image video) anatomy::(has_part*(synonyms(hippocampus)))

Computing with NIF Services

The PDSP <u>K_i database</u> is a unique resource in the public domain which provides information on the abilities of drugs to interact with an expanding number of molecular targets. The <u>K_i database</u> serves as a data warehouse for published and internally-derived K_i, or affinity, values for a large number of drugs and drug candidates at an expanding number of G-protein coupled receptors, ion channels, transporters and enzymes.



Which marijuana related genes are of interest to NCI? Let's just use PDSP as an example.

Which marijuana related genes are of interest to NCI? Let's just use PDSP as an example.

Computing with NIF Services

```
public static final String THC_QUERY = "cannabis thc marijuana";
```

```
public void demonstrateFederation() throws Exception {
    final String kiDatabaseId = "nif-0000-01866-1";
    FederationQuery query = FederationQuery.builder(kiDatabaseId, THC_QUERY).get();
    for (Facets facets: searcher.getFacets(query, 10, 0, 1)) {
        // Find all receptor (gene) facets
        if (!facets.getCategory().equals("Receptor")) {
            continue;
        }
        for (Facet facet: facets.getFacets()) {
            // Get grants related to these genes from NCI
            query = FederationQuery.builder("nif-0000-10319-1", "\"" + facet.getFacet() +"\"")
            .facet("Funding Institute", "national cancer institute")
            .exportType(ExportType.data)
            .rows(1000).get();
        TableData data = searcher.getTableData(query);
    }
}
```

for (FederationModelData model: data.getResult()) {
 System.out.println(facet.getFacet() + "," + model.get("project_number") + "," + model.get("project_title"));

Which marijuana related genes are of interest to NCI?

cannabinoid cb2	3R01CA142115-04S1	Cannabinoid CB2 Agonists for Treatment of Breast Cancer-Induced Bone Pain			
cannabinoid cb2	1R01CA142115-01A1	Cannabinoid CB2 Agonists for Treatment of Breast Cancer-Induced Bone Pain			
sigma	1R01CA163764-01	SIGMA-2/PEPTIDOMIMETIC CONJUGATES TARGET APOPTOSIS IN PANCREATIC CANCER			
sigma	1ZIABC008714-35	Bacterial Functions Involved in Cell Growth Control			
sigma	1ZIABC010632-09	Transcription Regulation in E. coli and H. pylori			
sigma	1ZIABC010632-08	Transcription Regulation in E. coli and H. pylori			
sigma	1ZIABC010632-07	Transcription Regulation in E. coli and H. pylori			
sigma	1ZIABC008714-32	Bacterial Functions Involved in Cell Growth Control			
sigma	1ZIABC008714-34	Bacterial Functions Involved in Cell Growth Control			
sigma	1ZIABC008714-33	Bacterial Functions Involved in Cell Growth Control			
sigma	1R21CA173887-01A1	Nanomicellar Formulation for Synergistic Targeting of Prostate Cancer			
sigma	1F32CA171543-01	Synthesis of Vinblastine Analogues with Improved Physiochemical Properties			
sigma	1ZIABC010378-13	Macromolecular Crystallography Research with Synchrotron Radiation			
sigma	1ZIABC011203-04	Proteolysis and Regulation of Bacterial Cell Growth Control			
sigma	1ZIABC011203-03	Proteolysis and Regulation of Bacterial Cell Growth Control			
sigma	1ZIABC010845-04	p53-induced Regulation of Transcription in the Chromatin Context			
sigma	1ZIABC011203-02	Proteolysis and Regulation of Bacterial Cell Growth Control			
sigma	1ZICBC010517-08	Large Databases of Small Molecules - Drug Development Tool and Public Resource			
sigma	2R56CA107510-06	The role of p53 and 14-3-3 in genomic instability			
sigma	1ZIABC011203-01	Proteolysis and Regulation of Bacterial Cell Growth Control			

What about ALL Databases?

