Relating some stuff to other stuff

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Abstract. Traceability in food and medicine supply chains has to handle stuffs—entities such as milk and starch indicated with mass nouns—and their portions and parts that get separated and put together to make the final product. Implementations have underspecified 'links', if at all, and theoretical accounts from philosophy and in domain ontologies are incomplete as regards the relations involved. To solve this issue, we define seven relations for portions and stuff-parts, which are temporal where needed. The resulting theory distinguishes between the extensional and intensional level, and between amount of stuff and quantity. With application trade-offs, this has been implemented as an extension to the Stuff Ontology core ontology that now also imports a special purpose module of the Ontology of units of Measure for quantities. Although atemporal, some automated reasoning for traceability is still possible thanks to using property chains to approximate the relevant temporal aspects.

1 Introduction

Part-whole relations have been investigated in fields such as ontologies, conceptual modelling, cognitive science, and natural language. The part-whole relation between stuffs like milk, mayonnaise, and alcohol—i.e., uncountable entities other in amounts and indicated in language with mass nouns—or particular amounts of stuff—e.g., the amount of milk in your mug—has been named also part of, but also portion of, piece of, sub quantity of, or ingredient of; e.g., [4, 10, 12, 14, 16, 18, 25]. This already raises the question as to what exactly is going on, and which of those relations are the same or different, so as to be able to choose the right one when developing an ontology or a conceptual model. This becomes crucial in particular when one would want to reason over it for, e.g., traceability in the food chain: the portion in your mug of milk *was* a portion of the amount of milk in the carton, which was again a portion from some batch in the food processing plant, and deriving their relatedness would aid food safety applications in traceability [9, 28]. Superficially similar examples are a piece of meat that is contaminated with *E. coli*, yet its fat that would be safe for consumption, and vaporising alcohol from an amount of wine during cooking.

That is, there is a need for making distinctions in how stuffs relate. While it has been recognised that there are differences between parts and portions and stuff and their quantities, this has not yet been fully addressed. Options proposed conflate knowledge at the type and the instance/particular level (the stuff universal and an amount of it) and the repeatable quantity [14], the temporal dimension has received little attention, or to the extent that it cannot be readily implemented [2, 10], and it is not clear whether all those relations are really variations on mereological parthood [18].

We aim to solve these problems by defining seven relations for portions, pieces, and stuff-parts, which are temporalised where needed. In addition, we make a clear distinction between the extensional and intensional levels (amounts vs stuff kinds) that are separate yet represented in the same ontology, and we distinguish portions from quantities. The resulting model with the relations are implemented by extending the Stuff Ontology core ontology of [17] accordingly and importing a special purpose module of the Ontology of units of Measure (OM) for quantities that was developed by domain experts in food [26]. Traceability is then aided by availing of the more precise representation and property chains. The ontologies are available from `http://www.meteck.org/stuff.html`.

The remainder of the paper first summarises related works (Section 2), which is followed by some preliminaries (Section 3). Section 4 describes the model and has the formal definitions of the stuff relations, which is subjected to implementation trade-offs in Section 5. We discuss in Section 6 and conclude in Section 7.

2 Related work

Many ontologies do have at least one relation to relate stuffs specifically. We cover a selection to exemplify the outcome of the assessment, which is that developers of the respective ontologies have struggled with the same questions and either opted for different 'workarounds' or ignored it by overloading parthood. Thereafter we zoom in on the two most recent papers from formal ontology.

2.1 Ontologies as artefacts

The taxonomy of part-whole relations [18] has a subQuantityOf relation, which the authors admit to be underspecified as lumping together portions of the same kind of stuff and part-stuff of a whole-stuff that are of a different kind of stuff. Elsewhere the latter is also called ingredient [16] and hasSubStuff [17]. The SIO [11] has only has proper part between objects, which may or may not be stuffs, though for liquids, there is also a 'liquid solution component' intended as a specific stuff-part, and mass (a quantity) as 'is attribute of' some 'material entity'. DOLCE-lite (based on [20]) also uses only part, but also has a way to represent the quantity of the amount-of-matter using the has-quality property. BioTop [5] has a temporal part (temporal in the name only, not in the logic, for OWL is atemporal), and therewith one can distinguish descriptively between contiguous and scattered portions, and likewise with portionOf and scatteredPortionOf in the Stuff Ontology [17]. SUMO has piece as "arbitrary parts of Substances" and its super property part for its superclass Object; there is no measure of quantity associated with Substance. It is not much better in domain ontologies that typically seek modelling guidance from foundational and core ontologies. For

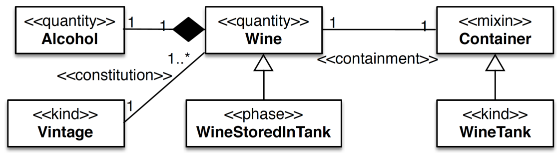

Fig. 1. Guizzardi's example for quantities [14].

instance, the Environment ontology uses the generic part_of relation from BFO. SNOMED CT's [27] Has active ingredient clearly has to do with a part-stuff of some medicine, but has no domain and range restrictions to enforce it.

A different angle is so-called pedigrees for traceability, notably for medicines, [28] that extends the provenance ontology PROV-O[1]. Currently, it focuses on the amounts and their properties and it states that there is a link between the steps, but not yet what type of relation that is.

