

Patterns for representing time-dependent information in OWL 2 ontologies

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Abstract

Background: OWL 2 is a popular ontology development language which is supported by a wide range of tools such as editors and reasoners. It is increasingly being adopted by large scale biomedical ontologies such as the Gene Ontology and ChEBI. A limitation of OWL is that it only allows for the expression of binary relationships (object properties). In the biomedical domain, much of the knowledge that is represented in ontologies is linked to time in some fashion. For example, different developmental stages of an organism have different anatomical properties. Representing this information accurately often requires the use of ternary relations (i.e. with an additional parameter), not supported in OWL 2.

Results: In this paper we present several design patterns for working around this limitation. Firstly, we describe the use cases motivating the need for an explicit representation of temporality in the context of OWL and biomedical ontologies. Secondly, we propose and discuss different design patterns and evaluate them against the given use cases in the context of their completeness, user friendliness, and performance profile for common reasoning tasks.

Conclusions: In conclusion, we present our recommendations.

Keywords: biomedical ontology, time, temporal reasoning, OWL, BFO

Background

Our primary point of reference is the BFO (Basic Formal Ontology) top-level ontology [1]. In the current work on a new release of BFO (BFO 2), ternary (time-indexed) instance-level relations have been formulated for the first order logic (FOL) variant of the ontology.

The specification of BFO 2 is contrasted with the language specifications of OWL, as a formalism requested by most users of (computable) ontologies. However, OWL conveys considerable limitations compared to FOL, which are however justified by the computational properties (decidability) of the former.

The objective of this paper is therefore the presentation and discussion of OWL design patterns that partly mitigate this limitation. It is organised as follows. In the remainder of this Background, we give an overview of the OWL language and BFO ontology into which our proposal will be embedded, and outline our use cases and competency questions. Thereafter, in our Results we survey the existing approaches to the representation of time-dependent information in we propose and discuss different design patterns and evaluate them against the given use cases in the context of their completeness, user friendliness, and performance profile for common reasoning tasks. The concluding section presents our recommendations for the community.

BFO

Basic Formal Ontology (BFO) is an upper level ontology designed to serve as a foundation from which domain ontologies can be built [1]. Use of a shared upper level ontology and shared relationships mitigates problems that arise when several ontologies are used together in a research pipeline. For example, the root structure of two ontologies might partially overlap, without explicit mappings clarifying the intended interrelationships (e.g. having classes such as ‘process’ and ‘event’; ‘object’ and ‘thing’). Or the ontologies may make use of similar sounding relationships without clarifying whether the relationships are intended to mean the same thing (e.g. **partOf**, **includedIn**,...). They may further re-implement or redefine classes that are defined differently elsewhere.

BFO offers a small set of foundational classes together with definitions, and a set of relationships intended to be used in multiple ontologies. Both classes and relationships are domain-independent, albeit it is clearly stated that BFO’s focus is on the representation of science. Thus, domain-specific relationships such as **isTautomerOf** (a chemical relationship used in ChEBI) or **isAbout** (a relation in the information artifact

ontology) are out of scope for BFO.

BFO subscribes to three-dimensionalism and therefore the uppermost partition in its class hierarchy reflects temporal mode of existence: between *continuant*, an entity that (1) exists in full at any time that it exists at all, and (2) continues to exist self-identically for as long as it exists; and *occurent*, an entity that unfolds over a period of time and thus has temporal parts. For example, you are a continuant, while your life is an occurrent. A cell is a continuant, while the process of cell division is an occurrent.

BFO is, primarily, seen as an ontology of types (universals), based on which an isomorphic structure of classes can be derived. E.g., the extension of the type *Material Object* is the isonomic class, all members of which are instances of this type. The realms of classes and individuals (or types and their instances) are strictly disjoint: no individual can be instantiated, and no class can be member another class.

Table 1 gives a selection of core BFO classes and their definitions.

BFO offers an extensive set of relations, including **partOf**, **participatesIn**, and **inheresIn**. Table 2 details these and others together with their definitions. Most of these relations relate individuals, not classes or types.

Web Ontology Language (OWL)

The Web Ontology Language (OWL), currently available as version 2 [2] is a popular ontology development language which is supported by a wide range of tools such as editors and reasoners. OWL is based on Description Logics (DL), a family of representation formalisms designed to build large scale ontologies [3], consisting of class and relation hierarchies, defining and constraining axioms (TBox) on the one hand and, optionally, assertions about individuals (ABox). There is a broad range of DL dialects all of which are decidable subsets of first-order logics (FOL).

OWL, and particularly its language profile OWL-DL it is increasingly being adopted by large scale biomedical ontologies such as the Gene Ontology [4] and ChEBI [5].

NEEDS IMPROVEMENT

A limitation of most DL-based languages, including all OWL profiles, is the restriction of relational expressions to binary relationships (object properties). However, in nearly all scientific domains numerous statements that are supposed to be expressed in ontologies are linked to time in some fashion. For example, different developmental stages of an organism have different anatomical properties. Material objects are located at different places at different times, atoms constitute different molecules at different times. Representing this information accurately requires the use of ternary relations.

But while there has been work on expressive description logics that try to transcend this limitation ([6]) and also on description logics that explicitly account for temporality (e.g. [7]), there is no strong push towards standardisation of those formalisms, and tools suitable for end users are not readily available. It has thus been acknowledged that there is a need for solutions that work within the confines of present technologies by [8], who juxtaposes a reification approach, in which ternary relations are expressed as OWL classes to a four-dimensionalist approach, which allows continuants to have temporal parts.

