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An Applied Calculus for Spatial Accessibility Reasoning

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Abstract: Recent attempts to perform formal knowledge representation and reasoning in cell biology have presented new challenges to spatial reasoning. In this paper we formalize two distinct notions of containment that were so motivated and which are relevant to reasoning about physical systems, a notion of being inside and a notion of being restricted. We develop a formal vocabulary for purposes of representing and reasoning about restrictive containment and formalize three kinds of accessibility that are each salient to attempts to reason about the possibility of interaction between pairs of objects in a system. We also consider the relation of this calculus to the well known Region Connection Calculus and related calculi for reasoning about containment. Finally, we discuss methods for implementing in a context of uncertainty, within a planning system and discuss an application to some simple representation and reasoning tasks in virology.

Keywords: qualitative spatial reasoning, molecular biology, spatial accessibility, Bayesian reasoning
Category: I.2.4

1 Introduction

In this paper we define a calculus for representing and reasoning about accessibility between objects in a system. The formalism is intended to be compatible with and an extension to existing qualitative spatial reasoning methods. We also discuss methods for simplifying reasoning and implementations of the calculus within a Bayesian reasoning system. It is motivated by a desire to extend work that has been done to represent central notions in biological structure [Cohn 01] and biological process simulation [Cui *et al* 92]. However, we anticipate that the formalism is sufficiently general to be applicable to any system in which containment is relevant, *e.g.*, computer network security, building security analysis, etc.

In the first section below, Section 2, we briefly discuss the knowledge representation issues that motivated this effort. In Section 3 we present a simple set of axioms for representing the relatively generic spatial relations required to define restrictive containment and accessibility. We compare this scaled-back spatial representation with the Region Connection Calculus (RCC-8) [Randell *et al* 92] and [Cohn *et al* 97] in Section 3.1. In Section 4 we extend the initial formalism for purposes of representation and reasoning about the restrictive containment and accessibility. We conclude in Section 5 with detailed examples that illustrate how the formalism could be implemented in a wide range of reasoning systems and contexts.

We assume a second order logic or a many-sorted first order universe containing physical objects partitioned into non-containers and potential containers, objects that could contain other objects. However, we do not separate out these sorts here, quantifying instead over all objects in our domain. The logic required for this representation becomes second-order because we quantify over first-order relations in two supplementary definitions that we introduce for type-level reasoning, see Section 4.3.

In the specification we reserve italicized lowercase variables from the end of the alphabet, *v,w,x,y,z*, to range over the physical objects in a physical system and italicized uppercase letters from the middle of the alphabet, *P,Q,R*, act as variables ranging over the first-order relations. We use *a,b,c,d* as constants denoting specific physical objects. We denote numbered axioms with an 'A', *e.g.*, (A2) is the second axiom, definitions with a D and provable propositions with a P.

2 Containment

Before we introduce containment vocabulary, it is useful to consider two notions of containment that are relevant to reasoning about physical systems. The first is a strictly spatial notion concerning the location of one object with respect to the boundaries of another. Something contains something else, depending on the context, if and only if the object is inside, located within the convex hull of, encircled by, wrapped by, or "located within" the second object. In this sense of containment, a car contains passengers, playgrounds contain children and a stew contains potatoes, etc. Let us call this the locational sense of containment. However, there is a second notion of containment corresponding to the notion that a prison contains a prisoner in a way that it does not contain a prison guard. This second sense of containment involves being constrained from exiting the object which may also contain it in a locational sense, *i.e.*, the second sense has to do with accessibility. Let us refer to this as the restrictive sense of containment. The restrictive sense of containment should be of interest in attempts to model dynamic physical systems. Useful models of such systems may require the ability to represent and reason about the accessibility of objects or spaces within the system.

In the rest of this paper, unless otherwise noted, we use 'containment' in this specialized "restrictive" sense. When we intend the locational sense of containment we simply use 'inside' or, if absolutely necessary, refer to "locational containment" to disambiguate from the restrictive notion of "contains".

Before launching into the formalization, it is useful to briefly consider the representational needs that motivate this effort. It is noteworthy that much useful work has been done in the area of qualitative spatial reasoning and topology for purposes of reasoning about the ability of the movement of objects in an environment. As noted in [Bennett *et al* 2000]:

> The fundamental problems of kinematics are of the forms: can a rigid body move between two locations within a confining environment and, if so, what is a possible path between the two locations?

This describes the problem with which we concern ourselves here. Existing approaches have done important work in giving a theory of kinematics in purely qualitative terms. In particular, [Bennett *et al* 2000] give a highly detailed qualitative calculus for representing and reasoning about the constraints on rigid bodies in a system and the extent to which the relative sizes and proximity of the objects in the system prevent or allow movement of such rigid bodies. The work in [Bennett *et al* 2000] generalizes and builds on earlier related efforts including [Schwartz *et al* 1983] [Davis 87], [Davis 88] and [Mukerjee *et al* 95]. In this paper we attempt to characterize the different kinds of accessibility that can exist between pairs of objects. Determining whether some of the relations we define below hold between a pair of objects may involve the implementation of methods and formalisms specified in the aforementioned articles. (However, below we discuss how cellular biology provides example of situations not easily analyzed in these terms.) We also focus on how one might use knowledge of the accessibility between pairs of objects to reason about cross system accessibility, *e.g.*, whether given the set of objects between *a* and *b* in some physical system and the accessibility relations that hold between any given pair of objects in our domain of interest, how do we efficiently determine whether and to what extent *a* is accessible to *b*?

Hence, we are less concerned with relative sizes of objects and more concerned with developing a formal system for representing the relative constraints that two objects can pose to each other, not necessarily on the basis of size and without necessarily assuming that pairs of objects maintain rigidity. Cell biology provides interesting examples such as cases of diffusion across lipid bilayers. In a standard cell biology textbook we encounter claims that small nonpolar molecules, unlike charged molecules, such as molecular oxygen and carbon dioxide, readily diffuse across a lipid bilayer.

