An Internet of “Computational Things”?

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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?”
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.

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.

"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

DASPOS: http://daspos.org
Gary Berg-Cross and David Carral

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

David Carral, Adila Krisnadhi, Michelle Cheatham, Pascal Hitzler
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

\[ T = \frac{2}{3k_B} \left\langle \frac{1}{N} \sum_{i=1}^{N} \frac{|p_i|}{2m_i} \right\rangle \]
But this definition depends on some **computational** model that captures the molecular behavior of water…
Water model - Wikipedia, the free encyclopedia
The potential for models such as TIP3P and TIP4P is represented by. E_{ab} = \sum_i\text{...}
Simple water models - 2-site - 3-site - 4-site

TIP4P model of water page on SklogWiki - a wiki for ...
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/def or lj/cut/coul/long or ...

[PDF] TIP4P-Ew - 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 ....

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
And some **software code** that implements the computational model by **algorithm**...
What is OpenMD?

OpenMD is an open source molecular dynamics engine which is capable of efficiently simulating liquids, proteins, nanoparticles, interfaces, and other complex systems using atom types with orientational degrees of freedom (e.g., “sticky” atoms, point dipoles, and coarse-grained assemblies). Proteins, zeolites, lipids, transition metals (bulk, flat interfaces, and nanoparticles) have all been simulated using force fields included with the code. OpenMD works on parallel computers using the Message Passing Interface (MPI), and comes with a number of analysis and utility programs that are easy to use and modify. An OpenMD simulation is specified using a very simple meta-data language that is easy to learn.

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”?
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!