An electrical engineering perspective on missed opportunities in computational physics

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October 11, 2018

We look at computational physics from an electrical engineering perspective and suggest that several concepts of mathematics, not so well-established in computational physics literature, present themselves as opportunities in the field. We emphasize the virtues of the concept of elliptic complex and highlight the category theoretical background and its role as a unifying language between algebraic topology, differential geometry and modelling software design. In particular, the ubiquitous concept of naturality is central. We discuss the Galerkin finite element method as a way to achieve a discrete formulation and discuss its compatibility with so-called cochain methods. Despite the apparent differences in their underlying principles, in both one finds a finite-dimensional subcomplex of a cochain complex. From such a viewpoint, compatibility of a discretization boils down to preserving properties in such a process. Via reflection on the historical background and the identification of common structures, forward-looking research questions may be framed.

1 Introduction

A finite formulation of the governing equations is necessary for computer simulations of physical phenomena. The traditional approach to this in continuum physics is a discretization – a way to transfer from continuum to discrete – for the spaces arising from the (partial) differential equations that describe the phenomenon in question. Another route is to use an algebraic formulation utilizing macroscopic quantities. In this paper, we discuss finite formulations from an electrical engineering perspective, reaching out especially to the engineering, computational physics, and applied mathematics communities. The topic of our interest is the nature of the process of obtaining finite, discrete descriptions of (continuum) physics. Through articulating physics via such concepts as natural differential operators and elliptic complexes, the framework of category theory (Adamek et al., 2009) provides a sense of synthesis to the seemingly scattered field. At first glance, the concepts of category theory may steer the reader’s thoughts towards foundations of mathematics. However, on a closer look, it is also the glue and common ground throughout computational physics. Evolving from such foundational questions as the distinction between sets and classes in

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order to resolve the paradoxes of set theory and the foundations of mathematics, category theory leads to the foundations of computer science. Unfortunately, these days, the foundations of computer science are largely eclipsed by the needs of computer engineering. However, computational electromagnetics has demonstrated a more direct role for category theory in linking engineering design to software methodology, as we will discuss in this paper.

The title of this paper is a deliberate reference to Freeman Dyson’s paper entitled *Missed opportunities* (Dyson, 1972). Throughout this paper, we aim to bring forth concepts of mathematics, which, at least in hindsight, present themselves as opportunities for computational physics but paths less traveled in this context. Certainly, we are not in the position to give such insightful advice as Dyson did in his aforementioned influential work, but we hope to be able to frame some future research with a fresh point of view stemming from our electrical engineering background.

1.1 Recent historical background and motivation

From an engineer’s viewpoint, the importance and practical value of considering foundational issues related to discrete descriptions of continuum physics is evident in the context of framing forward-looking research problems. In electrical engineering, albeit via arguably confusing terminology, Gabriel Kron was one of the pioneers to promote the use of both differential geometry and algebraic topology in applications, and for finding unifying concepts in discrete and continuous descriptions of electromagnetism (see e.g. (Kron, 1959a), (Kron, 1959b)). J. P. Roth would also follow up on Kron’s work, and discuss e.g. homological techniques for electrical engineering in a systematic manner (Roth, 1955), (Roth, 1959), (Roth, 1971). Later, Balasubramanian et al. explained Kron’s methods with more modern terms partially filling the gap between the languages used by Kron and mathematicians (1970).

Taking a view from the 1980s in the computational electromagnetics (CEM) community, the ideas initiated by Kron and his followers had still not quite penetrated the field. Finite element modelling was becoming more accessible due to development of computers. However, issues regarding spurious, unphysical solutions had plagued modelling in the finite elements setting since the 1960s, when Silvester brought finite elements to the context of CEM (Silvester, 1969). Meanwhile, methods of finite-difference time-domain (FDTD) type utilizing staggered grids, originally introduced by Yee (1966), were also being developed (Taflove, 1980). In the wake of recent developments by mathematicians such as Dodziuk (1976), (1981), Kotiuga’s works of the time (see e.g. (Kotiuga, 1984), (Kotiuga, 1989a)) presented a journey to the early mathematical literature, while connecting with and renewing the state-of-the-art of CEM, emphasizing topological aspects. Around the same time, Alain Bossavit described the framework of Whitney forms for finite element setting, introduced by Whitney long before the era of computer-aided modelling (Whitney, 1957), to the engineering community (Bossavit, 1988a), (Bossavit, 1988b), (Bossavit, 1988c). After the appearance of Kotiuga’s PhD thesis (Kotiuga, 1984), Bossavit noted the correspondence between Whitney forms and Nédélec elements (Nédélec, 1980) and their affine invariance, and that this was a key to resolving several outstanding problems in three-dimensional computational electromagnetics. In fact, Whitney forms first appeared in (Weil, 1952). This paper by André Weil, representing partially a foundation of algebraic topology and a category theoretical rationale for Whitney forms, was a source of considerable anxiety, initiating the final countdown for Bourbaki’s aspirations for a set-theoretic foundation of mathematics. In the meantime Whitney forms played a crucial role in some geometrically motivated mathematical works by, for example, Dodziuk. However, it was the engineering
community that finally revived Whitney forms in the 1980s, understanding their significance in the context of CEM. For engineering applications, Whitney forms, widely used today in the context of finite element computations, ensure nice continuity properties and help avoid unphysical, spurious solutions (Bossavit, 1990), thus redeeming some of the issues that were related to finite element methods. Later, Ralf Hiptmair re-formulated and generalized the framework to higher-order forms (Hiptmair, 1999), (Hiptmair, 2001a).

While the framework of Whitney forms discretizes metric-independent properties effectively, on the flip-side of the coin one has the problem of discrete constitutive relations, which tend to be metric-dependent (Tarhasaari et al., 1999), (Hiptmair, 2001b), (Kangas et al., 2011), (Auchmann and Kurz, 2006). As the search for compatible, structure-preserving discretizations led to the research program of discrete exterior calculus (DEC) (Arnold et al., 2006), Kotiuga brought some of the relevant historical mathematical questions in relation to such program together with present state of CEM (Kotiuga, 2008). In particular, the discrete star localization problem, which states that a discrete version of Hodge star operator, ubiquitous in constitutive laws of physics, cannot be local in the same sense as its continuum counterpart it mimics, casts a shadow on the hope of discretizing constitutive relations in a fully structure-preserving manner. Moreover, the so-called commutative cochain problem, related to the impossibility of finding a fully structure-preserving discrete analogue for the exterior product of differential forms, poses further limitations for the possibilities of DEC. Simply, some of the properties of continuum theory seem not to be reproduced in the discrete setting. The bottom line is that the (at least seemingly) inherent difference of discrete and continuum formulations is thus still largely unresolved: Is there a coherent theoretical framework which reveals a given discretization procedure as being canonical?