> The smaller the molecule and, more importantly, the fewer its favorable interactions with water (that is, the less polar it is), the more rapidly the molecule diffuses across the bilayer. [Alberts 98]

And

> … Lipid bilayers are highly impermeable to all ions and charged molecules, no matter how small. [Alberts 98]

These examples underscore some important facts about containment. First, whether or not an object restrictively contains another object is not solely a function of object size or easily characterized topological features. Hence, it is not possible to reason about containment solely in terms of the size of the objects and the size of the pores in the potential containers. An object's ability to exit another object may be based on its size or features of the contained object that have little to do with size-related or topological features of the container. Note, for instance, that an mRNA molecule in a eucaryotic cell is able to leave the cell after it has undergone capping and polyadenylation. These processes do not decrease the size of the molecule but they alter its stability and ability to pass out of the nucleus intact. A simpler example of how changes unrelated to "pore" size in a container can change its containment status is unlocking the door to a prison cell. The point is that state descriptions in a qualitative reasoning system will often have to pay explicit attention to issues of containment and permeability in any given state description. Process descriptions will similarly require consideration of how processes affect containment and permeability. It would be difficult to reduce these properties to the spatial properties typically considered in qualitative spatial reasoning and kinematics. Hence, in some applications the properties discussed below may simply be applied as primitive relations, *i.e.*, properties not easily subjected to further analysis, while in other situations it may be possible to use extant methods and reasoning calculi, such as those in [Randell *et al* 00], to determine whether or not the properties do or do not apply between a pair of objects.

3 Basic Spatial Relations

A prerequisite for restrictive containment is that the contained object be in the appropriate spatial relationship with potential container, *i.e.*, that the contained object be inside the potential container. The *inside* relation denotes the relationship of locational containment and as such is quite general by design. For example, we do not use mereological notions to clarify its intended meaning. Just as we allude to different senses of locational containment when we say that a "building contains people" as compared to when we say that the "salad contains carrots" or especially when we say things like "the firewall contains the entire network", we want to avoid imposing a very particular spatial implementation on the notion of *inside* as we develop it below.

The *inside* relation is given as a primitive of the system. *inside* is an irreflexive (A1) asymmetric (A2) and transitive (A3) relation as specified in 1-3 below:

(A1) $\forall x[\neg inside(x,x)]$
(A2) $\forall x \forall y[inside(x,y) \rightarrow \neg inside(y,x)]$
(A3) $\forall x \forall y \forall z[[inside(x,y) \wedge inside(y,z)] \rightarrow inside(x,z)]$

The second primitive relation is the *outside* relation. A good comparison point here is the "OUTSIDE" relation presented in [Randell *et al* 92]. In order to keep our vocabulary generally applicable we leave our definition more general but it should not be inconsistent with the more specific "OUTSIDE" definition. We discuss this further below. We intend that *outside* apply to most situations in which neither of two distinct objects bear the *inside* relation to the other, but see *overlaps* below. The *outside* relation is irreflexive, above, and symmetric. Also, *outside(x,y)* is inconsistent with *inside(x,y)*, *i.e.*, *inside* and *outside* cannot simultaneously hold of the same pair of objects.

(A4) $\forall x[\neg outside(x,x)]$
(A5) $\forall x \forall y[outside(x,y) \rightarrow outside(y,x)]$
(A6) $\forall x \forall y[inside(x,y) \rightarrow \neg outside(x,y)]$

For completeness sake, we introduce three other basic spatial relations as well: *overlaps*, *equals*, and $inside^{-1}$. *overlaps* is irreflexive (A6), symmetric (A7) and neither transitive nor antitransitive. Also,

(A7) $\forall x[\neg overlaps(x,x)]$
(A8) $\forall x \forall y [overlaps(x,y) \rightarrow overlaps(y,x)]$

(A9) $\forall x \forall y[overlaps(x,y) \rightarrow [\neg inside(y,x) \wedge \neg outside(y,x)]]$

Typically, in a RCC-8 implementation of such vocabulary, a necessary condition for the *overlaps* relation holding of two distinct objects is that some proper part of one of the object be found within the region defined by the convex hull of the other. *equals* is the equality relationship and is, of course, reflexive, symmetric and transitive.

(A10) $\forall x[equals(x,x)]$
(A11) $\forall x \forall y[equals(x,y) \rightarrow equals(y,x)]$
(A12) $\forall x \forall y \forall z[[equals(x,y) \wedge equals(y,z)] \rightarrow equals(x,z)]$
(A13) $\forall x \forall y[equals(x,y) \rightarrow [\neg overlaps(x,y) \wedge \neg inside(x,y) \wedge \neg outside(x,y)]]$

We introduce the relationship of inverse insideness, $inside^{-1}$, so as to round out the set of basic relations. It can be defined, however, in terms of the *inside* relation.

(D1) $inside^{-1}(x,y) \equiv_{def} inside(y,x)$
(A14) $\forall x \forall y[inside^{-1}(x,y) \rightarrow [\neg overlaps(x,y) \wedge \neg equals(x,y) \wedge \neg outside(x,y)]]$
(D2) $atLeastPartiallyInside(x,y) \equiv_{def} [inside(x,y) \vee overlaps(x,y)]$

From (D1) and (A1-A3) it follows that $inside^{-1}$ is irreflexive, asymmetric and transitive. The result is a set of relations, {*inside*, $inside^{-1}$, *outside, equals, overlaps*}, that is pair-wise disjoint and jointly exhaustive, *i.e.*,

(A15) $\forall x \forall y\ [inside(x,y) \vee outside(x,y) \vee overlaps(x,y) \vee equals(x,y) \vee inside^{-1}(x,y)]$

To facilitate reasoning about restrictive containment we introduce three other spatial relations. *dirInside* denotes the relation of being directly inside. *dirOutside* denotes the relation of being directly outside some other object and not encompassed by any other object. The *between* relation is ternary and holds when for a pair of objects there is some third object such that one element of the pair is outside of it while the other is inside it. The precise definition of these relations is below:

(D3) $dirInside(x,y) \equiv_{def} [inside(x,y) \wedge \neg\exists z[atLeastPartiallyInside(z,y) \wedge inside(x,z)]]$
(D4) $between(x,y,z) \equiv_{def} [inside(x,z) \wedge outside(y,z)]$
(D5) $dirOutside(x,y) \equiv_{def} [outside(x,y) \wedge \neg\exists z[between(x,y,z)] \wedge \neg\exists v[(between(y,x,v)]]$

(D4) and (D5) and (D2) allow us to demonstrate (P1). The proof is straightforward and we do not print it here.

(P1) $\forall x \forall y[[dirOutside(x,y) \wedge inside(y,z)] \rightarrow atLeastPartiallyInside(x,z)]$

Because *inside(x,y)* is implied by *dirInside(x,y)* we can demonstrate its irreflexivity (P2) and asymmetry (P3). For instance, consider the proof for irreflexivity. Suppose that *dirInside* was not irreflexive, *i.e.*, for some *a*, *dirInside(a,a)*. By (D3) *inside(a,a)* but by (A1), *¬inside(a,a)*. Hence, we can reject the hypothesis that *dirInside* is irreflexive. The proof for the asymmetry of *dirInside* would proceed similarly.