In addition, OWL-DL object properties are limited to the level of individuals.. This is not the case with other, graph-based formalisms which encapsulate quantification and time reference into class-to-class relations. The most prominent one in the biomedical domain is the OBO syntax ([9]), in which such relations are defined as follows:

$$\begin{aligned} Rel(A, B) =_{def} \forall a, t : \mathbf{inst}^3(A, a, t) \\ \rightarrow \exists b : (\mathbf{inst}^3(B, b, t) \wedge \mathbf{rel}^3(a, b, t)) \end{aligned} \tag{1}$$

Most work on OBO Foundry ontologies has been committed to this definition, which provided the intuitive class-to-class relations with a clear semantics rooted in FOL.

OWL syntax and semantics (mapping to FOL) for: classes (which are the extensions of BFO types or correspond to logical expressions formed by the extensions of BFO types, so-called defined classes) BFO types), individuals (the concrete entities that instantiate BFO types and / or are members of BFO classes). The semantics of OWL follows the principles of set theory. OWL object properties are binary predicates between OWL individuals. They can optionally be connected by so-called property chains. Well-formed class-level expression therefore require quantifiers when including object properties, such as `owl : allValuesFrom (only)` or `owl : allValuesFrom (only)`.

For instance, the class expression **partOf some** *Cell* contains all individual things that are part of at least one member of the class *Cell*. Main constructors of OWL ontologies are `rdfs : subClassOf` (class subsumption), `owl : equivalentClass` (class equivalence), and `rdf : Type` (class membership) statements. For example *CellMembrane* `subClassOf` **partOf some** *Cell* means that every member of the class *CellMembrane* is part of at least one member of the class *Cell*. The big advantage of OWL ontologies is their formal rigor, their well-studied computational behaviour, their rather intuitive syntax (compared to FOL), the presence of editing tools like Protégé, and their support by DL reasoners like Hermit and Fact++, which perform reasoning tasks like consistency and satisfiability checking.

The representation of time in DL axioms

In comparison to the OBO axiom

$$CellMembrane \textbf{partOf} Cell \quad (2)$$

to which the OWL axiom

$$CellMembrane \textbf{subClassOf partOf some } Cell \quad (3)$$

is commonly considered equivalent to, the latter is undefined with regard to time. This is not a side aspect, because it makes a difference whether, e.g., a cell membrane is always part of some cell or only at some time. The lack of temporal definition of OWL statements is especially unsatisfactory when it comes to transitive properties like **partOf** or **locatedIn**, where the suppression of the temporal factor can produce plainly wrong entailments, especially at the level of individuals like in the following example:

$$\begin{aligned} &\textbf{locatedIn}(\textbf{Thrombus\#39874}, \textbf{Heart\#431234}) \\ &\textbf{locatedIn}(\textbf{Heart\#431234}, \textbf{Patient\#900812}) \end{aligned} \quad (4)$$

Assuming that the thrombus was no longer in the heart when it was transplanted to Patient#115678, then the entailment

$$\textbf{locatedIn}(\textbf{Thrombus\#39874}, \textbf{Patient\#115678}) \quad (5)$$

which follows from the transitivity property of the relation **locatedIn** is obviously wrong. What follows from this is far-reaching, although it has rarely ever been accounted for in practical OWL engineering: The inability of OWL of expressing temporal contexts of the domain entities to be represented, produces ambiguous statements that may entail unintended reasoning consequences.

Strengths of Relatedness

We make the distinction between different temporal strengths of relatedness.

0.0.1 Temporary Relatedness (TR)

Informally: for all instances of A there is some time t and some instance b of B such that a is related to b at t . Examples:

- (a) for all apple seeds there is some apple such that the seed is part of the apple at some time.
- (b) for all trees there is some leaf such that the leaf is part of the tree at some time.

Formally:

$$\begin{aligned} \text{TemporarilyRelated}(A, B) =_{\text{def}} \forall a, t : \mathbf{inst}^3(A, a, t) \\ \rightarrow \exists b, t' : (\mathbf{inst}^3(B, b, t') \wedge \mathbf{rel}^3(a, b, t') \wedge \mathbf{within}(t', t)) \end{aligned} \quad (6)$$

0.0.2 Permanent Generic Relatedness (PGR)

Informally: for all instances a of A there is, at all times t that a exists, some instance b of B such that a is related to b at t , but not necessarily always the same b at all times t . Examples:

- (a) all cells have a water molecule as part at all times, but not always the same water molecule.
- (b) every bacteria colony has some bacteria as parts at all times, but not always the same bacteria.

$$\begin{aligned} \text{PermanentlyGenericallyRelated}(A, B) =_{\text{def}} \forall a, t : \mathbf{inst}^3(A, a, t) \\ \rightarrow \exists b : (\mathbf{inst}^3(B, b, t) \wedge \mathbf{rel}^3(a, b, t)) \end{aligned} \quad (7)$$

0.0.3 Permanent Specific Relatedness (PSR)

Informally, for all instances a of A there is, at all times t that a exists, an instance b of B such that a is related to b at t ; in this case it is always the same b at all times t . Examples:

- (a) a human being has a brain as part at all times, and it is necessarily the same brain.
- (b) a radioactively marked molecule of DNA has the radioactive isotope as part at all times, and it is necessarily the same atom.

$$\begin{aligned} \text{PermanentlySpecificallyRelated}(A, B) =_{\text{def}} \forall a, t : \mathbf{inst}^3(A, a, t) \\ \rightarrow \exists b : (\mathbf{inst}^3(B, b, t) \wedge \mathbf{rel}^3(a, b, t)) \\ \wedge \forall t' : (\mathbf{inst}^3(A, a, t') \rightarrow (\mathbf{rel}^3(a, b, t') \wedge \mathbf{inst}^3(B, b, t'))) \end{aligned} \quad (8)$$

Use Cases and Competency Questions

In which we set out our important and super relevant use cases. Straight from the biology.

We furthermore describe the points we are going to evaluate against.

1. completeness,
2. user friendliness, and
3. performance profile

The details of how we conducted the evaluation are described in our Methods section at the end.

