

MIxS as RDF: Fields as Object Properties

2020-11-09

Context: modeling of fields (e.g. altitude)

Ticket: <https://github.com/GenomicsStandardsConsortium/mixs-rdf/issues/9>

Possibilities

- Data Property: Range is a literal (e.g. xsd string)
- Class
- Annotation Property: Range is either literal or object
- Object Property: Range is an object

Note:

- This will not impact people using CSVs for metadata (it's all just columns)

NMDC rendering of mixs (via biolinkml)

The screenshot shows the Biocreative interface with the following details:

- Top Bar:** < > schema (<https://microbiomedata/schema>) Search...
- Left Sidebar:** attribute > alt
Active ontology x Entities x Individuals by class x DL Query x Individual Hierarchy Tab x
Datatypes x Individuals
Data properties x Annotation properties
Classes x Object properties
Object property hierarchy:
owl:topObjectProperty
acted on behalf of
activity id
activity set
add_date
alternate identifiers
attribute
_16s_recover
_16s_recover_software
abs_air_humidity
adapters
add_recov_method
additional_info
address
adj_room
aero_struct
agrochem_addition
air_temp
air_temp_regn
al_sat
al_sat_meth
alkalinity
alkalinity_method
alkyl_diethers
alt
aminopept_act
ammonium
amniotic_fluid_color
amount_light
ances_data
anno
annual_precpt
annual_temp
antibiotic_regn
api
arch_struct
...
- Middle Panel:** Annotations: alt
Annotations Usage
Annotations: alt
rdfs:label alt
skos:definition "Altitude is a term used to identify heights of objects such as airplanes, space shuttles, rockets, atmospheric balloons and heights of places such as atmospheric layers and clouds. It is used to measure the height of an object which is above the earth's surface. In this context, the altitude measurement is the vertical distance between the earth's surface above sea level and the sampled position in the air"
pattern {float} {unit}
skos:inScheme environment
- Bottom Panel:** Description: alt
Characteristics
Functional
Inverse functional
Transitive
Symmetric
Asymmetric
Reflexive
Irreflexive
Equivalent To
SubProperty Of
attribute
Inverse Of
Domains (intersection)
study or biosample
Ranges (intersection)
'quantity value'

<https://github.com/microbiomedata/nmd-c-metadata/tree/master/schema>

NMDC rendering of mixs (via biolinkml)

The screenshot shows the Biocreative interface with the following details:

- Annotations tab:** The `alt` annotation is selected.
- Annotations section:**
 - rdfs:label:** `alt`
 - skos:definition:** "Altitude is a term used to identify heights of objects such as airplanes, space shuttles, rockets, atmospheric balloons and heights of places such as atmospheric layers and clouds. It is used to measure the height of an object which is above the earth's surface. In this context, the altitude measurement is the vertical distance between the earth's surface above sea level and the sampled position."
 - pattern:** `{float} {unit}`
 - skos:inScheme:** environment
- Description tab:** The `alt` description is selected.
- Relationships:**
 - Functional:** Equivalent To → `attribute`
 - Inverse functional:** SubProperty Of → `attribute`
 - Transitive:**
 - Symmetric:**
 - Asymmetric:**
 - Reflexive:**
 - Irreflexive:**
- Domains (intersection):** `study or biosample`
- Ranges (intersection):** `'quantity value'`

A large yellow arrow points from the text "Regex for string" to the `skos:definition` field.

NMDC rendering of mixs (via biolinkml)

The screenshot shows the Biocreative interface for rendering a MixS schema. The top navigation bar includes buttons for back, forward, search, and tabs for schema, entities, individuals by class, DL Query, and Individual Hierarchy Tab. The main area displays the MixS schema with various annotations and usage details.

Annotations:

- rdfs:label**: alt
- skos:definition**: "Altitude is a term used to identify heights of objects such as airplanes, space shuttles, rockets, atmospheric balloons and heights of places such as atmospheric layers and clouds. It is used to measure the height of an object which is above the earth's surface. In this context, the altitude measurement is the vertical distance between the earth's surface above sea level and the sampled position in the air"
- pattern**: {float} {unit}
- skos:inScheme**: environment

Description: alt

- Functional**: Equivalent To
- Inverse functional**: SubProperty Of **attribute**
- Transitive**
- Symmetric**
- Asymmetric**
- Reflexive**
- Irreflexive**

Domains (intersection): study or biosample

Ranges (intersection): quantity value

Object Property; range is Quantity Value

Example range class: Quantity Value

The screenshot shows a semantic web editor interface with three main panels:

