OBI Data Prototype

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This is a prototype of the "value specification" approach to modelling data in OBI/IAO: the Ontology for Biomedical Investigations and the Information Artifact Ontology. It is based on discussing during the Philly2013 workshop and on the mailing list, but it does not (yet) reflect a consensus.

James used the new OBI build tool to convert this document into OWL and test it. See: http://obi.svn.sourceforge.net/viewvc/obi/trunk/src/tools/build/

History

This document has gone through several revisions – see SVN for details. Major changes include:

- 2013-06-10: first draft
- 2013-06-17: removed determinable/determinate distinction
- 2013-07-29: removed "information structural entity" and removed "has information structure" in favour of "has value specification"
- 2013-08-12: more conservative approach making fewer changes to the current OBI

Motivation

OBI's scope is biomedical investigations and it must be able to describe the data generated in investigations. Some of the oldest terms in OBI and IAO were designed to describe measurement. More recently we have recognized the need to describe predictions, simulations, and setting information. Superficially these are very similar to each other. "20g" could occur as:

- 1. a measurement of the mass of a particular mouse
- 2. a predicted mass of some future mouse after a treatment

- 3. an output of a simulation of mouse growth
- 4. a rule for selecting mice of a certain mass

Despite the superficial similarity, 1-4 are *about* very different things (if they're about anything at all):

- 1. a particular quality of a particular mouse at a particular time something that clearly existed
- 2. a calculated value that does not correspond to any existing particular quality, but may be compared with a particular quality of a particular mouse in the future if the treatment is carried out
- 3. a calculated value, perhaps about what the mass of mice in general would be like under certain conditions
- 4. a directive, perhaps about part of a particular plan (now) to select mice in the future

OBI is a realist ontology, where we try to build consensus by being as precise as we can be about what is going on in the world. *Aboutness* (in the sense used by IAO) is our primary way of distinguishing information content entities, and so we need to be clear in distinguishing measurements from predictions and settings, etc. This pushes our modelling toward greater complexity.

But we also want our modelling to be as simple as possible. We would like to factor out the similarities between 1-4, in order to reuse as much of our modelling as possible, and in order to reduce the number of asserted hierarchies we're dealing with.

In this proposal we distinguish the *content* that is about something from the "value specification" that is not. "20g" is a value specification, and is not about anything in particular. But we can use the "has value specification" relation to connect a measurement datum to "20g", and thereby say something about the mass that was measured.

The proposal is designed to add just enough complexity to allow us to model measurements, predictions, and simulations in a similar way, by factoring out the shared structure of a "value specification".

Here are some notes on previous discussions:

- Bjoern's summary and proposal
- ICBO 2012 working session
- Christian's summary and proposal
- Philippe and Alejandra's modelling tests
- Philly2013 data document

Upper Ontology

For clarity, we start from scratch rather than importing an existing ontology. Wherever possible, terms here have the same ID as in their source ontologies.

These are BFO classes and relations that we will need. NOTE: We don't include "dependent continuant", because it's not in BFO2 Graz and doesn't serve a purpose here.

```
Class: obo:BF0_0000001
  Annotations: rdfs:label "entity"
Class: obo:BFO_0000002
  Annotations: rdfs:label "continuant"
 SubClassOf: 'entity'
Class: obo:BF0_0000031
  Annotations: rdfs:label "generically dependent continuant"
  SubClassOf: 'continuant'
Class: obo:BFO_0000020
  Annotations: rdfs:label "specifically dependent continuant"
  SubClassOf: 'continuant'
Class: obo:BF0_0000004
  Annotations: rdfs:label "independent continuant"
  SubClassOf: 'continuant'
Class: obo:BF0_0000040
  Annotations: rdfs:label "material entity"
  SubClassOf: 'independent continuant'
Class: obo:BFO 0000019
  Annotations: rdfs:label "quality"
  SubClassOf: 'specifically dependent continuant'
ObjectProperty: obo:BFO_0000086
  Annotations: rdfs:label "has quality"
Class: obo:BF0_0000003
  Annotations: rdfs:label "occurrent"
 SubClassOf: 'entity'
Class: obo:BF0_0000015
  Annotations: rdfs:label "process"
  SubClassOf: 'occurrent'
```

