# Applications of Algebraic Topology to Compatible Spatial Discretizations

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*We provide a common framework for compatible discretizations using algebraic topology to guide our analysis. The main concept is the natural inner product on cochains, which induces a combinatorial Hodge theory. The framework comprises of mutually consistent operations of differentiation and integration, has a discrete Stokes theorem, and preserves the invariants of the DeRham cohomology groups. The latter allows for an elementary calculation of the kernel of the discrete Laplacian. Our framework provides an abstraction that includes examples of compatible finite element, finite volume and finite difference methods. We describe how these methods result from the choice of a reconstruction operator and when they are equivalent.*

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## Introduction

Compatible discretizations are model reduction techniques that replace continuum partial differential equation models by algebraic equations that mimic their fundamental structural properties. Spatial compatibility is especially relevant to coupled transient multiphysics simulations where unphysical modes from one model component may cause instability in the remaining components. In the context of hydrodynamics-transport applications spatial compatibility leads to locally conservative schemes that are consistent with integral forms of the conservation laws. It is well known that for weak solutions with shock waves the integral form is more relevant than the differential equation form. In particular, it leads to the Rankine-Hugoniot conditions that govern the speed and the form of the shock waves. As a result, compatible schemes are critical to obtain accurate approximation of shock speeds and positions; in contrast, non-compatible methods are not guaranteed to converge to weak solutions of the conservation law (Leveque, 2002).

We provide a common framework for compatible discretizations using algebraic topology (Flanders, 1989) to guide our analysis. This results in combinatorial operations of differentiation and integration that obey a discrete Stokes theorem. Furthermore, the invariants of DeRham cohomology groups (Dezin, 1995) are preserved in a discrete sense, which allows, among other things, for an elementary calculation of the kernel of the discrete Laplacian. One of the first applications of algebraic topology to compatible discretizations is due to (Hyman and Scovel, 1988). We draw upon many of the ideas proposed in that paper. Other works of note that use exterior calculus to develop compatible discretizations are (Mattiussi, 1997), (Dezin, 1995), (Hiptmair, 2001) and (Arnold, 2002). For further references in this area, we refer the reader to (Bochev and Hyman, 2005).

The key components of the framework are a restriction operator defined by the DeRham map and reconstruction operator. We show how some existing compatible finite element (Bossavit, 1998), finite volume (Nicolaides and Wu, 1997) and finite difference (Hyman and Shashkov, 1997) methods are obtained from the framework by specific choices of the reconstruction operator. This opens up a possibility to develop a common convergence and stability analysis across a range of discrete models (Berndt et al, 2001).

## Notation

We assume that the reader is familiar with the basic notions of exterior differential calculus as found in (Flanders, 1989). Below we briefly review notations that are used throughout the paper.

Let Ω denote a bounded region in three-dimensions. With $\Lambda^k(\Omega)$, $k$=0,1,2,3, we denote the set of all smooth differential forms $x \to \omega(x) \in \Lambda^k(T_x\Omega)$. Here $T_x\Omega$ is the tangent manifold to Ω at $x$. We recall the wedge product $\wedge : \Lambda^k(\Omega) \times \Lambda^l(\Omega) \mapsto \Lambda^{k+l}(\Omega)$ and the exterior derivative $d : \Lambda^k(\Omega) \mapsto \Lambda^{k+1}(\Omega)$. The exterior derivative satisfies $dd$=0 and gives rise to an exact sequence

$$\mathbf{R} \to \Lambda^0 \xrightarrow{\ d\ } \Lambda^1 \xrightarrow{\ d\ } \Lambda^2 \xrightarrow{\ d\ } \Lambda^3 \to 0 \tag{1}$$

called the De Rham complex. If Ω is a Riemannian manifold, the metric structure gives rise to an inner product $(\cdot,\cdot)$ on $\Lambda^k(\Omega)$ and an adjoint $d^*$ to $d$ defined by

$$(d\omega,\eta) = (\omega, d^*\eta). \tag{2}$$

The completion of $\Lambda^k(\Omega)$ with respect to the inner product is the Hilbert space of square integrable differential forms $\Lambda^k(L^2,\Omega)$. We also have the Sobolev spaces

$$\Lambda^k(d,\Omega) = \left\{\omega \in \Lambda^k(L^2,\Omega) \mid d\omega \in \Lambda^{k+1}(L^2,\Omega)\right\}. \tag{3}$$

We assume that the boundary of Ω consists of two disjoint, smooth, possibly empty components $\Gamma_1$ and $\Gamma_2$, respectively. At every boundary point, a differential form can be decomposed into its tangential and normal components, $\omega = \omega_t + \omega_n$. For the Sobolev spaces (3) we consider the boundary condition $\omega_t = 0$ on $\Gamma_1$.