Results

Survey of existing approaches

Histories in BFO 2

In BFO 2, work is under way to sketch out a more detailed theory of the relationship between continuants (SNAP objects) and occurrents (SPAN objects) they participate in. Specifically, BFO 2 make the assumption that for each material object there exists a special process, the *history* of the object, which encompasses „the totality of processes taking place in the spatiotemporal region occupied by the entity.“ ([10]) This means that there is a one to one correspondence between continuants and certain processes, which effectively provides a „bridge“ between the 3D and the 4D perspective. No complete formal theory of histories, which have previously been described in [11], is available as of yet.

Should we keep SNAP and SPAN. Or better continuant and occurrents?

0.1 Conventional Modellers' Strategy for Temporalised Relations in OWL 2

As explicit semantics for modelling temporal dynamics are not available in OWL 2, modellers tend to implicitly treat object properties as committing to a „for all times“ interpretation in order to avoid obvious problems with the entailed models. For instance, in an anatomy ontology like the FMA, the object property **hasPart** is transitive, and used in axioms such as

$$Lung \text{ subClassOf } \mathbf{hasPart} \text{ some } LobeOfLung \quad (9)$$

and

$$LobeOfLung \text{ subClassOf } \mathbf{hasPart} \text{ some } BronchiopulmonarySegment \quad (10)$$

If the underlying interpretation were „for some time“, transitivity of the binary **hasPart** could no longer be taken for granted, as two **hasPart** assertions to be chained could belong to two different SNAP ontologies.

Strategies Advanced in Related Work

Existing Design Patterns

Default Reinterpretation

On the default reinterpretation of the OWL direct semantics to preserve the RO generic relatedness default reading.

Obviously, the interpretation must be equivalent to the OWL 2 direct semantics [12] in as far as it preserves the syntactical structure and inferences and does not lead to additional expressivity. But it has – to our knowledge – never been made explicit what this substitution might consist of. This is even more significant as this does not constitute at all a side issue or an idiosyncrasy of biomedical ontologies. On the contrary, virtually all OWL ontologies contain axioms on classes of continuants using binary object properties and leave the exact interpretation unexplained.

To address this mismatch and try to understand it better we sketch here a possible elucidation which consists in a modification of the interpretation function. The general strategy of this interpretation is to augment the interpretations of class members and object properties in the OWL model with an additional time index t which specifies that the entity in question exists (object property holds) at t . Class instances then become pairs and object property instances triples. In order to keep the surface grammar and overall semantics intact, the interpretations of all OWL axioms will be prepended with a conditionalised universal quantification over t that specifies that the axiom should hold at all times that the entity in question exists. Time instants are hereby external to the domain. For example, the interpretation of a class assertion axiom that asserts that a is an instance of class C , as long as a exists, would then read (domain Δ , interpretation $\cdot^{\mathcal{I}}$):

$$\forall t : \langle a^{\mathcal{I}}, t \rangle \in \Delta^{\mathcal{I}} \rightarrow \langle a^{\mathcal{I}}, t \rangle \in C^{\mathcal{I}} \quad (11)$$

We implicitly assume that Δ contains individual/time-point pairs only for those times at which an individual exists. Notably, this is only sufficient to express rigid instantiation: Whenever an individual exists at all, it is also a member of the class it instantiates. The interpretation of temporality-sensitive relations will become clear when we spell out the semantic rules of existential quantification and value restriction, both of which assert permanent generic relatedness because they apply existential quantification over the object property range so that at each point in time a different individual of class B can serve as a relatum. We will use the canonical structural syntax [13] to ease comparison with the specified semantics [12].

Table 1: Syntactical representations of (permanent) relatedness expressions

OBO Syntax	OWL (Manchester Syntax)	First Order Logic
[Term] id: A relationship: rel ² B	A subClassOf rel ² some B	$\forall a, t : \mathbf{inst}^3(A, a, t) \rightarrow$ $(\exists b : \mathbf{inst}^3(B, b, t) \wedge$ $\mathbf{rel}^3(a, b, t))$

Existential quantification (**rel**² some B)

$$\begin{aligned} \text{ObjectSomeValuesFrom}(\mathbf{rel}^2, B)^{\mathcal{I}} &=_{def} \\ \{ \langle a^{\mathcal{I}}, t \rangle \in \Delta^{\mathcal{I}} \mid \exists b : \langle a^{\mathcal{I}}, b, t \rangle \in \mathbf{rel}^{3^{\mathcal{I}}} \wedge \langle b, t \rangle \in B^{\mathcal{I}} \} \end{aligned} \quad (12)$$

Value restriction (**rel**² only B)

$$\begin{aligned} \text{ObjectAllValuesFrom}(\mathbf{rel}^2, B)^{\mathcal{I}} &=_{def} \\ \{ \langle a^{\mathcal{I}}, t \rangle \in \Delta^{\mathcal{I}} \mid \forall b : \langle a^{\mathcal{I}}, b, t \rangle \in \mathbf{rel}^{3^{\mathcal{I}}} \rightarrow \langle b, t \rangle \in B^{\mathcal{I}} \} \end{aligned} \quad (13)$$

In OWL object property assertions the time index is bound through universal quantification again:

$$\text{ObjectPropertyAssertion}(\mathbf{rel}^2, a, b) =_{def} \forall t : \langle a^{\mathcal{I}}, t \rangle \in \Delta^{\mathcal{I}} \rightarrow \langle a^{\mathcal{I}}, b^{\mathcal{I}}, t \rangle \in \mathbf{rel}^{3^{\mathcal{I}}} \quad (14)$$

Hence, object property assertions specify permanent relatedness. Disregarding the difference between specific and generic permanent relatedness for the time being, this interpretation of OWL 2 at least successfully mimics the semantics of class level relations intended by the relations ontology (RO, [9]) and allows us to think of the syntactical forms represented in table 1 as equivalent.

