

Geovocamp Madison 2014

Material TRANSFORMATION ONTOLOGY DESIGN PATTERN

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University of Notre Dame

GeoVocamps

- Vocamps have been active since 2008. GeoVocamps since 2011
- I have participated in:
 - GeoVoCamp Dayton 2012
 - GeoVoCamp SOCoP DC 2012
 - GeoVoCamp Santa Barbara 2013
 - GeoVoCamp DC 2013
 - Decartes-Core GeoVoCamp Santa Barbara 2014

OPENMD

Molecular Dynamics in the Open

[About OpenMD](#)[Download](#)[Documentation](#)[Community](#)[Credits](#)[Re-use the code](#)[Examples](#)[News](#)

Download and
Build OpenMD



OpenMD Lab
(examples, etc.)



Ask Questions,
Share Tips, Get Help



Re-use the code



Read the Manual

What is OpenMD?

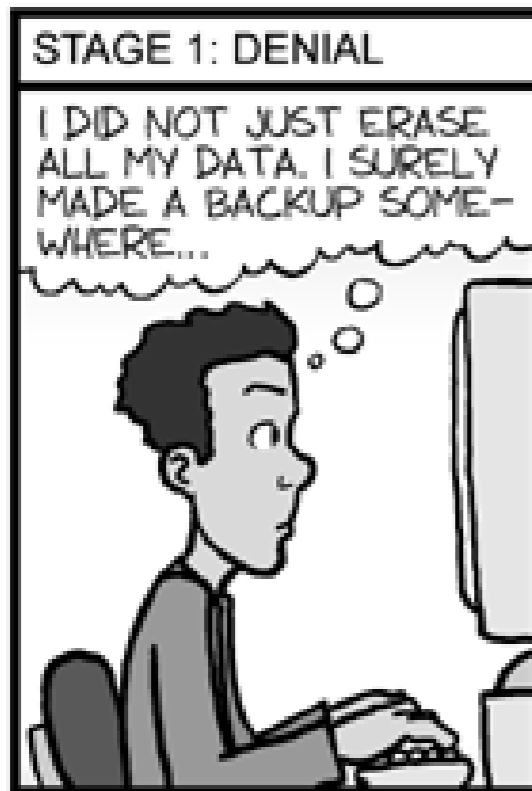
OpenMD is an open source molecular dynamics engine which is capable of efficiently simulating liquids, proteins, nanoparticles, interfaces, and other complex systems using atom types with *orientational* degrees of freedom (e.g. "sticky" atoms, point dipoles, and coarse-grained assemblies). Proteins, 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.

<http://www.openmd.org>

So, Why did a nice
Computational Scientist
like you...

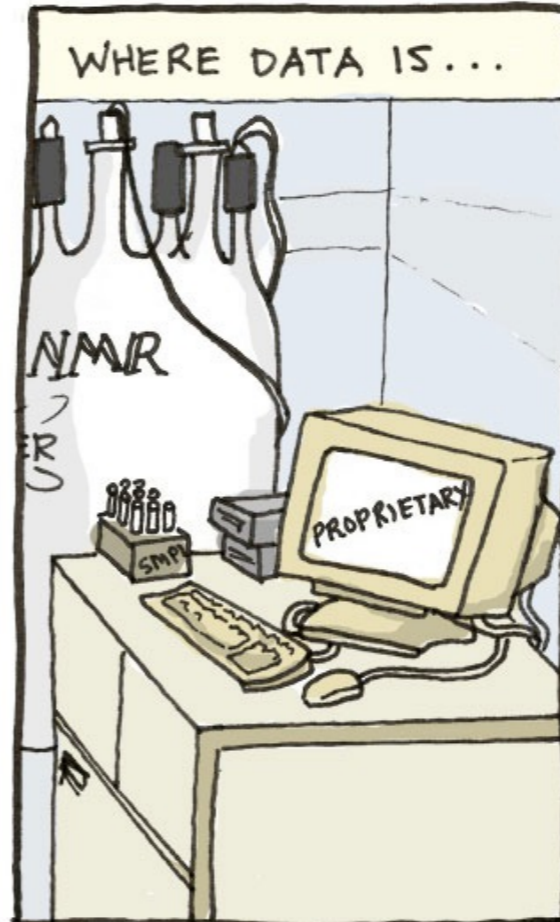
THE FOUR STAGES OF DATA LOSS

DEALING WITH ACCIDENTAL DELETION OF MONTHS OF HARD-EARNED DATA



JORGE CHAM © 2003

www.phdcomics.com



How Chuck imagines it should be:

