The Neuroscience External Resources Data Standard

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2023 NWB Developer Days
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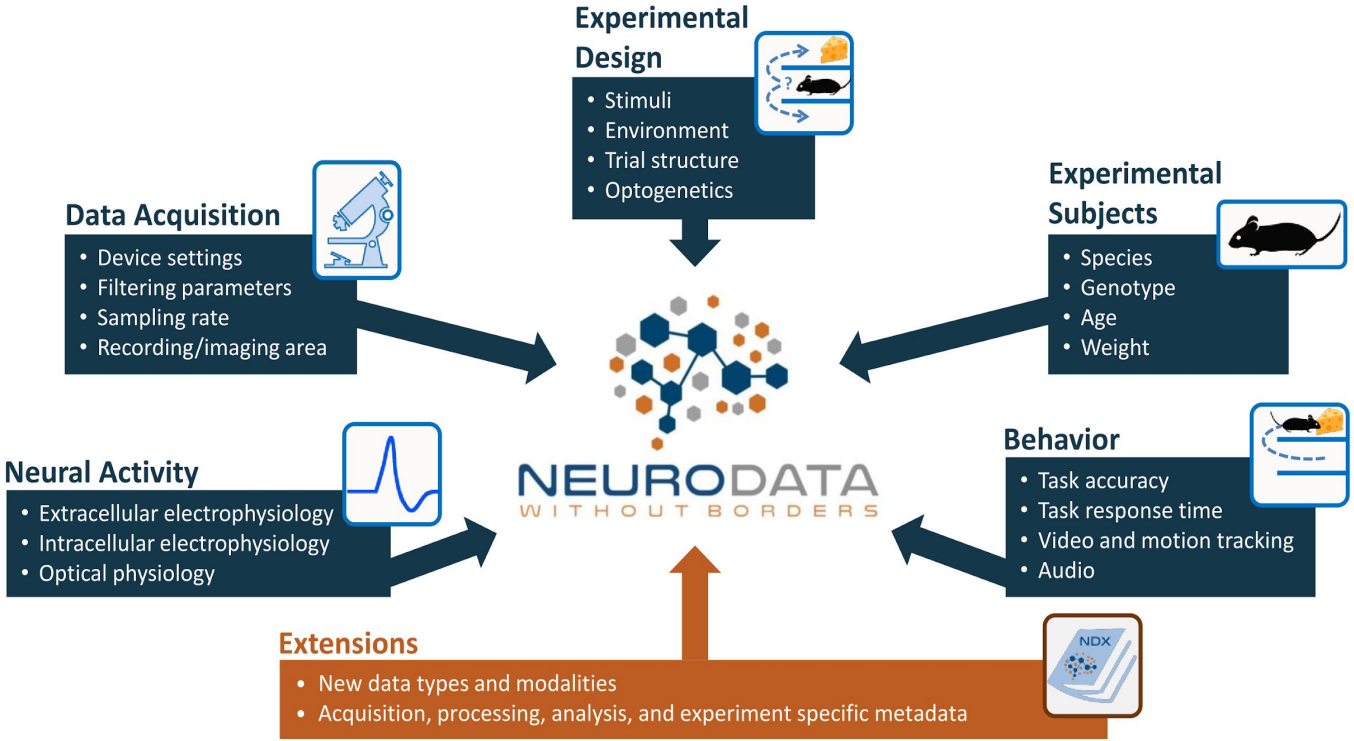
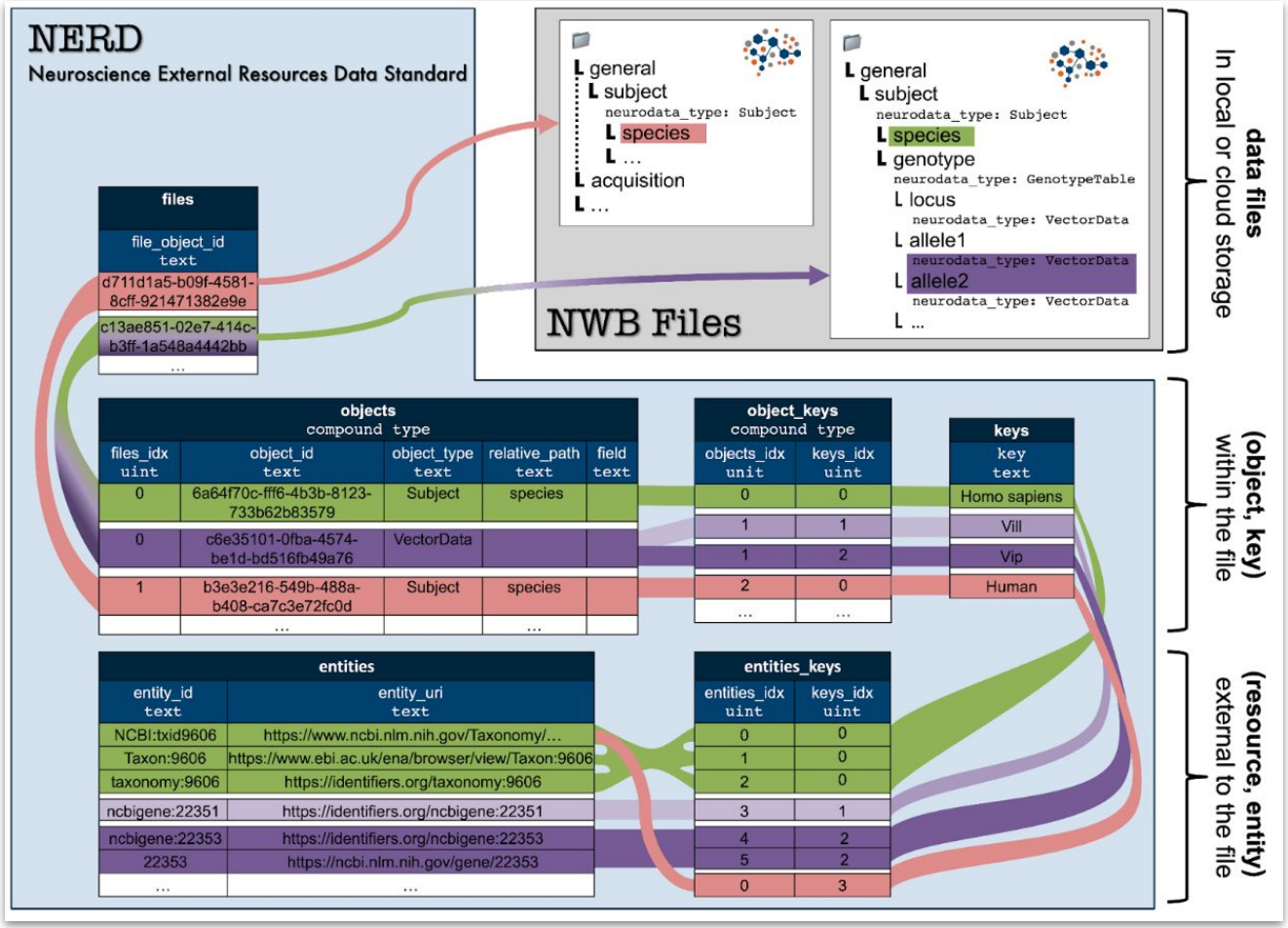
An Ecosystem for Neuroscience Data Standardization