This approach also retains standard transitivity semantics of OWL 2 object properties, so that quantification over time maintains transitivity of the relation in question. This can be shown, e.g. for the transitive relation **hasPart**: if an organism has some heart at any time, and if this heart has some heart valve at any time, then the organism has some heart valve at any time:

$$\frac{A \text{ subClassOf } \mathbf{hasPart}^2 \text{ some } B \quad B \text{ subClassOf } \mathbf{hasPart}^2 \text{ some } C}{A \text{ subClassOf } \mathbf{hasPart}^2 \text{ some } C}$$

And while there is nothing to be gained by actually modifying OWL 2 to use this interpretation, it is very important that ontology engineers are aware of the implications of their modelling decisions with regard to relations that are sensitive to the issue of temporal strength. However, this approach still has the consequence that „temporary relatedness“ cannot be expressed directly in an OWL 2 ontology, so we need to look for more involved solutions to the problem.

Reification

A common strategy to work around the limitations of description logics is to represent ternary relations through reification. Reification involves the introduction of a class $C_{\mathbf{rel}^3}$ for each ternary relation \mathbf{rel}^3 . The relata of \mathbf{rel}^3 are then connected to instances of $C_{\mathbf{rel}^3}$ by three new binary relations \mathbf{R}_1^2 , \mathbf{R}_2^2 , \mathbf{R}_3^2 . The instance-level assertion

$$\mathbf{rel}^3(a, b, t)$$

would then be transformed into the following statement:

$$\exists x : C_{\mathbf{rel}^3}(x) \wedge \mathbf{R}_1^2(x, a) \wedge \mathbf{R}_2^2(x, b) \wedge \mathbf{R}_3^2(x, t) \quad (15)$$

Changed
from list of
statements
to proper
axiom

Such proposals have, with a varying degree of sophistication, seen quite a bit of dissemination in the ontology engineering community [14], but they suffer from unavoidable drawbacks. Most obviously, they are rather complex. This bears the risk of errors in the ontology engineering process and decreases reasoning efficiency [15]. To address the complexity problem, it has been suggested to select reification classes based on what seems ontologically „fitting“ for the domain of an ontology [16].

Welty/Fikes: Fluents

The prototypical approach for dealing with temporally changing information in OWL within a four-dimensionalist framework was provided by [8]. And while they agree that the 4D approach is „clearly not something that immediately appeals to common sense“, they also claim that it „gives us another tool to use when solving a practical problem.“ To this end, they present an ontology that models fluents, i.e. „relations that hold within certain time interval but not in others.“ This works by considering all entities as four dimensional entities that have temporal parts (time slices), such that the material object property assertions hold (synchronously) between time slices. For example, temporary relatedness could be expressed as in (16).

$$Leaf \text{ subClassOf } \text{inverseOf}(\text{timeSliceOf}^2) \text{ some } \text{hasPart}^2 \text{ some } \text{timeSliceOf}^2 \text{ some } Tree \quad (16)$$

This is by far one of the most straightforward translations of the four-dimensionalist commitment, but it suffers from a certain verbosity. This increases even more if permanent relatedness is concerned. In this case, the above expression would have to be amended to include a „ $\text{inverseOf}(\text{timeSliceOf}^2)$ only“ clause to ensure that all time slices of the entity are appropriately related to a time slice of the other entity.

Zamborlini/Guizzardi: Moments, Relators and Qua-Individuals

The commitment that some relational expressions are in fact better accounted for as proper entities is also prominent in Zamborlini and Guizzardi treatment of contingent properties [17]. For them, certain „material relations“ only hold by virtue of a separate truthmaker, the so called *relator*, which is formed by combining the „qua individuals“ that partake in the relation. Qua individuals abstract away certain aspects of an individual so that only that information remains which is relevant for the individuals participation in the relation.

Both kinds of entities are examples of „moments“ in their nomenclature, which are said to inhere in individual entities and can thus be compared to dependent continuants or occurrents (respectively) in BFO parlance. But while relators might often be appropriately represented by BFO processes, the admissibility of qua individuals into BFO might be questionable since they can hardly be aligned with BFO’s realist commitment (where sheer abstractions could only be regarded as artefacts of a persons though process).

Underneath the level of qua individuals (e.g. „*LeafQuaPartOfTree*“) and relators, there is the assumption of an ontology of time slices not unlike the one in [8], such that temporal overlap between the qua individuals related by the relator can be enforced.

Zamborlini and Guizzardi cite as an advantage for this approach that it is capable of representing the persistence of a relationship across multiple time slices without mentioning each explicitly (because the relator is associated with the qua-individual and not its time slice). This is part of a set of requirements suggested for modelling temporally changing information:

1. Avoid duplication of the other time slices if one entity partaking in the relation changes.
2. Provide a consistent ontological interpretation of contingent (non-rigid) instantiation.
3. Avoid repeating persisting properties for each time slice
4. Ensure that immutable properties of an entity cannot be overridden by a time slice.

We believe these points to be a good starting point for the evaluation of any proposal to address the problem of time-dependent relation and should be used to supplement our initial requirements.

Gangemi: Descriptions and Situations

Aldo Gangemi’s DnS pattern [18] deserves mention because it treats time-dependence of relations as a special case of perspectivity which can be accounted for by the very heavy-duty reification mechanism of descriptions

and situations. In this case, the suggestion is to use the situation pattern in order to associate the relations and their temporal context with a common situation, which is effectively a reified assertion (a proposition). Again, such entities are figments of the mind and can only be admitted into a realist ontology such as BFO as such – rather than being a general way to refer to arbitrary facts.