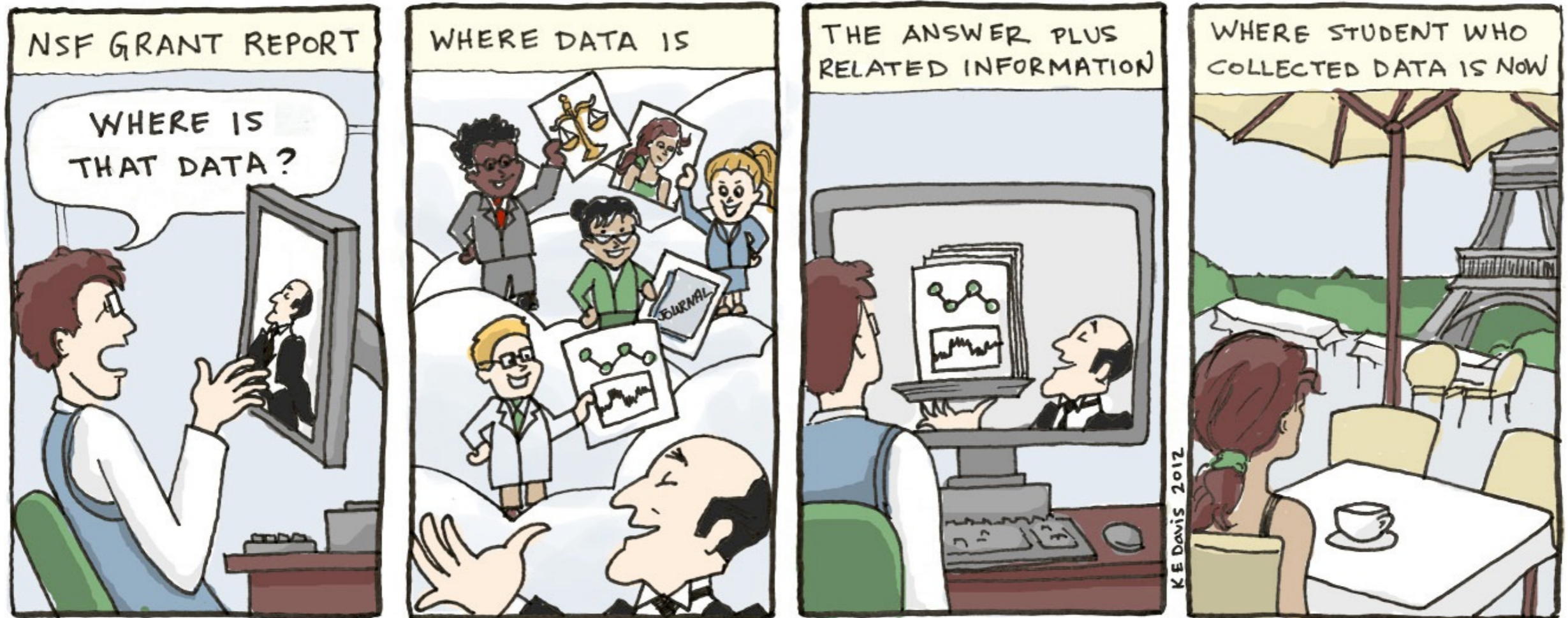


Image Design Credit: Kristina Davis (CRC)