ObjectProperty: obo:BFO_0000057

Annotations: rdfs:label "participates in"

Running Example

Our running example will involve measurements of a particular mouse named "Mickey" as part of a fictional investigation. Here we describe two universals and two particulars:

Class: obo:PATO_0000125

Annotations: rdfs:label "mass"

SubClassOf: 'quality'

Individual: mickey

Types: 'material entity'

Annotations: rdfs:label "Mickey", rdfs:comment "Mickey is a mouse." Facts: 'has quality' 'mass of Mickey'

Individual: mickey-mass

Types: 'mass'

Annotations: rdfs:label "mass of Mickey"

NOTE: In a previous draft of this document we used the determinable/determinate distinction to sub-class 'mass'. This made the modelling more complicated. Since a BFO OWL representation of determinable/determinate classes have not yet been discussed in detail, we decided to remove them from the current prototype.

- Barry's slides: http://ontology.buffalo.edu/bfo/2013/BFO-2-Smith.ppt
- BFO2 issue: https://code.google.com/p/bfo/issues/detail?id=42

NOTE: We aren't modelling time in this prototype.

Information Entities

Under "generically dependent continuant" we distinguish between information content entities (ICEs) that are necessarily *about* something, and information entities that are not necessarily about anything.

ObjectProperty: obo:IAO_0000136
Annotations: rdfs:label "is about"

ObjectProperty: obo:IAO_0000221

Annotations: rdfs:label "is quality measurement of"

SubPropertyOf: 'is about'

Class: obo:IAO_0000030

Annotations: rdfs:label "information content entity"

SubClassOf: 'generically dependent continuant'

SubClassOf: 'is about' some 'entity'

Units of Measurement

Under ICE we include "measurement unit labels" to connect to the Units of Measurement Ontology, and we have an ObjectProperty use with them:

Class: obo:IAO_0000009

Annotations: rdfs:label "datum label" SubClassOf: 'information content entity'

Class: obo:IAO_0000003

Annotations: rdfs:label "measurement unit label"

SubClassOf: 'datum label'

ObjectProperty: obo:IAO_0000039

Annotations: rdfs:label "has measurement unit label"

In OBI we have been modelling specific measurement units as OWL individuals. For our purposes we'll just need the SI unit "gram".

Class: obo:U0_0000002

Annotations: rdfs:label "mass unit label" SubClassOf: 'measurement unit label'

Individual: obo:U0_0000021
 Types: 'mass unit label'

Annotations: rdfs:label "gram"

Value Specifications

A "value specification" is a structure such as a number and a measurement unit, or a categorical classification. They are used for measurement data, predictions,

settings, simulations, etc. Rather than having duplicates classes for each of these different uses, instead we have one "value specification" hierarchy that gets reused for measurement, prediction, etc.

A "value specification" is not necessarily about anything. However, "information content entity" has been used for years as the ancestor class of all OBI and IAO's information entities, and an ICE must be about something. In previous drafts of this prototype and in the OBI Core review process we tried to pull OBI and IAO terms that are not clearly about anything out from under ICE and place the directly under GDC. We were unable to do this in a way that did not disrupt or break large parts of the existing hierarchy. We have therefore left the task of making these distinctions to future versions of IAO.

We will update OBI Core when those distinctions are made. For now we leave "value specification" under ICE.

Class: obo: OBI_0001933

Annotations: rdfs:label "value specification" SubClassOf: 'information content entity'

ObjectProperty: has-value-specification

Annotations: rdfs:label "has value specification"

Range: 'value specification'

DataProperty: obo:IAO_0000004

Annotations: rdfs:label "has specified value", rdfs:comment "was 'has measurement value'"

Domain: 'value specification'

If a value specification is about something, we use the "specifies value of" object property to state the relationship. But not all value specifications are about something in a way that OBI/IAO can currently model, and so this object property is not required.

