Selecting and customizing a mereology ontology for its reuse in a pharmaceutical product ontology

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The purpose of this paper

• This paper presents our experience in reusing mereology ontologies in a Pharmaceutical Product ontology, an ontology built by the EU NeOn project.

• The essential difference between our work and the one of former authors (e.g. Borst) is that we analyze, reuse and customize a mereology ontology already built, and that we do not develop a mereology ontology from scratch.
Outline

1. Scope of our study of mereology ontologies

2. Reusing a mereology ontology in a Pharmaceutical Product ontology

3. Results and future directions
Scope of our study of time ontologies

1. Scope of our study of mereology ontologies

2. Reusing a mereology ontology in a Pharmaceutical Product ontology

3. Results and future directions
Scope of our study of time ontologies. What we consider as an ontology

“An ontology is a formal, explicit specification of a shared conceptualization”

In a formal language with a formal semantics

Concepts, properties relations, functions, constraints, axioms, are explicitly defined

Agreed Knowledge

Abstract model and simplified view of some phenomenon in the world that we want to represent

Therefore, if we assume this definition, a mereology ontology is an agreed mereology implemented in a formal language with formal semantics (KIF, OWL, etc.)
Reusing a mereology ontology in a PPO

1. **Scope of our study of mereology ontologies**

2. **Reusing a mereology ontology in a Pharmaceutical Product ontology**

3. **Results and future directions**
Reusing a mereology ontology in a PPO

I. Ontology search

II. Selection of a mereology ontology

III. Customization of the chosen mereology ontology

IV. Integration of the chosen mereology ontology in the PPO
Ontology search

I. Ontology search

Mereology ontology 1

Mereology ontology 2

II. Selection of a mereology ontology

Mereology ontology i

III. Customization of the chosen mereology ontology

Customized mereology ontology i

IV. Integration of the chosen mereology ontology in the PPO

Integrated mereology ontology i
Ontology search process. Driven by the host ontology

I. Ontology search

I.a. Analysis of the PPO CQs

I.b. Identification of the features of the mereology ontology to be reused

Part of, direct part of, etc.

Which are the parts of the drug?, etc.

I.c. Search candidate mereology ontologies

Basic axioms and definitions + Weak supplementation principle

Mereology ontology 1

Mereology ontology 2

II. Selection of a mereology ontology

III. Customization of the chosen mereology ontology

IV. Integration of the chosen mereology ontology in the PPO
Analysis of the Pharmaceutical Product ontology CQs

I. Ontology search

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# Extracting terms from PPO CQs

<table>
<thead>
<tr>
<th>Identifier</th>
<th>Competency question</th>
<th>Extracted terms</th>
</tr>
</thead>
</table>
| CQ1        | What is the composition of the drug?                                                | - Drug  
- Component of                                       |
| CQ2        | Which is the main active ingredient (molecule) of the drug?                          | - Has main active ingredient  
- Molecule  
- Drug                                               |
| CQ3        | Which is the main substance of the composition?                                     | - Has main substance  
- Component of                                         |
| CQ4        | Does the drug have interaction with another drug?                                    | - Drug  
- Has interaction with                                |
|            | ...                                                                                 | ...                                                   |
| CQ61       | ...                                                                                 | ...                                                   |
Applying patterns to CQs to obtain mereology terminology

PATTERN. PARTIAL ORDER

Question to be answered: what relations are candidate to be renamed so that mereology definitions and axioms can be reused?

Guide to answer the question:

R.1. $R$ establishes a (partial) order $\rightarrow R$ is candidate to be a kind of part of

R.2. $R'$ establishes a (partial) order $\land R'$ is super-relation of $R$ $\rightarrow R$ is candidate to be a kind of part of
### Applying patterns to CQs to obtain mereology terminology