NERD
Neuroscience External Resources Data Standard
NWB Files
general
subject
neurodata_type: Subject
species
…
acquisition
…
general
subject
neurodata_type: Subject
species
genotype
neurodata_type: GenotypeTable
locus
neurodata_type: VectorData
allele1
neurodata_type: VectorData
allele2
neurodata_type: VectorData
…
data files
In local or cloud storage
files
file_object_id
text
d711d1a5-b09f-4581-8cff-921471382e9e
c13ae851-02e7-414c-b3ff-1a548a4442bb
…
objects
compound type
files_idx uint
object_id text
object_type text
relative_path text
field text
0
6a64f70c-fff6-4b3b-8123-733b62b83579
Subject
species
0
c6e35101-0fba-4574-be1d-bd516fb49a76
VectorData
1
b3e3e216-549b-488a-b408-ca7c3e72fc0d
Subject
species
object_keys
compound type
objects_idx unit
keys_idx uint
0
0
1
1
1
2
2
0
keys
key text
Homo sapiens
Vill
Vip
Human
(object, key)
within the file
entities
entity_id text
entity_uri text
NCBI:txid9606
https://www.ncbi.nlm.nih.gov/Taxonomy/…
Taxon:9606
https://www.ebi.ac.uk/ena/browser/view/Taxon:9606
taxonomy:9606
https://identifiers.org/taxonomy:9606
ncbigene:22351
https://identifiers.org/ncbigene:22351
ncbigene:22353
https://identifiers.org/ncbigene:22353
22353
https://ncbi.nlm.nih.gov/gene/22353
entities_keys
entities_idx uint
keys_idx uint
0
0
1
0
2
0
3
1
4
2
5
2
0
3
(resource, entity)
external to the file