As for continuum descriptions, theories of physics typically formalize our intuition of continuum by stating their principles in the form of differential equations required to hold in each point of the space. As a consequence, one is confronted with infinite-dimensional function spaces, when utilizing such theories to make predictions. Apart from very simple cases, approximative solutions to the arising field problems are needed: One is required to form a discretization for the function space to find a solution with a finite set of information. Numerical solution methods of field problems, such as the finite element method (FEM) (Oden and Reddy, 2011), (Reddy and Gartling, 2001), (Strang and Fix, 2008), rely on such discretizations: ways to transfer from continuum to a discrete space.

Modelling the world directly utilizing macroscopic quantities, in some sense, avoids the tedious limit process that is inevitable in the differential description of the world (Tonti, 2014). Moreover, one can argue that macroscopic quantities are the ones closer to our true experience, since they are the ones closer to measurements: Instead of electric fields we measure voltages, and instead of electric current densities we measure electric currents, for example.\footnote{Of course, this is not to say that we are claiming anything about direct measurability of any macroscopic quantity.} Hence, numerical methods starting from algebraic equations concerning macroscopic quantities, such as the cell method (CM) (Tonti, 2001), have been developed. The fundamental ideas leading to CM date back to Maxwell’s notions of analogies between different physical theories and were articulated by Tonti in terms of Tonti diagrams (Tonti, 1972), (Tonti, 1977).\footnote{Continuing this path, now applied category theory can be seen as a pervasive effort of transporting analogous ideas formally between mathematics and science as well as between different fields of science. For some striking analogies articulated via categories, see e.g. (Baez and Stay, 2011).} CM does not require a model to be represented in terms of discretized differential equations to obtain a finite formulation suitable for computers, as it avoids the
differential formulation altogether.

Methods such as the cell method, or the finite integration technique (FIT) (Weiland, 1977)\textsuperscript{3}, often referred to as cochain methods, are sometimes called directly discrete methods as they would seem to provide a discrete formulation directly, without resorting to a discretization of any sort. This view has been emphasized in the context of CM especially by Ferretti, for example in (Ferretti, 2013) and by Tonti to a lesser extent (Tonti, 2014). Although Tonti’s take on the issue is perhaps meant to be rather of pedagogical value than an ideological statement about the ontology of modelling, Ferretti goes even further in expounding that no discretization is needed in CM. This view has its justification and value in the sense that indeed no differential equations are discretized. However, in the formal sense, such a view is problematic: Neither the representation of laws of nature in terms of algebraic topology, as is the starting point for CM, nor in terms of differential geometry, as is the starting point for FEM\textsuperscript{4}, is directly suitable for a discrete formulation in physics of continuum. This critique is rooted in the mathematics of continuum physics.

1.2 Methodology and objectives

For the sake of simplicity, we will be concerned with representing physics with partial differential equations expressed in terms of differential forms and algebraic equations expressed in terms of cochains, a macroscopic counterpart for differential forms. Thus, e.g. mixed tensor physics is not explicitly considered. While pointing out several “missed opportunities” in computational physics of continuum, we shall discuss the contents of the diagram

\[
\text{Cochains} \xrightarrow{\text{Limit process}} \text{Differential forms} \xrightarrow{\text{Integration}} \text{Discrete formulation} \quad \text{Discretization} \\quad \text{Discrete formulation} \xrightarrow{\text{Discretization}}
\]

where nodes represent formulations of physics and arrows represent ways to travel between them. Cochains are the mathematical tool for representing macroscopic quantities of physics. There is a well-known one-to-one correspondence between cochains and differential forms. Through limit process, one obtains their differential form counterparts, defined pointwise, from which through integration over macroscopic $p$-volumes, one again

\textsuperscript{3}Even though FIT explicitly considers physical variables as integrals of field quantities, one is still effectively dealing with the physics macroscopically to begin with. Hence, we consider FIT a close relative of CM. FIT indeed started off dubbed as a FDTD-like method but was later explicitly set in a more geometric setting by Weiland (1996).

\textsuperscript{4}Differential geometry provides a modern framework and a suitable formalism for presenting FEM. The historical roots go back to “Dirichlet’s Principle”, which is one of Hilbert’s 23 problems from 1900. Historically, it is not due to Dirichlet but Riemann who attributed the principle to Dirichlet because he needed to assume the existence of solutions to Laplace’s equation in order to develop his theory of functions of a complex variable. Hilbert’s student, Ritz, attacked this problem from a constructive point of view in the early 1900s, but it was Richard Courant’s definitive treatment in the late 1920s that gave birth to both a constructive proof of Dirichlet’s principle, and to FEM. As a numerical method, FEM can be traced to the interactions between John Von Neumann and Courant close to two decades later in the early days of programmable computers. For the related history, see e.g. (Courant, 1943), (Gander and Wanner, 2012), (Gorkin and Smith, 2005) (Pelosi, 2007), (Taylor, 2002), and references therein.
obtains cochains. For example, in electromagnetism, the integral of the magnetic flux density differential 2-form $B$, related to infinitesimal surfaces, over a surface $S$ yields the magnetic flux cochain $\Phi$ through $S$. We emphasize the similarity of the two different routes to a discrete formulation depicted in the diagram.\footnote{For comprehensive studies of similarities between different numerical methods from a different viewpoint, see e.g. (Bochev and Hyman, 2006), (Mattiussi, 1997).} In particular, we discuss Galerkin FEM and cochain methods as examples. While cochain methods access the global macroscopic quantities directly unlike FEM, infinite-dimensional function spaces are inherently present in both before the discretization is made. This has implications for computational physics through the identification of structural similarities.

We will highlight the category theoretical background arising from algebraic topology and differential geometry within computational physics. In particular, the ubiquitous concept of naturality plays a central role (Kolar et al., 1993). There are many facets to such background. Category theory has been slowly penetrating modern physics and computation (Baez and Dolan, 1998), (Baez and Stay, 2011), (Coecke and Paquette, 2011), (Lal and Teh, 2015), (Nikolaus and Schweigert, 2012) and even engineering sciences (Baez and Erbele, 2015), (Baez and Fong, 2015). Semantics of computation may be articulated via category theory: Lambda calculus and functional programming sit naturally in this context (Baez and Stay, 2011), (Milewski, 2017). Common functional programming languages, such as Haskell\footnote{http://www.haskell.org}, can be seen as instances of the general theory. We aim to argue that category theory as a unifying language between concepts of algebraic topology and differential geometry, as well as the language of computer science and programming, may provide synthesis to the seemingly scattered field of computational physics and be beneficial in programming discrete solvers.

Hence, this is a paper about computational physics, written from the viewpoint of electrical engineers and meant to initiate discussion across disciplines and frame future research. As recent engineering history shows, rigorous identification of underlying structures is often the key for forward-looking research.

