Adjoint join volumes

Michael L. Connolly

1259 El Camino Real #184, Menlo Park, CA 94025, USA

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A simple geometrical identity, called the adjoint join formula, is introduced. It allows one to simplify the computation of the volumes of some unions of simple solid objects such as spheres and polyhedra. It involves cones and a generalization of a cone, called a join. In order to apply the adjoint join formula it is necessary to first compute the surface of the object. The volume of an object is equal to a cone of the object's surface over some point. This cone is the sum of the cones of each face of the surface over the point. The computation of the volume of each of these cones can sometimes be simplified by applying the adjoint join formula. The adjoint join formula states that if two geometrical objects in space have dimensions that sum to three, then the join of the boundary of the first object with the second object is equal to the join of the first object with the boundary of the second object (up to sign). There are occasions when the volume of the first join is difficult to compute, but the volume of the second join is easy to compute, so applying the adjoint join formula simplifies the volume computation. The method is applied to the union of a group of spheres. This provides a simple way to compute the volume of a molecule analytically, provided that one can compute its van der Waals surface analytically. This is not the first analytical and exact method to compute the volume of a hard-sphere representation of a molecule, but it is conceptually the simplest.

1. Introduction

When computing the volumes of solid objects, exact methods from solid and analytic geometry are used for simple objects such as polyhedra, spheres and volumes of revolution. Numerical approximations such as octrees [1] and Simpson's rule [2] are used for complex objects such as those from constructive solid geometry and boundary representations [3]. This paper introduces a geometric identity, called the adjoint join formula, that will help extend exact, analytic methods to objects of intermediate complexity. For example:

- unions of spheres,
- unions of spheres and polyhedra,
- volumes bounded by pieces of spheres and tori that meet at circular arcs.

The basic idea is to replace one description of a particular volume of space by another description whose volume computation is simpler. Although there are some algebraic equations and mathematical proofs in the paper, most of the paper is concerned with trying to convey the concepts involved. In particular, I hope to:

- make the geometric meaning of the adjoint join formula clear,
- make the fact that the adjoint join formula is true seem intuitively obvious.

In order to explain this topological method it is necessary to explain a number of ideas in common use in algebraic topology: cones, chains, joins, boundaries and adjoint operators. After this is done, the adjoint join formula will be stated and proved, and finally some examples of its application will be presented.

2. Cone

The topologist uses the word *cone* [4] to refer not only to the traditional cone with a circular base, but also many other, more general objects (fig. 1). The volume of a three-dimensional cone with a flat base is one-third the altitude times the area of the base. A cone does not need to be three-dimensional and it does not need to have a flat base. A sector of a circle is a cone of an arc over the circle center. A part of sphere lying between the center of the sphere and a region on the surface of the sphere is also a kind of cone fig. 1(d). The volume of this three-dimensional cone is one-third the area of the spherical region times the radius. The area of the spherical region can be computed from the Gauss–Bonnet formula [5,6]. A cone can have a base made up of several parts, each with a different altitude (fig. 1(e)). The area of a polygon may be computed by decomposing it as a cone of its boundary over some point in the interior (fig. 1(f)). The volume of a polyhedron may be computed analogously. All of these figures satisfy the mathematicians definition of a cone, which is the union of all lines connecting the vertex to a point on the base [2].

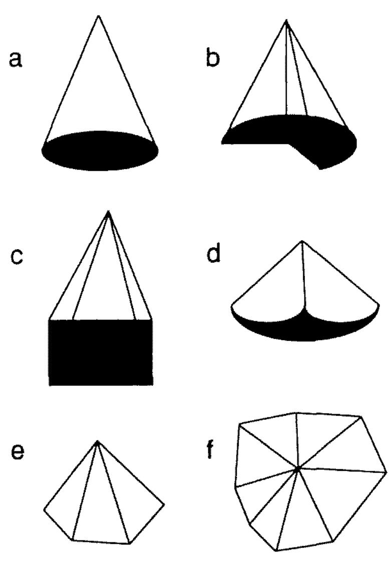

Fig. 1. Several different kinds of cones.