<table>
<thead>
<tr>
<th>Identifier</th>
<th>Competency question</th>
<th>Extracted terms</th>
<th>Candidate mereology terms</th>
</tr>
</thead>
<tbody>
<tr>
<td>CQ1</td>
<td><em>What is the composition of the drug?</em></td>
<td>- Drug</td>
<td>ORDER - Part of</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Component of</td>
<td></td>
</tr>
<tr>
<td>CQ2</td>
<td><em>Which is the main active ingredient (molecule) of the drug?</em></td>
<td>- Has main active ingredient</td>
<td>-Part of</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Molecule</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Drug</td>
<td></td>
</tr>
<tr>
<td>CQ3</td>
<td><em>Which is the main substance of the composition?</em></td>
<td>- Has main substance</td>
<td>ORDER IN SUPER-RELATION - Part of (y, x)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Component of</td>
<td>Sub-relation of</td>
</tr>
<tr>
<td>CQ4</td>
<td><em>Does the drug have interaction with another drug?</em></td>
<td>- Drug</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Has interaction with</td>
<td></td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td></td>
</tr>
<tr>
<td>CQ61</td>
<td>...</td>
<td>...</td>
<td></td>
</tr>
</tbody>
</table>
## Reformulation of CQs using mereology terminology

<table>
<thead>
<tr>
<th>Identifier</th>
<th>Competency question</th>
<th>Competency question using the vocabulary of mereology</th>
</tr>
</thead>
<tbody>
<tr>
<td>CQ1</td>
<td><em>What is the composition of the drug?</em></td>
<td>1.1) Which are the direct parts of the drug?</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.2) Which are the parts of the drug?</td>
</tr>
<tr>
<td>CQ2</td>
<td><em>Which is the main active ingredient (molecule) of the drug?</em></td>
<td>Which part of the drug is its main ingredient?</td>
</tr>
<tr>
<td>CQ3</td>
<td><em>Which is the main substance of the composition?</em></td>
<td>Which part of the drug is its main substance?</td>
</tr>
<tr>
<td>CQ4</td>
<td><em>Does the drug have interaction with another drug?</em></td>
<td>Are there parts of the drug that interact with parts of another drug?</td>
</tr>
</tbody>
</table>
Inheritance through part of

The interaction is inherited from the parts to the whole

Inspired from:

Identification of the features of the mereology ontology to be reused

I. Ontology search

I.a. Analysis of the PPO CQs

I.b. Identification of the features of the mereology ontology to be reused

Which are the parts of the drug?, etc.

Part of, direct part of, etc.

I.c. Search candidate mereology ontologies

Basic axioms and definitions + Weak supplementation principle

Mereology ontology 1

…

Mereology ontology 2

II. Selection of a mereology ontology

III. Customization of the chosen mereology ontology

IV. Integration of the chosen mereology ontology in the PPO
Candidate mereologies to provide features

General Extensional Mereology (MM)

Closure Extensional Mereology (MM)

Extensional Mereology (EM)
Strong supplementation

Minimal Mereology (MM)
Weak supplementation principle

Theory M
Part of is:
• Reflexive
• Antisymmetric
• Transitive

Closure Mereology (CM)
Sum principle
Product principle

General Mereology (GM)
Unrestricted fusion principle


I.a. Analysis of the PPO CQs

I.b. Identification of the features of the mereology ontology to be reused

I.c. Search candidate mereology ontologies

Part of, direct part of, etc.

Which are the parts of the drug?, etc.

Basic axioms and definitions + Weak supplementation principle

Mereology ontology 1

Mereology ontology 2

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## Candidate mereology ontologies

<table>
<thead>
<tr>
<th>Name</th>
<th>Source</th>
<th>Language</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOLCE mereology</td>
<td><a href="http://wonderweb.semanticweb.org/">http://wonderweb.semanticweb.org/</a></td>
<td>KIF, OWL</td>
</tr>
<tr>
<td>SUO mereology</td>
<td><a href="http://suo.ieee.org/">http://suo.ieee.org/</a></td>
<td>KIF</td>
</tr>
<tr>
<td>Mereology based on Smith and other authors</td>
<td><a href="http://suo.ieee.org/">http://suo.ieee.org/</a></td>
<td>KIF</td>
</tr>
<tr>
<td>Mereology based on Borgo and other authors</td>
<td><a href="http://suo.ieee.org/SUO/ontologies/Guarino.txt">http://suo.ieee.org/SUO/ontologies/Guarino.txt</a></td>
<td>KIF</td>
</tr>
<tr>
<td>Mereology based on Casati and Varzi</td>
<td><a href="http://www.ai.sri.com/daml/ontologies/sri-basic/1-0/Time.daml">http://www.ai.sri.com/daml/ontologies/sri-basic/1-0/Time.daml</a></td>
<td>KIF</td>
</tr>
</tbody>
</table>
Mereology ontology selection

I. Ontology search

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Mereology ontology 1

... Mereology ontology 2

Mereology ontology i

Customized mereology ontology i

Integrated mereology ontology i
Criteria to mereology ontology selection

Effort in the reuse

• Features covered by the MO currently needed
• Modifications needed in the definitions
• Etc.