NERD Example

root (NWBFile)
session_description: Data from monkey Haydn performing ready-set-go time interval reproduction task. This file contains continuous segments of the full session on 2016-12-11 that can be used for training models for the Neural Latents Benchmark.
identifier: 8969f328-3929-11ec-8077-43176b153428
session_start_time: 2016-12-11 00:00:00-05:00
timestamps_reference_time: 2016-12-11 00:00:00-05:00
▶ **file_create_date**
experimenter: ('Hansem Sohn',)
related_publications: ('http://dx.doi.org/10.1016/j.neuron.2019.06.012',)
▶ **keywords**
epoch_tags: set()
▶ **electrodes**
▼ **electrode_groups (3)**
  ▼ **electrode_group_1**
    description: Electrodes on a neural probe
    location: Dorsomedial frontal cortex
    ▶ **device**
  ▶ **electrode_group_2**
  ▶ **electrode_group_3**
▶ **devices (3)**
▶ **intervals (1)**
▼ **subject**
  age: P4Y
  sex: M
  species: Macaca mulatta
  subject_id: Haydn

Using add_ref

Create and Link ER

```
er = ExternalResources()
read_nwbfile.link_resources(er)
```

NWBFile Experimenter

```
er.add_ref(
    container=read_nwbfile,
    attribute="experimenter",
    key="Hansem Sohn",
    entity_id='ORCID:0000-0001-8593-7473',
    entity_uri='https://orcid.org/0000-0001-8593-7473')
```

Electrode_Group Location

```
er.add_ref(
    container=read_nwbfile.electrode_groups['electrode_group_1'],
    attribute="location",
    key="Dorsomedial frontal cortex",
    entity_id="DB09",
    entity_uri="https://scalablebrainatlas.incf.org/macaque/DB09")
```

Subject Species

```
er.add_ref(
    container=read_nwbfile.subject,
    attribute='species',
    key='Macaca mulatta',
    entity_id='NCBI_TAXON:9544',
    entity_uri='https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/id=9544')
```

NERD Visualized

	file_object_id	objects_idx	object_id	files_idx	object_type	relative_path	field	keys_idx	key	entities_idx	entity_id	
0	9c3a5c45-316c-493d-a712-03a01b662ee9	0	9c3a5c45-316c-493d-a712-03a01b662ee9	0	NWBFile	general/experimenter		0	Hansem Sohn	0	ORCID:0000-0001-8593-7473	
1	9c3a5c45-316c-493d-a712-03a01b662ee9	1	f8641805-f93c-446f-8194-5fce08d22dbb	0	ElectrodeGroup	location		1	Dorsomedial frontal cortex	1	DB09	https://s
2	9c3a5c45-316c-493d-a712-03a01b662ee9	2	5ee39486-8625-4ac3-9691-ce9d724812a4	0	Subject	species		2	Macaca mulatta	2	NCBI_TAXON:9544	https://ww

TermSet

- **Validation of Data**
  - Currently supports only data sets.
- **Streamlines the NERD user experience**
  - Reduces the number of required fields in the add_ref method.

```
id: notebooks/species_example
name: Experimenter
prefixes:
  ORCID: https://orcid.org/
imports:
  - linkml:types
default_range: string

enums:
  Experimenters:
    permissible_values:
      Dichter, Benjamin K.:
        description: The ORCiD
        meaning: ORCID:0000-0001-5725-6910
      Rubel, Oliver:
        description: The ORCiD
        meaning: ORCID:0000-0001-9902-1984
```