- Annotations: quantity value**: Shows annotations for the 'quantity value' class. It includes:
 - rdfs:label**: quantity value
 - skos:definition**: A simple quantity, e.g. 2cm
 - skos:exactMatch**: <http://schema.org/QuantityValue>
- Annotations: quantity value**: Shows annotations for the 'quantity value' class. It includes:
 - Equivalent To**: float
 - SubClass Of**:
 - 'attribute value'
 - 'has numeric value' **max 1 double**
 - 'has raw value' **max 1 string**
 - 'has unit' **max 1 unit**

Example range class: Quantity Value

The screenshot shows a semantic web editor interface with three main panels:

- Annotations Tab:** The top panel displays annotations for the 'quantity value' class. It includes:
 - rdflib:label:** quantity value
 - skos:definition:** A simple quantity, e.g. 2cm
 - skos:exactMatch:** <http://schema.org/QuantityValue>
- Description Tab:** The bottom panel displays the description of the 'quantity value' class. It includes:
 - Equivalent To:** (empty)
 - SubClass Of:** (empty)
- Navigation Bar:** The left sidebar shows the class hierarchy under 'owl:Thing', with 'quantity value' highlighted.

E.g. "2 cm" -- literal string representation

Example range class: Quantity Value

The screenshot shows a triple editor interface with three main tabs: Annotations, Class description, and SubClass Of.

Annotations: quantity value

- Annotations:**
 - rdflib:label:** quantity value
 - skos:definition:** A simple quantity, e.g. 2cm
 - skos:exactMatch:** <http://schema.org/QuantityValue>

Class description: quantity value

- Equivalent To:** (empty)
- SubClass Of:**
 - 'attribute value'
 - 'has numeric value' **max 1** double
 - 'has raw value' **max 1** string
 - 'has unit' **max 1** unit

SubClass Of:

- 'attribute value'
- 'has numeric value' **max 1** double
- 'has raw value' **max 1** string
- 'has unit' **max 1** unit

Structured;
broken into 3 sub-parts

Example range class: Quantity Value

The screenshot shows the Protégé ontology editor interface with three main panels:

- Left Panel (Navigation properties):** Shows the class hierarchy under "Classes". The path to "quantity value" is: owl:Thing > attribute value > quantity value. Other visible classes include activity, agent, boolean, controlled term value, geolocation value, integer value, person value, text value, timestamp value, url value, boolean, bytes, class_definition, database, date, datetime, decimal degree, double, float, integer, language code, named thing, ncname, nodeidentifier, objectidentifier, slot_definition, and string.
- Middle Panel (Annotations):** The "Annotations" tab is selected. It lists annotations for "quantity value":
 - rdfs:label:** quantity value
 - skos:definition:** A simple quantity, e.g. 2cm
 - skos:exactMatch:** <http://schema.org/QuantityValue>
- Bottom Panel (Description):** The "Description" tab is selected. It lists sub-class constraints:
 - Equivalent To:** (empty)
 - SubClass Of:** (empty)

A yellow callout box points to the "rdfs:label" annotation with the text "E.g. '2'^^xsd:double". Another yellow callout box points to the "skos:definition" annotation with the text "E.g. cm (UO)".

Other Object Property Ranges

The screenshot shows the Protégé ontology editor interface with the following details:

- Top Navigation:** schema (<https://microbiomedata/schema>)
- Toolbars:** Active ontology, Entities, Individuals by class, Individual Hierarchy Tab, DL Query.
- Left Sidebar:** Annotation properties, Datatypes, Individuals, Classes, Object properties, Data properties. The "Object property hierarchy: env_local" tab is selected.
- Middle Panel:** The "Annotations: env_local_scale" tab is selected. It displays the following annotations:
 - rdfs:label: env_local_scale
 - skos:definition: A detailed text definition of what the annotation means.
- Right Panel:** The "Annotations: controlled term value" tab is selected. It displays the following annotations:
 - rdfs:label: controlled term value
 - controlled term value: A detailed text definition of what the annotation means.
- Bottom Panel:** The "Description: controlled term value" tab is selected. It displays the following class descriptions:
 - Equivalent To: None
 - SubClass Of:
 - 'attribute value'
 - term max 1 'ontology class'
 - General class axioms:
 - SubClass Of (Anonymous Ancestor): 'was generated by' max 1 activity

Example instance data

Active ontology | Entities | Individuals by class | DL Query | Individual Hierarchy Tab