### 1.3 The structure of the article

In section 2, we discuss mathematical structures underlying continuum physics and its discrete descriptions. In particular, complexes of chains and cochains with some further structures imposed on them, as well as the concepts of ellipticity and naturality are discussed. Moreover, we address homology and cohomology of such complexes. In section 3, we examine the correspondence between cochains and differential forms. In these sections, we emphasize the category theoretical background rooted in these concepts. In section 4, we discuss how to achieve a discrete formulation of a partial differential equation description of continuum physics, using FEM as an example. Some background in differential geometry and algebraic topology is beneficial. For this, we refer the reader to e.g. (Gross and Kotinga, 2004) and (Frankel, 2012). In section 5, we discuss the unifying underlying structures present in the discretizations of cochain methods and FEM and thus point out problems related to the concept of directly discrete methods. In section 6 we make a few remarks on a categorical approach to simplicial complexes and how the discussion thus far and the chosen approach relate to programming discrete solvers for continuum physics. In section 7, we gather the “missed opportunities” together to present them as open research problems, and finally in section 8, conclusions are drawn.
2 Mathematical structures for discrete solvers

Physical quantities are related to geometrical objects. For example, we have force-like quantities related to paths, flows and fluxes through surfaces, and quantities contained by a volume. Formalizing this intuition in terms of mathematics, these geometrical objects are chains, formal sums of what we call cells, and the quantities related to them are called cochains. A thorough exposition of such algebraic topological concepts in the context of electromagnetic modeling can be found in (Gross and Kotiuga, 2004). Keränen’s thesis (2011) offers an accessible treatment of cochains, although it has an emphasis on electromagnetism on semi-Riemannian manifolds. For a classic exposition, we refer the reader e.g. to (Whitney, 1957).

Here, we shall recall the notions of chain and cochain complexes, and the relevant complexes with additional structures, elliptic complexes in particular. We will be rigorous but brief, leaving some details to be elaborated on in the references.

2.1 (Co)chain complexes.

To be able to model quantities related to geometric objects of different dimensions, we want to combine the (co)chains of different dimension in a single structure, a (co)chain complex on a topological space \( \Omega \), a sequence of Abelian groups or modules. As is often desirable in continuum physics, dealing with (co)chains with coefficients in \( \mathbb{R} \), the resulting spaces are vector spaces.

Combining the information we have in the spaces of chains of different dimensions \( C_i(\Omega) \) and the boundary operators \( \partial \) acting as mappings between them, we obtain the sequence

\[
0 \to C_n(\Omega) \overset{\partial}{\to} C_{n-1}(\Omega) \overset{\partial}{\to} \ldots \overset{\partial}{\to} C_0(\Omega) \to 0,
\]

with \( \partial \circ \partial = 0 \), defining a **chain complex** on \( n \)-dimensional \( \Omega, C_x(\Omega) \). Dually, a **cochain complex** on \( \Omega, C^x(\Omega) \), is the sequence

\[
0 \leftarrow C^n(\Omega) \overset{d}{\leftarrow} C^{n-1}(\Omega) \overset{d}{\leftarrow} \ldots \overset{d}{\leftarrow} C^0(\Omega) \leftarrow 0
\]

of cochain spaces of different dimensions \( C^i(\Omega) \) with coboundary operators \( d \) between them. Again, \( d \circ d = 0 \). Such complexes are **exact** if the images of the (co)boundaries match with the kernels of the following ones.

A **subcomplex of a chain complex**, or a **chain subcomplex** of \( C_x(\Omega) \) is a chain complex \( \kappa_x(\Omega) \) consisting of spaces \( \kappa_p(\Omega) \subset C_p(\Omega) \) with \( \partial \kappa_{p+1}(\Omega) \subset \kappa_p(\Omega) \) (Naber, 1980). Similarly, a **cochain subcomplex** \( \kappa^x(\Omega) \) of \( C^x(\Omega) \) consists of spaces \( \kappa^p(\Omega) \subset C^p(\Omega) \) with \( d \kappa^p(\Omega) \subset \kappa^{p+1}(\Omega) \). Note that a finite (co)chain complex arising from a cellular mesh complex on \( \Omega \) is a subcomplex of the infinite-dimensional (co)chain complex on \( \Omega \).

A **chain map** between chain complexes \( C_x(\Omega_1) \) and \( C_x(\Omega_2) \) is a sequence of structure-preserving mappings \( f_i: C_i(\Omega_1) \to C_i(\Omega_2) \) for all \( i \in \{0,1,...,n\} \) such that \( f_i \circ \partial = \partial \circ f_{i+1} \). That is, the boundary maps on the two complexes commute with \( f_i \). Dually a **cochain map** between cochain complexes \( C^x(\Omega_1) \) and \( C^x(\Omega_2) \) is a sequence of structure-preserving mappings \( f^i: C^i(\Omega_1) \to C^i(\Omega_2) \) for all \( i \in \{0,1,...,n\} \) such that \( f^i \circ d = d \circ f^{i-1} \). (Co)chain maps are thus induced by mappings between \( \Omega_1 \) and \( \Omega_2 \). (Co)chain complexes and (co)chain maps form the **category of (co)chain complexes**. \( C_x(\Omega) \) and \( C^x(\Omega) \) are functors from the category of topological spaces and continuous maps to this category, attaching a (co)chain complex to each topological space and a (co)chain map to each continuous mapping between such spaces.
2.2 Elliptic complexes

The elliptic complex was popularized over half a century ago by Donald Spencer, primarily through his student J. J. Kohn (Kohn, 1972). Advantageously, an elliptic complex gives rise to a Hodge theory which, when restricted to the de Rham Complex, yields the traditional Hodge theory of differential forms (see e.g. (Wells, 1980) for a more recent exposition).

To articulate what exactly is an elliptic complex, we need a few definitions. We shall follow the notation of (Gilkey, 1974), which is a standard reference for more details. Confining ourselves first to $\mathbb{R}^n$, with all functions complex-valued, a linear differential operator $P(x, D) = \sum_{|\alpha| \leq m} a_\alpha(x) D^\alpha$ has the associated symbol $\sigma(P) = p(x, \chi) = \sum_{|\alpha| \leq m} a_\alpha(x) \chi^\alpha$, with formal variables $\chi^\alpha$ replacing the partial derivatives $D^\alpha$ with respect to the multi-index $\alpha$, an ordered tuple of indices. Here, $|\alpha| = \sum_{i=1}^n \alpha_i$. Moreover, interpreting the pair $(x, \chi)$ as an element of the cotangent bundle, essentially, the symbol replaces partial derivatives with coordinates of the cotangent bundle. The highest-degree part of the symbol is called the leading-order symbol $\sigma_L P = \sum_{|\alpha| = m} a_\alpha(x) \chi^\alpha$.