### Translation of fields to forms

The relationship between forms and vector-scalar functions is determined as follows. Let $x,y,z$ be local coordinates. Then a 0-form is a function and a 3-form can be written as $\omega = f\, dx \wedge dy \wedge dz$. This defines the relation $\omega \leftrightarrow$ function. A 1-form can be written as $\omega = adx + bdy + cdz$ and a 2-form can be written as

$$\omega = ady \wedge dz + bdz \wedge dx + cdx \wedge dy\,. \tag{4}$$

Therefore, 1 and 2-forms are associated with vector fields. The action of the exterior derivative on 0,1 and 2-forms gives the action of the gradient, curl and divergence on the associated scalar or vector field. Furthermore, if $\omega_1$ and $\omega_2$ are two 1-forms with corresponding vector functions $v_1$ and $v_2$, then the wedge product $\omega_1 \wedge \omega_2$ is a 2-form with corresponding vector function $v_1 \times v_2$. If $\eta$ is a 2-form with corresponding vector function $v_3$, then the wedge product $\omega_1 \wedge \eta$ is a 3-form with scalar function $v_1 \times v_3$.

## Algebraic topology

In this section, we review some basic concepts in algebraic topology; see (Cairns, 1961), as they apply to deriving discrete approximations to differential operators. Our principal goal is to develop a framework that offers mutually consistent discrete notions of integration and differentiation and provides discrete operators that verify the basic vector calculus identities.

### Chain Complex

For simplicity, we restrict attention to computational grids that are simplicial complexes. However, all developments can be extended to general polyhedral chain complexes. For basic definitions and operations on simplexes, we refer to (Flanders, 1989). In particular, we recall the boundary operator $\partial$ with the property that $\partial\partial=0$.

A chain is a formal linear combination of *k*-simplexes. $C^k$ denotes the space of all k-chains. Thus, $c \in C_k$ if $c = \sum_i a_i s_k^i$ where $s_k^i$ are a *k*-simplexes and $a_i$ are real numbers. Boundary of a chain is defined by linearity. Assume that $K = (C_0, C_1, C_2, C_3)$ is a complex. Then, we have the exact sequence

$$0 \leftarrow C_0 \xleftarrow{\ \partial\ } C_1 \xleftarrow{\ \partial\ } C_2 \xleftarrow{\ \partial\ } C_3 \leftarrow 0. \tag{5}$$

In this sequence $C_0$ represents the set of all ordered vertices in the triangulation. The ordering of the vertices induces orientation of the edges $C_1$, the faces $C_2$ and the cells $C_3$ in the triangulation *K*.

### Cochain Complex

The space of all bounded linear functionals on $C_k$ is denoted by $C^k$. The elements of $C^k$ are called cochains and the duality pairing between chains and cochains is denoted by $\langle \cdot , \cdot \rangle$. The adjoint of $\partial$, $\delta : C^k \to C^{k+1}$ is defined by $\langle \partial c_{k+1}, c^k \rangle = \langle c_{k+1}, \delta c^k \rangle$. This operator, called coboundary, satisfies $\delta\delta=0$ and forms an exact sequence dual to (5):

$$0 \to C^0 \xrightarrow{\ \delta\ } C^1 \xrightarrow{\ \delta\ } C^2 \xrightarrow{\ \delta\ } C^3 \to 0. \tag{6}$$

Let $\{\sigma_k^i\}$ be a basis for $C_k$. The spaces $C_k$ and $C^k$ are isomorphic and we can identify the basis of $C^k$ with $\{\sigma_k^i\}$. Thus, $\langle \sigma_k^i, \sigma_k^j \rangle = \delta_{ij}$ and a cochain can be written as

$$c^k = \sum_i a_i \sigma_k^i . \tag{7}$$

The action of this cochain on a chain $c_k = \sum_i b_i \sigma_k^i$ is given by

$$\left\langle c^k, c_k \right\rangle = \sum_{i,j} a_i b_j \left\langle \sigma_k^i, \sigma_k^j \right\rangle = \sum_i a_i b_i . \tag{8}$$