(P2) $\forall x[\neg dirInside(x,x)]$
(P3) $\forall x \forall y[dirInside(x,y) \rightarrow \neg dirInside(y,x)]$

We can demonstrate that *dirInside* is anittransitive as follows:

Suppose that *dirInside* was not anittransitive, *i.e.*, for some *a,b,c, dirInside(a,b)*, *dirInside(b,c)* and *dirInside(a,c)*. Then *inside(a,c)* by (D3) and *¬∃v[atLeastPartiallyinside(v,c)* and *inside(a,v)]*. But, also from (D3) and the given information, *inside(b,c)* and *inside(a,b)*. Hence, there can be no such *a,b,c*. *dirInside* is antitransitive.

(P4) $\forall x \forall y \forall z\ [[dirInside(x,y) \wedge dirInside(y,z)] \rightarrow \neg dirInside(x,z)]$

Given (D5), (A4) and (A5) it is also easy to show that *dirOutside* is irreflexive and symmetric.

Figure 1 illustrates the difference between *dirInside* and *inside*. In the pair of ovals on the left, *dirInside(a,b)* but on the right, *¬dirInside(a,b)* because *between(a,b,c)*. Figure 2 helps to clarify the *between* relation. In Scenario 1 of Figure 2, *¬between(a,c,b)*, despite its consistency with natural language use of 'between', but the relation would apply to the objects in Scenario 2 because *inside(a,b)* and *outside(c,b)*

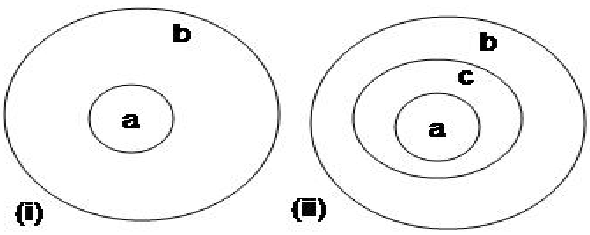

Figure 1: (i) dirInside(a,b) and (ii) not dirInside(a,b)

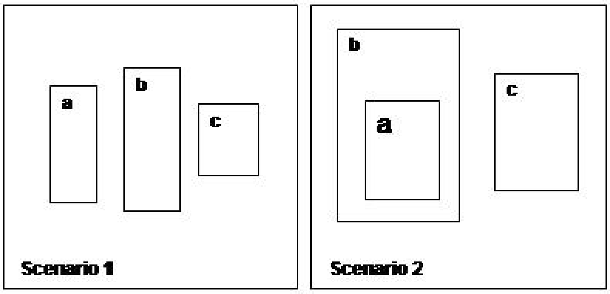

Figure 2: Illustration of the 'between' relation

3.1 Comparison with Other Meronymy Work

Many implementations of the locational sense of 'inside' may benefit from comparing the aforementioned primitive notion to the notions of insideness as spelled out in [Randell *et al* 92]. The authors offer an axiomatization that captures the typical meaning of 'inside'. Let '*RegionFn(x)*' denote the region occupied by x in our state description and '*ConvHullFn(x)*' denote the region encompassed by the convex hull of the object x while *discrete(x,y)* means that *x* and *y* have no parts in common. The domain in [Randell *et al* 92] is the set of spatial regions rather than objects so we translate their definition in (R).

(R) *inside(x,y)* $\equiv_{def}$ *[discrete(RegionFn(x),RegionFn(y))* $\wedge$ *part(RegionFn(x), ConvHullFn(y))]*

Presumably (R) will be consistent with many applications of the *inside* relation we offer here but it can be easily abandoned insofar as nothing in the remainder of the accessibility and containment formalization we develop depends on this. Howver, for purposes of illustrating some of these relations we assume that something like the (R) definition applies.

For most applications of this calculus, an object *a* is inside an object *b* when all or almost all of *a*'s parts are found inside the boundaries of object *b*. It suffices to note that whether or not an object *a* is inside an object *b* in a system at a given point in time will supervene on facts about *a*'s spatial location relative to *b* at that point in time. The necessary and sufficient conditions for insideness will depend on the kind of accessibility that we are interested in. In fact, perhaps the notion of spatial insideness isn't necessary for accessibility reasoning at all. One could imagine applying the reasoning system below to some network security system for bank accounts in which the notion of insideness is a metaphor for being guarded by some security system (*e.g.*, inside the firewall) in which case the spatial notion of insideness is irrelevant, so we should be careful not to unnecessarily restrict ourselves to spatial applications. Nevertheless, in systems in which we want to reason about containment some kind of insideness will be a prerequisite to being contained.

Finally, if we wish to relate this system to a system for reasoning in two dimensions and implement only the RCC-8 relations we might naturally map our relations as follows.

Let us assume that we are considering a fixed system, *i.e.*, a set of objects located at a specific space-time point.

$inside(x,y) \equiv_{def} properPart(RegionFn(x),ConvHullFn(y))$
$outside(x,y) \equiv_{def} discrete(RegionFn(x),ConvexHullFn(y))$
$overlaps(x,y) \equiv_{def} partiallyOverlaps(ConvexHullFn(x),ConvexHullFn(y))$

Note that if we were to implement the above definitions within our calculus, we would be able to prove the following assertion, (A16). However, we will posit it as an axiom:

(A16) $\forall x \forall y \forall z[[inside(x,y) \wedge inside(x,z)] \rightarrow \neg outside(y,z)]$

This axiom allows us to demonstrate the following theorem:

(P5) $\forall x \forall y[[dirInside(x,y) \wedge \neg inside(y,z) \wedge \neg equals(y,z)] \rightarrow \neg inside(x,z)]$

This proof would proceed from the fact that (D3) and the third conjunct in the theorem's antecedent entail that *outside(y,z*) and showing that *inside(x,z)* would thereby generate a contradiction because of (A16), *i.e.*, it would be the case that *inside(x,z)* and *inside(x,y)*, which would entail that $\neg outside(y,z)$.

It is also useful to attempt to relate the inside relation upon which we base our definition of containment with efforts to characterize the notion of parthood. Under many senses of 'parthood' it makes sense to infer that when *a* is part of *b*, *a* is contained by *b*. However, note that if two objects *x* and *y* are such that *inside(x,y)*, we can imagine many senses in which this did not imply a parthood relation. For example, a tourist in the Empire State Building is not necessarily a part of the Empire State Building, but only shares a part of its spatial location. Hence, it is only a limited sense of 'parthood' to which we would want *inside* to commit us. If we consider the taxonomy of parthood relations developed in [Winston *et al* 87], it is conceivable that our notion of containment would be relevant to the following part-whole relations: "component-object" (the components physically belong to the composite) "portion-mass" (components and composite are of the same nature), "place-area" (link an area to place or location) and, perhaps, "member-collection". The kinds of part-whole reasoning to which our containment formalization would most readily apply are those in which one can make clear sense of what it would be for the part to leave the whole and/or enter another for it is in terms of this ability that containment is defined. This conceptualization is difficult in the cases of the other kinds of part-whole relations identified in [Winston *et al* 87], *i.e.*, "feature-event", "phase-activity" and "stuff-object".