2.2 Theoretical aspects on representing stuff relations

There are multiple papers on relations between stuffs. We discuss in detail only the two most comprehensive proposals on parts and portions for stuffs, as they supersede the others.

Guizzardi [14]'s proposal zooms in on quantities (of stuff) and their parts; an example is shown in Fig. 1. The example is clearly about the extensional level—particular amounts of stuff—though the description of the UML extension less so, it forces all quantities to be in a container, part-quantities are essential, and it is atemporal. The limitation of atemporality is that one cannot fully represent scattered portions, like the glass of wine tapped from the wine in the wine tank, which is further delimited in [14] by the constraint of self-connectedness. For traceability in the food processing chain to ensure food safety, however, this is important; e.g., that the contaminated milk in the bottle on the shelf in the shop is a portion of the batch of milk processed on day x in processing plant y. Conflating the extensional and intensional is tricky with the 1:1 multiplicity between a whole-stuff and a part-stuff. It is the case that for some specific amount of wine, there is one specific amount of alcohol as part of it, and that specific amount of alcohol is part of that specific amount of wine. However, there are more drinks that have alcohol, so if we were to add a class, say, Vodka and a 1:1 association to Alcohol, we have a problem: a same amount of alcohol must be part of both some wine and some vodka, but it cannot be. The underlying issue is that quantification over the relations is different for extensional and intensional parts of stuff, so conflating them will violate either one. Further, while subQuantityOf for particular amounts is indeed essential insofar as it concerns the identity of the amount, this may not be the case for universals; e.g., alcohol-free beer is perhaps still beer, decaf coffee still coffee. Finally, it forces a quantity to be in a container, which need not be the case (e.g., a lump of clay).

[1] https://www.w3.org/TR/prov-o/

Donnelly and Bittner [10] do use a temporal mereology for portions of stuff, remain at the extensional level (i.e., no assertions about types of stuff), and with the various summation relations, can differentiate between pure and mixed stuffs. A tricky issue is that they adopted some of Barnett's [4] misconceptions of kinds of stuff. Donnelly & Bittner illustrate "unstructured stuff" ("discrete stuffs" [4], "pure stuffs" [17]) with water. However, by that example, then their and Barnett's "structured stuffs"/"non discrete stuff" is not, which affects the applicability of the summation relations and the feasibility to 'lift' it up to the intensional level. For instance, their examples include "milk, crude oil, graphite, quartz, and wood", but milk and crude oil are homogeneous mixtures, graphite is carbon-only (unstructured pure stuff), quartz without any qualifier (like Amethyst) are just SiO_2 molecules and if water is unstructured, then so must quartz be. Quartz would be structured pure stuff in the Stuff Ontology [17], and therewith obtain the appropriate axioms. Wood is a solid heterogeneous mixture and has its own issues with portions: for a homogeneous mixture, that is easy to establish (freezing or boiling point, sortal weight etc.), but not so for heterogeneous mixtures, due to the compartmentalisation of the different kinds of stuffs that are part of the whole stuff. These issues are not addressed in the formalisation of portions-as-portions (of the same kind of stuff as the whole) and portions-as-parts (of a different kind of stuff as the whole).

Thus, overall, some theoretical advances have been made regarding relating stuff to other stuff, as well as their quantities, but it is incomplete regarding the type/instance issue, the temporal dimension, and relation overloading issues.

3 Preliminaries

Before relating stuffs, three preliminaries have to be outlined: the Stuff Ontology is reused for the intensional level; a brief recap of mereology is included to keep the paper self-contained; and some formalisation considerations are discussed.

The Ontology of Macroscopic Stuff The Stuff Ontology refines the notion of stuff beyond the mere distinction between pure and mixed stuff [4, 7, 10], yet in less detail than the philosophy of chemistry [8, 24]. Fig. 2 includes its four top-level classes: pure and mixed stuff, which is homogeneous or heterogeneous. This is further specialised with classes such as Solution, Suspension, and the Colloids[2], which are all defined classes as well. The same underlying principles have been used as proposed in the philosophy and chemistry literature, including: a granule (also called grain or basis type) of the stuff that is at one finer-grained level than the stuff itself; homogeneous versus heterogeneous matter; and the macroscopic sameness criterion for the least portion, which is the smallest portion that still exhibits the macroscopic properties of that kind of stuff [8, 4]. Because its aim was practical usefulness, it is represented in OWL 2 DL, extensively annotated, and available online at `http://www.meteck.org/stuff.html`.

[2] Colloids are homogeneous mixtures where one phase is evenly dispersed in another; e.g., whipped cream (air in gaseous phase dispersed in cream in liquid phase).

