

Convergence in Computational Neuroscience 2012

# Introduction to CNO

an ontology for annotating computational neuroscience models

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## What is an ontology?

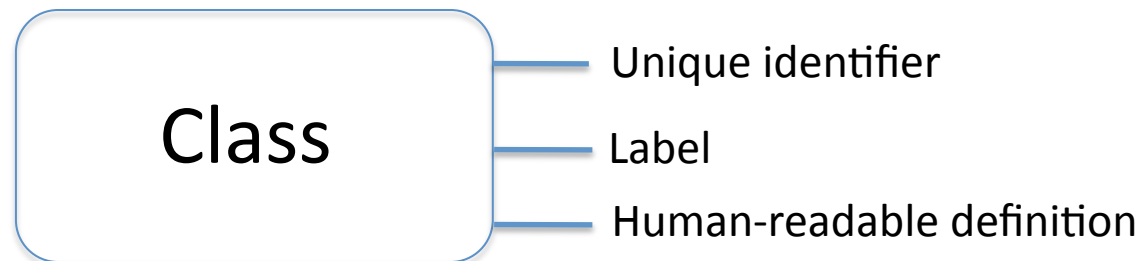
Ontologies are formal models of knowledge in a particular domain and composed of classes that represent concepts defining the field as well as the logical relations that link these concepts together