In summary, we have purposely kept our suite of spatial representation relations relatively unconstrained so as to facilitate application to a wider variety of applications, or in other words, to broaden the set of models that will be consistent with the formal rules. Our notions of accessibility do not rely on the ability to make fine grained spatial distinctions about juxtaposition and contact. We stress that the arguments for our spatial relations are the objects themselves rather than the regions occupied by the objects. This is essential because the permeability of barriers and containers requires consideration of the objects rather than the regions that they occupy.

4 Accessibility

Here we turn to the question of accessibility. Informally, when we claim that *b* is accessible to *a* we mean that either there is no object *z* such that *between(a,b,z)* or *between(b,a,z)* or the objects between *a* and *b* are unable to restrict *a* from getting at *b*. Formalizing the restrictiveness of objects requires the introduction of two more primitive relations, *inPerm* and *outPerm*. *inPerm(x,z)* is intended to represent the fact that the perimeter of z is permeable to x such that x could pass from being directly outside (*dirOutside*) z to being directly inside (*dirInside*) z. Similarly, *outPerm(x,z)* is intended to represent the fact that the perimeter of z is permeable to x such that x could pass from being directly inside (*dirInside*) z to being directly outside (*dirOutside*) z. Both relations are defined as irreflexive.

(A17) $\forall x[\neg inPerm(x,x)]$
(A18) $\forall x[\neg outPerm(x,x)]$

We require these extra notions because accessibility concerns not just the spatial configurations but the extent to which the configured objects present a barrier. The materials in the cupboard under the sink become accessible to the toddler if she is able to open the cupboard door, whether the door is closed is irrelevant to accessibility given the door-opening skill. We might spell out the meaning of these relations in modal terms, *e.g.*, *inPerm(x,y)* means that, given the current state of the system, *dirOutside(x,y)* and there exists some *z* such that *dirInside(z,y)*, $\Diamond[dirInside(x,y) \wedge contact(x,z)]$ where *contact* represents a disjunction of the relations PO (partially overlaps) and EC (externally connected) [Cohn *et al* 97]. However, we leave them as primitive notions for now. We also define *permeable(x,y)* as follows:

(D6) $permeable(x,z) \equiv_{def} [inPerm(x,z) \wedge outPerm(x,z)]$

Our thinking here is that permeability is best understood in terms of breaching. If an object is able to transverse another object only if a breach of some sort has occurred, then we would not deem the object permeable. If, as a default rule, object *a* is able to pass through object *b*, then we might apply the permeability relation

In many applications it is not felicitous to insist that either *inPerm(a,b)* or $\neg$*inPerm(a,b)* for any two objects *a* and *b* in the system. As our cell biology quotes above indicate, the ability of molecules to diffuse through a cell membrane is a state of affairs that requires representation of degree of permeability. In general, permeability often does in fact admit of degree. Within systems for which partial permeability is relevant to a state description we may need to implement this system in a Bayesian network, as we indicate in Section 5.1 below, so as to allow for the specification of probabilities of penetration for given objects or object types.

We also note the significance of the ability to tease out the inward-outward direction of the permeability relation. It is an important characteristic of many physical systems, not to mention an untold number of television programs involving characters stuck in storage closets, that objects are able to easily pass into a container but are able to leave the container only with great difficulty. In other words, $inPerm(x,z)$ and $\neg outPerm(x,z)$.

Given this notion of access and permeability, we can now define containment as follows:

(D7) $containedBy(x,y) \equiv_{def} [inside(x,y) \wedge \neg outPerm(x,y)]$
(D8) $blockedBy\ (x,y) \equiv_{def} [outside(x,y) \wedge \neg inPerm(x,y)]$

In the sections below, when discussing an object, *y*, we refer to the objects such that *blockedBy(x,y)* as a 'barrier' with respect to y and the objects such that *containedBy(x,y)* as a 'container' with respect to *y*.

These new relations give us a means by which to define accessibility for any two objects. Consider the following relation:

(D9) $inBarrierBetween(x,y,z) \equiv_{def} [blockedBy(x,z) \wedge inside(y,z])$

Assertions of the form *inBarrierBetween(a,b,c)* might be informally interpreted as "*a* cannot access *b* because *c* is between them and blocks its progress."

(D10) $outContainerBetween(x,y,z) \equiv_{def} [containedBy(y,z) \wedge\ outside(x,z)]$

Assertions of the form *outContainerBetween(a,b,c)* can be interpreted to mean that *b* cannot access *a* because *b* is contained by *c*. Finally we define the notion of accessibility of one object to another:

(D11) $acc(y,x) \equiv_{def} \neg\exists z[inBarrierBetween(x,y,z) \vee outContainerBetween(y,x,z)]$

As we would expect, from these definitions, we can prove assertions such as the following:

(P6) $\forall x \forall y \forall z[[inPerm(x,z) \wedge dirInside(y,.z) \wedge\ dirOutside(x,z)] \rightarrow acc(y,x)]$
(P7) $\forall x \forall y \forall z[[outPerm(x,z) \wedge dirOutside(y,z) \wedge\ dirInside(x,z)] \rightarrow acc(y,x)]$

We prove (P6), proof of (P7) would proceed similarly.

Proof. Consider some arbitrary *a,b,c*, such that the antecedent of (P6) holds, *i.e.*, *inPerm(a,c)*, *dirInside(b,c)*, *dirOutside(a,c)*.

Let us assume that $\neg acc(b,a)$. Hence, let us suppose that there is some *d* such that $[inBarrierBetween(a,b,d) \vee outContainerBetween(b,a,d)]$ (1)

Suppose that *inBarrierBetween(a,b,d)*

Then, by (D9) *blockedBy(a,d)* (2) and *inside(b,d)* (3). By (D8) and (2), *outside(a,d)* (4) and ¬*inPerm(a,d)* (5).

Consider the relationship between *d* and *c*. By (A15), either *inside(d,c)*, *outside(d,c)*, $inside^{-1}(d,c)$, *equals(d,c)*, *overlaps(d,c)*.

If *equals(d,c)*, then *inPerm(a,d)* and ¬*inPerm(a,d)*. So ¬*equals(d,c)*.

From (D2), (3) and the fact *dirInside(b,c)* we can infer that ¬*atLeastPartiallyInside(d,c)*, *i.e.*, ¬*inside(d,c)* and ¬*overlaps(d,c)*.