Parts and wholes As the relations between stuff concern parthood relations, we recap here briefly some important aspects of the various mereological theories, following [29]. Part p is a primitive relation, which is reflexive, antisymmetric, and transitive (Eqs. 1-3). Proper parthood, pp, is defined in terms of parthood (Eq. 4), and is irreflexive, asymmetric, and transitive (Eqs. 5-7):

$$\forall x(p(x,x)) \tag{1}$$
$$\forall x,y((p(x,y) \wedge p(y,x)) \rightarrow x = y) \tag{2}$$
$$\forall x,y,z((p(x,y) \wedge p(y,z)) \rightarrow p(x,z)) \tag{3}$$
$$\forall x,y(pp(x,y) \equiv p(x,y) \wedge \neg p(y,x)) \tag{4}$$
$$\forall x,y(pp(x,y) \rightarrow \neg pp(y,x)) \tag{5}$$
$$\forall x \neg(pp(x,x)) \tag{6}$$
$$\forall x,y,z((pp(x,y) \wedge pp(y,z)) \rightarrow pp(x,z)) \tag{7}$$

Because one needs to consider actual pieces and portions of stuff, i.e., the extensions of stuff universals, an extensional mereology may be of use, which looks at how to exhaustively define an object by its constituent parts, notwithstanding that this has its traps [10]. First, the theory Minimal Mereology (MM) has weak supplementation, saying that every proper part has to be supplemented by some other part (Eq. 8, where o is overlap), or phrased liberally: if a whole has a proper part, then there must be at least two different proper parts.

$$\forall x,y(pp(x,y) \rightarrow \exists z(p(z,y) \wedge \neg o(z,x))) \tag{8}$$

The alternative is strong supplementation in Extensional Mereology (EM): if an object fails to include another among its parts, then there must be a 'remainder'. EM is highly problematic, especially for colloids, because EM allows non-atomic objects with the same proper parts to be identical, yet sameness of parts tends not to be enough for identity: an amount of air plus an amount of liquid cream one pours into the bowl is surely not the same as whipped cream that one can make of it, yet they have the same parts, or oil and egg yolk versus mayonnaise, and so on. So, EM is a bad idea for stuffs, but MM may be of use.

The total or universal whole is the totality of the quantity of some stuff that exists at some point in time, which is not of interest. For instance, my lemonade I made at time t in Cape Town and your lemonade you made at time t in Bologna are independent and thus certainly not related through parthood. The opposite is either the 'atom'—smallest indivisible part that has no parts—or 'atomless gunk', i.e., infinite divisibility. While infinite divisibility may appear appealing for stuffs, there is, in fact, a relative notion of 'atom': the least portion.

On formalising it We have seen that 'pushing' everything there is to say about stuff universals and their amounts into one level—say, first order predicate logic—may be problematic, because things have to be said about stuffs themselves, like that a mixture is composed of at least two different kinds of stuff. This requires quantification over predicates, hence a second order logic.

With stuffs being different from objects, one can use a many-sorted logic, so as to quantify over stuffs and over objects [4, 10]. However, if one does not want to assert something about its constituent parts, alike a mass-quantity with no declared internal structure [12], then a many-sorted logic is not needed. Here, we delimit the scope to just relations between stuffs, rather than summations, so quantification is over stuffs and their particular amounts only.

Most accounts of portions are either atemporal or are temporal in name only, for it is easier to implement and practically use it. If one wants to be as precise as possible, one cannot avoid the temporal modality at the extensional level, alike in [10]. This lets one distinguish between a portion like the 'upper half of the wine in the tank' and 'the glass of wine just tapped from it' as well as between 'piece' and 'portion': a piece always and only *was* part of the whole, whereas a portion *is or was* part of the whole amount of stuff.

Thus, we end up with a second order logic, where at least the 'first order fragment' of it is temporal. Recalling some basic notation and features of second order logic, we can quantify over predicates, such as $\exists P(P(x) \land P(y) \land x \neq y)$ meaning 'there exists a property that two distinct entities share in common', and use them as variables; e.g., with, say, $Colour$ being a property, then $\neg\exists x \forall P(Colour(P) \rightarrow P(x))$ is the formalisation of 'no object has every colour'. In addition, we will use the usual shorthand notation of $\exists^{\theta x}$ with x an integer > 1 for cardinality constraints beyond simple mandatory/existential quantification, and θ being a comparison operator $\leq$, $=$, or $\geq$. Finally, the temporal modality. A first order LTL with the until and since operators suffices, or just ternaries. We use the latter, using a linear flow of time $\mathcal{T} = \langle \mathcal{T}_p, < \rangle$ where $\mathcal{T}_p$ is a set of time points (indicated with t) and $<$ is a binary precedence relation on $\mathcal{T}_p$ that is assumed to be isomorphic to $\langle \mathbb{Z}, < \rangle$.

4 Relating Stuff

An informal, high-level overview of the various entities and relations is shown in Fig. 2. It is drawn in EER diagram notation so as to avoid the complicating factor of UML's aggregation association, finding meaningful names for the association ends was distracting, and it may make it easier to morph it into a temporal ER, such as ER_{VT} [1], and convert it all to a temporal relational database if one so prefers. Note that inheritance of properties applies, so, among others, also Homogeneous Mixed Stuff has an instantiation relation (because Stuff has) and Portions and Pieces also have a measure of their quantity (because Amount of Stuff has). Those quantities (10ml etc.) have their own representation system, which is summarised into a Quantity extension. Regarding quantities, we concur with other ontologies that quantity kinds are things in their own right, i.e., the "quantity as a class" commitment (weight, length etc.) [13, 26] rather than as a property/attribute (hasLength etc.) or equating portion and quantity [14], for the identity of a quantity is independent of the entity that 'has' that quantity. For instance, one may rather have a quantity of 1 kg of gold as a present than 1 kg of soil. Put differently, quantities are reusable entities across amounts of matter.