ObjectProperty: obo:OBI_0001927

Annotations: rdfs:label "specifies value of"

Domain: 'value specification'

The most important of these is "scalar value specification", which is the pair of a number and a unit. Given the "measurement unit label" asserted hierarchy, we can create a hierarchy of *defined classes* as needed:

Class: obo:OBI_0001931

Annotations: rdfs:label "scalar value specification"

EquivalentTo: 'value specification' and

```
'has measurement unit label' some 'measurement unit label' and 'has specified value' min 1 xsd:float
```

```
Class: scalar-mass-value-specification
Annotations: rdfs:label "scalar mass value specification"
EquivalentTo: 'scalar value specification' and
'has measurement unit label' some 'mass unit label'
```

Here is an example of a particular scalar mass value specification, "20g":

```
Individual: 20g-specification
  Types: 'value specification'
  Annotations: rdfs:label "20g specification"
  Facts: 'has measurement unit label' 'gram',
    'has specified value' "20"^^xsd:float
```

Notice that we only assert that this is a 'value specification', and not that it is specifically a 'scalar mass value specification'. The reasoner will classify it correctly:

```
Fact: 20g specification is a scalar mass value specification Query: 'scalar mass value specification' Individuals: include '20g specification'
```

Measurement Data

Our primary goal is to model measurement data well. We assert this class in OBI:

```
Class: obo:IAO_0000109
Annotations: rdfs:label "measurement datum"
SubClassOf: 'information content entity'
```

Given the asserted hierarchy of value specifications, we can create a *defined* hierarchy of measurement classes.

```
Class: value-measurement-datum

Annotations: rdfs:label "value measurement datum"

EquivalentTo: 'measurement datum' and

('has value specification' some 'value specification')
```

Class: scalar-measurement-datum

```
Annotations: rdfs:label "scalar measurement datum"

EquivalentTo: 'measurement datum' and
    ('has value specification' some 'scalar value specification')

Class: scalar-mass-measurement-datum
    Annotations: rdfs:label "scalar mass measurement datum"

EquivalentTo: 'measurement datum' and
    ('has value specification' some 'scalar mass value specification') and
    ('is quality measurement of' some 'mass')
```

We define an instance of a measurement datum about Mickey's mass by linking the value specification "20g" (using 'has value specification') to the particular mass quality being measured (using 'is quality measurement of'):

```
Individual: scalar-measurement-of-mass-of-mickey
  Types: 'measurement datum'
  Annotations: rdfs:label "scalar measurement of mass of Mickey"
  Facts: 'has value specification' '20g specification',
    'is quality measurement of' 'mass of Mickey'
```

We just assert that this is a 'measurement datum', but the reasoner classifies it correctly as a 'scalar mass measurement datum':

Fact: mass measurement of Mickey is a scalar mass measurement datum Query: 'scalar mass measurement datum' Individuals: include 'scalar measurement of mass of Mickey'

Queries

Modelling the data correctly is important, but we also need to query the data and get useful answers. First of all, we can query for all mass measurements:

```
Fact: mass measurement of Mickey is a mass measurement datum

Query: 'measurement datum' and ('is quality measurement of' some 'mass')

Individuals: include 'scalar measurement of mass of Mickey'

Subclasses: include 'scalar mass measurement datum'
```

We can create this defined class to capture all mass measurements:

```
Class: mass-measurement-datum
Annotations: rdfs:label "mass measurement datum"
EquivalentTo: 'measurement datum' and
```

```
'is quality measurement of' some 'mass'
```

```
Fact: mass measurement of Mickey is a 'mass measurement datum' Query: 'mass measurement datum' Individuals: include 'scalar measurement of mass of Mickey' Subclasses: include 'scalar mass measurement datum'
```

Using SPARQL we can get the subject, value, and units for mass measurements:

```
FACT get subject, value, and units for mass of Mickey measurement
PREFIX obo: <a href="http://purl.obolibrary.org/obo/">http://purl.obolibrary.org/obo/</a>
PREFIX: <a href="http://purl.obolibrary.org/obo/obi/test.owl#">http://purl.obolibrary.org/obo/obi/test.owl#</a>
SELECT ?subject ?value ?unit
WHERE {
    ?mass rdf:type obo:PATO_0000125 . # PATO mass
    ?subject obo:BFO_0000086 ?mass_instance . # BFO has quality
    ?measurement rdf:type obo:IAO_0000109 . # IAO measurement datum
    ?measurement obo:IAO_0000221 ?mass_instance . # IAO is quality measurement of
    ?measurement :has-value-specification ?spec .
    ?spec obo:IAO_0000039 ?unit . # IAO has measurement unit label
    ?spec obo:IAO_0000004 ?value . # IAO has value
}
INCLUDE 'Mickey' "20" 'gram'
```

This query looks fairly complicated. However the only *added* complexity from using "value specification" is the 'has value specification' link:

?measurement :has-value-specification ?spec .