3. Orientation

For some cones there are problems with this simple definition (fig. 2). We want the cone of triangle ABC over vertex P to be independent of where the point P is located, but with our current definition, if P is inside the triangle we get a different cone than if P is outside the triangle. For P outside the triangle (fig. 2(b)), some points lie on more than one cone line connecting the cone vertex to the triangle. For example, points lying inside the shaded region, but outside the triangle lie in both the cone of AB over P and also the cone of BC + CA over P. This problem is generally handled by simply saying that the cone is undefined in such cases, but we are not willing to limit ourselves.

An idea that will enable us to achieve our objective is the idea of an *orientation* [7]. An orientation is a handedness. For a line segment, it is a direction, as in a vector or an edge of a directed graph. For a point it is a formal plus or minus sign. For a polygon, it is a clockwise or counterclockwise traversal of the edges. In this article we will follow the convention that a clockwise orientation gives a positive area and a counter-clockwise orientation gives a negative area. For a tetrahedron, it is the sign of the volume as determined by the triple product of three edges meeting at a vertex.

Another useful idea is that of a *chain* [7]. In algebraic topology, a chain is a collection of objects, for example polygons, each with a sign or orientation. In fact, one

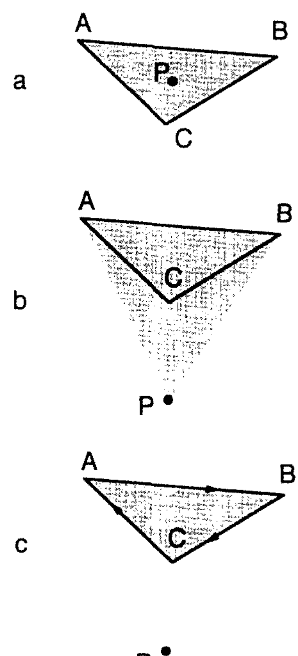

Fig. 2. Area of triangle described as cone of triangle boundary over a point.

can assign to each polygon of the chain not just a plus or minus sign, but any integer, positive, negative or zero. These integers are sometimes called coefficients, in analogy with polynomials. A coefficient of zero means that the polygon is not included in the chain. The simplest planar polygon is the triangle, and the simplest spatial polyhedron is the tetrahedron. The general term for the simplest polyhedron in each dimension is *simplex* [7]. A 0-simplex is simply a point. In this paper, chains will always have a homogeneous dimension. An n-chain is a finite set of n-dimensional simplices, each with an integer coefficient. Any polygon or polyhedron can be decomposed into simplices.

Since we are dealing with oriented geometrical objects, their areas and volumes will be signed areas and volumes. In fig. 2(c) triangle ABP is clockwise, which gives a positive area, but triangles BCP and CAP are counterclockwise, giving negative areas which cancel out part of triangle ABP. The sum of these three triangle areas is triangle ABC, as desired.

4. Join of two chains

A cone is a special case of a more general geometrical construction called a join [4,8]. Instead of considering all lines from a point to an object, we consider all lines from one object to another object. As before, it is best to represent geometrical objects as oriented chains. The join of two skew lines in space is a tetrahedron (fig. 3). The asterisk symbol is used to represent the join operation. If a simplex is represented by listing its vertices in some order, then the join of two simplices is the simplex defined by concatenating these two vertex lists. The join operation resembles a product and obeys the distributive law. That is, if F is one chain and G and H are two other chains, then $F * (G + H) = F * G + F * H$. It is also commutative, up to sign: $F * G = (-1)^{jk} G * F$, where j is the dimension of F and k is the dimension of G. The sign is due to the fact that we are dealing with oriented chains and reversing the order of the factors is a permutation that can be decomposed into jk transpositions of vertices. For non-oriented chains, the join operation is strictly commutative [7].

Curved objects can be handled using differentiable chains [9]. A differentiable chain is a formal sum of differentiable simplices, each with an integer coefficient. A differentiable simplex is a differentiable mapping from a straight simplex into

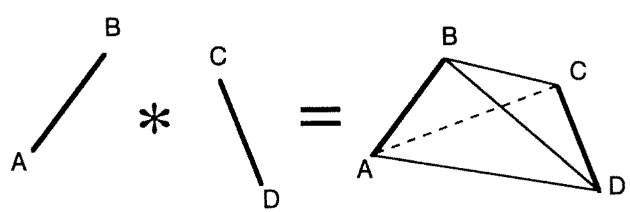

Fig. 3. The join of two line segments in general position is a tetrahedron.