But $inside^{-1}(d,c)$, means that *inside(c,d)* by (D1), so, given (4), we can show that *between(c,a,d)* contrary to the fact that *dirOutside(a,c)* which, by (D5) implies that ¬∃*z between(c,a,z)*. So ¬$inside^{-1}(d,c)$.

So, ¬*inBarrierBetween(a,b,d)*.

If (1) and ¬*inBarrierBetween(a,b,d)*, then, *outContainerBetween(b,a,d)*. Suppose *outContainerBetween(b,a,d)*, then, from (D10), *containedBy(a,d)* (6) and *outside(b,d)* (7) and from (6) and (D7), *inside(a,d)* (8) and ¬*outPerm(a,d)* (9).

Consider the relation between *d* and *c*.
If ¬*equals(d,c)*, then, from (D4), (7) and (8), *between(a,b,d)*. But *dirOutside(a,c)*, (hyp.)
so, from (D5), ¬∃*v[between(a,b,v)]*. Hence ¬¬(*equals(d,c)* or *equals(d,c)*.

But, consider *equals(d,c)*. From our initial hypothesis, *dirOutside(a,c)* and so, from (D5), *outside(a,c)*. But if *equals(d,c)* and (8), we can show *inside(a,c)*. But given (A6), this generates a contradiction. Hence, ¬*outContainerBetween(b,a,d)*.
Hence, the assumption that ¬*acc(b,a)* leads to a contradiction. So *acc(b,a*) and we demonstrate the theorem by universal generalization. *QED*.

The utility of the relations described in (D7)-(D11) is that they facilitate description of the state of a physical system at a given moment in time and the analysis of the system for potential problems and possibilities in terms of the accessibility of certain objects. For example, we can consider vulnerabilities in a computer network, the effectiveness of a security alarm system or perform more accurate *in silico* experiments about biological systems. Given a representation of a system in terms of the *inside* and *outside* relation as well as the expression of the capabilities of the objects in the system to easily transverse containers, we are now able to pose queries about unidirectional accessibility. Hence, if we are concerned about preventing object *a* from accessing object *b*, we can ask:

inbarrierBetween(a,b,?x)

In other words, "Which barriers block *a* from coming in to meet *b*?" If we want to query as to whether there is anything that keeps *b* in and prevents it from accessing *a*, we can ask

outContainerBetween(b,a,?y)

If there are no bindings for either of these we conclude *acc(a,b)*. Note that acc is not a symmetric relationship as there may be objects, *z* such that *inside(a,z)*, *inPerm(b,z)* but *¬outPerm(a,z)*. In other words, *a* is accessible to *b* but *b* is not accessible to *a*.

Observe that the above rules concerning accessibility assume that in the attempt to generate a path through containers and barriers, the barriers and containers cannot themselves be used to transport objects in the system and that the accessed object will not itself move so as to become more accessible. However, let us briefly consider how to reason about accessibility in the situations in which:

a) Both objects move: the containers and barriers remain fixed but the two objects of interest could both exploit permeability properties in generating a path to a state in which both objects are accessible to each other. We call this "weak accessibility."

b) Containers move: Some or all of the containers (in the locational sense, at least) and barriers do not remain stationary but are also able to exploit permeability properties and transports container contents such that contained objects become accessible to each other. For example, consider a border crossing that must be crossed by car and not on foot. We might say *outPerm(carA,BorderC)* or *outPermeableType(Car,BorderC)*(where 'Car' denotes the property "being a car", see below). The border is *outPerm* for the car but not for the pedestrian. However, since the car is *inPerm* and *outPerm* for the pedestrian, s/he can use this car to cross the border. Of course, this is the accessibility maneuver exploited in the Trojan Horse story of mythology. Let us call this "indirect accessibility."

4.1 Weak Accessibility

Suppose that we now want to consider two objects *a* and *b* from the perspective of determining whether or not they are able to exploit existing permeability properties in the various objects that serve as potential barriers and containers so as to be able to move to a state such that *¬∃x[between(a,b,x)]*. When it is possible for *a* and *b* to come into contact by moving from their respective initial location by traversing permeable boundaries, then we say that *weaklyAcc(a,b)*.

But when else can we claim that the *weaklyAcc* relation holds between two objects? We need to determine whether there are any objects in the system that are accessible to both of the objects in question.

(D12) $weaklyAcc(x,y) \equiv_{def} \exists z[[[dirInside(x,z) \rightarrow acc(x,y)] \wedge [dirInside(y,z) \rightarrow acc(y,x)]] \vee [[dirOutside(y,z) \rightarrow acc(y,x)] \wedge [dirOutside(x,z) \rightarrow acc(x,y)]]]$

This definition states that if there is some point in the system accessible to both *a* and *b*, *z* in the definition, then the objects are accessible to each other. From the definition of *weaklyAcc* it is straightforward to prove the symmetry of *weaklyAcc* and that *weaklyAcc(x,y)* is implied by *acc(x,y)* and *acc(y,x)*.

(P6) $\forall x \forall y[weaklyAcc(x,y) \rightarrow weaklyAcc(y,x)]$

(P7) $\forall x \forall y[[acc(x,y) \vee acc(y,x)] \rightarrow weaklyAcc(x,y)]$

4.2 Indirect Accessibility

The other accessibility problem that we want to address is that of the potential ability of objects to move objects that they contain. Consider Figure 3. Suppose that we wanted to know whether *acc(c,d)*. Further suppose that *outPerm(c,b)*, $\neg$*inPerm(d,a)* and that *outPerm(b,a)* but $\neg$*outPerm(c,a)*. This means that *c* would not be able to exit *b* and then pass through *a*. However, if *b* were to exit *a* while containing *c*, and then *c* were to exit *b*, *c* would be able to access *d*. Let us call such accessibility *indirectAcc*.

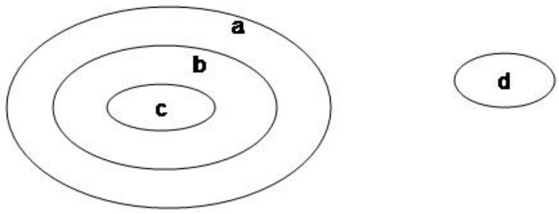

Figure 3: Illustration for explaining indirect (Trojan Horse) accessibility

We define indirect accessibility, *indirectAcc*, as follows:

(D13) $indirectAcc(x,y) \equiv_{def} \exists v \exists z[[[inside(x,v) \wedge inside(y,z) \wedge weaklyAcc(v, z)] \wedge [dirOutside(v,z) \rightarrow acc(y,x)] \wedge [dirOutside(z,v) \rightarrow acc(x,y)]] \vee [[inside(x,v) \wedge weaklyAcc(v,y)] \wedge [dirOutside(y,v) \rightarrow weaklyAcc(x,y)]] \vee [[inside(y,z) \wedge weaklyAcc(x,z)] \wedge [dirOutside(x,z) \rightarrow weaklyAcc(x,y)]]]$

The three main disjuncts in this lengthy definition correspond respectively to the situations in which both *x* and *y* could be transported by one of the objects to which they bear the *inside* relation, the situation in which just *y* would need to be transported by one of its containers and the situation in which just *x* would need to be transported by one of its containers. Of course, we can imagine this being iterated again so that we determine whether the containers of *x* and *y* are indirectly accessible, etc.

