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An Internet of "Computational Things"?

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Ontolog Summit 2015

Internet of Things: Toward Smart Networked Systems and Societies

Track B: Beyond Semantic Sensor Network Ontologies

March 5, 2015

"Linked Open Data for Computational Science?"

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DASPOS Data and Software Preservation for Open Science

ABOUT | PEOPLE | WORKSHOPS | RESEARCH | REPORTS

The massive data sets accumulated by High Energy Physics (HEP) experiments represent the most direct result of the often decades-long process of construction, commissioning and data acquisition that characterize this science. Many of these data are unique and represent an irreplaceable resource for potential future studies. Forward-thinking efforts for preservation are necessary now in order to achieve the relevant parameters, analysis paths and software to preserve the usefulness of these rich and varied data sets.

"Ten or 20 years ago we might have been able to repeat an experiment. They were simpler, cheaper and on a smaller scale. Today that is not the case. So if we need to re-evaluate the data we collect to test a new theory, or adjust it to a new development, we are going to have to be able to reuse it. That means we are going to need to save it as open data..."

Rolf-Dieter Heur 2008
Director General, CERN

Second Workshop Completed

The second DASPOS Workshop took place on Thursday, July 25, 2013, at ACM/IEEE JCDL in Indianapolis, Indiana.
More information

Data and Software Preservation for Open Science, DASPOS, represents an initial exploration of the key technical problems that must be solved to provide appropriate data, software and algorithmic preservation for HEP, including the contexts necessary to understand, trust and reuse the data. While the archiving of HEP data may require some HEP-specific technical solutions, DASPOS will create a template for preservation that will be useful across many different disciplines, leading to a broad, coordinated effort.

Discovery and Coordination

Series of highly-structured public workshops to define, discuss and document the details of data and software preservation

Prototyping and Experimentation

Key areas of research: data and query models and software sustainability models

The DASPOS Team

Computer science experts, experienced digital librarians, and experts in data-intensive fields, such as physics, astrophysics and

DASPOS:http://daspos.org

Gary Berg-Cross and David Carral

GeoVocamp SOCoP 2014: http://vocamp.org/wiki/GeoVoCampSOCoP2014

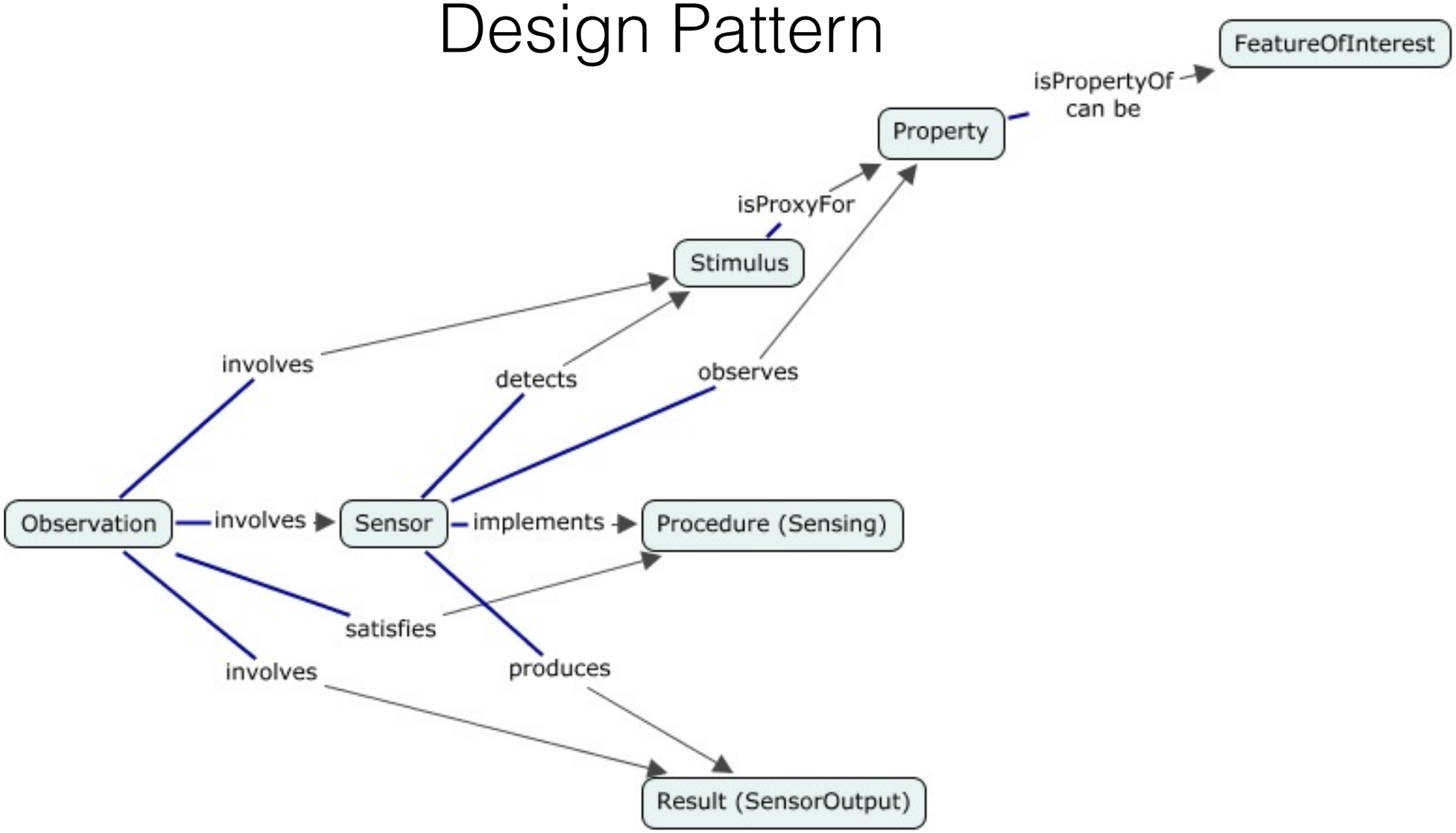
DaSe Lab, Kno.e.sis Center, Wright State University