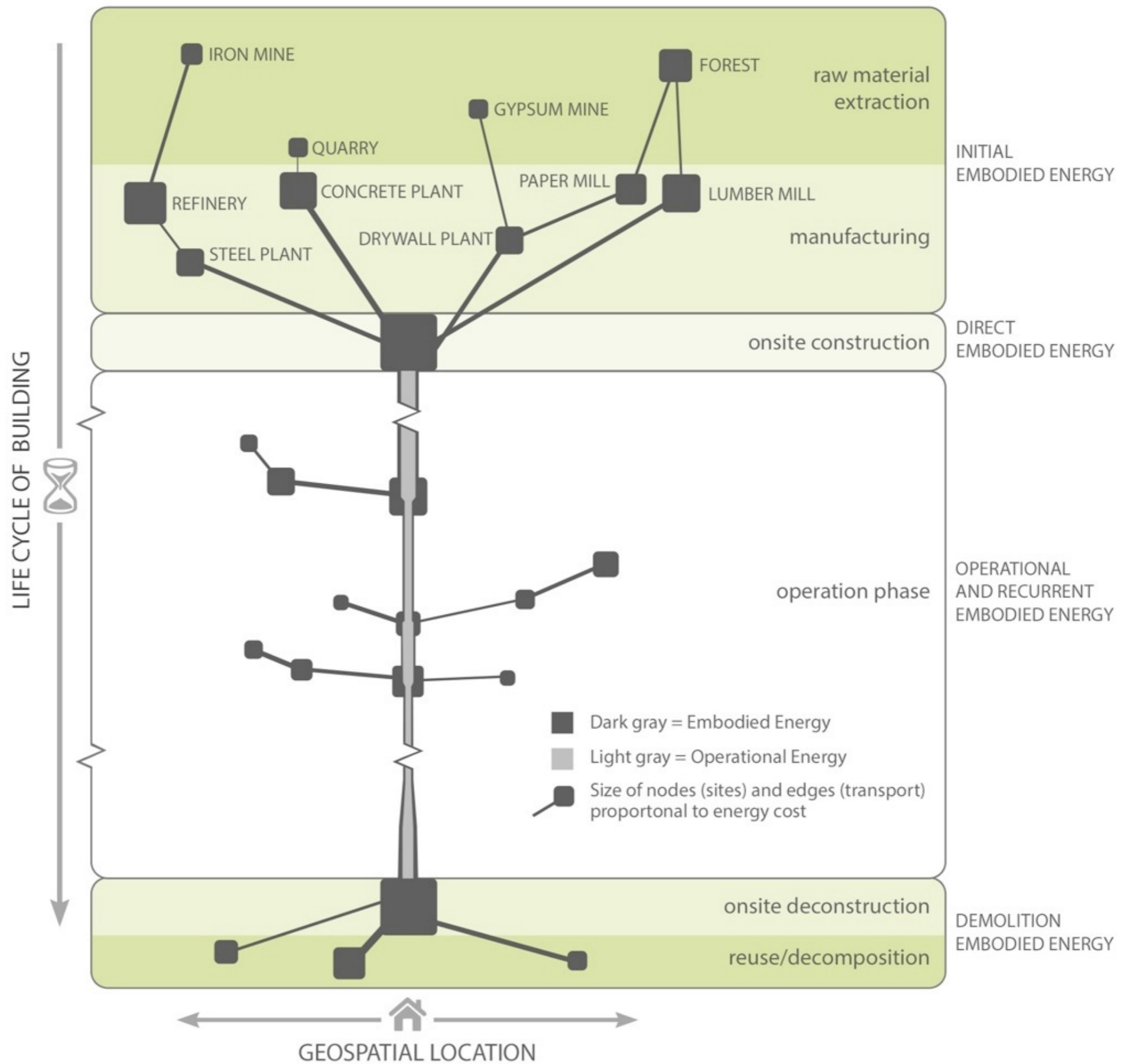


Image Design Credit: Kristina Davis (CRC)