Class hierarchy: biosample Annotations Usage

Asserted

Annotations: SAM1234

Annotations +
rdfs:label [language: en]
SAM1234

Description: SAM1234

Types +
biosample

Same Individual As +

Different Individuals +

Property assertions: SAM1234

Object property assertions +
alt 87afe5342e

Data property assertions +

Negative object property assertions +

Negative data property assertions +

Direct instances: SAM1234

For: biosample

SAM1234

SAM2345

The screenshot shows a semantic web interface with several tabs at the top: Active ontology, Entities, Individuals by class, DL Query, and Individual Hierarchy Tab. The Individuals by class tab is active. Below the tabs, there's a navigation bar with icons for creating, deleting, and editing entities. The main area is divided into sections: Class hierarchy, Annotations, Description, and Property assertions. The Class hierarchy section shows a tree of data types under the root 'biosample'. The Annotations section shows the rdfs:label annotation for individual SAM1234. The Description section shows that SAM1234 is of type biosample. The Property assertions section shows an object property assertion 'alt' with value '87afe5342e'. The bottom left shows direct instances of SAM1234, listing SAM1234 and SAM2345.

Example instance data

The screenshot shows the Protégé ontology editor interface with several tabs open:

- Class hierarchy: biosample**: Shows a tree view of classes under `biosample`, including `timestamp value`, `url value`, `boolean`, `bytes`, `class_definition`, `database`, `date`, `datetime`, `decimal degree`, `double`, `float`, `integer`, `language code`, `named thing`, and `biosample`.
- Annotations: SAM1234**: Shows annotations for individual `SAM1234`. It has an `rdfs:label` entry with the value `[language: en] SAM1234`.
- Description: SAM1234**: Shows the type `biosample` and a link to the individual `87afe5342e`.
- Property assertions: SAM1234**: Shows an object property assertion `alt 87afe5342e`.
- Direct instances: SAM1234**: Shows direct instances `SAM1234` and `SAM2345`.
- For: biosample**: Shows individuals `SAM1234` and `SAM2345`.
- Direct instances: 87afe5342e**: Shows direct instances `87afe5342e` and `87afe5342e`.
- Description: 87afe5342e**: Shows the type `'quantity value'` and a link to the individual `87afe5342e`.
- Property assertions: 87afe5342e**: Shows an object property assertion `'has unit' cm`.
- Data property assertions**: Shows entries for `'has raw value' "2 cm"` and `value "2.0"^^xsd:double`.

A red box highlights the `Object property assertions` section for `SAM1234` and the `Data property assertions` section for `87afe5342e`.

Yes I know 2cm is a silly value for alt...

Didn't have time to change example

Example instance data - as JSON-LD

The screenshot shows the Protégé ontology editor interface. On the left, the 'Class hierarchy' pane displays a tree of classes under 'biosample', including timestamp value, url value, boolean, bytes, class_definition, database, date, datetime, decimal degree, double, float, integer, language code, named thing, and biosample. The 'Direct instances' pane below shows two instances: SAM1234 and SAM2345. A red arrow points from the 'quantity value' instance in the bottom pane to the JSON-LD output on the right.

Active ontology x Entities x Individuals by class x DL Query x Individual Hierarchy Tab x

Class hierarchy: biosample

Annotations Usage

Asserted

Annotations: SAM1234

rdfs:label [language: en]
SAM1234

Description: SAM1234

Types +
biosample

Same Individual As +

Different Individuals +

Direct instances: SAM1234

For: biosample

SAM1234

SAM2345

Direct instances: 87afe5342e

For: 'quantity value'

87afe5342e

```
## JSON-LD
{@context": { ... },
{"id": "SAM1234",
"alt": {
"Has_raw_value": "2 cm",
"Value" : 2.0,
"Has unit": "cm"
},
...
}

Types +
'quantity value'

Same Individual As +
Different Individuals +
```

Object property assertions +

'has unit' cm

?

@

X

O

Data property assertions +

'has raw value' "2 cm"

value "2.0"^^xsd:double

?