David Carral, Adila Krisnadhi,
Michelle Cheatham, Pascal Hitzler

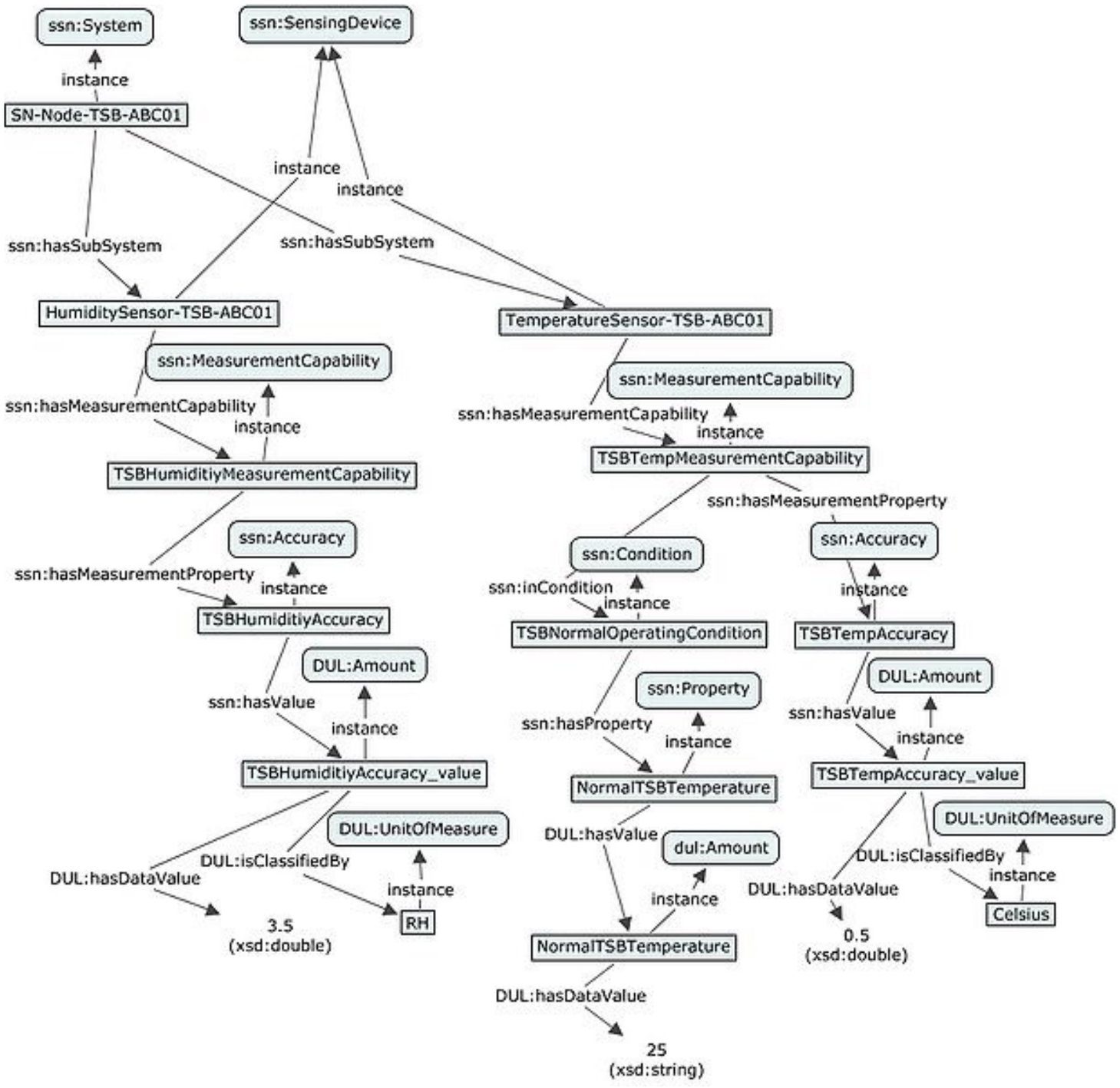
Credit: Beatrice Murch, Creative Commons License, https://www.flickr.com/photos/blmurch/2754681293/sizes/l/