By inverse Fourier transform and the properties of the Fourier transform we can write

$$P(x, D)u(x) = \int_{\mathbb{R}^n} e^{ix\chi} p(x, \chi) \hat{u}(\chi) d\chi,$$

where $\hat{u}$ denotes the Fourier transform of $u$. Then, a pseudo-differential operator $P(x, D)$ is defined to operate on the function $u(x)$ by (3). Here, $p(x, \chi)$, a smooth function in $x$ and $\chi$ with compact $x$-support, is a symbol of order $m$, such that for all multi-indices $\alpha$ and $\beta$ there exists a constant $C_{\alpha\beta}$, such that $|D^\alpha \chi^\beta p(x, \chi)| \leq C_{\alpha\beta}(1 + |\chi|)^{|\beta|}$. Then, the corresponding pseudo-differential operator is said to be a pseudo-differential operator of order $m$. Note how, essentially, (3) is composed of Fourier transform, multiplication by the symbol function and inverse Fourier transform. Thus, one may note the relation to filtering in signal processing.

Pseudo-differential operators form an algebra closed under composition and adjoints. An elliptic operator is essentially an invertible element in this algebra. More precisely a pseudo-differential operator is an elliptic operator if its symbol $p(x, \chi)$ is elliptic, which means that $p$ is invertible and there exists $C$ such that $|p(x, \chi)^{-1}| \leq C(1 + |\chi|)^{-m}$, for a $\chi$ large enough.

Finally, we note that all we have said above about pseudo-differential and elliptic operators generalizes nicely to a compact Riemannian manifold $\Omega$ by working with local coordinate charts (Gilkey, 1974). That is, an operator on smooth functions on a compact Riemannian manifold is a pseudo-differential operator, if the induced map on coordinate charts is a pseudo-differential operator for each chart $\psi_\alpha : U_\alpha \subset \Omega \to \mathbb{R}^n$. Moreover, this generalizes to vector bundles over $\Omega$: An operator $P : \Gamma(E_1) \to \Gamma(E_2)$ is a pseudo-differential operator of order $m$ if $P$ is locally expressible as a matrix, each component of which is a pseudo-differential operator of order $m$. Here, $\Gamma$ is the functor taking a vector bundle $E_i$ to the space of its smooth sections. Then, for each covector $\chi \in T^*_x \Omega$, $\sigma(P) : T^*_x \Omega \to \text{Hom}(E^*_1, E^*_2)$ can be written as a matrix. The symbol of $P$ can thus be viewed as a mapping taking covectors to morphisms between the fibers of $E_1$ and $E_2$ over $x$.

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7 Often, to facilitate certain computations involving complex numbers, these are multiplied by a constant; an exponent of $i$, the imaginary unit.

8 Why consider vector bundles in the first place? If we are to discuss field quantities, we are to discuss vector bundles. The field quantities we are solving for when modelling engineering problems are sections of vector bundles. For example, a vector field is a section of the tangent bundle, and a covector field, a differential 1-form, is a section of the cotangent bundle.
x. The operator \( P \) being elliptic translates to the leading order symbol \( \sigma_L P \) mapping \( E_1^x \) isomorphically to \( E_2^x \), for all \( x \in \Omega \) and \( 0 \neq \chi \in T^*_x \Omega \).

Then, consider the sequence of spaces of sections of vector bundles \( E_i \) over \( \Omega \) and differential operators \( D \) locally expressible as matrices of partial derivatives:

\[
\Gamma(E_n) \xrightarrow{D} \ldots \xrightarrow{D} \Gamma(E_1) \xrightarrow{D} \Gamma(E_0).
\]

At each point \( x \), we get the associated sequence of symbols

\[
0 \leftarrow E_n^x \xleftarrow{\sigma_L D} \ldots \xleftarrow{\sigma_L D} E_1^x \xleftarrow{\sigma_L D} E_0^x \leftarrow 0.
\]

The sequence (4) is a complex if \( D \circ D = 0 \) and it is an elliptic complex if (5) is exact for each \( x \) and for each \( \chi \neq 0 \). Moreover, for boundary conditions yielding a well-posed boundary value problem (the Shapiro-Lopatinski boundary conditions (Shapiro, 1953), (Lopatinski, 1953)), an elliptic complex becomes a Fredholm complex (Segal, 1970). Fredholm operators are characterized by finite-dimensional kernel and cokernel – the Hilbert spaces are separable, yielding a countable basis. Note that even though the Fredholm operators may act on infinite-dimensional spaces, we obtain a very tangible picture of such a complex in terms of the symbol sequence via finite-dimensional vector spaces and matrices. Computations are formulated in terms of finite-dimensional complexes coming from the symbol sequence. Moreover, all this should be rather intuitive for an engineer by a “generalization of the Laplace transform”.

Many elliptic operators of interest arise from elliptic complexes. From ellipticity of the complex, it follows that the sum of the differential operator and its adjoint \( D + D^* \) is an elliptic operator (Atiyah and Bott, 1967). Given an elliptic complex, the elliptic operator \( \Delta = DD^* + D^*D \) yields the harmonic sections of the complex, analogously to harmonic forms of the de Rham complex, and a generalized Hodge theory in this manner. Thus, with an elliptic complex, we are provided with an extremely useful set of tools for doing computational physics.

In general, complexes of Hilbert spaces, i.e. vector spaces equipped with an inner product that are complete with respect to the induced norm have been recently in the forefront within the context of numerical methods (Arnold et al., 2010). Such general complexes are not necessarily Fredholm or elliptic, and the spaces are not necessarily separable. A Hilbert complex \( H^x \) is the sequence of Hilbert spaces

\[
0 \leftarrow H^n \xleftarrow{d} H^{n-1} \xleftarrow{d} \ldots \xleftarrow{d} H^0 \leftarrow 0,
\]

with \( d \) representing here closed densely-defined linear operators between Hilbert spaces, with \( d \circ d = 0 \) (Arnold et al., 2010), (Brüning and Lesch, 1992), (Holst and Stern, 2012). An elliptic complex is a Hilbert complex. The most obvious example of a Hilbert complex of cochains is the de Rham complex \( F^x(\Omega) \) of differential forms on a smooth manifold \( \Omega \),

\[
0 \leftarrow F^n(\Omega) \xleftarrow{d} F^{n-1}(\Omega) \xleftarrow{d} \ldots \xleftarrow{d} F^0(\Omega) \leftarrow 0,
\]

with the exterior derivative acting as the coboundary mapping. Essentially, Hilbert complex can be viewed as an abstraction of the de Rham complex. A Hilbert subcomplex \( H^x_s \) of \( H^x \) consists of spaces \( H^s_s \subset H^s \) with \( dH_s^s \subset H^{s+1}_s \). For Hilbert subcomplexes, the subspaces are naturally understood as Hilbert subspaces.