Effort in future extensions

• Features covered by the MO
<table>
<thead>
<tr>
<th>Theory</th>
<th>Principles and definitions</th>
<th>CACTUS</th>
<th>DOLCE</th>
<th>SUO</th>
<th>Smith et al.</th>
<th>Borgo et al.</th>
<th>Casati and Varzi</th>
</tr>
</thead>
<tbody>
<tr>
<td>M</td>
<td>A.1) Reflexivity</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>A.2) Antisymmetry</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>A.3) Transitivity</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>D.1) Proper part</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>D.2) Direct part</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>D.3) Overlap</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>D.4) Underlap</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>D.5) Disjoint</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>MM = M + (P4)</td>
<td>A.4) Weak supplementation</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Inferred</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>A.5) Strong supplementation</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>EM = M + (A5)</td>
<td>(Let’s note that (A5) implies (A4))</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>CM = M + (A6) + (A7)</td>
<td>A.6) Sum principle</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>A.7) Product principle</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>CEM = CM + (A5)</td>
<td>D.6) Binary sum</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>D.7) Binary product</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>GM = M + (A8)</td>
<td>A.8) Unrestricted fusion principle</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>GEM = GM + (A5)</td>
<td>D.8) General sum</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>AX = (A9) + a mereology X</td>
<td>D.9) Atom</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>A.9) Atomicity</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>
Customization of the chosen ontology

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Mereology ontology 1

Mereology ontology 2

Mereology ontology i

Customized mereology ontology i

Integrated mereology ontology i
Customization of the chosen ontology

- Pruning the MO
- Enriching the MO
- Translating into OWL
- Evaluating

E.g. *part of* reflexivity
Integration of the MO in the PPO

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Integration of the MO in the PPO

R1) hasActiveIngredient(?x, ?y) → partOf(?y, ?x)
R2) hasMainSubstance(?x, ?y) → partOf(?y, ?x)
R3) chemicalSubstance(?chs1) ∧ chemicalSubstance(?chs2) ∧
    partOf(?chs11, ?chs1) ∧
    partOf(?chs21, ?chs2) ∧
    hasInteractionWith(?chs11, ?chs21) →
    hasInteractionWith(?chs1, ?chs2)
D.4) chemicalSubstance ⊆ mereologicalIndividualFWSPrinciple
D.5) drug ≡ chemicalSubstance ∩
    (> 1 hasActiveIngredient chemicalSubstance) ∩
    (> 1 hasMainSubstance chemicalSubstance)
Answers to the CQs (e.g. for Frenadol)

CQ_1.1. What is the composition of the drug? (direct parts)

frenadol_1 hasDirectPart: clorfenamine_1, paracetamol_1, dextrometorphan_1

CQ_1.2. What is the composition of the drug? (all parts)

frenadol_1 hasPart: aminoGroup_1, oxygen_1, clorfenamine_1, hydrogen_1, paracetamol_1, …

CQ_2. Which is the main active ingredient (molecule) of the drug?

frenadol_1 hasActiveIngredient: paracetamol_1

CQ_3. Which is the main substance of the composition?

frenadol_1 hasMainSubstance: paracetamol_1

CQ_4. Does the drug have interaction with another drug?

frenadol_1 hasInteractionWith: ethylAlcohol_1
Results and future directions

1. Scope of our study of mereology ontologies

2. Reusing a mereology ontology in a Pharmaceutical Product ontology

3. Results and future directions
Results

• The procedure for reusing mereology ontologies

• The study of mereology ontologies with regard to mereologies

• The OWL + SWRL mereology
Future directions

• Incorporate to the OWL + SWRL ontology axioms that imply extensionality to model the detailed structure of substances.

• Study of other types of part of, different to functional part of.

• Extend the repertory of reuse patterns.

• Extend the method for other common ontologies (e.g. topology ontologies).
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