How did you take it's temperature?

The Stimulus-Sensor-Observation Ontology Design Pattern



SSN: http://www.w3.org/2005/Incubator/ssn/wiki/SSN_Skeleton#The_Stimulus-Sensor-Observation_Ontology_Design_Pattern



SSN: http://www.w3.org/2005/Incubator/ssn/wiki/Report_Work_on_the_SSN_ontology

How might a Computational Scientist take it's temperature?

Temperature

$$T = \frac{2}{3k_B} \left\langle \frac{1}{N} \sum_{i=1}^{N} \frac{|\mathbf{p}_i|}{2m_i} \right\rangle$$

But this definition depends on some **computational** model that captures the molecular behavior of water…

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Water model - Wikipedia, the free encyclopedia

en.wikipedia.org/wiki/Water_model ▾ Wikipedia ▾

The potential for models such as TIP3P and **TIP4P** is represented by. E_{ab} = \ sum_{i} ^{\text{on. where kC, the electrostatic constant, has a value of 332.1 ...

Simple water models - 2-site - 3-site - 4-site

TIP4P model of water page on SklogWiki - a wiki for ...

www.sklogwiki.org/SklogWiki/index.php/**TIP4P**_model_of_water ▾

Jan 20, 2011 - The **TIP4P** model is a rigid planar four-site interaction potential for water, ... The **TIP4P** model consists of a Lennard-Jones site for the oxygen ...

Parameters - Phase diagram - Shear viscosity - Virial coefficients

Water models

www.lsbu.ac.uk/water/models.html ▾ London South Bank University ▾

Apr 1, 2014 - Water molecular models including SPC, SPC/E, TIP3P, **TIP4P**, TIP5P, PPC, POL5 , SSD and SWFLEX.

pair_style lj/cut/coul/long - Lammps

lammps.sandia.gov/doc/pair_lj.html ▾ Sandia National Laboratories ▾

style = lj/cut or lj/cut/coul/cut or lj/cut/coul/debye or lj/cut/coul/dsf or lj/cut/coul/long or lj/cut/coul/msm or lj/cut/**tip4p**/long; args = list of arguments for a particular ...

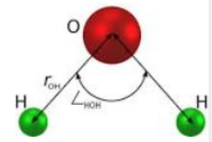
[PDF] TIP4P-Ew - Stanford University

www.stanford.edu/.../horn_**tip4p**EW_2004jcp.pdf ▾ Stanford University ▾

by HW Horn - 2004 - Cited by 557 - Related articles

May 22, 2004 - A re-parameterization of the standard **TIP4P** water model for use with Ewald techniques is introduced, providing an overall global improvement ...