So, we need to describe
Trajectories and
Transformations of Materials

A Geo-ontology Design Pattern for Semantic Trajectories

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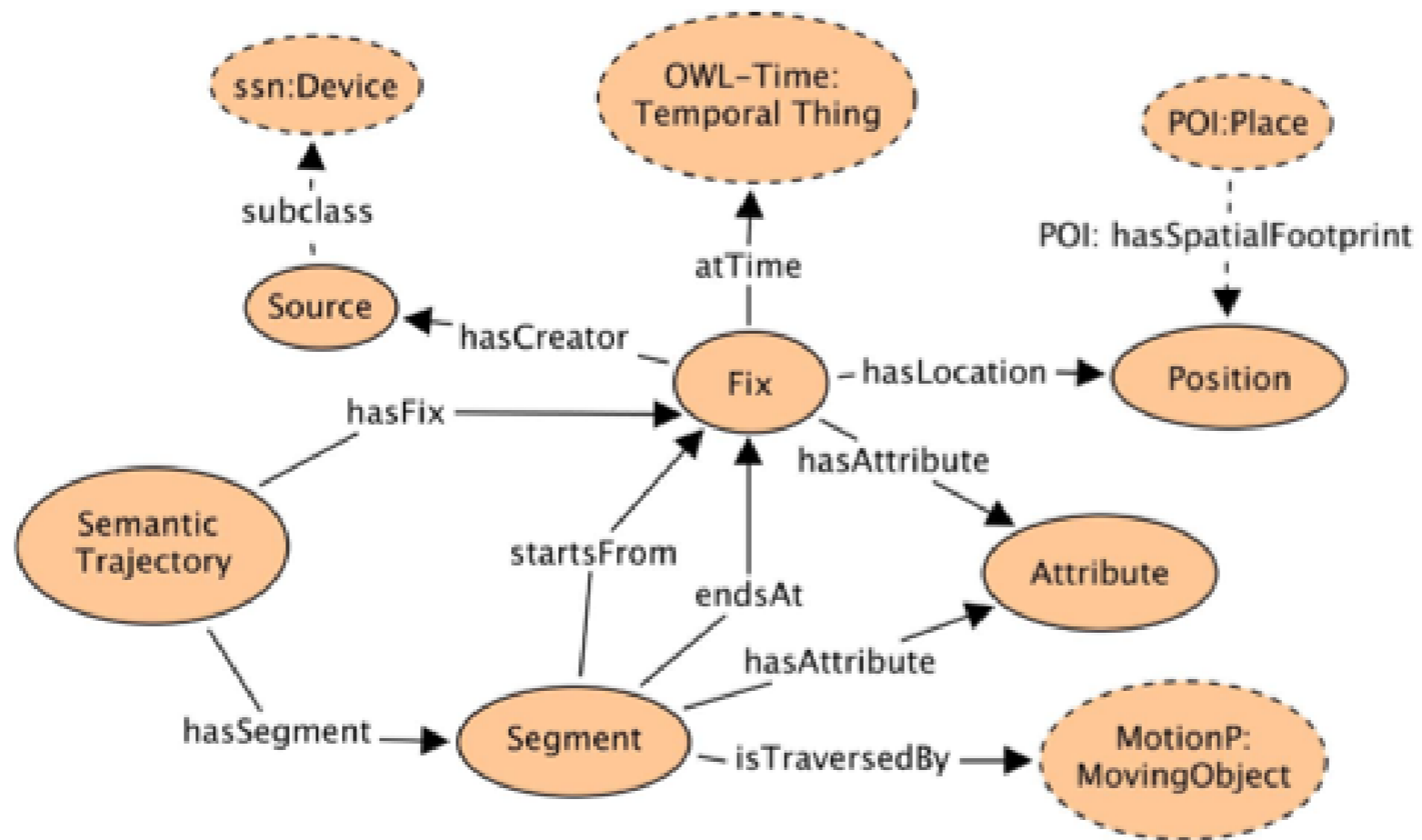
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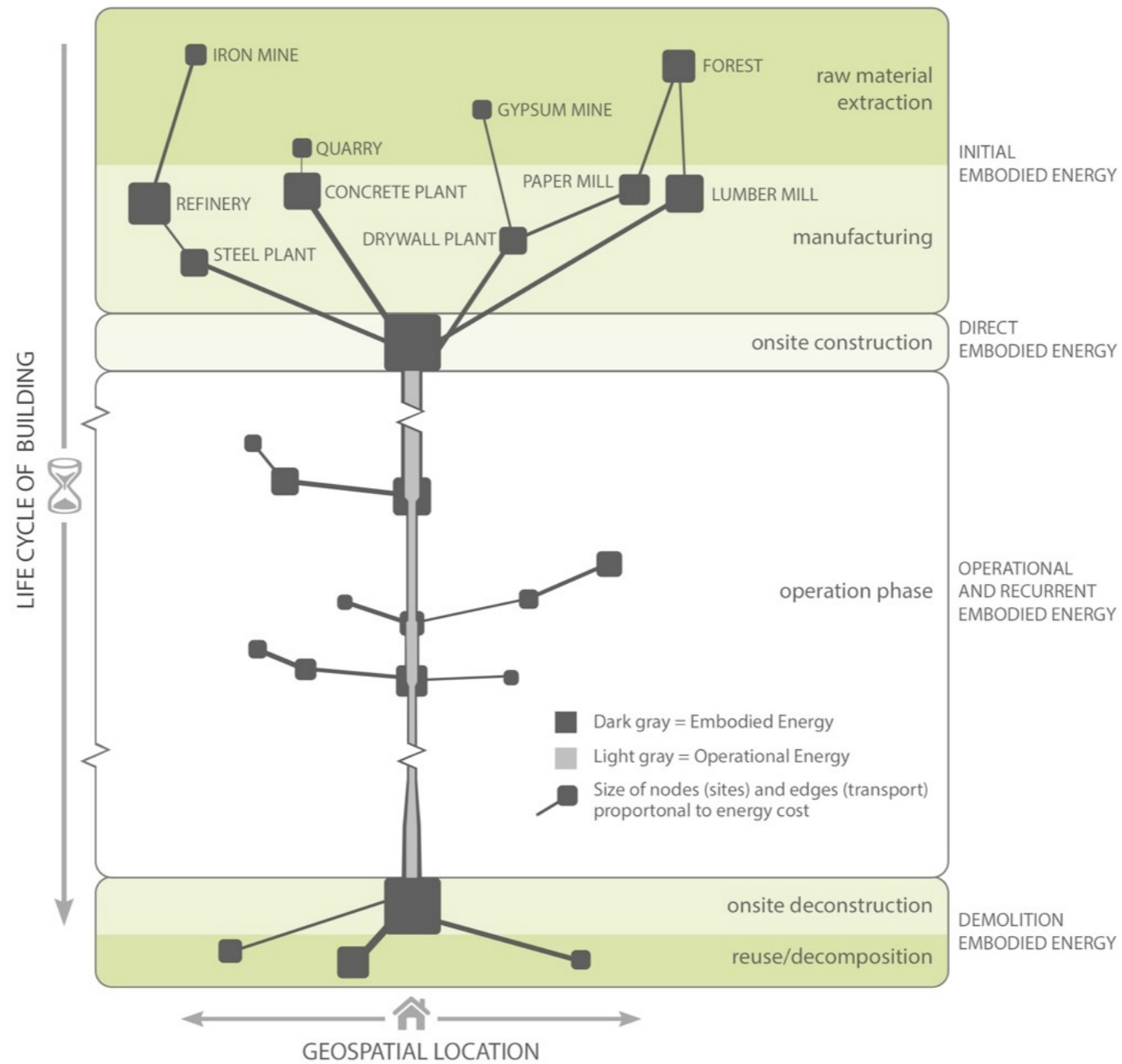
gbergcross@gmail.com