NERD TermSet Example

```
terms = TermSet(term_schema_path='./experimenter_term_set.yaml')
er = ExternalResources()
```

```
session_start_time = datetime(2018, 4, 25, 2, 30, 3, tzinfo=tz.gettz("US/Pacific"))

nwbfile = NWBFile(
    session_description="Mouse exploring an open field",
    identifier="Mouse5_Day3",
    session_start_time=session_start_time,
    session_id="session_1234",
    experimenter=["Dichter, Benjamin K.", "Rubel, Oliver"],
    lab="My Lab Name",
    institution="University of My Institution",
    related_publications="DOI:10.1016/j.neuron.2016.12.011",
)
nwbfile.subject = Subject(
    subject_id="001",
    age="P90D",
    description="mouse 5",
    species="Mus musculus",
    sex="M",
)
```

Using add_ref_term_set

add_ref

```
er.add_ref(
    container=read_nwbfile,
    attribute="experimenter",
    key="Hansem Sohn",
    entity_id='ORCID:0000-0001-8593-7473',
    entity_uri='https://orcid.org/0000-0001-8593-7473')
```

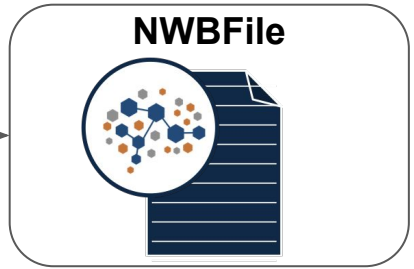
add_ref_term_set

```
er.add_ref_term_set(container=nwbfile,
                    attribute='experimenter',
                    term_set=terms
                   )
```

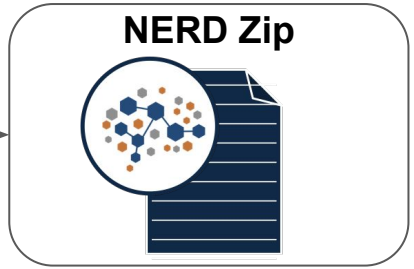
Write NWBFile and NERD

- The NWBFile and NERD are written separately.
  - NERD is written as a zip file containing the individual tables in the data structure.

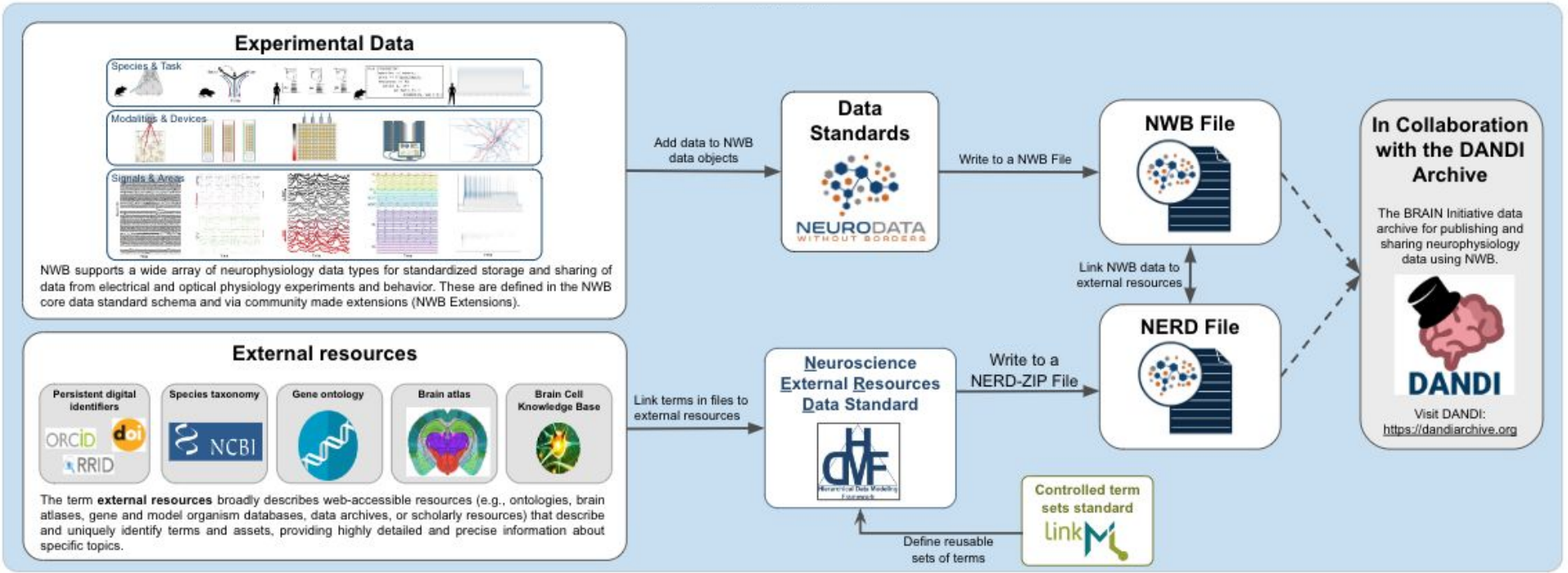
```
1 with NWBHDF5IO("NWBfile_ER_Example.nwb", "w") as io:
2     io.write(nwbfile)
```




```
1 er.to_norm_tsv(path='./')
```