However, for computational continuum physics when compact domains are considered, a Hilbert complex is often too abstract of a notion, since the more pedestrian approach of elliptic and Fredholm complexes would suffice. An elliptic complex, as a special case of a
Hilbert complex, yields thus in many cases a more concrete approach to our needs than a general Hilbert complex. The de Rham complex is indeed an elliptic complex. As also noted in (Gross and Kotiuga, 2004) and (Kotiuga, 1984), it is the framework of elliptic complexes that formalizes the ideas of analogies in physics expressed by Tonti via Tonti diagrams (Tonti, 1972), (Tonti, 1977): the de Rham isomorphism at one’s disposal in the complexes associated with the exterior derivative gives a concrete tool to answer questions about (co)homology of the complex.

2.3 Naturality

The concept of naturality is ubiquitous in mathematics. In particular, we are here interested in natural vector bundles and natural differential operators. Seminal early work in a context relevant for us includes that of Weil (1953) and Palais (1959). The book by Kolar et al. (1993) is a modern treatment fully set in the language of category theory.

2.3.1 Naturality associated with differentiable structure

A natural vector bundle is a functor $E$ from the category of $n$-dimensional smooth manifolds and local diffeomorphisms to the category of vector bundles and vector bundle homomorphisms that associates a vector bundle to each $n$-manifold $\Omega$ and to each $f : \Omega \to \Omega'$ a vector bundle homomorphism, i.e. a commutative diagram

$$
\begin{array}{ccc}
E(\Omega) & \xrightarrow{E(f)} & E(\Omega') \\
\pi_\Omega \downarrow & & \downarrow \pi_{\Omega'} \\
\Omega & \xrightarrow{f} & \Omega'
\end{array}
$$

which is a fiberwise linear isomorphism and covers $f$ (Kolar et al., 1993). Here, $\pi_\Omega$ and $\pi_{\Omega'}$ denote the canonical projections of the vector bundles. Many typical vector bundle constructions, such as bundles of tangent $p$-vectors and $p$-covectors, are natural: morphisms of certain type between manifolds are lifted to morphisms between vector bundles over the manifolds. For example, in the case of tangent bundles, in fact any smooth function between manifolds may be lifted to its push-forward between the corresponding tangent bundles. In this case, interpreting tangent vectors as differential operators, functoriality manifests itself in the chain rule. Moreover, a natural differential operator between natural vector bundles is, essentially, such that it commutes with local diffeomorphisms (Streder, 1975), (Terng, 1978), (Kolar et al., 1993). Moreover, if the associated vector bundles of an elliptic complex are natural vector bundles and the operators natural differential operators, we call the elliptic complex a natural elliptic complex.

For example, the exterior derivative $d$ of differential forms is a natural differential operator as it commutes with pullbacks by smooth functions. That is, the square

$$
\begin{array}{ccc}
DF^{p}(\Omega) & \xrightarrow{f^*} & DF^{p}(\Omega') \\
\downarrow d & & \downarrow d \\
DF^{p+1}(\Omega) & \xrightarrow{f^*} & DF^{p+1}(\Omega')
\end{array}
$$

commutes. Here, $DF^{p}(\Omega)$ is the space of smooth $p$-forms on $\Omega$ i.e. the space of smooth sections of the (natural) vector bundle of $p$-covectors, and $f^*$ is the pullback of a smooth
map \( f \) between the smooth manifolds \( \Omega' \) and \( \Omega \). This is to say that the exterior derivative is a natural transformation between the (contravariant) functors that assign the spaces of smooth \( p \)-forms and \((p + 1)\)-forms to \( \Omega \), respectively. In fact, it is essentially the unique natural differential operator between the associated natural vector bundles (Palais, 1959), (Kolar et al., 1993). As pointed out in (Kolar et al., 1993), linearity of \( d \) is thus also a consequence of naturality.

Another important natural operation commuting with pullbacks is the contraction of a differential \( p \)-form \( \eta \) with a vector field \( v \), \( i_v \eta \), producing a \((p - 1)\)-form. As an example, the contraction of magnetic flux density with the velocity field \( v \), \( i_v B \) is the geometrical way to represent the \( v \times B \) term of the Lorentz force. Thus, contraction is important in, e.g., modelling magnetohydrodynamics (MHD). Through Cartan’s formula

\[
\mathcal{L}_v = i_v \circ d + d \circ i_v, \tag{8}
\]

a structure-preserving discretization of contraction is also important for finding a discrete analogue for the Lie derivative \( \mathcal{L}_v \). Bossavit’s take on discretizing contractions is via the duality between the extrusion of a manifold (extruding along the flow of a vector field) and contraction of a differential form, utilizing Whitney forms, as discussed in (Bossavit, 2003).

2.3.2 Naturality associated with geometric structure

Different type of natural operations arise when a geometric structure, such as an inner product, on a vector bundle is considered (Kolar et al., 1993). Given an inner product, we have the associated connection and curvature, and the associated natural operations involve preservation of isometries and not just diffeomorphisms. In a sense, we need to restrict the category we are working in. We will see manifestations of such naturality later on in the context of FEM in section 4.

If we wanted to discuss mixed tensor physics, we would necessarily need more complicated operators than just the exterior derivative. Concretely, when compared to the exterior derivative, we would encounter operators for which not all the rest of the components of the covariant derivative vanish. As an example, small-strain elasticity may be articulated using the covariant exterior derivative \( d \nabla \) and vector- and covector-valued differential forms (Kovanen, 2016). In general \( d \nabla \circ d \nabla \neq 0 \), unless one is dealing with a flat connection. Thus, seeking naturality related to geometric structure, the notion of curvature is immediate.

2.4 Homology and cohomology

For modelling needs, chain and cochain complexes provide us with a way to discuss topological invariants. In particular, homology and cohomology capture the quantity and quality of holes in \( \Omega \). Intuitively speaking, take a 3-dimensional \( \Omega \) for example. There, 0-homology captures the quantity of connected components of \( \Omega \), 1-homology the number of tunnels through \( \Omega \) and 2-homology the number of voids. Cohomology can then be viewed as assigning values to these holes. In CEM, (co)homological considerations of the modelling domain \( \Omega \) are at the very heart of the science of modelling (Kotiuga, 1984); Consider for example, driving net currents through tunnels in the modelling domain in a magneto(quasi)static problem.\(^9\)

\(^9\)Exploiting cohomology can be a significant difference-maker in terms of efficiency of computations as well. As an example, see e.g. (Lahtinen et al., 2015) for making use of cohomology in non-linear magnetoquasistatic problems of superconductor modelling.
In terms of the chain complex and the kernel and the image of the boundary mapping $\partial$, the $p$th homology group may be defined as

$$H_p = \ker(\partial_p)/\im(\partial_{p+1}),$$

i.e. the quotient group formed by $p$-dimensional cycles (chains with empty boundaries) in $C_p(\Omega)$ modulo $(p + 1)$-dimensional boundaries ($(p + 1)$-chains that are boundaries for a $p$-chain) in $C_{p+1}(\Omega)$. Similarly, we can define the $p$th cohomology group as

$$H^p = \ker(\partial_p)/\im(\partial_{p-1}),$$

i.e. the quotient group formed by $p$-dimensional cocycles (cochains whose coboundary vanish) in $C^p(\Omega)$ modulo $(p - 1)$-dimensional coboundaries ($(p - 1)$-cochains that are coboundaries for a $p$-cochain) in $C^{p-1}(\Omega)$. Thus, a complex is exact if and only if its (co)homology vanishes.