## Compatible discretizations

We define all discrete structures in our framework by using two basic operators. The reduction operator $\mathcal{R} : \Lambda^k\left(L^2, \Omega\right) \to C^k$ translates forms to cochains and is given by the De Rham map

$$\left\langle \mathcal{R}\omega, \sigma \right\rangle = \int_\sigma \omega . \tag{9}$$

This map establishes discrete representation of *k*-forms in terms of global quantities associated with the chain complex *K*. Therefore; *k*-forms are encoded as *k*-cell quantities. The De Rham map has the important Commuting Diagram Property $\mathcal{R}d = \delta\mathcal{R}$.

The reconstruction operator $\mathcal{I} : C^k \to \Lambda^k\left(L^2, \Omega\right)$ translates cochains back to forms. Owing to the many possible ways in which global information can be used to obtain local representations, the choice of this operator is quite flexible. However, to obtain consistent discrete structures this operator must satisfy two conditions. Specifically, $\mathcal{I}$ must be a right inverse of $\mathcal{R}$

$$\mathcal{R}\mathcal{I} = id \tag{10}$$

and an approximate left inverse of that operator:

$$\mathcal{I}\mathcal{R} = id + O(h^s) . \tag{11}$$

In Eq. (11) *s* and *h* are positive real numbers that give the approximation order and the partition size in *K*, respectively. From Eq. (10) follows that

$$\ker \mathcal{I} = 0 . \tag{12}$$

The range of $\mathcal{I}$ is required to contain at least square integrable forms. When the range of $\mathcal{I}$ is a subspace of the Sobolev spaces in Eq. (3), we call $\mathcal{I}$ a conforming reconstruction operator.

### Combinatorial operations

The integral of $a \in C^k$ is defined on chains $\sigma \in C_k$ by duality:

$$\int_\sigma a = \langle a, \sigma \rangle . \tag{13}$$

To define a discrete derivative acting on cochains note that forms are dual to chains with respect to the pairing induced by integration and that, according to the Stokes theorem, *d* is the adjoint of $\partial$. We mimic this by using the duality of $C_k$ and $C^k$. Since $\partial$

is adjoint to δ, it follows that the discrete gradient, curl and divergence are given by the action of the coboundary.

**Natural and derived operations**

Natural operations are defined by composition of $\mathcal{I}$ with the desired analytic operation. Thus, they provide the best possible approximations of these operations on cochains. The natural inner product on cochains is given by

$$(a,b) = (\mathcal{I}a, \mathcal{I}b) \tag{14}$$

and the natural wedge product is defined by the formula

$$a \wedge b = \mathcal{R}(\mathcal{I}a \wedge \mathcal{I}b). \tag{15}$$

Nondegeneracy of the inner product follows from Eq. (12).

The derived operations are induced by the natural operations. The inner product on cochains in Eq. (14) gives rise to an adjoint $\delta^*: C^{k+1} \mapsto C^k$ of δ by virtue of $(\delta^* a,b) = (a,\delta b)$. This adjoint has the property that δ*δ*=0 and provides a second set of discrete gradient, curl and divergence operators. The use of δ or its adjoint δ* is determined by the encoding of scalar functions by 0 or 3-forms and of vector functions by 1 or 2-forms, respectively.

Using δ and δ* we define a discrete Laplacian $D: C^k \mapsto C^k$ by the formula

$$D = \delta^*\delta + \delta\delta^*. \tag{16}$$

The derived operations are necessary to avoid internal inconsistencies between the discrete operations in the framework. Because reconstruction is an approximate inverse of the reduction, using only natural definitions will lead to conflicts between the resulting set of operations. For example, the analytic adjoint is given by $d^* = (-1)^k * d\, *$. As a result, a natural definition of the discrete adjoint is

$$\delta^* = (-1)^k \mathcal{R} * d * \mathcal{I}. \tag{17}$$

Note that Eq. (17) requires $\mathcal{I}$ to be a conforming operator, a property that is not needed for the derived definition of the adjoint. More importantly, however, the natural definition of the adjoint is incompatible with the natural definition of the inner product in Eq. (14). One can show that $(\delta^* a,b) = (a,\delta b) + O(h^s)$ and so, the operator defined in Eq. (17) is not the adjoint of δ with respect to the inner product defined in Eq. (12).