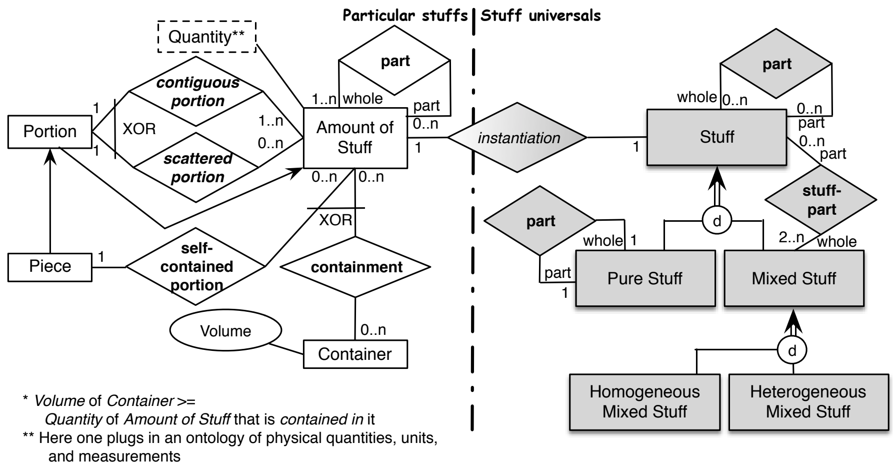

Fig. 2. Stuff relations, depicted informally (and incomplete) using EER Diagram notation, with part-whole relations in bold face and the universals-side in grey.

Which ontology is then chosen for the quantities, units, and measurements does not matter much.

The model is illustrated in the following example.

Example 1 As example, let us take 'a slice of cake': it is an instance of Piece, as it is a self-contained Amount of Stuff, and it is thus also a Portion. Given that it was cut off from some quantity of cake, it is a scattered portion of cake that is also a Amount of Stuff. The slice (and the cake) as Amount of Stuff is a kind of (instantiation of) a Homogeneous Mixed Stuff. Being a Homogeneous Mixed Stuff, it must have at least two stuff-parts (related through stuff-part), which are Flour, Sugar, Butter, Egg and Vanilla essence, where, e.g., Butter is an Emulsion, which is a homogeneous mixed stuff. A Quantity of 250g of Butter went in the particular cake the slice came from, which is a stuff-part of the Amount of Stuff that amounts to the whole amount of cake. That amount of butter was in a containment relation to a buttercup that is a Container with a Volume of 500g. Finally, the slice having a left and right contiguous portion, I break it in half and share it with my neighbour. ♢

This example is still incomplete: how much butter did I indulge in when eating my portion of the slice of cake? The whole quantity of cake had as part a quantity of 250g butter. Let's say the slice is 1/10th of the cake, so, by cake being homogeneous mixed stuff, the slice will also have 1/10th of the butter of the whole cake, or 25g. Splitting it into 2 portions, 12.5g of butter was part of the portion of cake I ate. All this can be formally represented with the model in Fig, 2, provided it has the appropriate temporal extensions, which we will address in the remainder of this section.

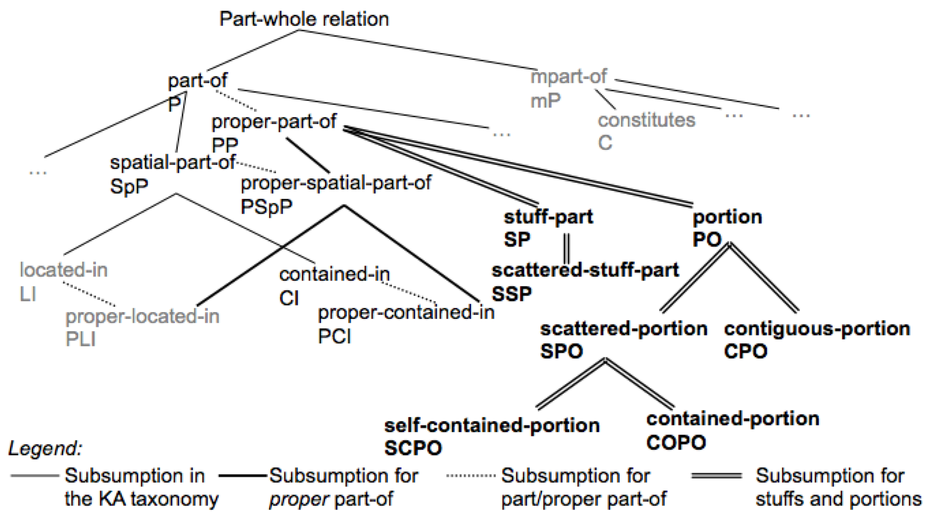

Fig. 3. Section of the basic taxonomy of part-whole relations of Keet and Artale [18] (less and irrelevant sections in grey or suppressed), extended with the stuff relations and their position in the hierarchy.