(Co)homology theories with seemingly different foundations abound. For example, cellular homology, simplicial homology, Cech homology and de Rham homology are homology theories dubbed under different labels, to name just a few. However, since the Eilenberg-Steenrod axioms were laid out, they can all be seen as instances of the general theory, and it turns out that homology is a homotopy invariant of the space (Eilenberg and Steenrod, 1952). The Eilenberg-Steenrod axioms, of which there are versions for both homology and cohomology (obtained from one another by reversing the arrows), assert that a homology theory is a sequence of functors from a suitable category of topological spaces (or from the category of chain complexes) to category of Abelian groups (or sequences of them), together with boundary operators $\partial$, which induce natural transformations between homology functors. This system is required to satisfy five properties, for which the reader is referred to (Eilenberg and Steenrod, 1952). These axioms allow us to talk about (co)homology theories without referencing to any concrete (co)chain realization.

But how do we view $H_p$ as functors? First of all, the assignment of a chain complex to the space $\Omega$ is functorial. Then, the homology is a (covariant) functor from the category of chain complexes to the category of sequences of Abelian groups satisfying the Eilenberg-Steenrod axioms. Dually, cohomology is a contravariant functor of the same kind from the category of cochain complexes. For homology, the functoriality means here, that given two chain complexes and a chain map $f$ between them, homology functor takes the chain spaces to the homology groups and the chain map to induced homomorphisms between the groups (as chain maps take cycles to cycles and boundaries to boundaries), in a way that respects identity maps and composition. Then, there is a composite functor which first assigns a chain complex to a space and then the homology groups to the complex. This is the homology of $\Omega$.

Moreover, the assignment of the $p$th homology group to a space may be viewed as a functor in its own right. Then, the boundary operators $\partial$ induce natural transformations between homology functors in the sense that for all $0 < p \leq n$ they assign to each $\Omega$ a homomorphism $\partial : H_p(\Omega) \to H_{p-1}(\Omega)$ such that for each morphism $f$ from $\Omega$ to $\Omega'$ the diagram

$$\begin{array}{ccc}
H_p(\Omega) & \overset{\partial}{\longrightarrow} & H_{p-1}(\Omega) \\
\downarrow H_p(f) & & \downarrow H_{p-1}(f) \\
H_p(\Omega') & \overset{\partial'}{\longrightarrow} & H_{p-1}(\Omega')
\end{array}$$

Relaxing one of these axioms, the dimension axiom, yields a generalized (co)homology theory. A standard example is the $K$-theory (Swan, 1968).
commutes.\footnote{Notation is slightly abused here by denoting the induced boundary homomorphisms with the same symbol as the boundary operators of chain complexes.} The existence of such a natural transformation can be articulated via the zig-zag lemma which yields a commutative diagram of long exact sequences of homology groups and group homomorphisms from a commutative diagram of short exact sequences of chain complexes and chain maps (see e.g. (Ghrist, 2014)). Note that even though we have considered the homology of chain complexes here for concreteness, this functoriality is at the heart of every homology theory. The dual results hold for cohomology: then, the coboundary operators \( d \) induce such natural transformations.

For the de Rham complex, we have the de Rham cohomology, where the role of cocycles is played by closed differential forms (those whose exterior derivative vanish) and exact forms (those that are exterior derivatives of another form) are the coboundaries. Then, utilizing the induced Hodge theory, the representatives of cohomology classes are harmonic forms: There is a unique harmonic differential \( p \)-form with prescribed periods on the homology basis for \( p \)-cycles on \( \Omega \) with coefficients in \( \mathbb{R} \). As the de Rham isomorphism can be utilized, cohomology of this complex becomes tangible, and Tonti diagrams obtain a clear formal meaning (Gross and Kotiuga, 2004). Clearly, the same thing cannot be said about a general Hilbert complex (Arnold \textit{et al.}, 2010). However, for a general elliptic complex, it is guaranteed that we have an analogous cohomology theory: The space of harmonic sections, the kernel of \( \Delta = DD^* + D^*D \), of the complex is isomorphic to the cohomology of the complex of corresponding degree (Gilkey, 1974). That is, the dimension of the space of harmonic sections of order \( p \) on \( \Omega \) is the \( p \)th Betti number of \( \Omega \). Thus, elliptic complexes are the framework to formalize Tonti’s analogies in physics.

2.5 An electrical engineering interlude

The relevant data structure for computational physics of continuum is that of a (co)chain complex. With the additional structure of an elliptic complex and naturality of the associated differential operators, one has a machine that produces a Hodge theory, extremely effective for articulating physical theories and essential for numerical methods in continuum physics. This framework is also essential in formalizing Tonti diagrams (Gross and Kotiuga, 2004). Moreover, (co)homological information of the complex as a topological invariant is essential for computations. Thinking in terms of traditional electrical engineering, via Hodge theory, homology is the bridge between field theory and circuit theory: The periods of harmonic forms are the variables that appear in Kirchoff’s laws, while the lumped parameters have a Hilbert space interpretation (Kotiuga, 1984). Thus, elliptic and Fredholm complexes, naturality and (co)homology are at the very heart of engineering. In this light, a general Hilbert complex often appears as an excessive abstraction in compact domains, without the benefits of ellipticity or separability (Arnold \textit{et al.}, 2010). Note also how the concept of naturality comes up at different levels. Desirably, such structures should be preserved in discretizations, too.

3 Correspondence between cochains and differential forms

The basic question addressed by André Weil in 1952 was the fact that cohomology theories satisfying the Eilenberg-Steenrod axioms (Eilenberg and Steenrod, 1952) had isomorphic cohomology groups (Weil, 1952). However, the axiomatic method made no mention of chains or cochains, and in the process, had nothing to say about possible correspondences between cochains in concrete realizations of cohomology theories such as those of de Rham
and Čech, or simplicial cohomology theory. In the process of devising tools for addressing this issue, Weil developed the spectral sequence and an interpolation formula now known as Whitney forms. Hassler Whitney developed these tools for the purposes of analysis on manifolds, and published his results in his monograph entitled Geometric Integration Theory in 1957 (Whitney, 1957).