Euclidean space. Let S_1 and S_2 be two straight simplices. Let p_1 be a point in S_1 and let p_2 be a point in S_2. Let two curved simplices be defined by two mappings m_1 and m_2 from S_1 and S_2, respectively, into Euclidean space. Let a line segment from $m_1(p_1)$ to $m_2(p_2)$ be parametrized by the real variable t running from 0 to 1. The join of these two curved simplices is defined by

$$j: S_1 \times [0,1] \times S_2 \to E,$$

$$j(p_1, t, p_2) = (1-t)m_1(p_1) + tm_2(p_2).$$

5. Boundary of a chain

Some chains are the boundaries of other chains. For example, the polygons of the surface of a polyhedron form the boundary of the solid polyhedron. The partial derivative symbol ∂ is used in topology to mean "the boundary of". The boundary of a line segment from point A to point B is $B-A$, that is, $\partial AB = B - A$. Let 0 mean the empty chain. For triangle ABC let us compute the boundary of its boundary:

$$\begin{aligned}\partial^2(ABC) &= \partial\partial(ABC) = \partial(AB + BC + CA)\\ &= \partial AB + \partial BC + \partial CA = (B-A) + (C-B) + (A-C) = 0.\end{aligned}$$

In fact, it is proven in homology theory that $\partial^2 = 0$ always [10]. This is generally stated as: the boundary of a boundary is zero, or a boundary has no boundary.

We are interested in the relationship between boundaries and joins. In particular, note that the volume of any solid object can be written as the cone of its boundary over a point in the interior (fig. 1(f)). In fact, due to the use of orientations and cancellations of areas and volumes (fig. 2(c)), one could just as well use a point *outside* the object as the cone vertex.

6. Boundary of a join

There is a simple formula for the boundary of the join of two chains F and G:

$$\partial(F * G) = (\partial F) * G + (-1)^{k+1} F * \partial G,$$

where k is the dimension of the chain F. It resembles the coboundary formula in cohomology theory [7], except that here there is a factor of $(-1)^{k+1}$ instead of $(-1)^k$, due to the extra dimension introduced by the line segment from a point of F to a point of G. The proof of this equation for the case of a tetrahedron involves examining fig. 3. The join of line segment AB with line segment CD is the tetrahedron $ABCD$. The boundary of AB is $B-A$. The boundary of CD is $D-C$. The boundary of the tetrahedron can be determined by omitting each vertex in turn and alternating the sign: $\partial(ABCD) = BCD - ACD + ABD - ABC$. If we cyclically permute (rotate) the vertices of a triangle, the sign does not change, but a transposition of two vertices corresponds to a reflection and reverses the sign.

$$\begin{aligned}\partial(AB * CD) &= \partial(ABCD)\\ &= BCD - ACD + ABD - ABC\\ &= (BCD - ACD) + (ABD - ABC)\\ &= (B * CD - A * CD) + (AB * D - AB * C)\\ &= (B - A) * CD + AB * (D - C)\\ &= \partial(AB) * CD + AB * \partial(CD)\\ &= \partial(AB) * CD + (-1)^{k+1} AB * \partial(CD), \quad \text{where } k = 1\,.\end{aligned}$$

The proof for simplices in other dimensions is analogous. The proof for chains made up from more than one simplex is clear, because the boundary operator (∂) and the join operator ($*$) are both linear. The proof for curved chains is also a straightforward generalization, because they are differentiable chains and differentiation is linear.

7. Boundary of a degenerate join

If one chooses two random line segments in space, almost always they will be skew to each other and define a tetrahedron of non-zero volume. Mathematicians call this being in "general position" [4]. But it is possible that the two line segments will lie in a common plane, thus defining a degenerate tetrahedron. Degenerate joins always occur if the sum of the dimensions of the two chains is greater than or equal to the dimension of the ambient Euclidean space. For example, two line segments in a plane each have dimension one, and $1 + 1 \geqslant 2$ (the dimension of the plane), so their join must be degenerate, regardless of how they are positioned. Since $1 + 1 = 2$, rather than being greater than 2, the boundary of the degenerate tetrahedron, namely four flattened triangles, is not itself degenerate.