Class

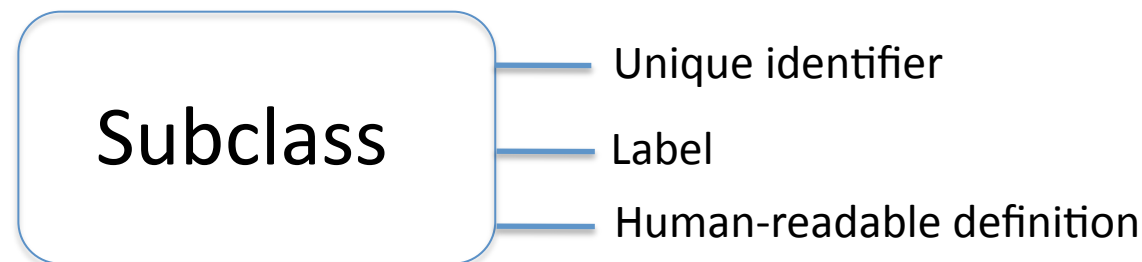
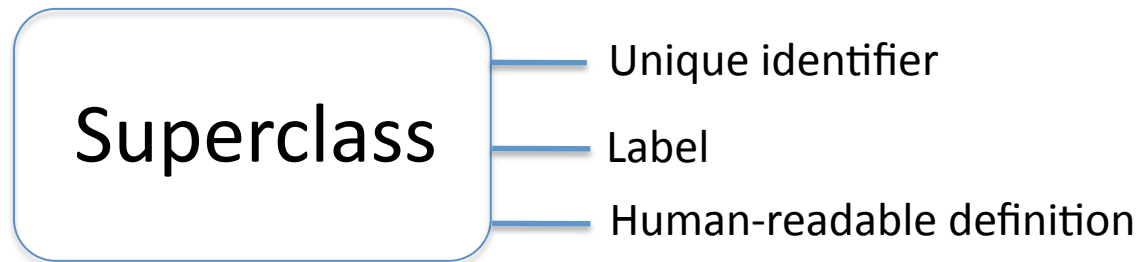
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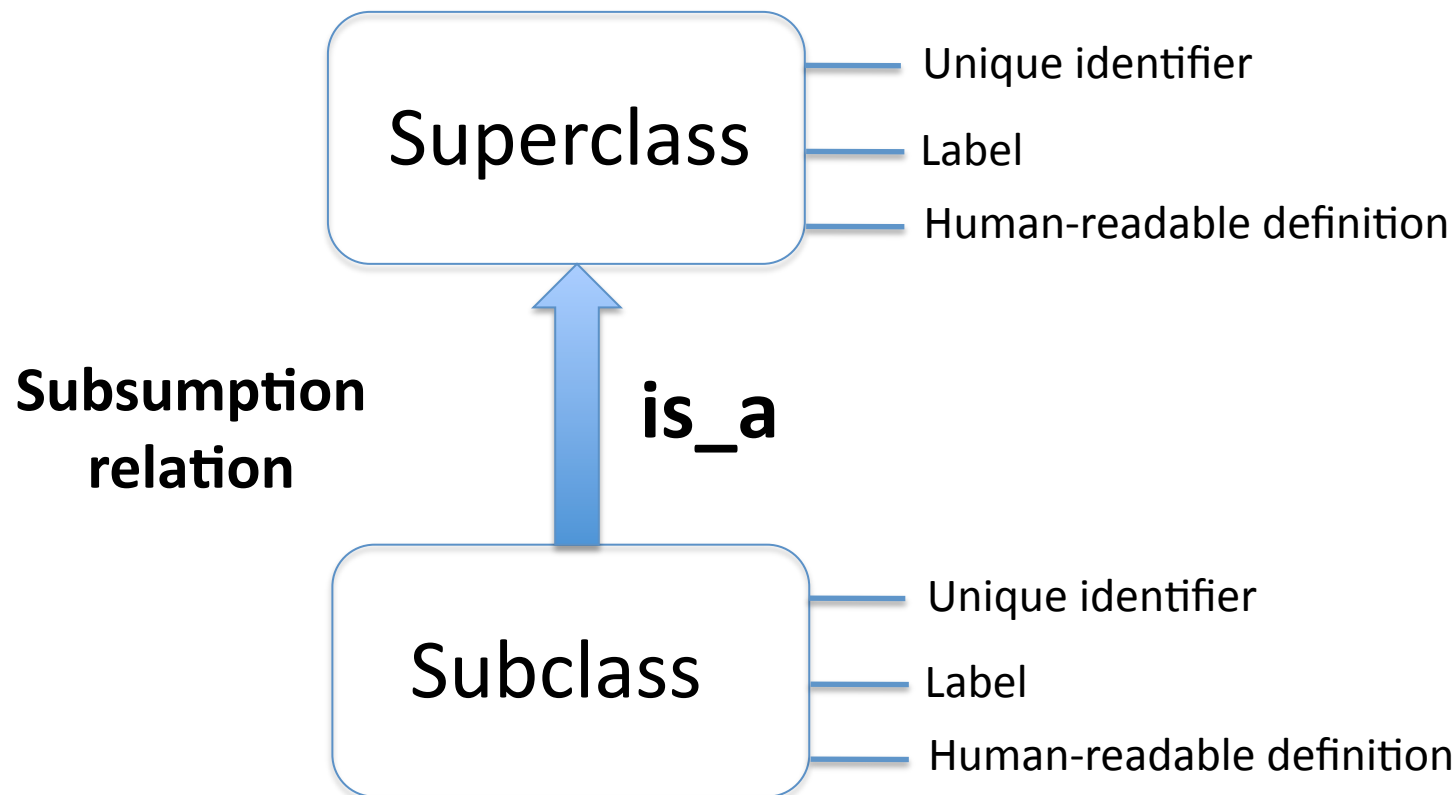
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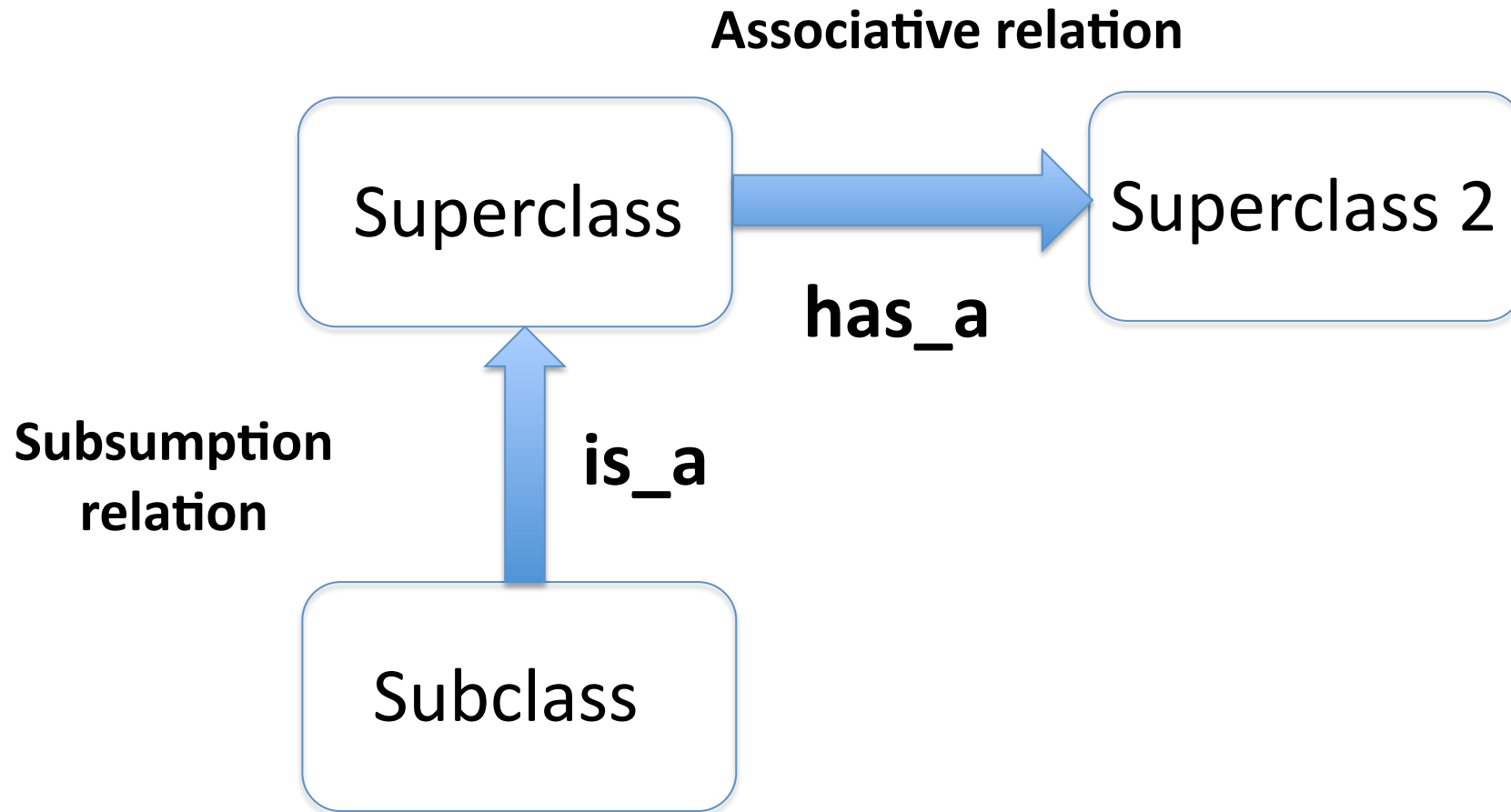
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These **classes** and **relations** have unique identifiers and definitions that allow **unambiguous** annotation of digital resources such as web pages or model source code