TODO: Add a Turtle example. Because Turtle has a nicer syntax for specifying anonymous entities, it might look cleaner than have OWL individuals for the measurement datum and the value specification.

Measurement Processes

When modelling measurements, it's also important to be able to trace which processes produced which results. We'll extend the current model to include an assay that measures Mickey.

```
Class: obo:OBI_0000011
  Annotations: rdfs:label "planned process"
  SubClassOf: 'process'
```

Of course, this could be more complicated. The assay will involve some protocol, that we have not specified here. It might involve a device with a measurement function, and an investigation agent, etc. Here we show that it is simple to query for the assay, and then it should be straightforward to extend the query to other aspects of the assay.

Now we extend the query above to include the assay that generated the measurement datum:

We can query forward from Mickey to the results about him:

```
FACT get the results of assays with Mickey as input
PREFIX obo: <a href="http://purl.obolibrary.org/obo/">
PREFIX : <http://purl.obolibrary.org/obo/obi/test.owl#>
SELECT ?value ?unit
WHERE {
  ?assay obo:OBI_0000293 :mickey . # OBI has specified input
  ?assay obo:OBI_0000299 ?measurement . # OBI has specified output
  ?measurement :has-value-specification ?spec .
  ?spec obo:IAO_0000039 ?unit . # IAO has measurement unit label
  ?spec obo:IAO_0000004 ?value . # IAO has value
INCLUDE "20" 'gram'
We can query backward from a given measurement datum to the assay and its
input:
FACT get the input of the assay that generated a particular measurement
PREFIX obo: <a href="http://purl.obolibrary.org/obo/">
PREFIX : <a href="http://purl.obolibrary.org/obo/obi/test.owl">http://purl.obolibrary.org/obo/obi/test.owl</a>
SELECT ?assay ?input
WHERE {
  ?assay obo:OBI_0000299 :scalar-measurement-of-mass-of-mickey . # OBI has specified output
  ?assay obo:OBI_0000293 ?input . # OBI has specified input
INCLUDE 'assay of mass of Mickey' 'Mickey'
If a value specification is unique, then we can query back from it to the assay
and inputs:
FACT get the input of the assay that generated a particular value specification
PREFIX obo: <a href="http://purl.obolibrary.org/obo/">
PREFIX : <http://purl.obolibrary.org/obo/obi/test.owl#>
SELECT ?assay ?input
WHERE {
  ?measurement :has-value-specification :20g-specification .
  ?assay obo:OBI_0000299 ?measurement . # OBI has specified output
  ?assay obo:OBI_0000293 ?input . # OBI has specified input
}
INCLUDE 'assay of mass of Mickey' 'Mickey'
However, we might want to reuse the same value specification for all our "20g"
measurements (which is the approach used in this prototype), in which case this
query might not return a unique assay and input. Or we might want to use an
```

anonymous individual (i.e. blank node) for the value specification, which could

also make the reverse query difficult. The best idea may be to focus on the measurement datum, then query back to the assay or investigation, and forward to the value specification.

Predictions

If value specifications were only used for measurement data, then we could simplify this modelling by collapsing the distinction between them. But there are several cases other than measurement where we want to use a value specification. One such case is prediction.

We have just begun to include predictions in OBI, and the details are not yet settled. The goal here is to show one approach that works with value specifications. OBI has a term 'prediction' (OBI_0302910), but for the current purpose we define a more specific term. (For simplicity, we do not specify the input.) we also use a new term for the result of the process, and place it as a child of GDC, because the aboutness of the prediction is not clear. The labels are admitted ugly, but hopefully clear. The modelling parallels the assay above.

```
Class: testable-prediction-generation
  Annotations: rdfs:label "testable prediction generation"
  SubClassOf: 'planned process'
  SubClassOf: 'has specified output' some 'predicted measurement result'
Class: predicted-measurement-result
  Annotations: rdfs:label "predicted measurement result"
  SubClassOf: 'generically dependent continuant'
Once we assert 'predicted measurement result' we can define child classes just
as we did with 'measurement datum':
Class: predicted-measurement-value
  Annotations: rdfs:label "predicted measurement value"
  EquivalentTo: 'predicted measurement result' and
    ('has value specification' some 'value specification')
Class: predicted-scalar-measurement-value
  Annotations: rdfs:label "predicted scalar measurement value"
  EquivalentTo: 'predicted measurement result' and
    ('has value specification' some 'scalar value specification')
Class: predicted-scalar-mass-measurement-value
  Annotations: rdfs:label "predicted scalar mass measurement value"
  EquivalentTo: 'predicted measurement result' and
    ('has value specification' some 'scalar mass value specification')
```