4.1 Relating portions

Concerning all those part and portion relations in the example and in Fig. 2, let us start with the axioms of Minimal Mereology for parthood relations part, p, and proper part, pp, which are subsumed by some generic top-relation, pw (part-whole), so we obtain the hierarchy of relations as depicted in Fig. 3. Linking this extended hierarchy to Fig. 2, one can see on the right-hand side of the figure the generic part p with its sub-relationships, and in particular stuff-parts, sp for short, and portions, po. The stuff-part will be discussed in Section 4.3. Portions, together with the hierarchy, induces its definition, which is formulated as:

$$\forall \mathsf{x}, \mathsf{y} \exists^{=1} \mathsf{S}(\mathsf{po}(\mathsf{x}, \mathsf{y}) \leftrightarrow \mathsf{pp}(\mathsf{x}, \mathsf{y}) \wedge \mathsf{S}(\mathsf{x}) \wedge \mathsf{S}(\mathsf{y}) \wedge \mathsf{Stuff}(\mathsf{S})) \quad (9)$$

That is, portions are of the same type of stuff as the whole.

While portion is atemporal, the time dimension has to be introduced to distinguish between scattered (spo) and contiguous (cpo) portions, for the former *was* a (contiguous) part of the whole portion, whereas the latter *is* a part of the whole portion. The latter being a contiguous part, it then also means that contiguous portion is properly contained in the whole portion, whereas the scattered portion is not. To this end, we take the containment relation from [18], make it proper containment (pci), which is included here as (Eq. 10), where R is DOLCE's region, ED is DOLCE's endurant [20], and has_3D a shorthand for DOLCE's qualities and qualia to denote something has a physical region. Contiguous portion can then be temporally defined (Eq. 11), so $cpo(x, y, t)$ then reads as "x is a contiguous portion of y at time t". This is in contrast to scattered portion (Eq. 12) that states, informally, that x is a scattered portion of y

at time t if it was at some time t'—which is before time t—a contiguous portion of y and at t it is not a contiguous portion of y.

$$\forall \mathsf{x}, \mathsf{y}(\mathsf{pci}(\mathsf{x}, \mathsf{y}) \rightarrow \mathsf{pp}(\mathsf{x}, \mathsf{y}) \wedge \mathsf{R}(\mathsf{x}) \wedge \mathsf{R}(\mathsf{y}) \wedge \exists \mathsf{z}, \mathsf{w}(\mathsf{has\_3D}(\mathsf{z}, \mathsf{x}) \wedge \mathsf{has\_3D}(\mathsf{w}, \mathsf{y}) \wedge \mathsf{ED}(\mathsf{x}) \wedge \mathsf{ED}(\mathsf{y}))) \tag{10}$$

$$\forall \mathsf{x}, \mathsf{y} \exists \mathsf{t}(\mathsf{cpo}(\mathsf{x}, \mathsf{y}, \mathsf{t}) \leftrightarrow \mathsf{po}(\mathsf{x}, \mathsf{y}, \mathsf{t}) \wedge \mathsf{pci}(\mathsf{x}, \mathsf{y}, \mathsf{t})) \tag{11}$$

$$\forall \mathsf{x}, \mathsf{y} \exists \mathsf{t}, \mathsf{t}'(\mathsf{spo}(\mathsf{x}, \mathsf{y}, \mathsf{t}) \leftrightarrow \mathsf{cpo}(\mathsf{x}, \mathsf{y}, \mathsf{t}') \wedge \neg \mathsf{cpo}(\mathsf{x}, \mathsf{y}, \mathsf{t}) \wedge \mathsf{t}' < \mathsf{t}) \tag{12}$$

The last two special relations distinguish between relating self-contained portions that are described with designated pieces like lumps and drops and slices, and relating portions that are housed in a container[3]. The ontological investigation into the entity 'container' is not the scope here, and we appeal to the reader's common sense understanding of it: an object with a cavity such that one can put something in that cavity; e.g., a bottle or a glass that can be filled with an amount of wine, a silo or a bag that store an amount of soy beans. So, if we have a self-contained portion then it is a piece that was part of some amount of stuff (which may be a portion) (Eq. 13) and if we have a contained portion, then it is scattered in a container C from the whole amount (e.g., the glass of wine taken from the wine in the wine bottle) (Eq. 14). For the self-contained portion, one cannot say that it is never in a container, for one could have, say, a lump of clay that is put in a sealed container for later use. Therefore, we use only the weak statement that a piece is not necessarily (the "$\neg\Box$") in a container:

$$\forall \mathsf{x}, \mathsf{y} \exists \mathsf{t}, \mathsf{t}'(\mathsf{scpo}(\mathsf{x}, \mathsf{y}, \mathsf{t}) \rightarrow \mathsf{spo}(\mathsf{x}, \mathsf{y}, \mathsf{t}) \wedge \neg\Box \mathsf{z}(\mathsf{pci}(\mathsf{x}, \mathsf{z}) \wedge \mathsf{C}(\mathsf{z}))) \tag{13}$$

$$\forall \mathsf{x}, \mathsf{y} \exists \mathsf{t}, \mathsf{t}'(\mathsf{copo}(\mathsf{x}, \mathsf{y}, \mathsf{t}) \rightarrow \mathsf{spo}(\mathsf{x}, \mathsf{y}, \mathsf{t}) \wedge \Box \mathsf{z}(\mathsf{pci}(\mathsf{x}, \mathsf{z}) \wedge \mathsf{C}(\mathsf{z}))) \tag{14}$$

This concludes the specification of the basic set of relations for portions.