# An example: System Biology Ontologies

From Courtot M. and al., Mol Sys. Biol, 2011



```
<reaction id="E1" reversible="false" sboTerm="SB0:0000182" >
  <listOfReactants>
    <speciesReference species="S" sboTerm="SB0:0000015" />
  </listOfReactants>
  <listOfProducts>
    <speciesReference species="P" sboTerm="SB0:0000011" />
  </listOfProducts>
  <listOfModifiers>
    <modifierSpeciesReference species="E" sboTerm="SB0:0000013" />
  </listOfModifiers>
  <kineticLaw sboTerm="SB0:0000029">
    <math xmlns="http://www.w3.org/1998/Math/MathML" >[...]</math>
    <listOfParameters>
      <parameter id="K" value="1" sboTerm="SB0:0000027" />
    </listOfParameters>
  </kineticLaw>
</reaction>
```

Conversion

Substrate

Product

Catalyst

Henri-Michaelis-Menten rate law

Michaelis constant

# An example: System Biology Ontologies

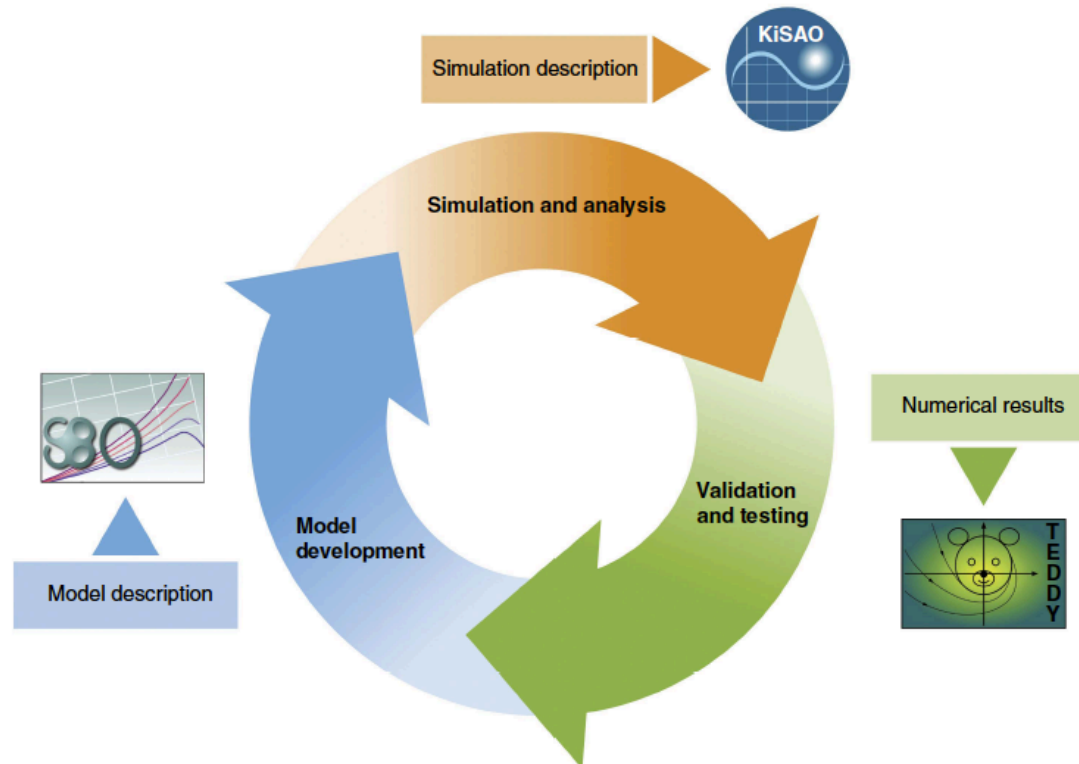
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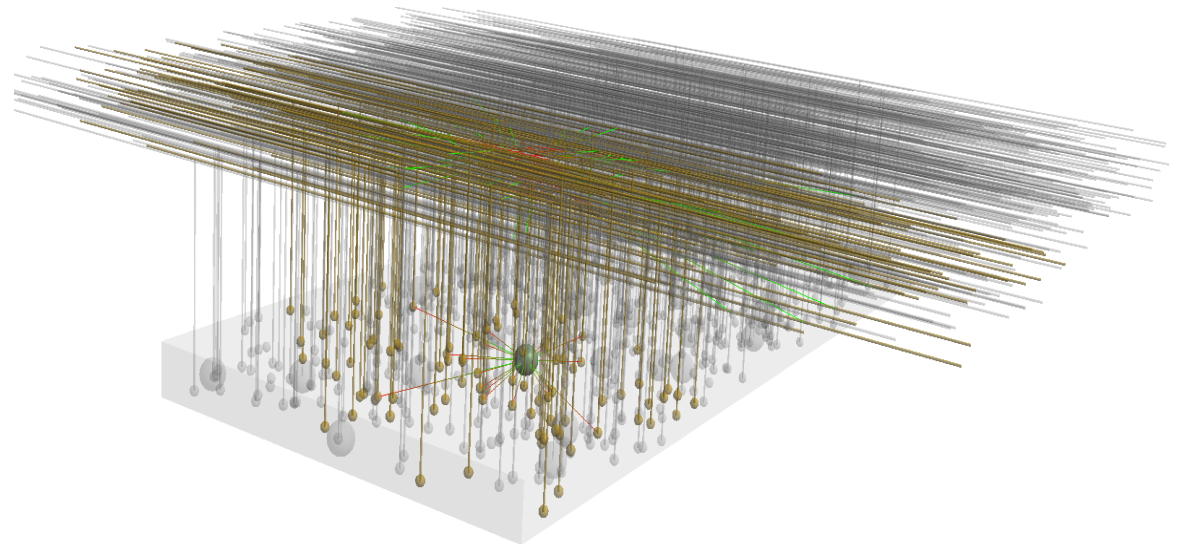
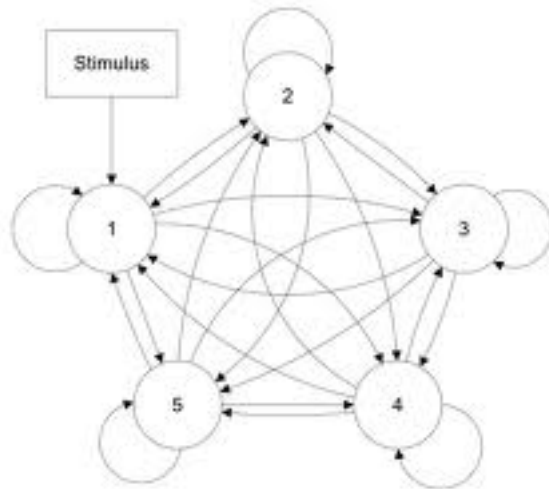
# An ontology for Computational Neuroscience: why?