Because $C^k$ are finite dimensional spaces, all discrete operations can be realized by matrices acting on vectors of coefficients formed by the quantities associated with the *k*-cells of the complex *K*. For further details about this aspect of the discrete framework, we refer the reader to (Bochev and Hyman, 2005).

**Mimetic properties**

The combinatorial, natural and derived operations defined in the last section, mimic the properties of their analytical counterparts. Discrete integration and differentiation satisfy a discrete Stokes theorem:

$$\left\langle \delta c^{k-1}, c_k \right\rangle = \left\langle c^{k-1}, \partial c_k \right\rangle. \tag{18}$$

Eq. (18) is a consequence of the definition of the discrete derivative as the adjoint of the boundary operator. The discrete derivative and its adjoint and the discrete wedge product satisfy the standard vector calculus identities $\delta\delta = \delta^* \delta^* = 0$ , $a \wedge b = (-1)^{kl} b \wedge a$, and

$$\delta(a \wedge b) = \delta a \wedge b + (-1)^k a \wedge \delta b \tag{19}$$

Note that Eq. (19) requires a conforming reconstruction operator.

The inner product in Eq. (12) induces a combinatorial Hodge theory on cochains (Dodziuk, 1973). We can define the set of harmonic cochains

$$H^k(K) = \left\{ c^k \in C^k \mid \delta c^k = \delta^* c^k = 0 \right\} \tag{20}$$

and then obtain a discrete Hodge decomposition $a = \delta b + h + \delta^* c$ on $C^k$. Using this decomposition it is possible to show (Dodziuk, 1973), (Hyman and Scovel, 1988), (Bochev and Hyman, 2005), that the size of the kernel of the analytic Laplacian is the same as the size of the kernel of the discrete Laplacian. This remarkable property of the discrete Laplacian is a consequence of using the derived, rather than the natural definition of the adjoint δ* in Eq. (16).

**The choice of the primary operation**

In our framework, the primary discrete operation is the natural inner product on cochains. Other approaches; see e.g., (Hiptmair, 2001) or (Bossavit, 1998) make the discrete $*$ the primary discrete operation and its construction is the central problem. In (Bochev and Hyman, 2005) it is demonstrated that a natural definition of this operator is not compatible with the natural inner and wedge product operations, while a derived $*$ operation is not compatible with the reconstruction and the reduction mappings. Furthermore, both the derived and the natural $*$ are not compatible with the derived adjoint δ*. Therefore, in a consistent discrete framework the primary operation can be either the natural inner product or the discrete $*$ operation. Our choice is motivated by the complications that arise in the definition of a good discrete $*$ and the fact that the inner product is sufficient to induce a combinatorial Hodge theory on cochains.

Most often, a discrete $*$ is required to discretize material laws. Because of the difficulties with this operation, we prefer either to incorporate material laws in the definition of the natural inner product, or to enforce them in a weak sense. In the first case we use the adjoint δ* and in the second we translate the problem into an equivalent constrained optimization problem. This approach guarantees that the discrete Laplacian is always a symmetric and semi-definite operator.

## Applications

In this section we discuss two basic types of models that arise in the discrete framework. Then we provide examples of reconstruction operators that lead to finite element, finite volume and finite difference realizations of the discrete models.

As a model problem, we consider the eddy current equations written in invariant form as a first-order system with material laws,

$$de = -d_t b; \quad dh = j; \quad *_{\mu^{-1}}\, b = h; \quad *_{\sigma^{-1}}\, j = e. \tag{21}$$

as a first-order system in terms of codifferentials

$$de = -d_t b; \quad e = *_{\sigma^{-1}}\, d *_{\mu^{-1}}\, b \tag{22}$$

and as a second order system

$$d *_{\sigma^{-1}}\, d *_{\mu^{-1}}\, b = -d_t b. \tag{23}$$

We assume that Eqs. (21)-(23) are augmented by the appropriate boundary conditions.