Water model



In computational chemistry, classical water models are used for the simulation of water clusters, liquid water, and aqueous solutions with explicit solvent. These models use the approximations of molecular mechanics. Wikipedia

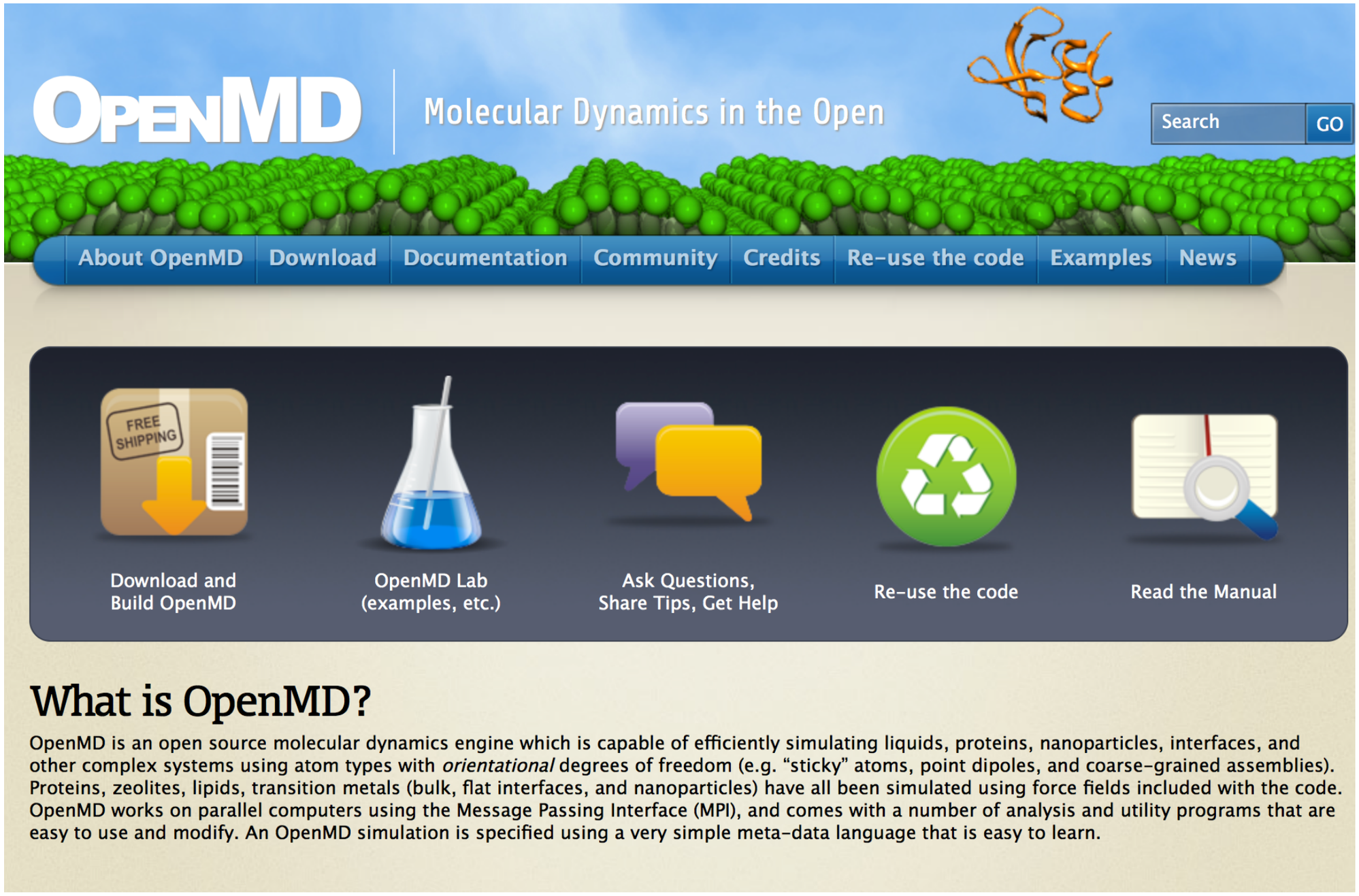
Related topics

In most water models, the **Lennard-Jones** term applies only to the interaction between the oxygen atoms. Wikipedia
Explore: Lennard-Jones potential

In-silico (see: water models), cyclic **water clusters** . . . are found with n = 3 to 60. Wikipedia
Explore: Water cluster

