An Ontology Design Pattern for Material Transformation

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Abstract. In this work we discuss an ontology design pattern for material transformations. It models the relation between products, resources, and catalysts in the transformation process. Our axiomatization goes beyond a mere surface semantics. While we focus on the construction domain, the pattern can also be applied to chemistry and other domains.

1 Introduction & Motivation

According to the United Nations, the construction industry and related support industries are leading consumers of natural resources. Consumption of these natural resources result in the emission of energy, and thus carbon and other greenhouse gases, which are then“embodied” in the consumption process. Efforts have been made to quantify these emissions through measures of embodied energy, carbon and water but are lacking due to poor quality of data sources, lack of understanding of uncertainty in the data, lack of geospatial attributes necessary for proper calculation of embodied properties, understanding regional and international variation in data, incompleteness of secondary data sources and variation in manufacturing technology that lead to significant variation calculated values [2]. One methodology for quantification of embodied energy is through input-output life cycle analysis utilizing process data that compile a life cycle inventory of a construction product. By analyzing a “cradle to grave” path of individual building components, the embodied energy sequestered in all building materials during all processes of construction, in on-site construction and final demolition and disposal of a buildings constituent components gives a measure of total embodied energy for a given structure. Sources of embodied energy include the amount of the energy consumed in construction, prefabrication, assembly, transportation of materials to a building structure, initial manufacturing building materials, in renovation and refurbishment of the structure through it’s lifetime [1]. The Green Scale Project[1] is studying the feasibility of creating a

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[1] http://www.greenscale.org

geospatial-temporal knowledge base (KB) which facilitates mapping of national energy and fuel production to individual construction site localities and construction material manufacture localities as linked open data. Such a knowledge base would facilitate the calculation of embodied energy for a given construction component as a query of the embodied energy required for manufacture and transportation of it's constituent parts. This KB will use ontology design patterns to formally describe the transportation and transformation processes.

Transportation of a manufacturing component from location to location and the energies associated with that transportation can be modeled via the Semantic Trajectory pattern (STODP) [3]. The remaining contribution to the total embodied energy is the energy required for transformation or assembly of one or more components into the desired manufactured artifact.

In this work we discuss the development of a Material Transformation pattern[2] to contextualize this transformation process from raw components and the required equipment to a final manufactured artifact. Chaining this pattern with STODP will facilitate understanding of a complete manufacturing process from raw material extraction to assembly of all components needed for that product. The presented work was done in two 2-day sessions involving domain experts from architecture, computational chemistry, and geography, as well as ontology engineers at GeoVoCampDC2013[3] and GeoVoCampWI2014[4]. We present a full axiomatization that goes beyond mere surface semantics [4] (e.g., a simple type hierarchy). During the development, several competency questions that a domain expert may ask were discussed. These include:

- *"What material resources were required to produce a product?"*
- *"Where did the transformation take place?"*
- *"What was the time necessary for the transformation?"*
- *"What materials or conditions were necessary for the transformation to occur?"*

2 Material Transformation Pattern

The Material Transformation pattern is visualized in Fig. 1, including the extension with entities relevant for representing energy information, which are green-colored and use dashed line. For formalization, we use the Description Logic (DL) notation, which can easily be encoded using syntax of the OWL 2. The core part of the pattern is intended to describe change(s) that occur between the input material of the transformation and its output. In this core part, the `MaterialTransformation` class represents concrete instances of material transformation. We distinguish inputs of a material transformation into `Resource`, which represents types of material that may undergo a change (into a different type of material) in the transformation, and `Catalyst`, which represents types of material needed by the transformation, but remain unchanged by it. A `MaterialTransformation` has some `Resource` as input (1), and some `Product`, which is also some type of material, as output (2). Axiom (5) asserts

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[2] http://ontologydesignpatterns.org/wiki/Submissions:Material_Transformation

[3] http://vocamp.org/wiki/GeoVoCampDC2013

[4] http://www.ssec.wisc.edu/meetings/geosp_sem/

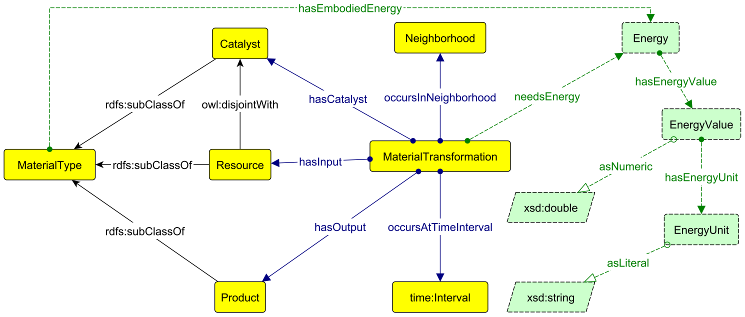

Fig. 1. Material Transformation Pattern with Energy Information

that every `Resource`, `Catalyst` and `Product` is some `MaterialType`, while (6) and distinguishes `Resource` from `Catalyst`. Axiom (3) and (4) assert that a `MaterialTransformation` occurs in a spatial `Neighborhood`[5] and a time interval, modeled using the `Interval` class from the W3C's OWL Time ontology[6].