4.2 Portions and pieces

The previous section alluded to one's intuition regarding portions and pieces. While related works do talk about portions, we could not find a formal definition in [7, 10, 14, 17]. Here, we make a first step in that direction, taking the notion of portions from philosophy, in particular the afore-mentioned macroscopic sameness, which implies that a portion of some amount of stuff is of the same type of stuff as the whole amount (Eq. 15), and the least portion would then amount to the equivalent of *Atom*, but then for stuffs. With *Atom* defined as (Eq. 16) (from [29]), the 'least portion type of atom' (LP) then follows from both (Eq. 17). These can have their temporal counterparts (by adding t, i.e., $Portion(x, t)$, $po(x, y, t)$, and $LP(x, t)$).

$$\forall \mathsf{x} \exists^{=1} \mathsf{S}(\mathsf{Portion}(\mathsf{x}) \leftrightarrow \mathsf{po}(\mathsf{x}, \mathsf{y}) \wedge \mathsf{S}(\mathsf{x}) \wedge \mathsf{S}(\mathsf{y}) \wedge \mathsf{Stuff}(\mathsf{S})) \tag{15}$$

$$\forall \mathsf{x}(\mathsf{Atom}(\mathsf{x}) \leftrightarrow \neg \exists \mathsf{pp}(\mathsf{y}, \mathsf{x})) \tag{16}$$

$$\forall \mathsf{x} \exists^{=1}(\mathsf{LP}(\mathsf{x}) \leftrightarrow \mathsf{Portion}(\mathsf{x}) \wedge \neg \exists \mathsf{po}(\mathsf{y}, \mathsf{x}) \wedge \mathsf{S}(\mathsf{x}) \wedge \mathsf{S}(\mathsf{y}) \wedge \mathsf{Stuff}(\mathsf{S})) \tag{17}$$

[3] pieces and portions as objects do differ, which we will discuss in the next subsection

Pieces—e.g., a lump of clay, a chip of wood, a drop of blood—are self-contained portions, i.e., they are neither currently contained in the whole amount nor are they necessarily in a separate container:

$$\forall x(\mathsf{Piece}(x,t) \leftrightarrow \mathsf{scpo}(x,y,t)) \tag{18}$$

4.3 Stuff parts

Stuff part, also called ingredient, was already specified in [17], where at the type level, a pure stuff has as ingredient stuff the same stuff it is, whereas mixed stuffs have at least two other kinds of stuff as part. The issues to examine are whether stuff parts are proper part or just part, temporality, and essentialism.

For pure stuffs as universals, the parthood relation that holds can be considered reflexive, because the domain and range are of the same stuff type, and likewise it is antisymmetric (and obviously transitive); thus, the regular parthood relation p holds. For pure stuffs at the particular level (amounts of pure stuff, like a glass of water), then the parts are of the same type, but it is obviously a smaller amount, so then we obtain proper parthood. One optionally could change the names of part and proper part to other ones to make sure that those two relations only have stuffs as domain and range. However, there is nothing of interest to assert about pure stuffs in that regard as it states the obvious already when it is asserted as being a kind of a pure stuff, like 'gold has as part gold and only gold'. A possible pitfall may be that then on paper there may be confusion, but this ought not to occur in praxis provided one has the taxonomy of part-whole relations imported or DOLCE: if one of the two participants is an object and the other some stuff, then it is a constitution relation by its definition, which would alert the modeller something is amiss, which OntoPartS-2 already does [19].

For mixed stuffs, we end up with proper part both at the universal and particular levels. Because one can say 'interesting' things about mixtures, it does make sense to introduce a separate named relation as a type of proper parthood. For instance, then one can define the part-stuffs a type of mixture is made up of, infer the possible product based on its stuff-ingredients, and play with substitutes in a recipe for case-based reasoning (e.g., soy milk instead of cow's milk, speckled beans instead of kidney beans, etc.); i.e., it serves in automated reasoning. Therefore, the stuff-part, *sp* and scattered-stuffpart, *ssp*, relations were added in Fig. 3, which are defined as:

$$\forall x,y \exists S,S'(\mathsf{sp}(x,y) \leftrightarrow \mathsf{pp}(x,y) \wedge S(x) \wedge S'(y) \wedge \mathsf{Stuff}(S) \wedge \mathsf{Stuff}(S') \wedge S \neq S') \tag{19}$$

$$\forall x,y \exists S,S'(\mathsf{ssp}(x,y,t) \leftrightarrow \mathsf{pp}(x,y,t') \wedge S(x) \wedge S'(y) \wedge \mathsf{Stuff}(S) \wedge \mathsf{Stuff}(S') \wedge S \neq S' \wedge t' < t) \tag{20}$$

The *sp* refines the relations hasSubStuff of [17] and sub-quantity-of of [18] into a full definition, as both had only domain and range axioms. It is different from Guizzardi's subQuantityOf [14], in that there is no strong supplementation (recall

Section 2), it is for designated stuffs and amounts thereof (cf. quantities), and it is not essential. Essentialism at the universal level may apply on a case-by-case basis; e.g., alcohol may be considered to be an essential part of vodka, but not of beer. Whether it is essential at the level of particulars in general, is not entirely clear, unless one defines and identifies a particular amount of stuff as the mereological sum of its quantities (for complications with that, see [10]) and excludes some convoluted corner cases (e.g., distilling the alcohol and putting it back in). Either way, if one assumes that both a portion and a part-stuff are essential to some amount of stuff, then it can be added easily with a temporal logic that has $\top$, $\bot$ and the $\mathcal{U}$ntil and $\mathcal{S}$ince operators [2].