4.3 Relations for Second Order Objects

Much reasoning about accessibility and containment occurs at the type level. For example, that a lipid bilayer can allow a particular water molecule to pass through should be derivable from a more general law relating cells with lipid bilayer membranes and water rather than from an explicit assertion about each water molecule in the system we're representing. Hence, we appeal to second order objects or relations in our domain. We posit relations that hold first between first order objects and unary relations and between pairs of relations. These second order terms would be introduce only for easing representation, *i.e.*, representing a relation once for an entire class or pair of classes rather than once for each individual member. They do not add extra containment reasoning functionality.

(D14) $inPermeableType(P,x) \equiv_{def} \forall y[P(y) \rightarrow inPerm(y,x)]$

and we would define *outPermeableType(P,x)* in a similar manner, substituting *outPerm* in for *inPerm* in the definition in (D14).

This instance-type level definition would be useful if we wanted to note that a particular object has achieved inward or outward permeability for a certain kind of object. For example, a leaky raincoat allows water to go through it. However, permeability is typically easily represented as a relation between types. For example, let the relation C be the property of being a cell, or perhaps being encompassed by a lipid bilayer. Let the relation 'IM' denote the property of being an ionic molecule. Then we note, *inPermeableTypes(IM,C)*. More generally, we define the *outPermeableTypes* in (D15) and this applies, mutatis mutandis, to *inPermeableTypes* and *permeableTypes* as well.

(D15) $outPermeableTypes(P,Q) \equiv_{def} \forall x \forall y\ [[P(x) \wedge Q(y)] \rightarrow outPerm\ (x,y)]$

5 Implementations and Applications of the Formalism

In this section we consider possible implementations of the calculus outlined above. In Section 5.1 we explore a method for implementing the formalism within a Bayesian network so as to reason about systems in which permeability is probabilistic. In Section 5.2 we consider an implementation of the calculus in a planning vocabulary. Finally in Section 5.3 we consider an application of the calculus to some simple representation and reasoning problems in cell biology.

5.1 Uncertainty Reasoning for Accessibility

Let us reconsider our earlier cell biology textbook quotation. Some may have objected that the ability of a molecule to "diffuse" across a bilayer is not a Boolean-valued question as the heretofore presentation of our calculus appears to assume. Presumably, cell biologists would argue that this is a question of degree. We can imagine this being true of many accessibility analyses.

Hence, let us consider a probabilistic system for representing and reasoning about accessibility when whether or not *inPerm(x,y)* or *outPerm(x,y)* is uncertain for many ordered pairs, $<x,y>$ in our system. Let us illustrate the approach by addressing the question of determining *acc(x,y)* for some pair of objects in a system, *i.e.*, is y able to traverse all potential containers or barriers between it and *x*? One commences by constructing a list of all potential containers and barriers for *x* and *y* by taking the set of objects $Obj=\{z|between(a,b,z) \vee between(b,a,z)\}$. Let us then define the "impediment list" for <*x,y*> as an ordering of the elements of *Obj* such that the first element is the object *a∈Obj* such that *dirInside(y,a)* or *dirOutside(y,a)*, and then define the (n+1)th element as the object *z* such that that the nth element bears the relation *dirInside* or *dirOutside* to it. Hence, if *a* is the first element in <*x,y*>'s impediment list, then the next element is the object *b*, such that either *dirInside(a,b)* or *dirOutside(a,b)*. We can then determine *y*'s ability to access *x* by determining its ability to pass through each of the elements in the <*x,y*> impediment list.

Note that for any element in <*x,y*>'s impediment list, whether or not *y* can pass through it depends on the permeability of the element and on whether or not *y* can pass through the preceding element in the impediment list. Where the permeability is deterministic, this is a relatively simple query. However, it is more complicated where the permeability of any or all of the impediment list elements is uncertain. To address this we construct a Bayesian network (BN) for calculating *y*'s capability to pass through a potential barrier or container *z* that appears on an impediment list, as illustrated in Figure 4. The key node in such a BN is the one representing the random variable for whether or not *y* can pass through *z* ("Obj z Permeable" in Figure 4). The parent nodes for this node will be a node whose possible values are determined by whether or not y passes through the item preceding z in the <*x,y*> impediment list ("Prior Obj Permeable") and a node whose values are the possible permeability states of z with respect to *y*, ("Permeability State"), *i.e.*, whether *inBarrierBetween(y,x,z)* or *outContainerBetween(x,y,z)*. Whether *z* is a barrier or container depends, of course, on whether the *inside* or *outside* relation hold between *y* and *b* and whether or *inPerm(x,z)* or *outPerm(x,z)*, so the permeability node in our BN has parent nodes whose values are determined by the relative location of *x* and *z* ("RelativeLocation", and nodes whose values are determined respectively by whether or not *inPerm(x,z)* ("inPerm(y,z)") and whether *outPerm(x,z)* ("outPerm(y,z)"). The conditional probability table for "Permeability State" is defined deterministically and is shown in Table 1. We can see that it implements the definitions specified in (D9) and (D10).

RelativeLocation	**inPerm(y,z)**	**outPerm(y,z)**	**PermeabilityState**
inside(y,z)	true	true	PermeableTo
inside(y,z)	true	false	outContainerBetween
inside(y,z)	false	true	PermeableTo
inside(y,z)	false	false	outContainerBetween
outside(y,z)	true	true	PermeableTo
outside(y,z)	true	false	PermeableTo
outside(y,z)	false	true	inBarrierBetween
outside(y.z)	false	false	inBarrierBetween

Table 1: Deterministic Conditional Probability Table for "Permeability State" Variable

This BN can be applied successively to each list element where the probabilities on the values for "Obj z Permeable" for element n are the inputs to the "Prior Obj Permeable" node for element n+1. Equivalently, as we discuss below, we can generate a single BN that reasons over the entire impediment list. Note that the utility of this representation is that at each step we are able to express uncertainty about *z*'s permeability with respect to *y*. For example, in Figure 4 the BN allows us to assert that '*(probability(outPerm(y,b) .9)'* and to indicate that the calculated probability of *y* being able to permeate all elements prior to *z* in the relevant impediment list is .85.