$$\texttt{MaterialTransformation} \sqsubseteq \exists\texttt{hasInput}.\texttt{Resource} \tag{1}$$

$$\texttt{MaterialTransformation} \sqsubseteq \exists\texttt{hasOutput}.\texttt{Product} \tag{2}$$

$$\texttt{MaterialTransformation} \sqsubseteq \exists\texttt{occursInNeighborhood}.\texttt{Neighborhood} \tag{3}$$

$$\texttt{MaterialTransformation} \sqsubseteq \exists\texttt{occursAtTimeInterval}.\texttt{time:Interval} \tag{4}$$

$$\texttt{Resource} \sqcup \texttt{Catalyst} \sqcup \texttt{Product} \sqsubseteq \texttt{MaterialType} \tag{5}$$

$$\texttt{Resource} \sqcap \texttt{Catalyst} \sqsubseteq \bot \tag{6}$$

We express changes occurring within a material transformation, using first-order logic, that it has an input that is not part of the output (7); and an output that is not part of the input, in a formula analogous to (7).

$$\forall x(\texttt{MaterialTransformation}(x) \rightarrow \exists y(\texttt{hasInput}(x,y) \land \neg\texttt{hasOutput}(x,y))) \tag{7}$$

These formulas, however, cannot be expressed in the OWL framework, but there are extensions of DL that can express them. For example, using boolean constructors on properties [5], axiom (7) is expressed in DL as:

$$\texttt{MaterialTransformation} \sqsubseteq \exists(\texttt{hasInput} \sqcap \neg\texttt{hasOutput}).\top$$

Meanwhile, for the remaining properties of the core part of the pattern, we assert the guarded domain and range restrictionsas exemplified for the `hasInput` property in (8) and (9) below. Such guarded restrictions are preferable over the unguarded versions (i.e., of the form $\mathsf{dom}(P) \sqsubseteq A$ and $\mathsf{range}(P) \sqsubseteq B$) as they introduce weaker ontological commitments and thus foster reuse.

$$\exists\texttt{hasInput}.\texttt{Resource} \sqsubseteq \texttt{MaterialTransformation} \tag{8}$$

$$\texttt{MaterialTransformation} \sqsubseteq \forall\texttt{hasInput}.\texttt{Resource} \tag{9}$$

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[5] Neighborhood provides a toplogical definition for specifing nearness. This could be specified in different ways such as using positional coordinates, a bounded area on a map, or a named region such as a place, city or factory.

[6] http://www.w3.org/TR/owl-time/

For the scenario where we need to calculate the embodied energy in the output of a material transformation, we can extend the pattern with additional energy information as depicted in Fig. 1. In the axiomatization, we then assert that a `MaterialTransformation` needs some `Energy` (10), while each material type has some embodied energy (11). Energy itself is abstracted as an instance of the `Energy` class, which has some energy value and unit.

$$\texttt{MaterialTransformation} \sqsubseteq \exists \texttt{needsEnergy}.\texttt{Energy} \tag{10}$$

$$\texttt{MaterialType} \sqsubseteq \exists \texttt{hasEmbodiedEnergy}.\texttt{Energy} \tag{11}$$

$$\texttt{Energy} \sqsubseteq \exists \texttt{hasEnergyValue}.\texttt{EnergyValue} \tag{12}$$

$$\begin{aligned} \texttt{EnergyValue} \sqsubseteq\ & \exists \texttt{hasEnergyUnit}.\texttt{EnergyUnit} \\ & \sqcap \exists \texttt{asNumeric.xsd:double} \end{aligned} \tag{13}$$

$$\texttt{EnergyUnit} \sqsubseteq \exists \texttt{asLiteral.xsd:string} \tag{14}$$

Embodied energy in the output as a result of a material transformation can be calculated by aggregating embodied energy of the input and catalyst, together with energy requirement of the material transformation itself. This cannot be done within OWL, but is relatively straightforward to implement in the application as all the necessary information are easily retrievable from the populated pattern. Furthermore, if the application allows updates on the data populating the pattern, we can chain two instantiations of this pattern and include STODP.

3 Conclusion and Future Work

Although it is beyond the scope of the present work, the Material Transformation pattern should be sufficiently generic to describe other types of transformation processes ranging from chemical reactions to creation-annihilation events in high energy physics. We believe the pattern to be of general use to broader product life cycle inventories outside the construction domain.

Acknowledgements. We are grateful for the inputs from Lamar Henderson, Deborah MachPherson, Laura Bartolo, and Damian Gessler to improve the pattern. Vardeman, Buccellato and Ferguson would like to acknowledge funding from the University of Notre Dame's Center for Sustainable Energy, School of Architecture, College of Arts and Letters and Center for Research Computing in support of this work. Gary Berg-Cross acknowledges funding from the NSF grant 0955816, INTEROP-Spatial Ontology Community of Practice. Vardeman would like to acknowledge funding from NSF grant PHY-1247316 "DASPOS: Data and Software Preservation for Open Science." Adila Krisnadhi, Michelle Cheatham, and Pascal Hitzler acknowledge support by the National Science Foundation under award 1017225 "III: Small: TROn – Tractable Reasoning with Ontologies."

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