Notably, though, Gangemi reminds us of the fact that OWL 2's **hasKey** axiom can be used to circumvent the problem of possible duplication of instances for the same relational n -tuple: If a situation S were to use the properties **hasTimeStamp**², **hasSubject**², and **hasObject**², the axiom

$$S \text{ hasKey}(\text{hasTimeStamp}^2, \text{hasSubject}^2, \text{hasObject}^2) \quad (17)$$

would ensure that duplicate entities would be coalesced in the model.

Proposed Design Patterns

Temporalized Relations

Of the three patterns *temporary relatedness* (TR), *permanent generic relatedness* (PGR), and *permanent specific relatedness* (PSR), TR and PSR have in common that they can be asserted between individuals: a token a can be temporarily related to a token b , such as a specific leaf is temporarily part of a specific plant, or a specific human, e.g. Barack Obama, is temporarily located at a specific place, e.g. in his plane Air Force One.

In a similar way, two individuals can be permanently related, such as, e.g., my body mass is permanently inherent in my body, or the planet Earth is permanently part of our solar system.

This allows, in both cases to hide the time argument within a so-called temporalized relation. The TR pattern is introduced as follows:

$$\text{rel_at_some_time}^2(a, b) =_{def} \exists t : \text{rel}^3(a, b, t) \quad (18)$$

This relation can be used in description logics axioms like the a-box axiom

$$\text{locatedIn_at_some_time}^2(\text{Obama}, \text{Air_Force_One}) \quad (19)$$

or in the t-box axiom

This section describes Alan's approach and the BFO 2 Graz release

$$Leaf \text{ subClassOf } \mathbf{partOf_at_some_time}^2 \text{ some } Plant \quad (20)$$

The PSR pattern is introduced as follows:

$$\mathbf{rel_at_all_times}^2(a, b) =_{def} \forall t : (\mathbf{exists_at}^2(a, t) \rightarrow \mathbf{exists_at}^2(b, t) \wedge \mathbf{rel}^3(a, b, t)) \quad (21)$$

This relation can be used in description logics axioms like the a-box axiom

$$\mathbf{locatedIn_at_all_times}^2 (Earth, Solar_System) \quad (22)$$

or in the t-box axiom

$$Vertebrate \text{ subClassOf } \mathbf{hasPart_at_some_time}^2 \text{ some } Spine \quad (23)$$

There are several properties that have to be considered for the practical use of temporalized relations. In case a ternary relation is transitive, e.g.

$$\mathbf{rel}^3(a, b, t) \wedge \mathbf{rel}^3(b, c, t) \rightarrow \mathbf{rel}^3(a, c, t) \quad (24)$$

the derived binary TR relation is not, because the implied time argument (cf. 18) is not the same for the conjoints in a transitive chain. If Obama is in Air Force One at some time, and Air Force One is in Oklahoma City Air Logistics Center at some time this does not imply that Obama was that Center t any time. There is no problem with inverse TR relations, yet.

$$\mathbf{rel}^3(a, b, t) = \mathbf{inv_rel}^3(b, a, t) \quad (25)$$

trivially entails

$$\mathbf{rel}^2(a, b) = \mathbf{inv_rel}^2(b, a) \quad (26)$$

If Obama is contained in Air Force One at some time, then Air Force One is the container of Obama at some time.

It is quite different with PSR. Here, it can be shown that transitivity is maintained: As the relation holds, according to formula 21 for all times in which the first argument exists, this is also the case for the second argument which becomes the first one in a transitivity chain. However, we cannot assume that the inverse relation of a ternary relation carries over to the binary PSR relation. According to 21, the scope of the quantification over time is only the first argument. It entails the existence of the second argument for the time of the existence of the first one, which, however, does not preclude that the second one outlives the first one. If we say that a certain vertebrate has always a spine this does not preclude the spine may still exist centuries after the animal's death. This means that the inverse of **hasPart_at_some_time²** is not **partOf_at_some_time²** but something like **partOf_at_some_time_at_which_the_whole_exists²**.

We have not considered, so far the PGR case. Not that this has been introduced as the standard interpretation of class-to-class relations in OBO, which means that it has influenced the development of biomedical ontologies over nearly a decade. On a closer scrutiny there is some evidence that many instance of OBO relation assertions would rather correspond to TR, such as in the foundational model of anatomy under real-world conditions: every human brain was part of some human organism, but after the death of the organism it may still have a limited existence. Every human may have had teeth, but toothless humans are still humans. In other cases PGR may be interpreted as PSR, especially in the case of dependent continuants: the redness of a red blood cell always inheres in it. Or the surface of my body cannot jump to a different body. Nevertheless there are enough cases in which PGR is the only acceptable interpretation, especially if we consider PSR as a specialization of PGR.

A major drawback here is the fact that PGR cannot be expressed by a relation between individual entities. For instance, the statement "every cell nucleus is part of some cell at any time" does not mean that a certain cell nucleus part of a certain cell. It may become part of a different cell if the original cell fuses with another one and thus becomes a different individual. It is therefore counterintuitive to assert PGR at the level of individuals. Therefore, the OBO "standard case" cannot be expressed via temporalized relations.

Yet there is a way to use temporalized relations to represent at least an important portion of the knowledge for which PGR would be the most correct one.

The reasoning is the following: If we want to express that the classes *A* and *B* are related by a permanent generic relationship, such as *A obo : hasPart B*, we may resort to *histories*, which are occurrents and

can therefore be related by binary relations. A history of a continuant c corresponds to four-dimensional spacetime “worm” with a temporal extension that equals the timespan t during which c exists and a three-dimensional spatial extension indexed by each point $t_i \in t$.

Histories can be related by occurrent parthood relations, such as every phase (temporal part) of the history of a cell nucleus is part of the history of some cell (not necessarily of the same cell).