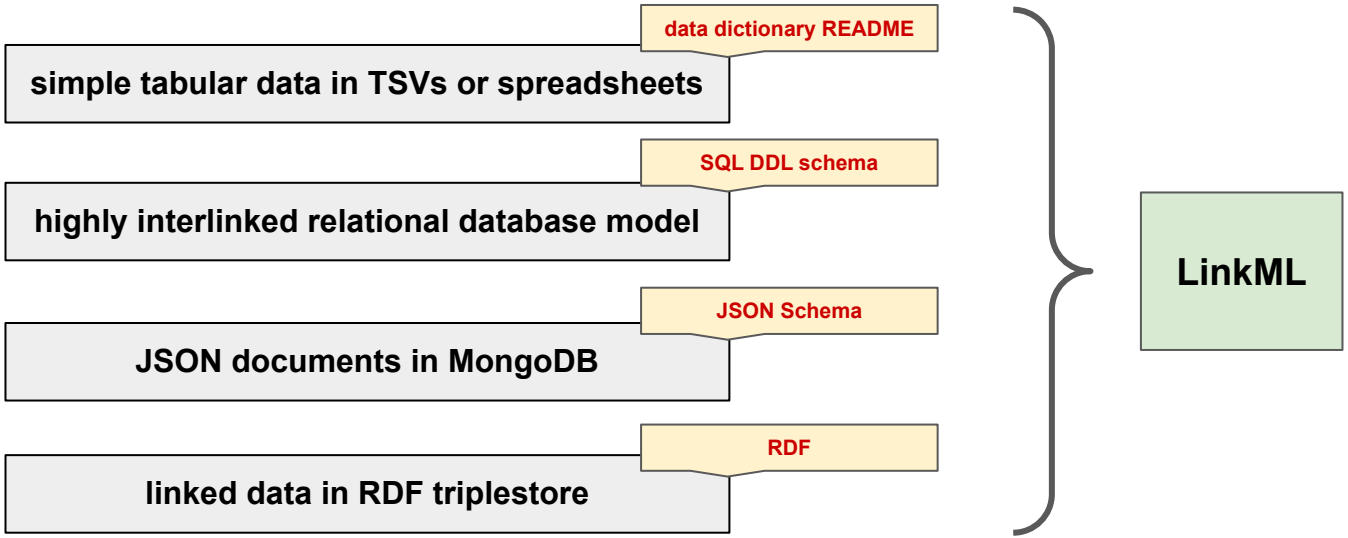


User Workflow



Introduction to LinkML

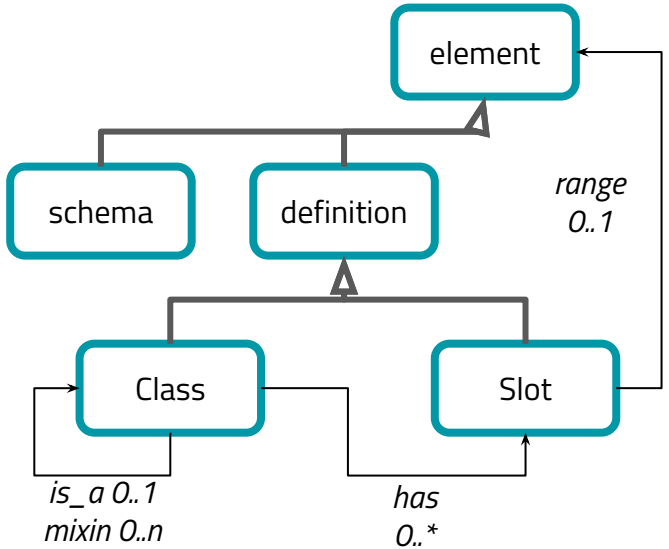
- All data follows some kind of schema / data model (“blueprint”)
- LinkML is a flexible modeling language that allows you to author schemas (“data models”) in YAML that describe the structure of your data