Eqs. (22)-(23) do not involve explicit material laws and can be discretized without any further transformations. A direct mimetic discretization translates the forms in Eqs. (22)-(23) to cochains and then uses the available discrete derivatives to mimic the original equations. Thus, the direct mimetic models of Eqs. (22) and (23) are given by

$$\delta e^1 = -\delta_t b^2; \quad e^1 = \delta^* b^2 \tag{24}$$

and

$$\delta \delta^* b^2 = -\delta_t b^2, \tag{25}$$

respectively. If the discrete time derivative $\delta_t$ commutes with the discrete derivative from Eq. (24) we see that $b$ stays divergence free if it was divergence free at the initial time moment.

A conforming mimetic discretization restricts Eqs. (22)-(23) to the range of $\mathcal{IR}$. This requires $\mathcal{I}$ to be a conforming reconstruction operator so as to obtain finite dimensional subspaces of the appropriate Sobolev spaces. For examples of such methods, we refer to (Bochev and Hyman, 2005) where it is shown that for conforming reconstruction operators direct and conforming mimetic methods are equivalent.

Eq. (21) involves material laws and its straightforward discretization would require a discrete $*$ operation for their approximation. To avoid construction of this operation we first translate Eq. (21) to an equivalent constrained optimization problem

$$\min \frac{1}{2}\left( \left\| j - *_\sigma e \right\|^2 + \left\| b - *_\mu h \right\|^2 \right) \quad \text{subject to} \quad de = -d_t b \;\; \text{and} \;\; dh = j \tag{26}$$

and then discretize Eq. (26). A direct mimetic model of Eq. (26) is obtained by translating the forms to cochains and then solving the discrete optimization problem

$$\min \frac{1}{2}\left( \left\| j^2 - e^1 \right\|^2 + \left\| b^2 - h^1 \right\|^2 \right) \quad \text{subject to} \quad \delta e^1 = -\delta_t b^2 \;\; \text{and} \;\; \delta h^1 = j^2. \tag{27}$$

We can also define a conforming discretization of Eq. (26) by restricting minimization to the range of $\mathcal{IR}$. As before, this requires $\mathcal{I}$ being a conforming reconstruction operator.

Let us now provide some examples of reconstruction operators. For simplicity, we consider two-dimensional grids and reconstruction of 1-forms from 1-cochains. To define the covolume reconstruction operator (Trapp, 2004) each triangle is divided into three subregions by connecting the circumcenter to the nodes as shown in Fig. 1

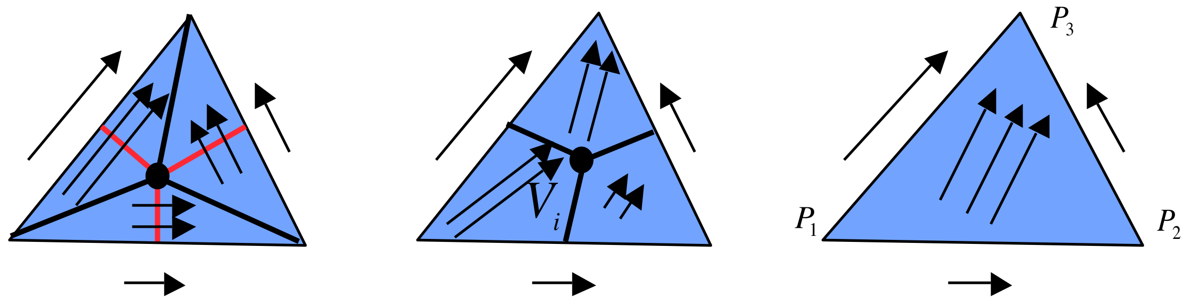


**Figure 1.** Examples of reconstruction operators: covolume (left), mimetic (center) and Whitney (right).

The covolume reconstruction operator maps the 1-cochain associated with the edges of the triangle to a picewise constant field. On each sub-triangle the image is the constant vector field that is parallel to the edge of the triangle and has circulation given by the cochain value. The range of this reconstruction operator is in the Hilbert space $\Lambda^k(L^2,\Omega)$ but not in the Sobolev space $\Lambda^k(d,\Omega)$. Therefore, covolume reconstruction is not conforming and can only be used in direct discretizations. A unique property of covolume reconstruction is that derived operators have local stencils and there is a discrete $*$ star operation that is compatible with the natural inner product. This property follows from the fact that covolume reconstruction can be associated with cochains on a Voronoi-Delaunay grid complex; see (Trapp, 2004), (Nicolaides and Wu, 1997). This association also implies that existence of the covolume reconstruction is contingent upon the existence of the Voronoi regions and so the simplexes must satisfy an angle condition (Nicolaides and Wu, 1997).