⁵ Raytheon BBN Technologies, USA

{mdean, dkolas}@bbn.com

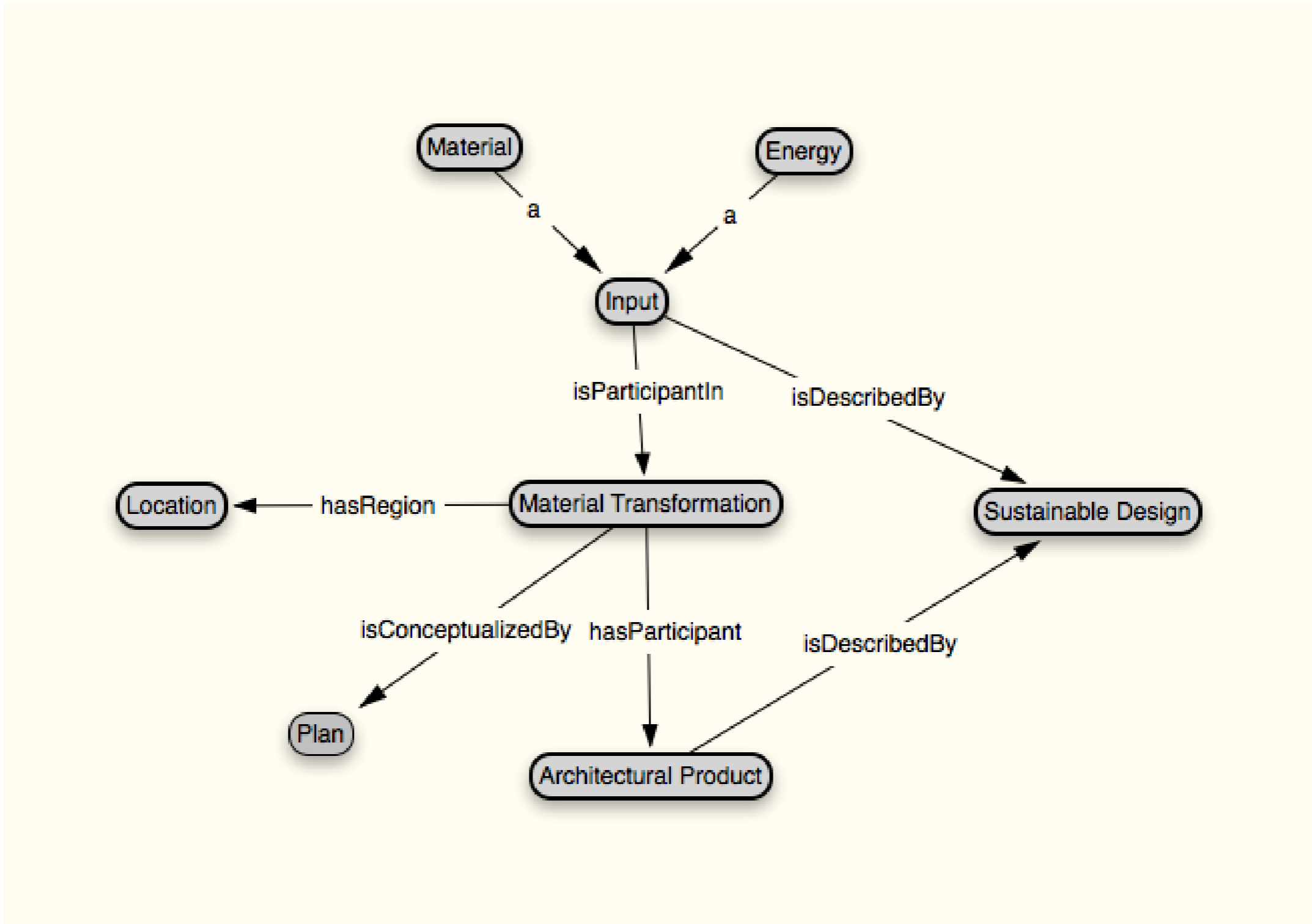


Back to...