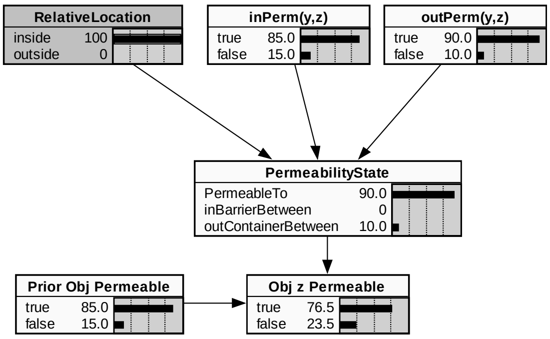

Figure 4: Bayesian network to calculate permeability of a potential barrier or container with respect to an object

A full BN for an impediment list would involve the combination of BN fragments of the sort illustrated in Figure 4. Consider an impediment list <*u,v,w*> for some pair <*x,y*>. Suppose *dirInside(y,u), inside(y,v)* and *outside(y,w)* and further suppose that *(probability (outPerm(y,u)) .6*), and that *(probability (outPerm(y,v)) .43)*, and that *(probability (inPerm(y,w)) .9)*. Implementing these probabilities in conjunction with the definitional rules on *inBarrierBetween* and *outContainerBetween* shows that the probability that y will be capable of gaining successive access through all of the elements in the relevant impediment list is .36. See Figure 5.

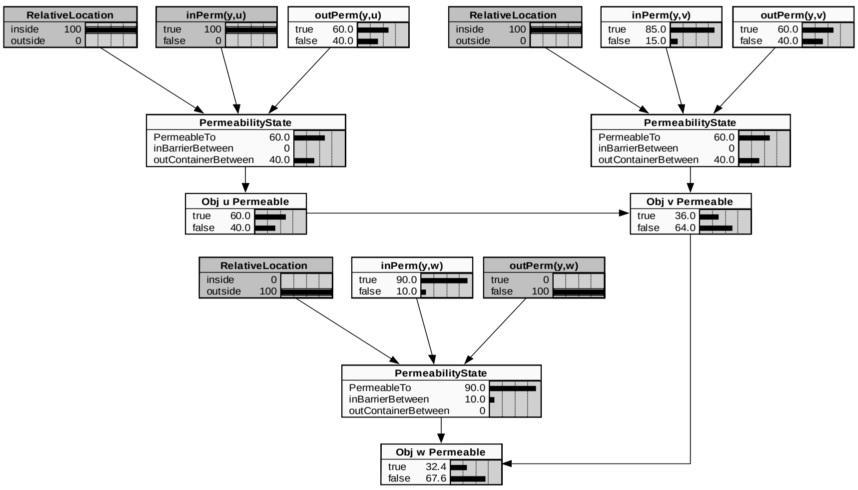

Figure 5: Bayesian network to calculate probability that the objects listed in a-chain (<u,v,w>) are of permeability and configuration such that acc(x,y).

It should be fairly clear how we might go about implementing similar BNs for reasoning about *weaklyAcc(x,y)*. This would involve checking points on the impediment list for <*x*,*y*> or <*y*,*x*> that are potentially accessible to *x* and *y*.

Also, note that an another useful feature of a BN representation such as the one illustrated above is that we can implement learning techniques to refine or learn the probabilities for *inPerm(x,y)* and *outPerm(x,y)* for pairs in the system.

5.2 Application for Process Reasoning

Finally, we have presented these relations as binary and ternary relations that hold between ordered pairs and ordered triplets of objects. These relations describe system states at a given moment in time. However, it is also important to note that the accessibility and permeability relations are best understood as constraints on how the system can progress over time assuming no changes in permeability relations. For example, when we say that *acc(a,b)* we mean that given the current state of the system there is a possibility that a future state of the system will have *a* and *b* in contact with each other. Similarly, *inPerm(a,b)* means that future states requiring a passage from *a* into *b* are not ruled out. As such we want to be more explicit about how these relations might be implemented in a planning or process-reasoning environment in which the accessibility of objects may change. Below we give some examples of how the vocabulary used above might be implemented in actual process reasoning. We indicate how a STRIPS-like planning vocabulary might implement the accessibility vocabulary and some examples of how the vocabulary above might help in representing some example process descriptions in virology and cell biology.

operation: *gainsShell (A, B)* (a new container is generated.)
precondition:
add: *(inside A,B)*

operation: *enters (A,B)* (an object enters another objects)
precondition: (overlaps(A,B) ∨dirOutside(A,B)), inPerm(A,B)
add: inside(A,B)
delete: outside(A,B)

operation: *losesShell (A,B)* (some container is removed from the system. This kind of operation is particularly salient to cell biology where membranes often dissolve or dissipate.)
precondition: inside(A,B)
add:
delete: inside(A,B)

operation: *(exits A,B)* (Object A leaves B, but B still exists.)
precondition: *dirInside(A,B),outPerm(A,B)*
add: *outside(A,B)*
delete: *inside(A,B)*

operation: *losesContainmentStatus (A,B)* (B becomes permeable to A, *i.e.*, will allow A to exit if A is inside B.)

precondition:

add: *outPerm(A,B)*

delete: $\neg$*outPerm(A,B)* (if that was stated in the system)

operation: *losesBarrierStatus (A,B)* (B becomes permeable to A, *i.e.*, will allow A to enter if A is outside B.)

precondition:

add: *inPerm(A,B)*

delete: $\neg$*inPerm(A,B)* (if that was stated in the system)

5.3 A Simple Knowledge Representation Example

We conclude by briefly readdressing the issue that motivated this work initially. We noted that this calculus was motivated by knowledge representation requirements in cell biology and so it is fitting to consider how it could be used in representing key cell biology concepts. We briefly consider some aspects of the viral life cycle. Virus life cycles require consideration of membrane components and virus types in order to reason about the *inPerm* relation with respect to the virus and a cell. The viral life cycle involves the formation of several new containers and the destruction or penetration of the old ones and the abilities of various parts of the cell or virus change rapidly with respect to their ability to enter or exit various parts of the cell. Consider the following passage from a virology textbook.

> **Passage A**: The mechanisms by which vaccinia virus attaches to and enters susceptible host cells are not well understood. The result is release of the core into the cytoplasm, indicating that entry requires fusion of viral with cellular membranes. [Flint 00]

Many parts of our calculus would be implemented to represent this passage. To start, we would represent this passage by noting:

inPermeableType (Cell, VacciniaVirus)

where '*Cell'* denotes the property of being a cell and '*VacciniaVirus*' denotes the property of being a vaccinia virus. The second sentence might be represented as:

$$\forall x \forall y \forall z\ [[Cell(x) \wedge VacciniaVirus(y) \wedge attached(x,y)] \rightarrow inPerm(y,x)]$$

A second interesting passage from a knowledge representation perspective is the following.