It is sometimes helpful to think of a degenerate object as a result of projecting a non-degenerate object from a higher-dimensional space to a lower-dimensional space. Non-degenerate boundaries of degenerate objects are especially interesting because they have zero area, as will be proved below. For example, if we project the sphere centered at the origin in three-dimensional space onto the XY plane, we now have a flattened sphere where the upper hemisphere is now a circular disk with area πr^2 and the lower hemisphere is now a circular disk with area $-\pi r^2$ (negative because the orientation is reversed by the projection mapping). So the total area of the projected sphere is $\pi r^2 - \pi r^2 = 0$.

That the area of a non-degenerate boundary of a degenerate object is zero is basically due to the idea of the degree of a map [11]. The degree of a map means the number of times a geometrical mapping wraps one object around another. It is always an integer. For example, the mapping $z \to z^2$ wraps the unit circle in the complex number plane around itself twice. There are actually two degrees of a map, the global degree and the local degree. The global degree is defined for the object as a whole, and the local degree is defined at each point. The local degree is computed by taking a point projected onto and adding up a finite number of plus and minus ones, where there is a plus one for each time the map preserves orientation, and a minus one for each time the map reverses orientation. For points in the second object that are not projected onto by any point in the first object, the local degree is defined to be zero. The global degree is defined only when the local degree is the same at all points, in which case it is simply defined to be this common local degree. This is the only case that is of interest to topologists, but since we are geometers, the local degree is also of interest. In particular, the area of the projected figure is simply the integral of the local degree of the projection map.

One can also use the local degree to describe a region of space in a manner that generalizes the characteristic function of a set from measure theory [2]. The characteristic function is defined to be 1 for points inside the set, and 0 for points outside the set. The local degree simply generalizes the characteristic function from having two possible values (0 or 1) to having any integer as a possible value. If the local degree is zero everywhere, this corresponds to the empty set. In chemical applications, it is acceptable for this local degree or *generalized characteristic function* to have values other than 0 or 1 in intermediate steps in the calculation, but at the end of the calculation, the local degree will have to have values of only 0 or 1 in order to correspond to the traditional characteristic function and so define a region of space.

A degenerate object in the plane can be thought of as the projection of a non-degenerate object in space onto the plane. The area of a projected boundary is obtained by integrating the local degree of the projection map over all points. In fig. 4, the projected boundary is drawn edge-on and not quite completely flat, so that four points actually superposed on each other can be distinguished. In the figure this is shown as 2 dots on segments with the arrows pointing to the right and 2 dots on segments with the arrows pointing to the left. At any point in the plane, the number of points where the projection map keeps the same orientation is equal to the number of points where the projection map reverses the orientation. This means that the degree of the projection map from the boundary in space onto the plane is zero.

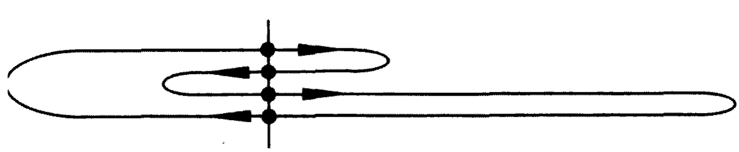

Fig. 4. The degree of a projection mapping of a boundary onto a plane, seen edge on.

It is easy to show that this statement holds in general. The global degree of a map is defined only for objects that have no boundaries, such as circles, spheres and the surfaces of polyhedra [11]. This requirement is necessary to ensure that the degree is the same at each point (it would change if a boundary were crossed). Since a boundary has no boundary, the projection mapping from any boundary onto the plane has a well-defined global degree. Since there are obviously some points in the plane that the boundary is not projected onto, the degree of the map at these points must be zero. Putting these two facts together shows that the global degree of the projection map is zero. This implies that the local degree is zero at each and every point, so not only is the signed area of a projected boundary zero, but the projected boundary has the same generalized characteristic function as the empty set. That is, the area cancellation occurs *at each point*; it is not simply a case of a positive area in one part of the projected boundary cancelling a negative area in another part of the projected boundary.

These same ideas hold in higher dimensions and for curved objects (differentiable chains). If we have a boundary of a degenerate object in space, it can be thought of as a projection of a non-degenerate object from four-dimensional space, and so the boundary volume is zero. The more subtle point at the end of the last paragraph carries over too: the degenerate boundary corresponds to the empty set, because its generalized characteristic function vanishes everywhere. Actually, only "almost everywhere", because the set of critical values of the degenerate boundary has measure zero due to Sard's theorem [11]. The local degree of a map is not defined at these points. Since the critical set has measure zero, it will not affect the volume.