Introduction continued

THE STANDARD

*A **meta-standard** for structuring your data*



TOOLS

Pragmatic developer and curator friendly tools for working with data

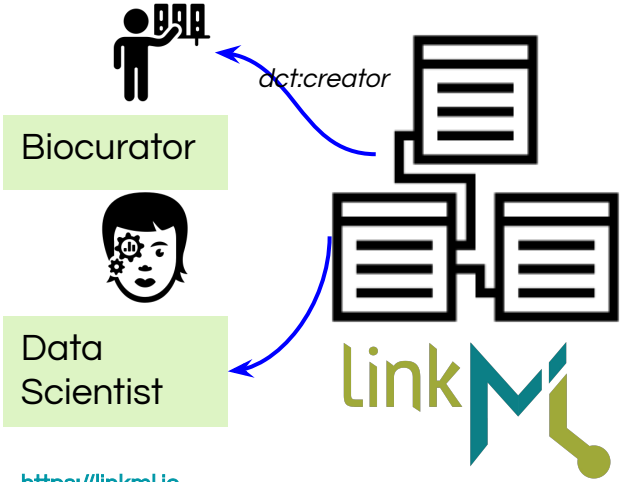
- **Validators**
- **Data Converters**
- **Compatibility tools**
- **Data entry**
- **Schema inference**

The LinkML landscape

Create data models / standards in simple YAML files, optionally annotated using ontologies

Compile to other frameworks

Choose the right tools for the job, no lock in



https://linkml.io
https://github.com/linkml/linkml

OWL
ShEx, SHACL
JSON-LD Contexts
JSON-Schema
Python Dataclasses
SQL DDL
Java
TSVs

Semantic Web Applications And Infrastructure

RDF

JSON-LD

"Traditional" Applications and Infrastructure

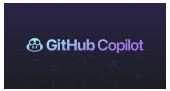
pandas

JSON

Authoring schemas in YAML

Option A: Author YAML *directly*

Optional productivity tools




```yaml
id: https://example.org/linkml/hello-world
title: Really basic LinkML model
name: hello-world
version: 0.0.1

prefixes:
 linkml: https://w3id.org/linkml/
 sdo: https://schema.org/
 ex: https://example.org/linkml/hello-world/

default_prefix: ex
default_curi_maps:
 - semweb_context

imports:
 - linkml:types

classes:
 Person:
   description: Minimal information about a person
   class_uri: sdo:Person
   attributes:
     id:
       identifier: true
       slot_uri: sdo:taxID
     first_name:
       required: true
       slot_uri: sdo:givenName
       multivalued: true
     last_name:
       required: true
       slot_uri: sdo:familyName
     knows:
       range: Person
       multivalued: true
       slot_uri: foaf:knows
```

Metadata

Namespaces

Dependencies

Actual data model

YAML conformant to LinkML standard

Schemasheets

Option B: Author using *schemasheets*

a person,living or dead

record	field	key	multiplicity	range	parents	desc	schema.org	wikidata	be
> class	slot	identifier	cardinality	range	is_a	description	exact_mappings	exact_mappings	in_
>								curie_prefix: wikida	
	id	yes	1	string		any identifier	identifier		
	description	no	0..1	string		a textual description	description		
Person		n/a	n/a	n/a		a person,living or dead	Person	Q215627	
Person	id	yes	1	string		identifier for a person	identifier		
Person|Organiza	name	no	1	string		full name	name		
Person	age	no	0..1	decimal		age in years			
Person	gender	no	0..1	decimal		age in years			
Person	has medical hist	no	0..*	MedicalEvent		medical history			
Event						grouping class for events		Q1656682	a
MedicalEvent		n/a	n/a	n/a	Event	a medical encounter			b
ForProfit					Organization				
NonProfit					Organization			Q163740	

SCHEMASHEETS
easy LinkML from spreadsheets

```
id: https://example.org/linkml/hello-world
title: Really basic LinkML model
name: hello-world
version: 0.0.1

prefixes:
 linkml: https://w3id.org/linkml/
 sdo: https://schema.org/
 ex: https://example.org/linkml/hello-world/

default_prefix: ex
default_curi_maps:
```

```
: a person
```

```
multivalued: true
slot_uri: foaf:knows
```