This concludes the sets of relations that relate stuffs to other stuffs.

5 Applying implementation trade-offs

Given the theoretically optimal formal characterisation of parts and portions of stuff presented in the previous section, the next step is to assess how this can be implemented practically with the state of the art technologies. The options are:

1. Use a system that supports a second order language and reasoner and implement it as formalised; e.g., with the *He*terogeneous *t*ool *s*et Hets [23].
2. Squeeze into OWL 2 DL what can be done:
   - Get rid of the second order axioms; either:
     (a) Drop the second order aspects altogether (simply ignore);
     (b) Push that to first order and the first order aspects to instance-level;
     (c) Create two branches in the TBox for the universals and for the particulars, alike in GFO [15].
   - Remove all modal aspects, i.e., the necessity and the temporality, and indicate its intention in the name of the object property only.
3. Use a temporally extended OWL:
   - Second order issue, and options, as above;
   - Choose a temporal trade-off, for the need for temporalising relations already results in an undecidable language [1]; e.g., use concrete domains as workaround, as in tOWL that extends $\mathcal{SHIN}(D)$ [21], or disallow temporal constructors on the right-hand-side of inclusions, as in TQL that extends OWL 2 QL [3].
4. Morph it into a relational database or integrate it with RDF as a Linked Data application such as VacSeen [6].

Option 1 is good for toy examples to verify and validate it with a few examples, but never will be for industry-grade implementations due to the high undecidedability of second order logic. The other three options list several viable usability trade-offs that favour computation over expressiveness, where the ultimate decision lies with the requirements of the use case. Option 2 permits some automated reasoning, but not fully the tracing of some amount of stuff over time. The time dimension is favoured in Option 3, but this is at the cost of, mainly, transitivity and/or qualified cardinality constraints so that one cannot fully represent mixed stuffs, pure stuffs, (solid) heterogeneous mixtures, and colloids, and therewith lose the ability to automatically classify a stuff into its right kind. In addition, TQL and tOWL are preliminary results and are not at the same level of robustness as the technologies of Option 2. Both options, for being in OWL, easily can import the Ontology of units of Measure (OM) that is also represented in OWL and developed by domain experts in food [26]. Finally, one could focus even more on implementation with Option 4, which is good for industry-level applications, but some unenforceable assumptions have to be made regarding its correctness and comprehensiveness and any automated reasoning is limited to what can be done with queries. Therefore, at present, the most straightforward choice seems to be Option 2-c by refining the Stuff Ontology [17] and importing the OM [26], with as future work the data-oriented Option 4 with TQL.

Integrating quantities. OM is 5 MB and is merged with bibliographic information and FOAF, and including units that are irrelevant to stuff, such as the vase end life of flowers, acceleration, and micro degree Celcius, but also specific ones relevant for food stuffs, such as the lactose_mass_fraction (as stuff-part of, e.g., milk powder). Other models for quantities are also not ideal; e.g. UCUM[4] and EngMath [13] are not available in OWL and QUDT[5] has similar excess baggage as the OM. Therefore, a module was created manually: we reduced the 5MB OM from 25253 axioms (1148 classes, 25 object properties, and 2622 individuals) to 1472 axioms (131 classes, 25 object properties, and 104 individuals) in the 216KB OMmini module. This module was imported into the extended Stuff Ontology, and bridge axioms added. These bridge axioms include alignments, such as $\mathsf{om{:}phenomenon} \equiv \mathsf{stuff{:}PhysicalEndurant}$, $\mathsf{om{:}`unit\ of\ measure'} \sqsubseteq \mathsf{Abstract}$, and $\mathsf{om{:}quantity} \sqsubseteq \mathsf{Region}$, thus also commencing with aligning OM to a foundational ontology—which was still the intention by [26]—as $\mathsf{stuff{:}PhysicalEndurant} \equiv \mathsf{dolce{:}PhysicalEndurant}$, and likewise for Abstract and Region. Further, the formal counterpart of the dashed 'Quantity**' and 'Container' entity types from Fig. 2 were added; among others:

$$\mathsf{stuff{:}AmountOfStuff} \sqsubseteq\ = 1\, \mathsf{om{:}quantity.om{:}quantity} \tag{21}$$

$$\mathsf{Container} \sqsubseteq \forall \mathsf{containedIn}^{-}.(\mathsf{PhysicalObject} \sqcup \mathsf{AmountOfStuff}) \tag{22}$$

$$\mathsf{Portion} \sqsubseteq \exists \mathsf{portionOf.AmountOfStuff} \tag{23}$$

$$\mathsf{Piece} \sqsubseteq \exists \mathsf{isSelfContainedScatteredPortionOf.AmountOfStuff} \tag{24}$$

$$\mathsf{AmountOfMatter} \sqsubseteq \exists \mathsf{instantiation.Stuff} \tag{25}$$

where Eq. 21 then further avails of the quantities from OM, and therewith also AmountOfMatter's subclass Portion and its subclass Piece, and instantiation in Eq. 25 is typed with AmountOfMatter and Stuff, addressing the two-layer issue in the same way as GFO [15]. This resulted in a combined ontology of 1831 axioms (logical axiom count 718), 193 classes, 57 object properties, and 104 individuals) which is in $\mathcal{SROIQ}(D)$, i.e., OWL 2 DL.