NOTE: Perhaps we could specify "and ('is quality measurement of' only 'mass')" for this class.

Then we can instantiate a prediction process and its result. We'll say that the prediction result is "20g", and reuse the same value specification:

```
Individual: prediction-of-mass-of-mice
  Types: 'testable prediction generation'
  Annotations: rdfs:label "testable prediction generation of mass of mice"
  Facts: 'has specified output' 'predicted mass of mice'

Individual: predicted-mass-of-mice
  Types: 'predicted measurement result'
  Annotations: rdfs:label "predicted mass of mice"
  Facts: 'has value specification' '20g specification'
```

We just assert that this is a 'predicted measurement result', but the reasoner classifies it correctly as a 'predicted scalar mass measurement value':

```
Fact: mass measurement of Mickey is a scalar mass measurement datum Query: 'scalar mass measurement datum' Individuals: include 'scalar measurement of mass of Mickey'
```

Using SPARQL we can get the value and units for the prediction. Instead of querying for measurements of mass, here we query for predictions that use mass units:

```
FACT get value and units for predictions of mass
PREFIX obo: <a href="http://purl.obolibrary.org/obo/">http://purl.obolibrary.org/obo/</a>
PREFIX: <a href="http://purl.obolibrary.org/obo/obi/test.owl#">http://purl.obolibrary.org/obo/obi/test.owl#</a>
SELECT ?prediction ?value ?unit
WHERE {
    ?unit rdf:type obo:U0_00000002 . # U0 mass unit
    ?prediction rdf:type :predicted-measurement-result .
    ?prediction :has-value-specification ?spec .
    ?spec obo:IAO_0000039 ?unit . # IAO has measurement unit label
    ?spec obo:IAO_0000004 ?value . # IAO has value
}
INCLUDE 'predicted mass of mice' "20" 'gram'
```

Settings

Settings are another case distinct from measurements where we want to use value specifications. For our current purpose, a setting is part of the instructions for performing an investigation.

Our example will be a material acquisition process involving a selection rule for picking mice for the investigation. We'll assert that the selected mice must weigh less than 20g. First we need to include terms for plans and rules.

```
Class: obo:BF0_0000017
  Annotations: rdfs:label "realizable entity"
  SubClassOf: 'specifically dependent continuant'
ObjectProperty: obo:BFO 0000055
  Annotations: rdfs:label "realizes"
 Domain: 'process'
 Range: 'realizable entity'
ObjectProperty: obo:BFO 0000059
  Annotations: rdfs:label "concretizes"
 Domain: 'specifically dependent continuant'
 Range: 'generically dependent continuant'
Class: obo: OBI_0000260
  Annotations: rdfs:label "plan"
  SubClassOf: 'realizable entity'
Class: obo:IAO_0000033
  Annotations: rdfs:label "directive information entity"
  SubClassOf: 'information content entity'
NOTE: Directive information entity might be better as a direct child of GDC,
but here we leave it under ICE.
Class: obo: OBI_0001755
  Annotations: rdfs:label "selection rule"
  SubClassOf: 'directive information entity'
Class: obo: OBI_0600008
  Annotations: rdfs:label "acquisition"
  SubClassOf: 'planned process'
  SubClassOf: 'realizes' some ('concretizes' some 'selection rule')
Class: obo: OBI 0600010
  Annotations: rdfs:label "material acquisition"
  SubClassOf: 'acquisition'
  SubClassOf: 'has specified output' some 'material entity'
```