Another way to show that the area (or volume) of the boundary of a degenerate object is zero is to use Stoke's theorem in its modern formulation due to Elie Cartan [9]. Let M be an n-dimensional differentiable chain in $(n-1)$-dimensional space. Then ∂M is its $(n-1)$-dimensional boundary chain in $(n-1)$-dimensional space. Let ϕ be a volume form for $(n-1)$-dimensional Euclidean space. The volume of ∂M can be computed by integrating the volume form ϕ over it:

$$\int_{\partial M} \phi = \int_M \mathrm{d}\phi = \int_M 0 = 0 .$$

The first equality is due to Stoke's theorem. The second equality follows from the dimension argument that since $\mathrm{d}\phi$ is an n-form in $(n-1)$-dimensional space, it is zero [9]. This shows that the volume of the boundary of a degenerate object is zero. The more subtle point that the volume cancellation occurs at each point can also be proved using Stoke's theorem, but instead of having ϕ be a volume form, let it be a distributional form [12]. In particular, let ϕ be the Dirac delta function for a particular point.

By abuse of notation, we allow ∂M to mean not only a differentiable chain, but also the generalized characteristic function defined by the local degree of the projection mapping onto $(n-1)$-dimensional space. That is, ∂M describes a region of space, with an integer assigned to each point to say how many times it is counted. Then the idea that the non-degenerate boundary of a degenerate object is empty can be written more simply as: $\partial M = 0$.

8. Adjoint joint formula

We now have developed enough machinery to state and prove the main theorem:

$$(\partial F) * G = (-1)^k F * \partial G,$$

where F and G are chains whose dimensions sum to the dimension of the ambient Euclidean space, and k is the dimension of F. The proof is simple. Because of the dimensional hypotheses on F and G, $F * G$ is degenerate, but $\partial(F * G)$ is not degenerate. This means we can apply the result of the previous section, $\partial M = 0$, with $M = F * G$. That is, we imagine that F and G have been projected from analogous chains in general position in a higher dimensional space. This gives us

$$\partial(F * G) = 0$$

If we next apply the earlier equation for the boundary of a join, we get

$$(\partial F) * G + (-1)^{k+1} F * \partial G = 0.$$

Moving the right-hand term to the right of the equals sign gives the desired formula.

In the formula $(\partial F) * G = (-1)^k F * \partial G$ the boundary operator ∂ is self-adjoint, up to sign. The word adjoint is generally applied to operators that are dual to each other with respect to a product or pairing [13]. Therefore, I have decided to call $(\partial F) * G$ and $(-1)^k F * \partial G$ adjoint joins, even though this is not standard mathematical terminology. Similarly, I call this formula $(\partial F) * G = (-1)^k F * \partial G$ the adjoint join formula.

A simple example of an application of the adjoint join formula is given by fig. 5. The degenerate join of line segment AB with line segment CD is a projection of a tetrahedron onto the plane. Since $k = 1$, we have

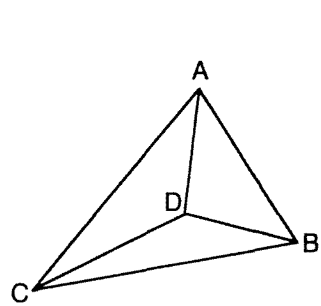

Fig. 5. The degenerate join of two line segments in the plane.

$$(\partial CD) * AB = -CD * \partial AB ,$$

$$(D - C) * AB = -CD * \partial AB ,$$

$$(C - D) * AB = CD * \partial AB ,$$

$$C * AB = D * AB + CD * \partial AB .$$

This can be interpreted to read that the join of C and AB (which is the triangle ABC) is equal to the join of D and AB plus the join of the line segment CD with the boundary of AB. The line segment CD is the "anti-boundary" of $D - C$, in analogy with the concept of an anti-derivative. So the join of C and AB is equal to the join of D and AB, plus the anti-boundary of the difference of C and D with the boundary of AB. This idea is not needed in a figure as simple as fig. 5, but it is useful in fig. 6, where the area of the join of C and the arc AB is not immediately calculable, but the area of the join of D with the arc AB is immediately calculable because D is the center of the circle that the arc lies on. Now you may say that one could simply, by inspection, partition fig. 6 into two triangles and a sector of a circular disk, and that is true, but the analogous statement in three dimensions is not true. There is no obvious way to compute the volume of the cone of a region on a sphere over a point other than the center. In this case, it is necessary to use the adjoint join formula. The value of being able to compute this volume will be shown in the next section, on computing the volume of a molecule.