If we want to express that all instances of the class A are always located in some instance of the class B we can express it, in OWL in the following way:

$$\begin{aligned} & \text{temporalPartOf some (historyOf some } A) \text{ subclassOf} \\ & \text{occurrentPartOf some (temporalPartOf some (historyOf some } B)) \end{aligned} \quad (27)$$

In a similar way, the converse case can be expressed:

$$\begin{aligned} & \text{temporalPartOf some (historyOf some } C) \text{ subclassOf} \\ & \text{hasOccurrentPart some (temporalPartOf some (historyOf some } D)) \end{aligned} \quad (28)$$

In the case of cell nuclei and cells their generic parthood could be formalized as follows:

$$\begin{aligned} & \text{temporalPartOf some (historyOf some } CellNucleus) \text{ subclassOf} \\ & \text{occurrentPartOf some (temporalPartOf some (historyOf some } Cell)) \end{aligned} \quad (29)$$

Transitivity would be maintained, e.g. every nucleolus is part of some cell because every nucleolus is part of some cell nucleolus

$$\begin{aligned} & \text{temporalPartOf some (historyOf some } Nucleous) \text{ subclassOf} \\ & \text{occurrentPartOf some (temporalPartOf some (historyOf some } CellNucleus)) \end{aligned} \quad (30)$$

as it can be trivially shown.

However, the inclusion of history phases does not allow a distinction between location and parthood [?], so that the relation between a pregnant organism and an embryo or foetus would not be distinguished between the relation between an organism and its brain.

Temporally Qualified Continuants

We can define a *temporal qualification* of a continuant as the result of regarding the continuant in as far as it exists only within a certain portion of time. A temporal qualification is characterised by its spatial co-extension with its continuant over the time period that it qualifies.

A temporally qualified continuant (TQC) is thus a way of referring to a continuant during a portion of time. Formally, we can describe it as a tuple $\langle a, t \rangle$ where a is an instance of a continuant and t is a portion of time.

There are several axioms needed to link TQCs to the continuants that they are temporal qualifications of and to ensure that TQC portions of time do not exceed the allowed portion of time that the corresponding continuant instance spans over (most of these are similar to the proposals presented above). Instantiation of a TQC is thus not time-indexed, while normal instantiation of continuants is time indexed as in the examples above.

We will use the notation TQC_A to denote the class of temporally qualified continuants which range over continuants of type A .

$$\forall x : (\mathbf{inst}^2(TQC_A, x) \rightarrow \exists a, t_0, t_1 : (\mathbf{inst}^3(A, a, t_0) \wedge \mathbf{equals}(x, a, t_1) \wedge \mathbf{within}(t_1, t_0))) \quad (31)$$

The intended meaning of the predicate **equals** is identity. We further introduce a relation **continuantOf** to link a TQC to the continuant that it is a TQC of. That is,

$$\forall x \mathbf{inst}^2(TQC_A, x) \rightarrow \exists a, t : (\mathbf{inst}^3(A, a, t) \wedge \mathbf{continuantOf}^2(a, x)) \quad (32)$$

In the next sections, we will discuss the representation of the three different temporal strengths, linking from the standard representation in BFO FOL through the introduction of temporally qualified continuants to the standard representation in OWL, showing how these different temporal strengths can be implemented through this method in a binary relationship framework such as OWL, though this representation will require relations that refer to ternary predicates in the FOL model, such as **continuantOf²**, to remain primitive.

Temporary Relatedness

We rephrase the definition (6) given above by inserting temporally qualified continuants and derive the form that the relationship takes for temporally qualified continuants and a binary relationship. This is a fairly

transparent translation:

$$\begin{aligned} \text{TemporarilyRelated}(A, B) =_{def} \forall a, t : \mathbf{inst}^2(A, \langle a, t \rangle) \\ \rightarrow \exists b, t_1 : (\mathbf{inst}^2(B \langle b, t_1 \rangle) \wedge \mathbf{rel}^2(\langle a, t \rangle, \langle b, t_1 \rangle) \wedge \mathbf{within}(t_1, t)) \end{aligned} \quad (33)$$

We then use the **continuantOf²** relation and the TQC notation to eliminate the tuples:

$$\begin{aligned} \text{TemporarilyRelated}(A, B) =_{def} \forall x : \mathbf{inst}^2(TQC_A, x) \rightarrow \exists a, y, z, t_1 : (\mathbf{inst}^2(TQC_A, y) \wedge \\ \mathbf{inst}^2(TQC_B, z) \wedge \mathbf{continuantOf}^2(a, x) \wedge \mathbf{continuantOf}^2(a, y) \wedge \mathbf{rel}^2(y, z)) \end{aligned} \quad (34)$$

This means that the logical form of the expression of temporary relatedness is that at least one temporal qualification of A is related to some temporally qualified B instance. However, we need another axiom to constrain **rel²** in the above to ensure that the portions of time are appropriately overlapping, since **rel³** holds at one time only:

$$\begin{aligned} \forall x, y : \mathbf{rel}^2(x, y) \rightarrow \exists a, b, t, t_1 : (\mathbf{equals}(x, \langle a, t \rangle) \wedge \mathbf{equals}(y, \langle b, t_1 \rangle) \\ \wedge \mathbf{continuantOf}^2(a, x) \wedge \mathbf{continuantOf}^2(b, y) \wedge \mathbf{rel}^3(a, b, t_1) \wedge \mathbf{within}(t_1, t)) \end{aligned} \quad (35)$$

Now we have derived a binary expression **rel²** we are free to use this in OWL axioms. We introduce the relation **hasSameContinuant²** between temporally qualified continuants to express that they are TQCs of the same continuant, expressed in the above axiom (34) as $(\mathbf{continuantOf}^2(a, x) \wedge \mathbf{continuantOf}^2(a, y))$, which allows us to express temporary relatedness in OWL as follows:

$$TQC_A \text{ subClassOf } \mathbf{hasSameContinuant}^2 \text{ some } (\mathbf{rel}^2 \text{ some } TQC_B) \quad (36)$$