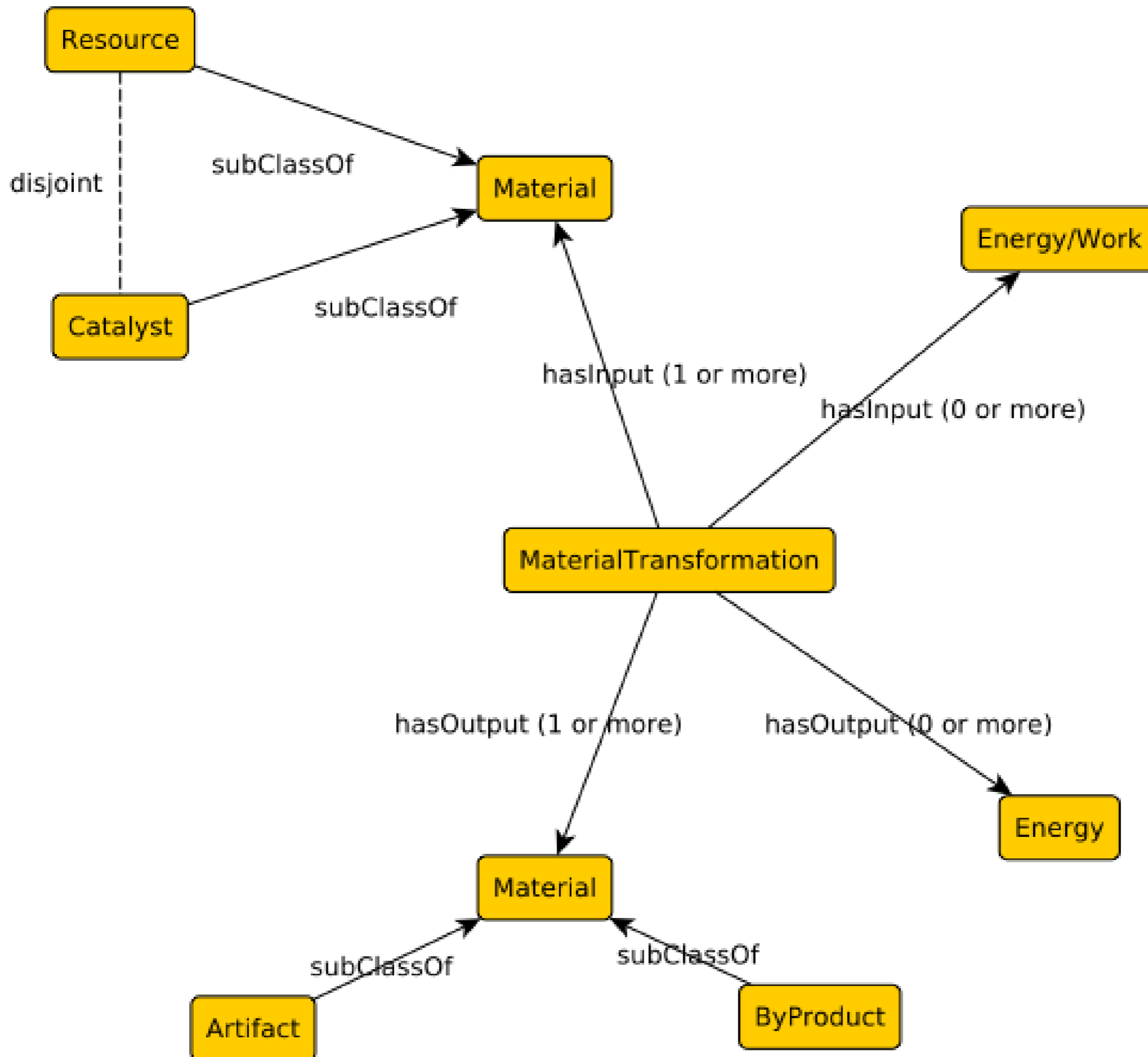


We need to describe what
(transformation) happens
at a POI!

GreenScale Proposed Topic for GeoVocamp DC 2014— Material Transformation



After the GeoVocamp
Process...





About 18,800,000 results (0.32 seconds)

cat·a·lyst

/ˈkɑtəl-ɪst/

noun

a substance that increases the rate of a chemical reaction without itself undergoing any permanent chemical change.

- a person or thing that precipitates an event.

"the governor's speech acted as a catalyst for debate"

synonyms: [stimulus](#), stimulation, [spark](#), sparkplug, [spur](#), incitement, impetus [More](#)



Syntactic Sugar

$$Energy \sqsubseteq \top \quad (1)$$

$$Material \sqsubseteq \top \quad (2)$$

$$Neighborhood \sqsubseteq \top \quad (3)$$

$$MaterialTransformation \sqsubseteq \top \quad (4)$$

$$hasInput \sqsubseteq U \quad (5)$$

$$hasOutput \sqsubseteq U \quad (6)$$

$$\top \sqsubseteq \neg \exists N. \top \quad (7)$$

Surface Semantics

$$Resource \sqsubseteq Material \quad (8)$$

$$Catalyst \sqsubseteq Material \quad (9)$$

$$Artifact \sqsubseteq Material \quad (10)$$

$$Byproduct \sqsubseteq Material \quad (11)$$

Deep Semantics

$$Resource \sqcap Catalyst \sqsubseteq \perp \quad (12)$$

$$Material \sqcap MaterialTransformation \sqsubseteq \perp \quad (13)$$

$$hasOutput \sqcap hasInput \sqsubseteq N \quad (14)$$

$$Material \sqsubseteq \exists partOf. Neighborhood \quad (15)$$

$$Resource \sqsubseteq \exists partOf. (Neighborhood \sqcap \exists partOf^{-}. Catalyst) \quad (16)$$

$$MaterialTransformation \sqsubseteq \exists hasOutput. (Material \sqcup Energy) \quad (17)$$
$$\sqcap \exists hasInput. (Resource \sqcup Catalyst$$
$$\sqcup Energy)$$

Deep Semantics

$$\textit{Resource} \sqcap \textit{Catalyst} \sqsubseteq \perp \quad (1)$$

$$\textit{Material} \sqcap \textit{MaterialTransformation} \sqsubseteq \perp \quad (2)$$