But first let us consider another application of the adjoint join formula. In fig. 7 we have the join of a line segment and a circular arc, skew to each other in space. They are not actually coplanar, they just look that way because the illustration is two-dimensional. To apply the adjoint join formula we must find the chain one object bounds, and then take the boundary of the other object. Now we can compute the boundary of any chain, but we can compute the "anti-boundary" of a chain only if it is a boundary. Since neither the line segment nor the arc is a boundary, we must find a way to make one of them a boundary. We look for a chain that will complete the boundary. In fig. 7(a) we see that the chain is simply the two radial line segments joining the arc end points to the arc center. This introduces a new join on the right-hand side of the equation, which is simply two tetrahedra, the

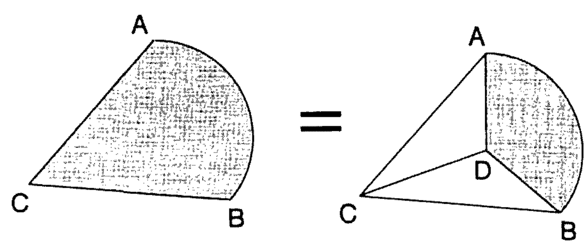

Fig. 6. The cone of an arc over a point not its center.

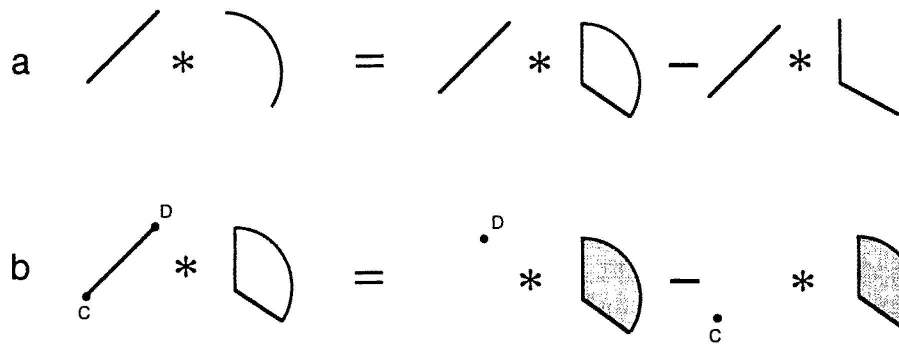

Fig. 7. Applying the adjoint join formula to the join of a line segment and an arc.

volumes of which are easily computed. The modified join, that of a line segment with the boundary of a sector, is now amenable to the adjoint join formula (fig. 7(b)). We replace the line segment by its boundary (one end point minus the other end point), and the sector boundary by its anti-boundary, the sector area. In both fig. 7(a) and fig. 7(b) we have implicitly used the distributive law. The volume of the cone of a sector area over a point is simply one-third the area of the sector times the altitude. This completes the calculation. The volume of the segment-arc join will be used in the molecular application below.

Applying the adjoint join formula is analogous to integration by parts: we must "integrate" one object and "differentiate" the other. By "integrate", I mean find the chain it bounds, and by "differentiate", I mean take its boundary. There are also analogies with parts of differential topology. The boundary of a join is analogous to the boundary of a product [14]. The boundary of a product is the boundary of the first factor times the second factor plus the first factor times the boundary of the second factor. This Leibniz rule for the boundary of a product is used in the idea of a spherical modification [15], also called surgery [16]. For both the adjoint join formula and a spherical modification one replaces the first factor by what it bounds and the second factor by its boundary.

Let us consider a simpler application of the adjoint join formula. Let S be a complete surface in space and let P and Q be any two points in space. By S being a complete surface, I mean that it has no boundary.

$$\begin{aligned} Q * S - P * S &= (Q - P) * S = (\partial PQ) * S \\ &= (-1)^k PQ * \partial S = (-1)^k PQ * 0 = 0 \end{aligned}$$

so

$$Q * S = P * S .$$

That is, the volume of the cone of a compete surface over a point is independent of the position of the point.