@

X

O

ShEx

```
<Biosample> CLOSED {
  $<Biosample_tes> ( &<NamedThing_tes> ;
    rdf:type [ <NamedThing> ] ? ;
    <https://microbiomedata/schema/mixs/env_package> @<TextValue> ? ;
    <lat_lon> @<GeolocationValue> ;
    <https://microbiomedata/schema/mixs/geo_loc_name> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/collection_date> @<TimestampValue> ? ;
    <env_broad_scale> @<ControlledTermValue> ;
    <env_local_scale> @<ControlledTermValue> ;
    <env_medium> @<ControlledTermValue> ;
    <ecosystem> @<AttributeValue> ? ;
    <ecosystem_category> @<AttributeValue> ? ;
    <ecosystem_type> @<AttributeValue> ? ;
    <ecosystem_subtype> @<AttributeValue> ? ;
    <specific_ecosystem> @<AttributeValue> ? ;
    <depth> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/tot_org_carb> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/alt> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/elev> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/salinity> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/diss_oxygen> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/nitrate> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/chlorophyll> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/cur_land_use> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/cur_vegetation> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/cur_vegetation_meth> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/previous_land_use> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/previous_land_use_meth> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/crop_rotation> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/agrochem_addition> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/tillage> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/fire> @<TimestampValue> ? ;
    <https://microbiomedata/schema/mixs/flooding> @<TimestampValue> ? ;
    <https://microbiomedata/schema/mixs/extreme_event> @<TimestampValue> ? ;
    <https://microbiomedata/schema/mixs/horizon> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/horizon_meth> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/sieving> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/water_content> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/water_content_soil_meth> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/samp_vol_we_dna_ext> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/pool_dna_extracts> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/store_cond> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/link_climate_info> @<TextValue> ? ;
    <https://microbiomedata/schema/mixs/season_temp> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/annual_temp> @<QuantityValue> ? ;
    <https://microbiomedata/schema/mixs/season_precpt> @<QuantityValue> ? ;
```

JSON-Schema

```
},
  "Biosample": {
    "additionalProperties": false,
    "description": "A material sample. It may be environmental (encompassing many organisms) or isolate or tissue. An environmental sample containing genetic material from multiple individuals as a biosample.",
    "properties": {
      "agrochem_addition": {
        "$ref": "#/definitions/QuantityValue",
        "description": "\"Addition of fertilizers, pesticides, etc. - amount and time of applications\""
      },
      "al_sat": {
        "$ref": "#/definitions/QuantityValue",
        "description": "Aluminum saturation (esp. For tropical soils)"
      },
      "al_sat_meth": {
        "$ref": "#/definitions/TextValue",
        "description": "Reference or method used in determining Al saturation"
      },
      "alt": {
        "$ref": "#/definitions/QuantityValue",
        "description": "\"Altitude is a term used to identify heights of objects such as airplanes, space shuttles, rockets, atmospheric balloons and heights of places such as atmospheric used to measure the height of an object which is above the earth's surface. In this context, the altitude measurement is the vertical distance between the earth's surface above sea level and the ground\""
      },
      "alternate_identifiers": {
        "description": "The same biosample may have distinct identifiers in different databases (e.g. GOLD and EMSL)",
        "items": [
          {
            "type": "string"
          }
        ],
        "type": "array"
      },
      "annual_prcpt": {
        "$ref": "#/definitions/QuantityValue",
        "description": "\"The average of all annual precipitation values known, or an estimated equivalent value derived by such methods as regional indexes or Isohyetal maps. \\\""
      },
      "annual_temp": {
        "$ref": "#/definitions/QuantityValue",
        "description": "Mean annual temperature"
      },
      "chlorophyll": {
        "$ref": "#/definitions/QuantityValue",
        "description": "Concentration of chlorophyll"
      },
      "collection_date": {
        "$ref": "#/definitions/TimestampValue",
        "description": "\"The time of sampling, either as an instance (single point in time) or interval. In case no exact time is available, the date/time can be right truncated i.e. all 2008-01-23T19:23:10+00:00; 2008-01-23T19:23:10; 2008-01-23; 2008-01; 2008; Except: 2008-01; 2008 all are ISO8601 compliant\\\""
      },
      "crop_rotation": {
        "$ref": "#/definitions/TextValue",
        "description": "\"Whether or not crop is rotated, and if yes, rotation schedule\\\""
      },
      "cur_land_use": {
        "$ref": "#/definitions/TextValue",
        "description": "Present state of sample site"
      },
      "cur_vegetation": {
        "$ref": "#/definitions/TextValue",
        "description": "\"Vegetation classification from one or more standard classification systems, or agricultural crop\\\""
      }
    }
  }
}
```

Summary

- Using Object Properties allows us to have complex objects as values
 - Have our cake and eat it: one value can be the raw string value
 - E.g. “2 cm”, “ENVO:nnnnn mangrove biome”
 - Extensible to including provenance
- Will not affect majority of MIxS users