> **Passage B**: a spherical particle that is believed to possess a double membrane acquired upon wrapping of the membranes of the cellular components of the *cis*-Golgi network about the assembling particle. The virus particle then matures into the brick-shaped intracellular mature virions (IMV), which is released only upon cell lysis. [Flint 00]

Two of the salient points from Passage B can be represented as:

$\forall x[SphericalParticle(x) \rightarrow \exists x \exists y[Membrane(x) \wedge Membrane(y) \wedge dirInside(x,y)) \wedge dirInside(z,y)]$
$\forall x \forall y\ [[Cell(x) \wedge inside(y,x) \wedge\ IMV(y) \wedge CellLysis(z) \wedge patient(x,z)] \rightarrow holdsAfter(z, outPerm(y,x)]$

Given the ability to represent the various accessibility relationships, one might ask about the kinds of reasoning tasks that these kinds of representations would facilitate. An area of interest in cell biology concerns viral life cycles. Processes of infection, replication and transmission in cellular biology typically involve the passages of objects of interest across various sorts of boundaries. The malaria life cycle, for example, involves the passage of sporozoites from a mosquito's salivary gland into the bloodstream of a human, then into the human's liver at which point they must penetrate hepatocytes, multiply, leave the cells they have entered, reenter the blood stream, penetrate other blood cells, producing either merozoites or micro and macrogametocytes. Gametocytes may then leave the human blood stream into a mosquito vector where the gametocytes are further "processed" and the resulting ookinette penetrates the wall of a cell in the midgut, where, after further processing, oocysts develop from which new sporozoites emerge and penetrate the host's salivary gland. [Sherman 98] Obviously, entrance and exit across various membranes is essential to this process. Hence, the ability to reason about the feasibility or existence of such passage seems to be a necessary precursor to the development of effective tools for formal reasoning about cellular biology. Let us briefly consider, in a simplified example, how the containment calculus might be implemented in reasoning about viral life cycles.

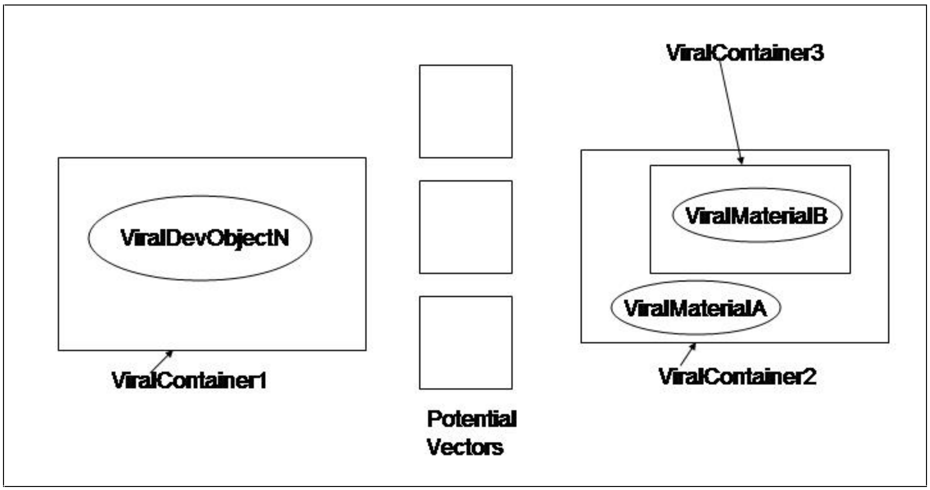

Figure 6: Identifying Potential Viral Life Cycle Links

Consider the rudimentary scenario depicted in Figure 6. Suppose one wants to determine potential vectors in this particular potential viral replication process. First, as depicted, suppose one knows that the virus at development stage N

(*ViralDevObjN*) will or may be inside of *ViralContainer1*, *e.g.*, a particular kind of organ or cell. A potential reasoning task would be to determine whether *ViralDevObjN* is capable of passing from that "container" to any of the potential vectors in which we are interested. In other words, it would involve finding values of ?POTVEC in the following query:

(∧ (type ?POTVEC PotentialVector) (acc ViralDevObjN ?POTVEC))

Secondly, suppose that one knows that viruses at development stage p (*ViralDevObjP*) can be further incubated given access to *ViralMaterialA* and/or that viruses at development stage m (*ViralDevObjM*) can be further developed given *ViralMaterialB*. An important reasoning task then becomes one of determining whether there is a potential vector that could be the source of viruses at development stage p or m that would be accessible to the *ViralContainer2* or *ViralContainer3*. In other words, given the scenario in Figure 6, we might attempt to find values of ?POTVEC such that:

(→
(∧
(inside ViralDevObjP ?POTVEC)
(type ?POTVEC PotentialVector))
(acc ViralMaterialA ViralDevObjP))

or

(→
(∧
(inside ViralDevObjM ?POTVEC)
(type ?POTVEC PotentialVector))
(acc ViralMaterialB ViralDevObjM))

The separate reasoning challenge, of course, concerns the identification of the possible vectors identified in such queries that would be capable of incubating viruses from stage N (*ViralDevObjN*) to stage M or P, *i.e.*, *ViralDevObjM* and *ViralDevObjP*. However, the formal vocabulary developed here could presumably be usefully implemented in identifying the vectors suitable for such further analysis.

6 Concluding Remarks

Above we have noted that existing approaches to qualitative spatial reasoning allow us to represent and reason about the fact that objects are located inside container objects. However, such representation methods will not allow us to represent containment in the sense of restriction. We have attempted to define this important notion in terms of the objects and permeability properties of physical systems and in terms of different ways in which objects can contain other objects, *e.g.*, inward vs. outward permeability. We have also teased out three different notions of accessibility between objects within a given physical system and suggested methods for investigating whether or not two given objects in a system bear these three kinds of accessibility relations.

We contend that the ability to perform this kind of knowledge representation could be useful in a very wide range of reasoning contexts. This includes computer security, cell biology, virology, building security analysis, chemical storage. We have also attempted to show how we might implement the tools of Bayesian networks to address some of the uncertainties inherent in accessibility and containment representation.

Future work will include an exploration of what we have called "indirect accessibility" with respect to a highly dynamic system in which no objects are stationary. We will also investigate how reasoning about the stationary status of objects and an ontology of physical objects designed in terms of containment capabilities could further facilitate reasoning in this area.

Acknowledgements

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