Additionally, we ensure that sharing a temporal qualification amounts to being the same continuant:¹

$$A \text{ hasKey}(\mathbf{continuantOf}^2) \quad (37)$$

Usability and simplification

Since the above axiom (36) makes a claim about the class TQC_A , it is less ideal from a usability perspective. We would rather like to say something about the target continuant classes A and B in our OWL version, for ease of use by the end user. Thus, we introduce a new relationship, **rel^{Temp}**, which obtains between continuants, and should be interpreted as follows:

$$\begin{aligned} A \text{ subClassOf } \mathbf{rel}^{\text{Temp}} \text{ some } B \rightarrow \\ TQC_A \text{ subClassOf } \mathbf{hasSameContinuant}^2 \text{ some } (\mathbf{rel}^2 \text{ some } TQC_B) \end{aligned} \quad (38)$$

¹Implementers should note that OWL 2 only mandates this for *named* individuals.

Unfortunately, the above statement cannot be formulated in OWL 2 due to its strict constraints on object properties. Neither can it be implemented in a rule language, since it would induce the generation of new individuals in its consequent, which violated DL safety. Still there is an avenue for hiding the complexity by using a macro processing engine, such as OPPL ([19]), in which processing instructions such as these could be employed:

```
?x:CLASS[subClassOf Continuant],
?y:OBJECTPROPERTY?MATCH("temporarily_(.*)"),
?z:CLASS[subClassOf Continuant]
SELECT ?x subClassOf ?y some ?z
BEGIN
  ADD ?x subClassOf continuantOf some ?y.GROUPS(1)
  some hasContinuant ?z,
  REMOVE ?x subClassOf ?y some ?z
END;
```

This can easily be adopted or parameterised for other axiom types or types of temporal sensitivity (e.g. permanent generic relatedness) Additional measures that alleviate the burden of this approach would be making **rel**² a sub-object-property of **rel**^{Temp}, which quite natural and obvious: If something is related at all times to some entity, it is related to that entity at some time.

Permanent Generic Relatedness

Permanent generic relatedness is considered by some to be the most common interpretation of temporally unspecified relations in biology. We have previously defined it in (7), which can now be rephrased using the TCQ approach as follows:

$$\forall x : \text{inst}^2(TQC_A, x) \rightarrow \exists y : \text{inst}^2(TQC_B, y) \wedge \text{rel}^2(x, y) \quad (39)$$

Informally, this means that, whatever temporal qualification of an instance of A we choose, it will always be **rel**-related to some temporal qualification of type B , but we neither care nor enforce which one.

This is the easiest and most elegant translation case from the FOL perspective. Moving to OWL, the above axiom (39) appears as:

$$TQC_A \text{ subClassOf } \text{rel}^2 \text{ some } TQC_B \quad (40)$$

Again, we can use a kind of macro expansion to bridge a shorthand for this type of relatedness (e.g. **rel**^{PG}) back to the underlying relationship. Thus we would use (40) to replace every occurrence of axioms

such as the following:

$$A \text{ subClassOf } \mathbf{rel}^{\mathbf{PG}} \text{ some } B \quad (41)$$

By replacing, we mean to imply that we advise against using $\mathbf{rel}^{\mathbf{PG}}$ as an object property, which would not be harmful in itself, but at least counter-intuitive. Instances of A satisfying (41) would require a pair of instances $\langle a, b \rangle$, where a is said to be permanently generically related to b , which is (a) meaningless since generic relatedness pertains to a type, not an instance and (b) misleading since it is not enforced by the model.

Still, the availability of permanent generic relatedness is noteworthy because it would not be possible in OWL 2 in absence of temporally qualified continuants (not only instantiation of classes, but also of object property tuples is rigid). This is afforded by the fact that we do not introduce an explicit object property for generic permanent relatedness.

Since permanent generic relatedness matches the presumed default interpretation of \mathbf{rel}^2 in most existing biomedical ontologies, upgrade paths for these ontologies need to be considered. We believe that, from a user perspective, the most convenient way would be to relegate all relations that require temporalisation into a specific branch (say, **temporallySensitivelyRelated²**) and employ something like the following preprocessing instruction:

```
?x:CLASS[subClassOf Continuant],
?y:OBJECTPROPERTY?[subPropertyOf temporallySensitivelyRelated],
?z:CLASS[subClassOf Continuant]
SELECT ?x subClassOf ?y some ?z WHERE
  FAIL ?x subClassOf hasContinuant some Continuant,
  ?y MATCH("^(.(?!temporarily_))*\$")
  FAIL ?z subClassOf hasContinuant some Continuant,
BEGIN
  ADD hasContinuant some ?x subClassOf ?y some continuantOf some ?z,
  REMOVE ?x subClassOf ?y some ?z
END;
```

This allows users to do away with $\mathbf{rel}^{\mathbf{PG}}$ and have expressions about continuants converted into expressions about temporal qualifications transformed seamlessly. There are two downsides to this. Firstly, this approach moves ontology engineering even more towards procedures that are familiar to software engineers but not to scientists from the field of application. Secondly, the above expression requires a reasoner to work, which might be costly to do after every edit.

On the other hand, it is subject to debate whether adopting an edit-compile-test approach in ontology engineering could in fact be useful for improving ontology quality.

Permanent Specific Relatedness

If we do introduce an explicit object property, could we hope to arrive at implementing something like permanent specific relatedness (8)? Unfortunately, this assumption proves to be too naïve.