$$\textit{hasOutput} \sqcap \textit{hasInput} \sqsubseteq N \quad (3)$$

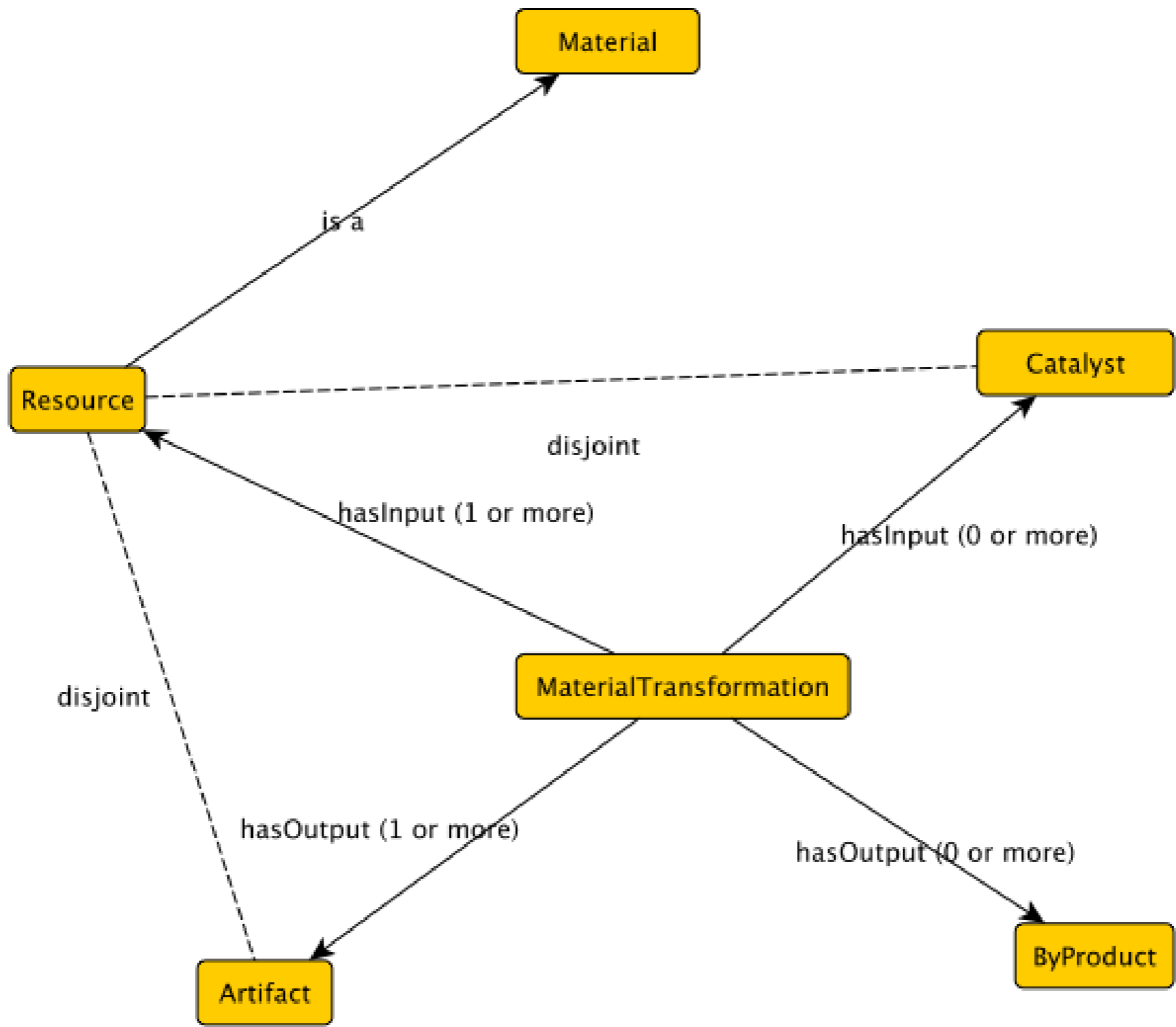
$$\textit{Material} \sqsubseteq \exists \textit{partOf} . \textit{Neighborhood} \quad (4)$$

$$\textit{Resource} \sqsubseteq \exists \textit{partOf} . (\textit{Neighborhood} \sqcap \exists \textit{partOf}^- . \textit{Catalyst}) \quad (5)$$

$$\begin{aligned} \textit{MaterialTransformation} \sqsubseteq \exists \textit{hasOutput} . (\textit{Material} \sqcup \textit{Energy}) \quad (6) \\ \sqcap \exists \textit{hasInput} . (\textit{Resource} \sqcup \textit{Catalyst} \\ \sqcup \textit{Energy}) \end{aligned}$$

Krzysztof Janowicz Remarks

- As we discussed before, do we need *Material*?
- 14 may be too strong



On Classifying Material Entities in Basic Formal Ontology

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ABSTRACT. Basic Formal Ontology (BFO) was created in 2002 as an upper-level ontology to support the creation of consistent lower-level ontologies, initially in the subdomains of biomedical research, now also in other areas, including defense and security. BFO is currently undergoing revisions in preparation for the release of BFO version 2.0. We summarize some of the proposed revisions in what follows, focusing on BFO's treatment of material entities, and specifically of the category *object*.

Where does time come in?
partOf is time dependent?

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