Let us go back to the diagram introduced in the first section of this paper. Here we scrutinize, what is behind the upper part

\[ \text{Cochains} \xleftarrow{\text{Limit process}} \text{Integration} \xrightarrow{} \text{Differential forms} \]

of the diagram introduced in Section 1. Let us concentrate on the simplicial case. Given a simplicial complex \( M \) on a smooth manifold \( \Omega \), the Whitney map \( W \) interpolates a cochain in a piecewise linear manner creating a Whitney form. Dually, the de Rham map \( R \) integrates a differential form \( \eta \) to provide a cochain. The composite \( RW \) is the identity mapping on cochains. Moreover, there is a precise sense in which \( \eta \) is homotopic to \( WR\eta \), and the composite \( WR \) tends to identity with the refinement of the simplicial complex (Dodziuk, 1976).

Formally, given the barycentric coordinates \( \lambda_i \) of the nodes of the simplicial complex \( M \), the Whitney map \( W \), which takes a simplicial \( p \)-cochain to a differential \( p \)-form, gives a Whitney \( p \)-form on a \( p \)-simplex \( \sigma \) via

\[
W \sigma = p! \sum_{k=0}^{p} \lambda_{ik} d\lambda_{i0} \wedge \ldots \wedge \hat{d}\lambda_{ik} \wedge \ldots \wedge d\lambda_{ip}, \quad p > 0. \tag{11}
\]

For \( p = 0 \) we have simply \( W \sigma = \lambda_i \). Here, \( \wedge \) is the exterior product of differential forms, which, given a \( p \)-form and a \( q \)-form, produces a \( p + q \)-form, and \( \hat{\cdot} \) denotes that we omit the factor under the hat sign. Moreover, the de Rham map \( R \) takes a differential \( p \)-form \( \eta \) to a simplicial \( p \)-cochain by integrating it on a \( p \)-chain \( c \):

\[
R \eta = \int_c \eta. \tag{12}
\]

Functors \( C^x \) and \( F^x \) assign the simplicial cochain complex \( C^x(M, \Omega) \) and the de Rham complex \( F^x(\Omega) \) to \( \Omega \). Then, the Whitney map is a cochain map between the simplicial cochain complex

\[
0 \leftarrow C^n(M, \Omega) \xrightarrow{d} C^{n-1}(M, \Omega) \xrightarrow{d} \ldots \xrightarrow{d} C^0(M, \Omega) \leftarrow 0 \tag{13}
\]

and the de Rham complex

\[
0 \leftarrow F^n(\Omega) \xrightarrow{d} F^{n-1}(\Omega) \xrightarrow{d} \ldots \xrightarrow{d} F^0(\Omega) \leftarrow 0. \tag{14}
\]

Moreover, the de Rham map is a cochain map in the other direction. Since \( W \circ d\hat{c} = d \circ W\hat{c} \), where \( \hat{c} \) is a simplicial cochain and \( d \) on the left denotes the coboundary on simplicial cochains and the exterior derivative of a differential form on the right, the isomorphism of de Rham cohomology groups of \( \Omega \) and simplicial cohomology groups related to \( M \) is implied, as cochain maps induce maps on cohomology functorially (Gross and Kotiuga, 2004), (Dodziuk, 1976), (Müller, 1978). Note that then the coboundary mappings induce natural transformations on cohomology.

All this suggests an interpretation for Whitney forms and the correspondence of cochains and differential forms as parts of a higher-categorical structure. The fact that chain homotopic chain maps induce the same maps on homology is the core of the isomorphism of de
Rham and simplicial cohomology groups (Bott and Tu, 1982). In fact, one could say that such chain homotopy was the reason Whitney forms were conceived (Weil, 1952). By considering chain complexes, chain maps and chain homotopies between them, one obtains a 2-category with chain homotopies acting as morphisms between morphisms: 2-morphisms. Furthermore, one can consider chain homotopies between chain homotopies, iterating this construction to infinity to obtain an $\infty$-category with an infinite number of “layers” of morphisms.\(^{12}\)

4 The Path to Discrete: Finite element method

Now, we are ready to discuss how to achieve a discrete formulation of physics. We will use the familiar FEM as an example. In this section, we will introduce the relevant details of FEM.

The Galerkin FEM (from now on we will refer to Galerkin FEM as just FEM) is likely the most utilized numerical solution method of partial differential equations in natural sciences. FEM is a discretization method: A way to discretize the function space from which the solution is sought. This is achieved by finding a finite-dimensional Hilbert subspace $H_s$ of the Hilbert space $H$ in which the solution of the original problem resides. Or, as formalized in (Arnold et al., 2010) and (Holst and Stern, 2012), it abstracts to finding a finite-dimensional subcomplex of a Hilbert complex on a compact manifold $\Omega$. However, in such compact domains with the Shapiro-Lopatinskii boundary conditions (Shapiro, 1953), (Lopatinskii, 1953), we are indeed dealing with Fredholm complexes and thus the theory of elliptic complexes guarantees that the Hodge theory we need falls in our laps, and we have a complex of separable spaces for the needs of functional analysis, as discussed in section 2.

4.1 Weak formulation

Now we consider how to obtain the relevant Hilbert spaces and the weak formulation utilized in FEM. For simplicity, we will only consider elliptic problems here. For further details, see e.g. (Arnold et al., 2010), (Bossavit, 1998) and (Brenner and Scott, 2008). For a thorough introduction to the required Sobolev spaces in the context of electromagnetism see (Kurz and Auchmann, 2012).

In a Hilbert space $H$ with inner product $\langle \cdot, \cdot \rangle$, it holds that (Yosida, 1980)

$$\gamma \in H, \quad \gamma = 0 \quad \iff \quad \langle \gamma, \gamma' \rangle = 0, \quad \forall \gamma' \in H.$$  \hspace{1cm} (15)

This is the backbone of FEM: using the inner product of $H$ we can test whether an equation holds. In FEM, we approach a discrete formulation from the typical direction, i.e., we are discretizing a problem formulated in terms of partial differential equations. We consider the equations to be formulated in terms of differential forms. Introducing the standard $L^2$ inner product in the space of piecewise smooth differential $p$-forms ($\langle \eta, \gamma \rangle = \int_{\Omega} \eta \wedge \star \gamma$), we can define the $L^2$ Hilbert space of such forms $L^2 F^p(\Omega)$, for whose elements $\gamma$, $\langle \gamma, \gamma \rangle < \infty$ holds. Then, we define the Sobolev spaces of differential forms

$$L^2 F^p(\partial, \Omega) = \left\{ \gamma \in L^2 F^p(\Omega) \mid \partial \gamma \in L^2 F^{p+1}(\Omega) \right\}$$  \hspace{1cm} (16)

\(^{12}\text{Such considerations lead us to the foundations of homotopy type theory (Univalent Foundations Program, 2013).}\)
and
\[ L^2F^p(\tilde{\gamma}, \Omega) = \left\{ \gamma \in L^2F^p(\Omega) \mid \tilde{\delta}\gamma \in L^2F^{p-1}(\Omega) \right\}, \tag{17} \]
where \( \tilde{d} \) and \( \tilde{\delta} \) denote the weak exterior derivative and the weak co-derivative, respectively. The Hodge operator \( \ast \) (see e.g. (Frankel, 2012) section 14), induced by the metric on \( \Omega \), is an isomorphism between \( L^2F^p(\tilde{d}, \Omega) \) and \( L^2F^{n-p}(\tilde{\delta}, \Omega) \). The ubiquity of \( \ast \) in constitutive equations of physical theories underlines the importance of both (16) and (17).

