Extending the Ontology of Physics for Biology with Thermodynamics

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ABSTRACT

We have extended the Ontology of Physics for Biology (OPB) to represent the entities and relations of classical thermodynamics. We describe key subclasses of OPB:*Thermodynamic entity* such as OPB:*Thermodynamic property,* and OPB:*Thermodynamic dependency* in the context of the OPB's overall representational schema. We are motivated by practical utility of energy bond-graph theory, a thermodynamics-based formalism used in the domain of system dynamical modeling and analysis of biological physical processes. We also intend OPB to extend available upper biomedical ontologies to encompass entities and theories of classical physics and thermodynamics.

1 INTRODUCTION

The Ontology of Physics for Biology (OPB, 2016) extends available biomedical ontologies to represent the biophysics of biological entities, their observable physical properties and the physical dependencies—the laws of classical physics—that determine how property values depend upon one another. OPB is based on engineering system dynamics — the study of stocks and flows of material, charge, etc. — used to qualitatively explain and to quantitatively analyze biological processes over domains such as chemical kinetics, fluid dynamics and electrophysiology and spatial scales from molecular to organismal. To our knowledge, no comparable ontology exists.

Our SemGen application[1] uses OPB semantics to derive and analyze SemSim models (sem antic sim ulation) to input, parse, and annotate biosimulation model code. Furthermore, SemGen can decompose SemSim models into reuseable fragments, merge the fragments as a new SemSim model and export new computational model code . A *SemSim* model is a light-weight OWL ontology that annotates each variable as an instance of an OPB:*Physical property* and each equation as an instance of OPB:*Physical dependency* to create a "property dependency graph" (OPB:*Property dependency graph*). We have recently applied SWRL rules to SemSim models and OPB to infer qualitative changes of model variables on other property values in the model (Neal, et al., 2016).

OPB parses system dynamical abstractions into 4 high-level classes. First, OPB:*Dynamical entities* are energy-bearing physical continuants such as portions of fluid, chemical, charge. Second, OPB:*Dynamical processes* are flows of material, charge, etc. as in chemical reactions, fluid flows, etc. Third, OPB:*Physical properties* (Cook, et al, 2011) are the observable or inferrable attributes of entities and processes. And fourth, OPB:*Physical dependencies* (Cook, et al, 2013) are physical laws (e.g., Ohm's law) and constraints (e.g., conservation of mass).

2 NEXT STEP: THERMODYNAMICS

To formally represent and constrain models of such dynamical phenomena, we have extended OPB to explicitly represent thermodynamic entities, properties, and dependencies. Whereas properly derived system dynamical models will constrain models to the universal rules of thermodynamics (e.g., conservation of energy, in particular), such constraints are only implicit in model equations. To explicitly satisfy both dynamical and thermodynamic laws and constraints, thermodynamics-based *energy bond graph* modeling was first described for biological systems (Perelson, 1975), adapted to engineering practice (Karnopp, 1979) and has been recently formalized by others (Gawthrop and Crampin, 2014; Lefèvre, et al., 1999) to model biological dynamical networks.

We have extended OPB to represent the entities and principles of classical thermodynamics in support of thermodynamic-based computational modeling as well as to extend the scant representation of physical and thermodynamical concepts in prevailing upper biomedical ontologies.

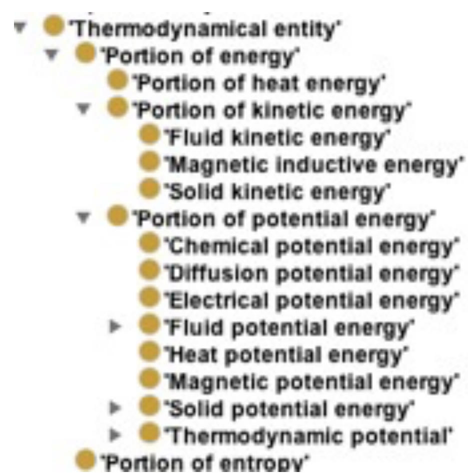

Fig. 1 OPB:*Thermodynamic entity* classes.

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[1] http://sbp.bhi.washington.edu/projects/semgen

2.1 OPB:*Thermodynamical entity*

In parallel to OPB system dynamical classes that represent stocks/flow of material, charge, etc., OPB thermodynamic classes represent stocks/flows of energy and entropy (Figure 1). Thus, an instance of OPB:*Mechanical solid* has (via OPB:*hasThermodynamicEntity*) a portion of OPB:*Solid potential energy* if stretched or compressed and/or a portion of OPB:*Solid kinetic energy* if in motion.

2.2 OPB:*Thermodynamical property*

Thermodynamical entities have OPB:*Thermodynamical properties*: (1) **rate** properties (e.g., OPB:*Energy flow rate*, OPB:*Entropy flow rate*), (2) **state** properties (e.g., OPB:*Energy amount*, OPB:*Entropy amount*) and (3) **constitutive** properties (e.g., OPB:*Thermal capacity*, OPB:*Thermal conductivity*).

2.3 OPB:*Thermodynamical dependency*

OPB:*Thermodynamical dependencies* (Fig. 2) define OPB:*Thermodynamical properties* in terms of other such properties or in terms of OPB:*Dynamical properties* (e.g., fluid volume or pressure).

Fig. 2. OPB:*Thermodynamic dependency* classes.

2.4 Overview and conclusion

Figure 3 is an overview of OPB classes showing the scope and depth of the OPB's representation of physics of biological processes. We have aimed to, first, extend upper ontologies to encompass entities and relations of physics as used by bioengineers and biophysicists, and now, to encompass thermodynamic entities and laws that govern biological processes. OPB is a reference ontology of biophysics that extends available "upper ontologies" (e.g, BFO, GFO), complements domain ontologies such as FMA, GO, ChEBI, and provides a computational resource for annotating biophysical models and datasets for reuse and integration.

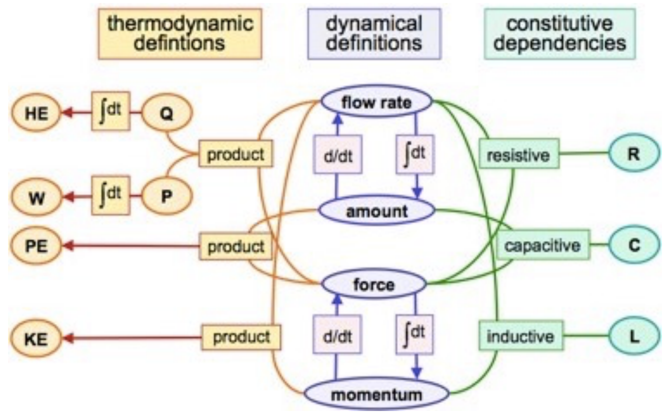

Fig. 3. Overview of OPB schema for relating thermodynamic classes (left) to observable state and rate dynamical properties (middle) and the constitutive properties of empirical dependencies (right).

2.5 Acknowledgements

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