It would require an additional axiom to ensure that only TQCs of the same instance are involved for the second relatum. Unfortunately, we cannot provide an accurate translation of this kind of relatedness into OWL 2, though we can achieve the following first order translation in TQC-talk:

$$\begin{aligned} \forall x : \mathbf{inst}^2(TQC_A, x) \rightarrow \\ \exists y : \mathbf{inst}^2(TQC_B, y) \wedge \mathbf{rel}^2(x, y) \wedge \\ \forall x_1, a : ((\mathbf{inst}^2(TQC_A, x_1) \wedge \mathbf{continuantOf}^2(a, x) \wedge \mathbf{continuantOf}^2(a, x_1)) \wedge \\ \exists y_1, b : (\mathbf{inst}^2(TQC_B, y_1) \mathbf{continuantOf}^2(b, y) \wedge \mathbf{continuantOf}^2(b, y_1) \wedge \\ \mathbf{rel}^2(x_1, y_1))) \end{aligned} \quad (42)$$

This would require three variables (x, y, y_1) to be bound at the same time, which is incompatible with any OWL translation.

Nice and good evaluation of the different approaches goes here

Conclusions

Summary

Recommendations of which approach to follow under which circumstances

Methods

All the boring stuff goes here

Author's contributions

Every author made very important contributions to everything.

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References

1. BFO 2 OWL Group: **BFO 2 OWL Preview Release**[<http://purl.obolibrary.org/obo/bfo/2012-11-15-bugfix/bfo.owl>].
2. Grau BC, Horrocks I, Motik B, Parsia B, Patel-Schneider P, Sattler U: **OWL 2: The next step for OWL**. *Web Semantics* 2008, **6**:309–322, [<http://portal.acm.org/citation.cfm?id=1464505.1464604>].
3. Baader F, Calvanese D, McGuinness D, Nardi D, Patel-Schneider P: *Description Logic Handbook, 2nd Edition*. Cambridge University Press 2007.
4. The Gene Ontology Consortium: **Gene ontology: tool for the unification of biology**. *Nat. Genet.* 2000, **25**:25–9.
5. Hastings J, de Matos P, Dekker A, Ennis M, Harsha B, Kale N, Muthukrishnan V, Owen G, Turner S, Williams M, Steinbeck C: **The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013**. *Nucleic Acids Research* 2013, **41**(Database issue):D456–63.
6. Calvanese D, De Giacomo G, Lenzerini M: **Conjunctive Query Containment in Description Logics with n-ary Relations**. In *Proceedings of the 1997 Description Logic Workshop (DL'97)*. Edited by Brachman R, et al. 1997:5–9.
7. Wolter F, Zakharyashev M, Mosurovicz M: **Temporalizing Description Logic: a point based approach**. *Bulletin of the Italian Association for Artificial Intelligence* 2001, **14**:16–20.
8. Welty C, Fikes R: **A Resuable Ontology for Fluents in OWL**. In *Proceedings of FOIS-2006*. Edited by Bennett B, Fellbaum C 2006:226–236.
9. Smith B, et al.: **Relations in biomedical ontologies**. *Genome Biology* 2005, **6**(5):R46, [<http://genomebiology.com/2005/6/5/R46>].
10. Smith B, et al.: **Basic Formal Ontology 2.0. Draft Specification and User's Guide** 2012, [<http://purl.obolibrary.org/obo/bfo/2012-07-20/Reference>].
11. Smith B, Grenon P: **The Cornucopia of Formal-Ontological Relations**. *Dialectica* 2004, **58**(3):279–296.
12. Motik B, Patel-Schneider P, Cuenca Grau B: **OWL 2 Web Ontology Language Direct Semantics** 2009, [<http://www.w3.org/TR/2009/REC-owl2-direct-semantics-20091027/>].
13. Motik B, Patel-Schneider P, Parsia B: **OWL 2 Web Ontology Language Structural Specification and Functional-Style Syntax** 2009, [<http://www.w3.org/TR/2009/REC-owl2-syntax-20091027/>].
14. Aranguren M, et al.: **Nary Relationship**. In *Ontology Design Pattern Public Catalog* 2009[http://www.gong.manchester.ac.uk/odp/html/Nary_Relationship.html].
15. Grewe N: **A generic reification strategy for n-ary relations in DL**. In *Proceedings of the 2nd workshop of the GI-Fachgruppe 'Ontologien in Biomedizin und Lebenswissenschaften' (OBML) : Mannheim, Germany, Sep 9–10*. Edited by Herre H, et al. 2010:N1–5.
16. Severi P, Fiadeiro J, Ekserdjian D: **Guiding Reification in OWL through Aggregation**. In *Proceedings of the 2010 Description Logic Workshop (DL2010)*. Edited by Haarslev V, Toman D, Weddell G 2010:416–427.
17. Zamborlini V, Guizzardi G: **On the Representation of Temporally Changing Information in OWL**. In *EDOCW*, IEEE Computer Society 2010:283–292, [<http://dblp.uni-trier.de/db/conf/edoc/edoc2010w.html#ZamborliniG10>].
18. Gangemi A: **Super-duper Schema: an OWL2+RIF DnS Pattern**. In *Proceedings of DeepKR Challenge Workshop at KCAP11*. Edited by Chaudry V 2011[<http://www.ai.sri.com/halo/public/dkrckap2011/Gangemi.pdf>].
19. Egaña M, Stevens R, Antezana E: **Transforming the Axiomisation of Ontologies: The Ontology Pre-Processor Language**. In *Proceedings of OWLED 2008 DC OWL: Experiences and Directions* 2008.

Figures

Figure 1 - Sample figure title

A short description of the figure content should go here.

Figure 2 - Sample figure title

Figure legend text.

Tables

Table 1 - BFO Classes

In this table we present the core BFO classes with their definitions.

BFO Classes	
A1	B2
A2	...
A3	..

Table 2 - BFO Relations

In this table we present a selection of BFO relations together with their definitions.

BFO Relations		
A1	B2	C3
A2
A3	..	.