## INCF Multi Scale modeling program

adding semantic information to NineML models

=> Extensible to other model descriptions: NeuroML, PyNN, ...

## Scope: Initial Annotating models of spiking neural network



=> Extended scope to Computational Neurosciences

# How to design CNO?

Constrain 1: being compatible and interoperable with other ontologies.

Design based on OBO community recommendations:

Label: cno\_7digits

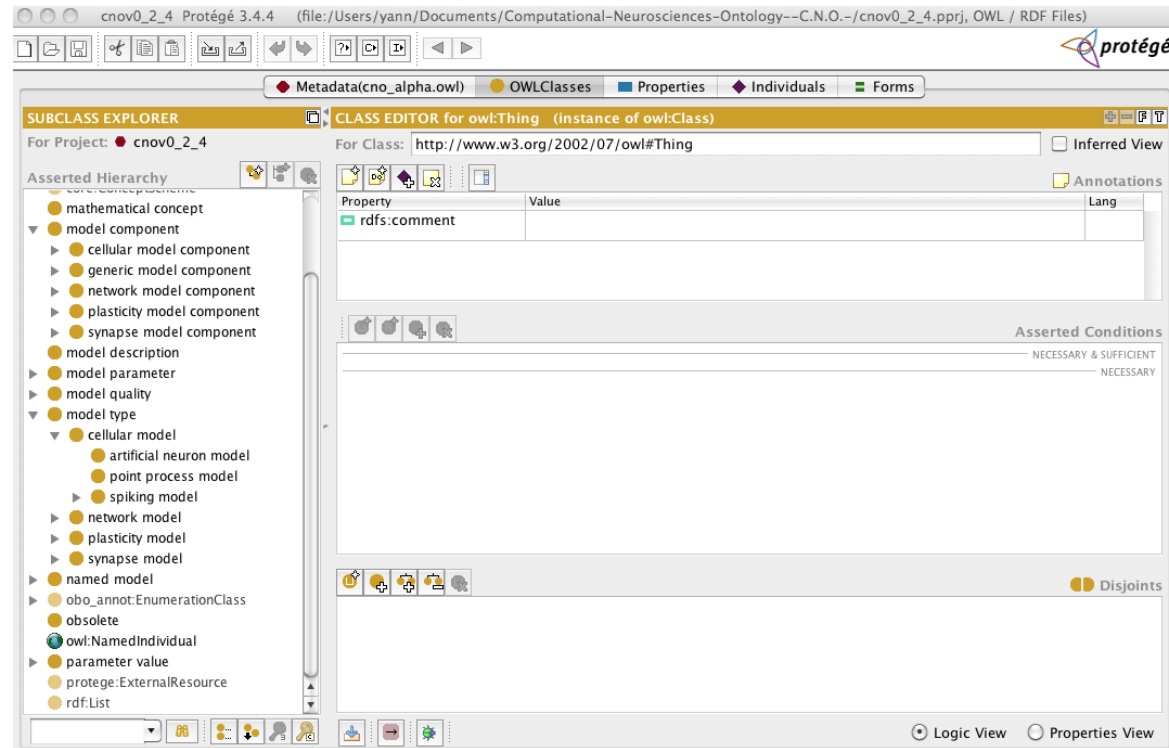
Definition: based on Aristotelician definition: *genis vs. qualia*