Feedback

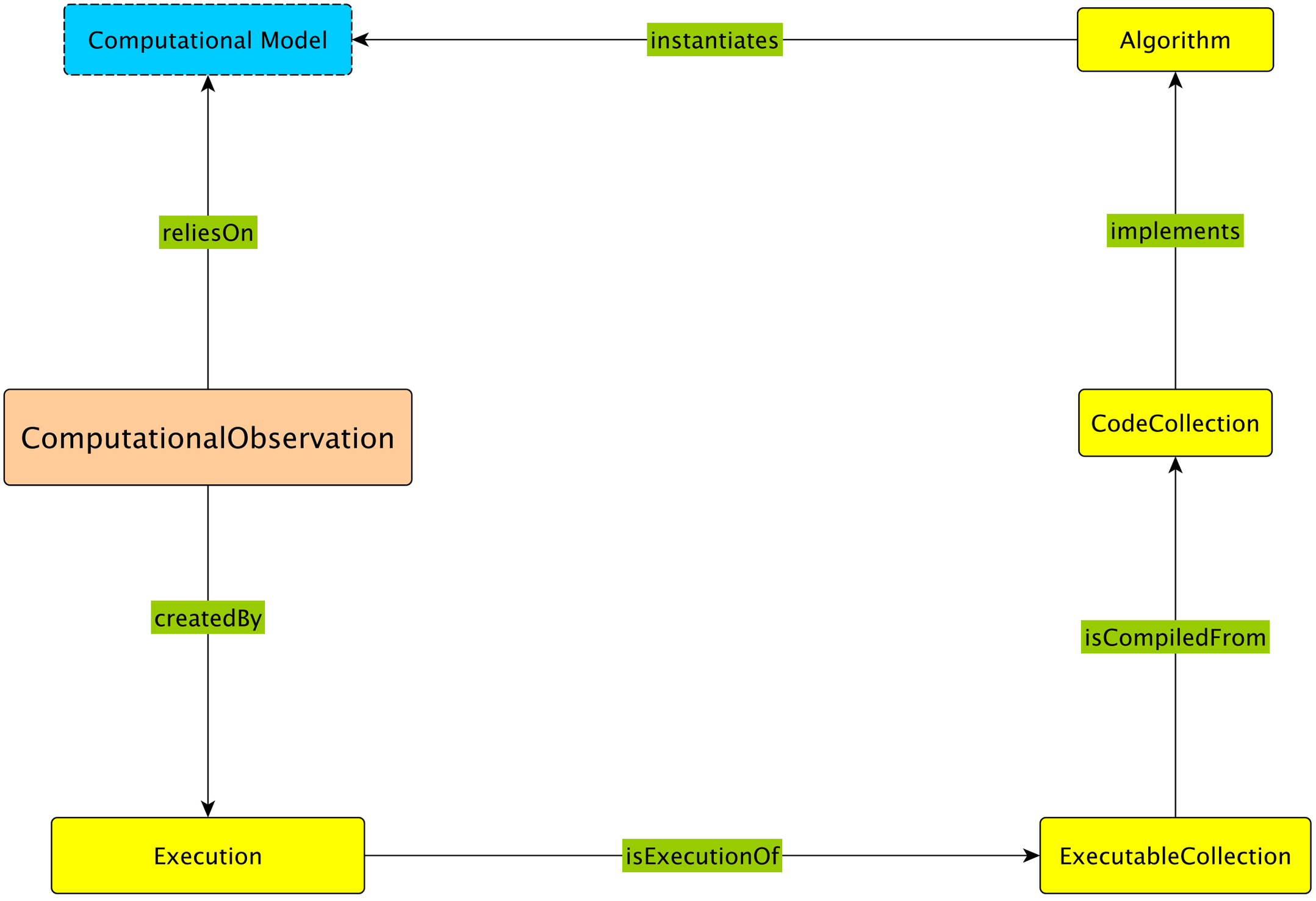
And some **software code** that implements the computational model by **algorithm**…