Now we instantiate the material acquisition and the selection rule. The modelling of the rule is very basic, and will need to be improved, but serves the current purpose of connecting the rule to the value specification.

```
Individual: select-small-mice-rule
  Types: 'selection rule'
Annotations: rdfs:label "select small mice rule",
    rdfs:comment "Select mice with mass less than 20g."
Facts: 'has value specification' '20g specification'
```

NOTE: We have not provided axioms to constrain the rule to just mice. We have not provided axioms for the "less than" part of the rule. It might be better to say that the rule has a part that has the value specification, but the current modelling is simpler.

```
Individual: select-small-mice-plan
  Types: 'plan'
  Annotations: rdfs:label "select small mice plan"
  Facts: 'concretizes' 'select small mice rule'

Individual: acquisition-of-mice
  Types: 'material acquisition'
  Annotations: rdfs:label "acquisition of mice"
  Facts: 'realizes' 'select small mice plan'
```

Now we can query for processes that realize some concretization of a mass setting, and the value and units:

TODO: It will be important to model ranges of values, including the significant figures in scientific notation.

Other Sorts of Measurement

The main use of value specifications is to handle scalar measurements with units. But we can also handle categorical classifications as another sort of value

specification, and measurements that don't use value specifications.

Categorical Measurements

Here is an example of a 'categorical value specification' that is used to classify a mouse in the "mouse with average mass" category:

```
Class: obo: OBI_0001930
  Annotations: rdfs:label "categorical value specification"
  SubClassOf: 'value specification'
Individual: mouse-with-average-mass-specification
  Types: 'categorical value specification'
  Annotations: rdfs:label "mouse with average mass value specification",
    rdfs:comment "Applies to mice with a mass of ~20g."
Individual: average-mass-measurement
  Types: 'measurement datum'
  Annotations: rdfs:label "categorical measurement of mass of Mickey"
 Facts: 'has value specification' 'mouse with average mass value specification',
    'is quality measurement of' 'mass of Mickey'
We can define subclasses of 'measurement datum' to demonstrate the correct
classifications:
Class: categorical-measurement-datum
  Annotations: rdfs:label "categorical measurement datum"
  EquivalentTo: 'measurement datum' and
    ('has value specification' some 'categorical value specification')
Class: categorical-mass-measurement-datum
  Annotations: rdfs:label "categorical mass measurement datum"
  EquivalentTo: 'measurement datum' and
    ('has value specification' some 'categorical value specification') and
    ('is quality measurement of' some 'mass')
Fact: average mass measurement is a categorical mass measurement datum
Query: 'categorical mass measurement datum'
Individuals: include 'categorical measurement of mass of Mickey'
Fact: average mass measurement is a mass measurement datum
Query: 'mass measurement datum'
Individuals: include 'categorical measurement of mass of Mickey'
```

Note: We defined 'scalar mass value specification' by means of 'mass unit label' above, but we don't currently have a way to define a parallel "categorical mass value specification".

Unstructured Measurements

Class: IAO_0000300

There can also be measurements that do not make use of 'value specification'. As an example, we can have a "free text" description of the mass of Mickey, which I model here as both a textual entity and an measurement datum.

```
Annotations: rdfs:label "textual entity"
  SubClassOf: 'information content entity'
Individual: free-text-mass-measurement
  Types: 'textual entity', 'measurement datum'
  Annotations: rdfs:label "free text description of mass of Mickey",
   rdfs:comment "Mickey's mass seems to be about average for a mouse."
 Facts: 'is quality measurement of' 'mass of Mickey'
Now we have a 'measurement datum' that is not a 'value measurement datum':
Fact: the description is a 'measurement datum'
Query: 'measurement datum'
Individuals: include 'free text description of mass of Mickey'
Fact: the description is not a 'value measurement datum'
Query: 'value measurement datum'
Individuals: exclude 'free text description of mass of Mickey'
Fact: the description is a 'mass measurement datum'
Query: 'mass measurement datum'
Individuals: include 'free text description of mass of Mickey'
Class: textual-mass-measurement-datum
  Annotations: rdfs:label "textual mass measurement datum"
  EquivalentTo: 'measurement datum' and
    'textual entity' and
    ('is quality measurement of' some 'mass')
Fact: the description is a 'textual mass measurement datum'
Query: 'textual mass measurement datum'
Individuals: include 'free text description of mass of Mickey'
```