Constrain 2: being able to make inference => OWL-DL

```
<owl:Class rdf:about="#cno_0000001">
  <rdfs:label rdf:datatype="http://www.w3.org/2001/XMLSchema#string">model type</rdfs:label>
  <rdfs:comment rdf:datatype="http://www.w3.org/2001/XMLSchema#string">
    This general class includes the most common types of models classified based on the level of
    description of the nervous system.</rdfs:comment>
  <owl:disjointWith rdf:resource="#cno_0000004"/>
  <owl:disjointWith rdf:resource="http://www.w3.org/2004/02/skos/core#Collection"/>
  <owl:disjointWith rdf:resource="#cno_0000175"/>
  <core:definition rdf:datatype="http://www.w3.org/2001/XMLSchema#string"
  >Representation of the different types of models.</core:definition>
  <owl:disjointWith rdf:resource="#cno_0000040"/>
  <owl:disjointWith rdf:resource="#cno_0000176"/>
  <rdfs:subClassOf>
    <owl:Restriction>
      <owl:onProperty>
        <owl:ObjectProperty rdf:about="#cno_0000005"/>
      </owl:onProperty>
```

# How to design CNO?

Protégé (<http://protege.stanford.edu/>)



Pizza tutorial



What if a model is a special kind of pizza?

# How to design CNO?

## Textbooks



## Journals



## What is CNO?

Version 0.2.4

-> 210 classes

-> 8 Object Properties

-> 4 Datatype Properties

Accessible on Bioportal

<http://bioportal.bioontology.org/ontologies/3003>

Owl File on Github

<https://github.com/INCF/Computational-Neurosciences-Ontology--C.N.O.-/tree/gh-pages>

## CNO: 3 main classes

**Model type:** proposing a taxonomy of model



**Model component:** selecting the toppings to add to describe the model

**Named model:** creating classical pizzas





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**Model type:** proposing a taxonomy of model



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**hasComponent**

**Named model:** creating classical pizzas



## CNO: 3 main classes

Classification: restrictions

**Model type:** proposing a taxonomy of model



**Model component:** selecting the toppings to add to describe the model



**hasComponent**

**Named model:** creating classical pizzas







Let's have a look at CNO

## CNO: What about model components?

**Model component ?**

Parameter

Variable

Functions



## CNO: What about model components?

Model component

Model parameter

Functions

Variable

Parameter

Should we list all the specific named parameters?

Do we actually know them?

How do we call them usually?

=> Necessity of disambiguation

Gathering the variability of parameter naming and the parameter values

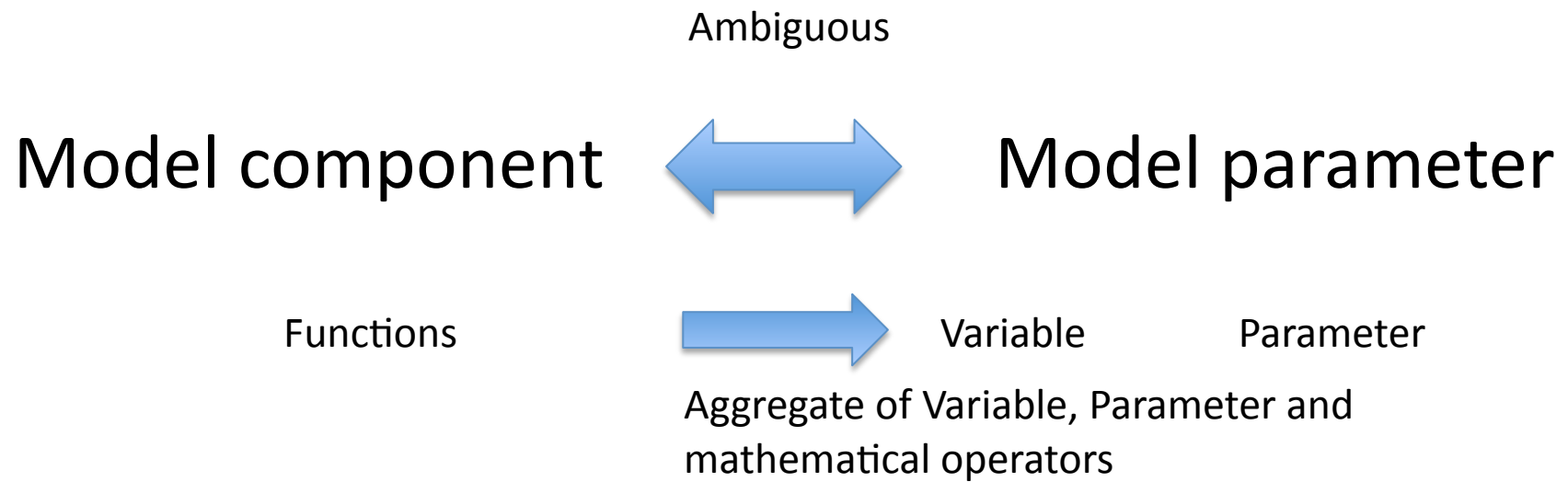
hasValue



Datatypes:

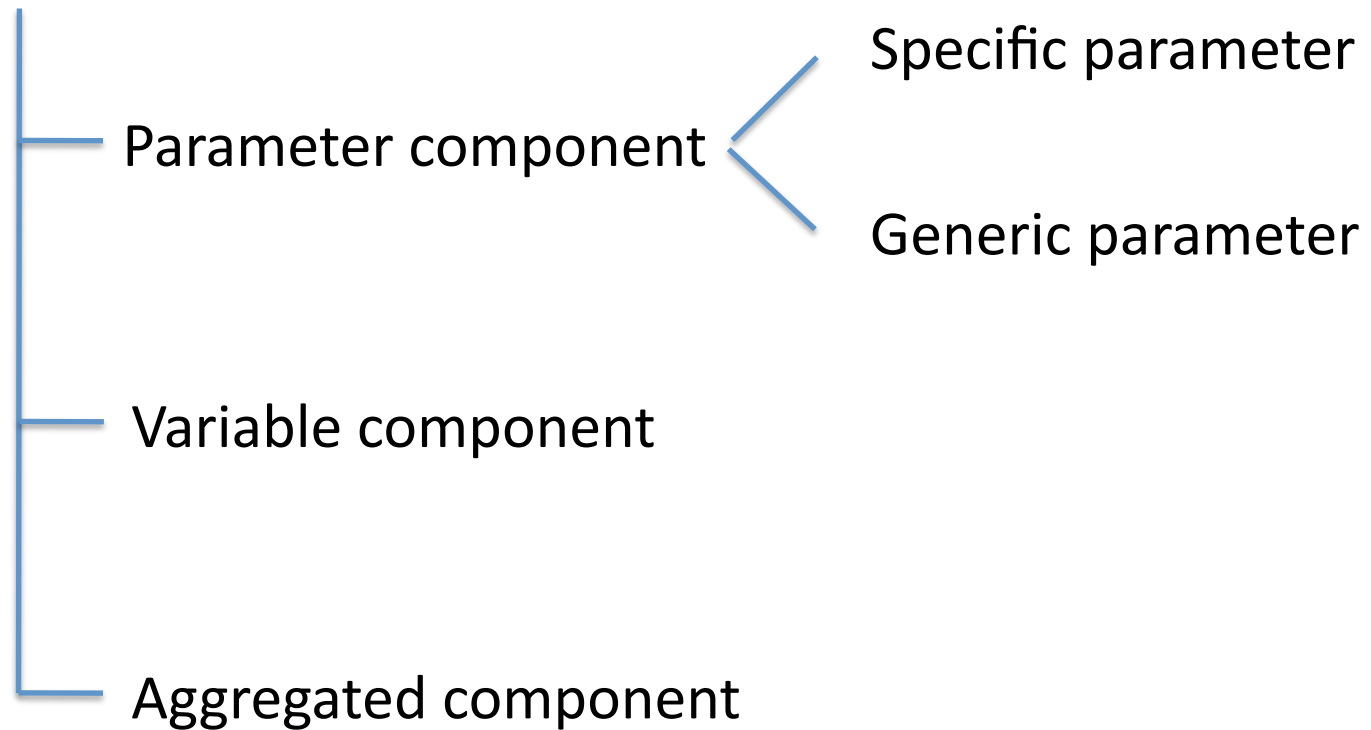
Name, Notation, Numerical Value, units

# CNO: What about model components?



## CNO: What about model components?

### Model component



# CNO: What is next?

Mapping with Biomedical Ontologies

 **BFO** Basic Formal Ontology

**IFOMIS**



 **science commons**

**The Ontology for Biomedical Investigations**

Search



**information-artifact-ontology**

The Information Artifact Ontology (IAO) is an ontology of information entities based on the BFO