9. Molecular application

The volume of a molecule will be computed using the adjoint join formula. First we consider a two-dimensional figure (fig. 8), which illustrates the basic ideas. The area of a union of circular disks (fig. 8(a)) can be described as the cone of the boundary of the union over some (any) point in the plane. Let us call this cone vertex the central point. The method by which the boundary is computed is not described, but it is not difficult. The cone of the boundary is simply the sum of a set of cones over this central point, one cone for each arc of the boundary (fig. 8(b)). The method used in fig. 6 can be used to compute the areas of each of these cones (fig. 8(c)).

The three-dimensional case is similar. The boundary is the van der Waals surface, which may be computed analytically by a lengthy, complex algorithm [5]. Instead of arcs, we have regions on a sphere. The volume of each cone of a spherical face over the central point can be computed using the adjoint join formula to express this cone as the sum of a cone over the atom's sphere center plus the join of a line segment from the central point to the atom center with the boundary of the spherical face (analogously to fig. 6). The volume of the cone over the atom center is one-third the product of the sphere radius with the spherical region area, whose area may be computed using the Gauss–Bonnet formula [5,6]. The join of the line segment with the spherical face boundary is the sum of the joins of the line segment with each arc of the boundary. But we showed how to compute the join of a straight line segment with a circular arc in the previous section. So we are finished.

The adjoint join formula is related to an earlier method of mine [17] for computing van der Waals and solvent-excluded volumes of molecules. It is not hard to see that the non-shaded polygon region in fig. 8(c) can also be decomposed as in fig. 8(d), where there is an interior polygon with accessible atom centers as its

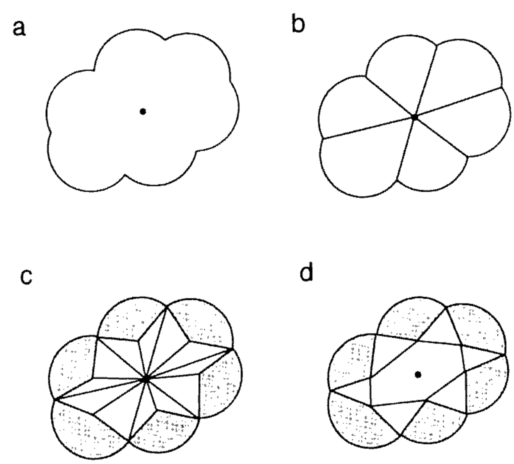

Fig. 8. Application to the union of circular disks indicates how to compute the volume of a molecule.

vertices. Figure 8(d) resembles fig. 2(b) of my earlier article. The current article's method for computing van der Waals volume is essentially equivalent to the one presented in the earlier article, except that the application-specific ad hoc construction used there is now seen to be an example of a general property of joins.

Another method for computing the van der Waals volume exactly has been developed by Gibson and coworkers [18–20]. It uses the inclusion-exclusion principle, which relates the volumes of unions to the volumes of intersections. It also uses the non-obvious fact that regardless of the number of spheres in the union, it is necessary to be able to compute intersections only up to order six.

The computation of the solvent-excluded volume, in which the van der Waals surface is smoothed by rolling a probe sphere over it, can also be performed using the adjoint join formula, once the solvent-accessible molecular surface has been computed. Unfortunately, this latter surface is difficult to compute, and for molecules with complex topographies, it is complicated by self-intersecting reentrant surfaces that produce cusps. Since my methods for handling cusps [21] cannot handle all possible cases, the exact and analytical computation of the solvent-excluded volume is still not completely solved.

10. Advantages and limitations of the method

The main advantages of the adjoint join formula are that it is:

- simple,
- general,
- analytic (exact).

Computing the volume of the union of simple geometrical objects using the adjoint volume formula involves these four steps:

- computing the boundary of the union,
- determining how to apply the formula to each face and its boundary,
- applying the adjoint formula to simplify the description of the cone over each face,
- computing the volume of the simplified geometrical objects using solid geometry and calculus.

These first two steps are more combinatorial in nature and require computer algorithms, not equations. This article does not present a general algorithm for either of the first two steps. It is also not completely clear how to specify what kinds of boundaries can be simplified. For example, unions of cones and cylinders generally produce faces whose boundaries are made up of non-circular arcs. The adjoint join formula can be used to move the cone vertex from the central point to a point lying on the axis of a cone or cylinder, but once this is done, there is no simple way to compute the volume of the part of the cone or cylinder delimited by these non-circular arcs. So for most solid-modeling applications, numerical methods are still required.

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