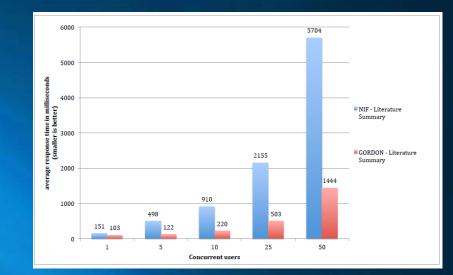
1	gene	projNum	projTitle
2	bptf	1ZIABC005263-28	Eukaryotic Chromatin Structure and Gene Regulation
3	bptf	1ZIABC005263-29	Eukaryotic Chromatin Structure and Gene Regulation
4	bptf	1ZIABC005263-31	Eukaryotic Chromatin Structure and Gene Regulation
5	bptf	1ZIABC005263-30	Eukaryotic Chromatin Structure and Gene Regulation
6	itk	1ZIABC011267-03	Preclinical drug development in pancreatic cancer
7	itk	1R41CA167907-01	Calibrated Methods for Quantitative PET/CT Imaging
8	itk	1ZIABC009281-26	Receptor Mediated T and B Cell Activation
9	itk	1ZIABC010304-14	Biochemical Basis of T Cell Activation
10	itk	1ZIABC009281-25	Receptor Mediated T and B Cell Activation
11	itk	1ZIABC010304-13	Biochemical Basis of T Cell Activation
12	itk	1ZIABC010944-04	Control of the immune response for cancer vaccine development
13	itk	1ZIABC009281-24	Receptor Mediated T and B Cell Activation
14	itk	1ZIABC010304-12	Biochemical Basis of T Cell Activation
15	itk	1ZIABC010944-03	Control of the immune response for cancer vaccine development
16	itk	1ZIABC010304-11	Biochemical Basis of T Cell Activation
17	itk	1ZIABC010944-02	Control of the immune response for cancer vaccine development
18	itk	3R01CA112663-10S1	T-bet and Tumor Immunity
19	crkl	1ZIASC006892-23	Molecular Biology of Pediatric Tumors
20	crkl	1ZIASC006892-24	Molecular Biology of Pediatric Tumors
21	crkl	1ZIASC006892-22	Molecular Biology of Pediatric Tumors
22	crkl	1ZIASC006892-21	Molecular Biology of Pediatric Tumors
23	tetrahydrocannabinol (thc)	3R01CA111196-04S1	MODULATION OF ONCOGENIC AGENTS BY MARIJUANA
24	brca1	2R01CA089239-13A1	Analysis of BRCA1 function in DNA Repair
25	brca1	7R01CA111436-04	Regulation of BRCA1 Function by Protein Phosphatase 1
26	brca1	1R01CA137023-01A1	The Role of BRCA1/BARD1 in Basal-like Breast Cancer
27	brca1	4R01CA129440-03	ROLE OF BRCA1/AKT1 PATHWAY IN THE TUMORIGENESIS
28	brca1	1R01CA129440-01A2	ROLE OF BRCA1/AKT1 PATHWAY IN THE TUMORIGENESIS
29	brca1	7R01CA089239-11	Analysis of BRCA1 Function in DNA Repair
30	brca1	1R01CA174904-01	Roles of Chromatin Modification in BRCA1 Dependent DNA Repair
31	brca1	1ZIABC010847-06	Gene-specific Mechanisms of BRCA1 transcriptional Control
	2013 Summ	er Institute: Discover Big	Data, August 5-9, San Diego, California

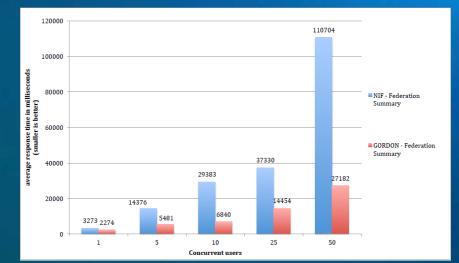
Where is SDSC in all of this?

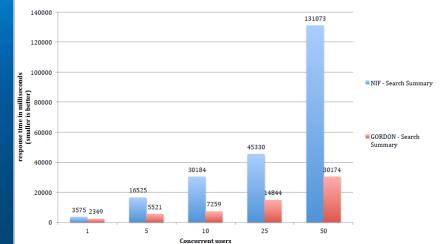
Running on Gordon (with no tweaking)

Configuration

- 1 server
 - 98 GB RAM
 - 24 core Intel Xeon CPU @2.8GHz
- RAID 5 SSD
- 2 Solr instances serving the
- Federation and literature cores.







Conclusion

The Neuroscience Information Framework is not really dependent on Neuroscience

Applying it to

- Diabetes and kidney diseases
- Model organisms
- Earthcube for geo-science data
- (Hopefully) social science data for economists

🧕 We need

- More scalability
- Improved complex query handling
- A distribution framework