[4] `http://www.unitsofmeasure.org/trac`

[5] `http://qudt.org/`

Automated reasoning. For traceability, transitivity of portionOf and property chains yield the most useful results. Take, e.g., the following property chains:

$$\mathsf{scatteredPortionOf} \circ \mathsf{portionOf} \sqsubseteq \mathsf{scatteredPortionOf} \quad (26)$$

$$\mathsf{stuffPart} \circ \mathsf{contiguousPortionOf} \circ \mathsf{SelfContainedScatteredPortionOf} \sqsubseteq \mathsf{scatteredStuffPartOf} \quad (27)$$

$$\mathsf{scatteredPortionOf} \circ \mathsf{scatteredPortionOf} \circ \mathsf{scatteredPortionOf} \sqsubseteq \mathsf{scatteredPortionOf} \quad (28)$$

The chain in Eq. 26 enables one to infer that a scattered portion—say, my glass of wine d.d. 9-7-'16—of a portion (bottle #1234 of organic Pinotage wine) of an amount of matter (cask #3 with wine from wine farm X of Stellar Winery from the 2015 harvest) is a scattered portion of that amount of matter (that cask). Reconsidering the slice of cake from Example 1, the property chain in Eq. 27 can be used to infer that that 12.5g of butter is a scatteredStuffPartOf the cake: the 12.5g of butter is a stuffPart of the left-hand side contiguousPortionOf of the slice of cake that, in turn, is a SelfContainedScatteredPortionOf the cake. This same chain in Eq. 27 also can be applied to other use cases; e.g., the amount of alcohol I would consume drinking half a glass of wine is a scatteredStuffPartOf the original amount of wine in the wine bottle. For the pharmaceutical supply chain in [28], we obtain that a portion (on a 'pallet') of the quantity of medicine produced by the manufacturer goes to the warehouse, of which a portion (in a 'case') goes to the distribution centre, of which a portion (as 'items') ends up on the dispensing shelf. Then tracing the customer's portion of medicine can be inferred with Eq. 28. Thus, then one can *infer* the chain of portions in the supply chains, and therewith start tracing it automatically from one amount at home back to the manufacturer (and all the way back to the farm, in case of food).

Note that, because the ontology also has scatteredPortionOf $\sqsubseteq$ portionOf, this combination would result in a cycle and therewith not be a 'regular' RBox, which is not allowed in OWL 2 DL. Making scatteredPortionOf and portionOf siblings does permit the chain. Because DL reasoners do not do much with the hierarchy in the RBox and the semantic differences between these properties—temporality—cannot be represented in OWL anyway, they are made siblings, for the inferences with the property chains are deemed more important. Likewise, due to the declaration of the chains, scatteredStuffPartOf's inverse hasScatterPartStuff is made a sibling of hasPartStuff because the latter was needed more in cardinality constraints for mixtures.

6 Discussion

To the best of our knowledge, this is the first attempt to systematically disentangle the parts and portions, having identified 7 different interactions between stuffs, and named them so for clarity. While the implementation is not a perfect match with the theory presented in Section 4, it still has several advantages of the other proposals to date. Notably, 1) there is a clear distinction between the extensional and intensional level; 2) it distinguishes between the (non-repeatable) amounts of stuff and the repeatable quantities; and 3) both are present in the same ontology and immediately usable for ontology development thanks to substantially extending the Stuff Ontology.

A shortcoming is the omission of the temporal dimension, which does not lend itself well for scalable automated reasoning. This is mitigated to some extent by availing of property chains, so that one still can trace a portion to the original amount. This is a limited solution, indeed, but preferable over no such inferences. It might be possible to have it 'both ways' with the Distributed Ontology Language [22]—currently being standardised with OMG—and its technological infrastructure, which breaks up the whole theory into modules based on expressiveness. Then one could have slow automated reasoning where acceptable and fast reasoning where needed. This is an avenue of future work.

The proper treatment of the stuff relations now opens up the opportunities for deployment in the intended use case with food processing, and, for it being a core ontology, also in other domains, such as stuffs in medicine (e.g., pills and vaccines [6, 28]) and engineering (e.g., the use cases in [13, 16]).

7 Conclusions

Seven relations for portions, pieces, and stuff-parts were defined and formalised in the logic it required, availing both of the temporal dimension and second order. The orchestration with stuffs and amounts of matter make a clear distinction between the extensional and intensional levels (amounts and stuff kinds) and between amount of stuff and its quantity. The implementable components were added to the Stuff Ontology core ontology and a module of the Ontology of units of Measure for the quantities was imported. Some useful automated reasoning was shown to be still possible thanks to property chains.

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