⇒ Interoperability with Biomedical ontologies especially NIFSTD: allow linking with Neurosciences terms

# CNO: What is next?

## Publication on NeuroLex: community tool to develop the ontology

The screenshot displays the NeuroLex website interface. On the left, there is a navigation menu with the NeuroLex logo and links for 'ABOUT', 'WHAT'S NEW', 'FAQS', 'NIFSTD ONTOLOGIES', 'HOW TO CONTRIBUTE', 'CURATION POLICIES', 'SUBSCRIBE', 'BACK TO NIF HOMEPAGE', and 'REGISTER A RESOURCE'. The main content area features a search bar with the text 'Find a Term!', a 'Show me a Random Term!' button, and a list of 'All Categories' from A to Z. Below this, there are four buttons for creating new terms: 'Create a new cell', 'Create a new brain region', 'Create a new resource', and 'Create a new generic'. Each button is accompanied by an input field. On the right side, there is a 'NIF incf' logo, a search bar for the wiki, and a 'MediaWiki' dropdown menu. A 'NIF NAVIGATOR' sidebar lists various data types and their counts, such as 'Animals (271504)', 'Connectivity (132460)', 'Dataset (611)', 'Pathways (497035)', 'Models (705)', 'Grants (2686257)', 'Brain Activation Foci (56581)', 'Antibodies (935642)', 'Biospecimen (35833)', 'Clinical Trials (107560)', 'Microarray (312252579)', 'People (377)', 'Multimedia (14005)', 'Software (1116)', 'Images (591097)', 'Drugs (656465)', 'Disease (27067)', and 'Plasmids (21152)'. Below the sidebar, there is a 'NERVOUS SYSTEM LEVEL' section with links to 'Genes (64754164)', 'Multi-Level (2850991)', 'Brain Regions (50083)', 'Molecular Level (697691)', 'Cellular Level (29509)', and 'Nervous System Function (66226)'. At the bottom, there is a 'Contribution Scores' section with a link to 'Last 30 days (Top 10)'. The footer contains the text: 'The NeuroLex project, supported by the Neuroscience Information Framework project, is a dynamic lexicon of neuroscience terms. Unlike an encyclopedia, a lexicon provides the meaning of a term, and not all there is to know about it. The NeuroLex is being constructed to help improve the way that neuroscientists communicate about their data, so that information systems like the NIF can find data more readily and provide more powerful means of integrating data that come across distributed resources. One of the big challenges to data integration is...

# CNO: What is next?

## Importing terms from SBO using MIREOT: Minimum information to reference an external ontology term

The image displays two web-based ontology interfaces. On the left is the 'Systems Biology' ontology, and on the right is the 'Kinetic Simulation Algorithm Ontology'. Both interfaces feature a 'Jump To:' search bar and a hierarchical tree view of terms. The 'Systems Biology' tree shows categories like 'mathematical expression', 'modelling framework', and 'systems description parameter'. The 'Kinetic Simulation Algorithm Ontology' tree shows categories like 'modeling and simulation algorithm' and 'modeling and simulation algorithm parameter'. The right interface also includes a 'Details' tab with a table of term information.

Details	Visualization	Notes (0)	Term Mappings (0)	Term Resources
Preferred Name				modeling and simulation algorithm
Definitions ( <i>skos:definition</i> )				Algorithm used to instantiate a simulation from a mathematical model.
ID				kisao:KISAO_0000000
Full Id				<a href="http://www.biomodels.net/kisao/KISAO#KISAO_0000000">http://www.biomodels.net/kisao/KISAO#KISAO_0000000</a>
Created				2008-05-26
Creator				dk
Is Organizational				true
Label				modeling and simulation algorithm
Definition				Algorithm used to instantiate a simulation from a mathematical model.
Disjoint With				<a href="#">modeling and simulation algorithm parameter</a> <a href="#">modeling and simulation algorithm characteristic</a>



## Making use of CNO

Annotation of LEMS and NeuroML

Annotation of PyNN

Annotation of ModelDB

Annotation of scientific publication

## CNO: What for?

- \* Model consistency checking

- \* Source code annotation

- \* Modelpedia:

  - ⇒ federate and organize specific information about particular types of model

  - ⇒ create a platform to compare model variants and establish mathematical links between the different model types

Many thanks to...

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Jeff Grethe, UCSD