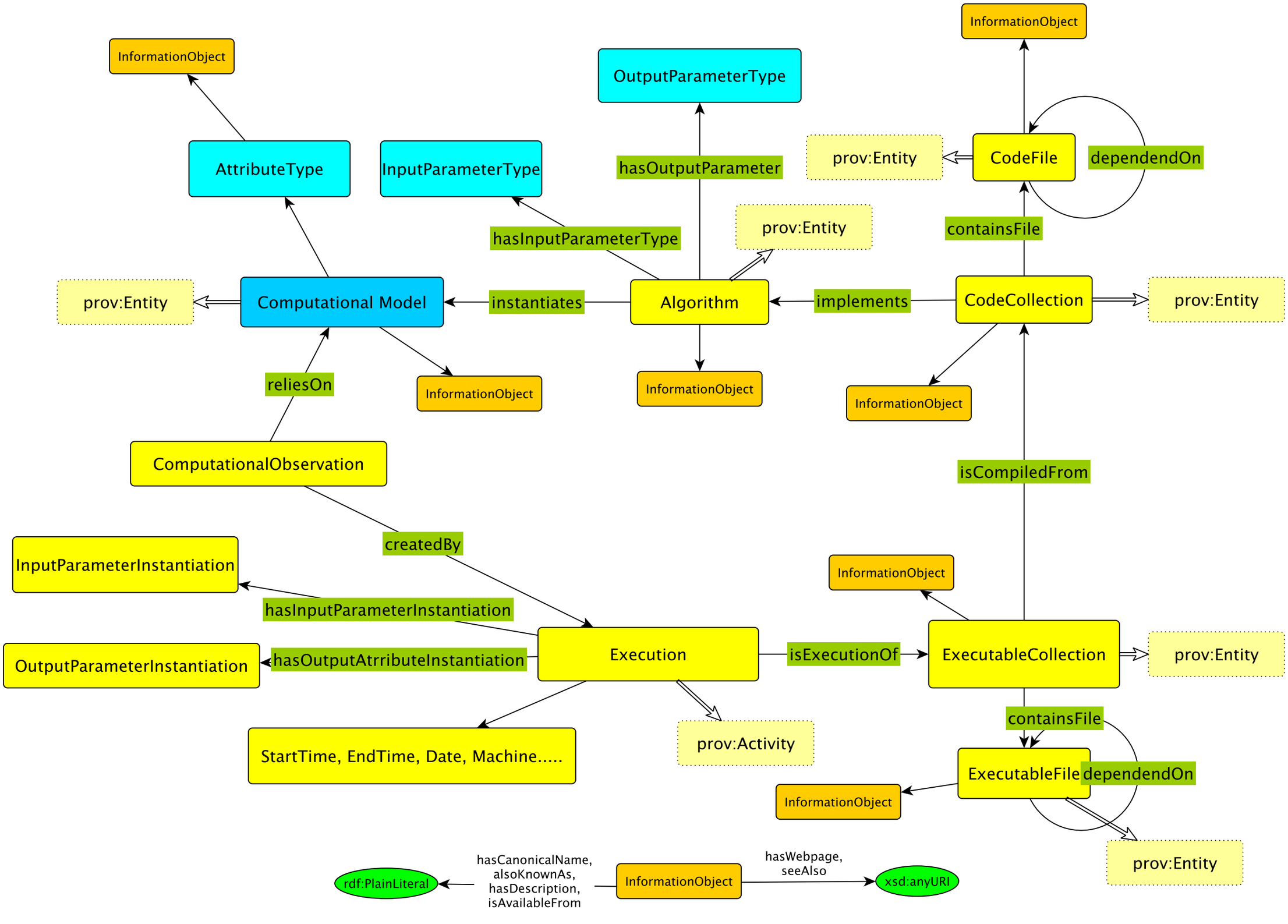


OpenMD: http://www.openmd.org

And some and some **execution** of the code that produces the data needed for a observation…

How to Connect “Physical Experimental Observation” to “Computational Experimental Observation”?


Computational Model
instantiates
Algorithm
reliesOn
implements
ComputationalObservation
CodeCollection
createdBy
isCompiledFrom
Execution
isExecutionOf
ExecutableCollection


InformationObject
OutputParameterType
InformationObject
AttributeType
InputParameterType
hasOutputParameter
prov:Entity
CodeFile
dependendOn
hasInputParameterType
prov:Entity
containsFile
prov:Entity
Computational Model
instantiates
Algorithm
implements
CodeCollection
prov:Entity
reliesOn
InformationObject
InformationObject
InformationObject
ComputationalObservation
isCompiledFrom
createdBy
InputParameterInstantiation
InformationObject
hasInputParameterInstantiation
OutputParameterInstantiation
hasOutputAtrributeInstantiation
Execution
isExecutionOf
ExecutableCollection
prov:Entity
containsFile
StartTime, EndTime, Date, Machine.....
prov:Activity
ExecutableFile
dependendOn
InformationObject
prov:Entity
rdf:PlainLiteral
hasCanonicalName,
alsoKnownAs,
hasDescription,
isAvailableFrom
InformationObject
hasWebpage,
seeAlso
xsd:anyURI

Application to IoT?

- Comments on the pattern itself?
- Examples from IoT to which the pattern could be applied?
- Potential Hackathon Topic?
- March 28th and 29th as potential dates?

Thank you!