Metadata

Namespaces

Dependencies

Actual Datamodel

YAML conformant to LinkML standard

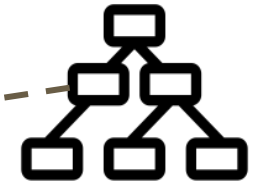
NEURODATA WITHOUT BORDERS

Enumerations in LinkML allow ontology mapping

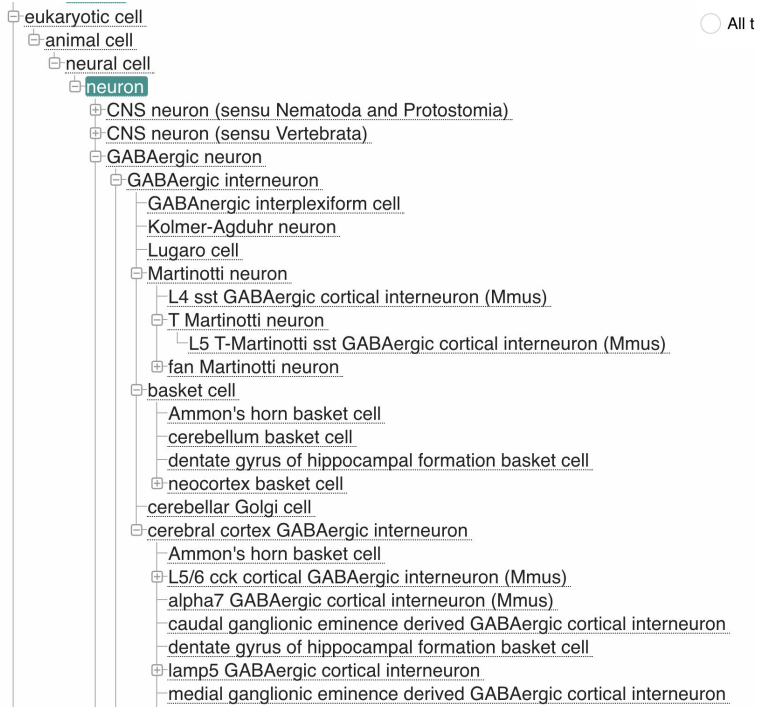
```yaml
prefixes:
  COB: http://purl.obolibrary.org/obo/COB_
  BFO: http://purl.obolibrary.org/obo/BFO_
  RO: http://purl.obolibrary.org/obo/RO_
  CHEBI: http://purl.obolibrary.org/obo/CHEBI_
  CHEMINF: http://semanticscience.org/resource/CHEMINF_
  SIO: http://semanticscience.org/resource/SIO_
  PUBCHEM.ELEMENT: https://pubchem.ncbi.nlm.nih.gov/element/
  LANL.ELEMENT: https://periodic.lanl.gov/
```

```yaml
enums:

  nanostructure_morphology_enum:
    permissible_values:
      nanotube:
        meaning: CHEBI:50796
      nanoparticle:
        meaning: CHEBI:50803
      nanorod:
        meaning: CHEBI:50805
      nanotubosome:
        meaning: CHEBI:50806
      quantum dot:
        meaning: CHEBI:50853
      nanofibre:
        meaning: CHEBI:52518
      nanocrystal:
        meaning: CHEBI:52529
      nanoribbon:
        meaning: CHEBI:52530
      nanosheet:
        meaning: CHEBI:52531
      nanowire:
        meaning: CHEBI:52593
```



Dynamic Enumerations in LinkML




```
enums:
  NeuronTypeEnum:
    reachable_from:
      source_ontology: obo:cl
      source_nodes:
        - CL:0000540 ## neuron
      include_self: false
      relationship_types:
        - rdfs:subClassOf
```

Topics to Start Discussion

1. Any questions in general?
2. Changes Just Around the Corner:
   a. HDMF_Zarr supporting the most up-to-data NERD tools (Next Release)
   b. Customize NERD Zip File name (Next Release)
3. Community Feedback Topics:
   a. Version Control on NERD
   b. NERD and NWBFile “write”
4. LinkML demo material walkthrough:
   https://github.com/sujaypatil96/nwb-dev-days-linkml-hdmf