Mimetic reconstruction (Hyman and Shashkov, 1997) acts in a similar way and recovers a piecewise constant field that is in $\Lambda^k(L^2,\Omega)$ but not in $\Lambda^k(d,\Omega)$. The main difference is that mimetic reconstruction uses subregions associated with the vertices of the triangle; see Fig. 1, and so, they are bordered by two edges. The constant field on each subregion is defined to be the linear combination of the edge vectors with coefficients equal to the values of the 1-cochain on the edges. Mimetic reconstruction is less restrictive than the covolume one because existence of the subregions is not contingent upon the circumcenter being inside the triangle. However, mimetic reconstruction gives rise to non-local derived operators.

The Whitney map (Whitney, 1957), (Dodziuk, 1973) is an example of a conforming reconstruction operator whose range is in the Sobolev space $\Lambda^k(d,\Omega)$. Let $P_i$; $i$=1,2,3 be the vertices of the triangle (see Fig. 1) and $\{\lambda_i\}_{i=1}^{3}$ their barycentric coordinates. The Whitney 1-forms on the triangle are given by

$$\omega_{ij} = \lambda_i d\lambda_j - \lambda_j d\lambda_i; \quad 1 \le i < j \le 3. \tag{28}$$

Let $c^1 = (c_{12}, c_{13}, c_{23})$ be a 1-cochain where $c_{ij}$ is the value associated with the edge whose endpoints are $P_i$ and $P_{i,}$. Whitney reconstruction maps $c^1$ to a differential 1-form according to the formula

$$\mathcal{I}c^1 = \sum_{i<j} c_{ij}\omega_{ij} = \sum_{i<j} c_{ij}\left(\lambda_i d\lambda_j - \lambda_j d\lambda_i\right). \qquad (29).$$

It is not hard to see that the right hand side in Eq. (29) is indeed a differential 1-form with polynomial coefficients. It is possible to show that gluing together reconstructions from all triangles gives rise to a piecewise polynomial 1-form that is in the Sobolev space $\Lambda^k(d,\Omega)$ (Dodziuk, 1973).

The covolume reconstruction is most often encountered in finite volume type discretizations (Nicolaides and Wu, 1997), (Trapp, 2004). Mimetic reconstruction has been used in the so-called mimetic finite difference methods (Hyman, Shashkov, 1997). Whitney map, on the other hand is an example of reconstruction that leads to discrete models of the finite element type. It has been extensively used in finite element methods for the Maxwell's equations (Bossavit, 1998).

## Conclusions

In this paper, we described a general framework for mimetic discretizations that uses two basic operators to define all discrete structures. In this framework cochains approximate scalars and vectors. Differentiation and integration are combinatorial operations induced by the De Rham map. Inner product and wedge product are natural operations defined by a reconstruction operator. The inner product induces an adjoint derivative and a discrete Laplacian. Together with the combinatorial and natural operations, these derived operations comprise the basis of the mimetic framework.

The choice of the natural and derived operations is governed by the internal consistency of the framework. In particular, a consistent discrete framework requires a choice of its primary operation. In our approach, this operation is the natural inner product on real cochain spaces. In other approaches, the key concept is the discrete $*$ operation and its construction is the principal computational task.

The choice of the inner product instead of the $*$operation is motivated by the complications that arise in the construction of the latter and the fact that the inner product is sufficient to induce a combinatorial Hodge theory on cochains. For problems that require approximations of material laws, we propose to consider constrained optimization formulations that enforce the laws weakly. In all other cases, our framework offers the choice of direct and conforming methods. Direct methods are representative of the type of discretizations that arise in finite volume and finite difference methods while conforming methods are typical of finite element methods. For conforming reconstruction operators direct and conforming methods are equivalent. This opens up a possibility to carry out error analysis of direct mimetic methods by using variational tools from finite elements. A recent example is the analysis in (Berndt et al, 2001).

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