\( L^2F^p(\tilde{d}, \Omega) \) and \( L^2F^{n-p}(\tilde{\delta}, \Omega) \) are the kind of spaces we want physical quantities to live in when using FEM: We need the quantities and their weak exterior derivatives and weak co-derivatives to be sufficiently well-behaved. The weakness of these operators ensures that they get along with piecewise smooth differential forms, too. In fact, for smooth forms, the weak and strong versions of these operators coincide. The piecewise-smoothness is often crucial in physics, as e.g. material boundaries can exhibit jumps in the derivatives of field quantities. The operation of the strong co-derivative on a \( p \)-form can be defined using the Hodge operator \( \ast \) and the (strong) exterior derivative \( d \) as \( (-1)^p \ast^{-1} d \ast \). This suggests us the definition of the weak exterior derivative \( \tilde{d} \), which is defined to satisfy \( \langle d\gamma, \eta \rangle = \langle \gamma, (-1)^p \ast^{-1} d \ast \eta \rangle \), \( \forall \eta \in D^{Fp+1}(\Omega) \), with vanishing boundary terms. Then, the weak co-derivative \( \tilde{\delta} \) obeys \( \langle \tilde{\delta}\gamma, \varpi \rangle = \langle \gamma, d\varpi \rangle \), \( \forall \varpi \in D^{Fp-1}(\Omega) \). Here \( D^{Fp}(\Omega) \) is the space of smooth \( p \)-forms supported by \( \Omega \). So, we can define the operation of these weak operators on piecewise smooth forms through operation of the strong operators on smooth forms, utilizing the inner product. Often, it is customary to make no notational difference between the weak operators and their strong counterparts, so that, for example simply \( d \) is used to denote both strong and weak exterior derivative.

Working in \( L^2F^p(\tilde{d}, \Omega) \), we can now re-state an equation of the form \( L\alpha = \nu \), where \( L \) is a linear operator, and \( \alpha \) is a differential form with \( L\alpha \in L^2F^p(\tilde{d}, \Omega) \), using (15), as
\[ \langle L\alpha, \gamma' \rangle = \langle \nu, \gamma' \rangle, \quad \forall \gamma' \in L^2F^p(\tilde{d}, \Omega). \tag{18} \]
From this weighted residual formulation of the problem one typically approaches the weak formulation via integration by parts, which utilizing \( d \) and \( \ast \) can be stated as
\[ \langle d\gamma, \eta \rangle = \langle \gamma, (-1)^p \ast^{-1} d \ast \eta \rangle + \int_{\partial \Omega} \gamma \wedge \ast \eta, \forall \eta \in D^{Fp+1}(\Omega). \tag{19} \]
Thus, the metric-dependent co-derivative can be converted into the metric-independent exterior derivative in this process. This is favourable in terms of commutative properties of the operators. Namely, the exterior derivative commutes with pullbacks by smooth functions while the co-derivative only commutes with pullbacks by isometries (Gerritsma et al., 2014). Commutation under pullbacks is an essential testing ground for a discretization: We want to preserve naturality. Note how the naturality of the exterior derivative is that of subsection 2.3.1 (related to differentiable structure) and the naturality of the co-derivative is that of subsection 2.3.2 (related to geometric structure).

This weak formulation process leads to
\[ a(\alpha, \gamma') = \langle \nu, \gamma' \rangle, \quad \forall \gamma' \in L^2F^p(\tilde{d}, \Omega), \tag{20} \]
where \( a(\cdot, \cdot) \) is a coercive and bounded bilinear form (Brenner and Scott, 2008).

4.2 The FEM discretization

The solution to the weak formulation (20) lies in an infinite-dimensional Hilbert space. The problem is yet to be discretized. As already mentioned, in FEM this is done by finding
a finite-dimensional subspace for $L^2F^p(\tilde{d}, \Omega)$ (supposing $\alpha$ resides there) with which to approximate the solution space. This is achieved through what is called meshing: covering of $\Omega$ with a cellular mesh complex and attachment of a set of basis functions to the cells of desired dimension, so that the basis functions span a Hilbert subspace $W^p(\Omega)$ of $L^2F^p(\tilde{d}, \Omega)$. Then, the unknown is approximated as a sum of these functions, and the weak formulation is tested with the basis of $W^p(\Omega)$, and not with all $\gamma' \in L^2F^p(\tilde{d}, \Omega)$. Thus, a finite, discrete formulation of the original problem, which due to Galerkin orthogonality (see (Brenner and Scott, 2008, p. 58)), results in an optimal approximation, is obtained.

4.2.1 Differentiable structure

As formalized by Arnold in (Arnold et al., 2010), this discretization can be seen as, not only as finding a subspace of a Hilbert space, but finding a Hilbert subcomplex of the $L^2$ de Rham complex

$$0 \leftarrow L^2F^n(\tilde{d}, \Omega) \xleftarrow{\tilde{d}} L^2F^{n-1}(\tilde{d}, \Omega) \xleftarrow{\tilde{d}} \ldots \xleftarrow{\tilde{d}} L^2F^0(\tilde{d}, \Omega) \leftarrow 0. \tag{21}$$

However, on a compact $\Omega$, this is indeed an elliptic complex, and the higher abstraction level of Hilbert complexes offers us no tangible benefits. Moreover, with Shapiro-Lopatinskii boundary conditions, we indeed have a Fredholm complex: a prototypical Hilbert complex with separable Hilbert spaces. Given a simplicial cellular mesh complex $M$ on $\Omega$, a viable and widely utilized option for the subcomplex is the Whitney complex

$$0 \leftarrow W^n(M, \Omega) \xleftarrow{\tilde{d}} W^{n-1}(M, \Omega) \xleftarrow{\tilde{d}} \ldots \xleftarrow{\tilde{d}} W^0(M, \Omega) \leftarrow 0, \tag{22}$$

consisting of Hilbert spaces of Whitney forms (Bossavit, 1988a). The Whitney complex is the restriction of $L^2F^p(\tilde{d}, \Omega)$ to Whitney forms, obtained via the Whitney map. At the continuum limit, as $M$ is refined, Whitney complex approaches the de Rham complex. The coboundary mappings commute with the inclusions and there is a bounded cochain mapping projecting the de Rham complex to the Whitney complex, ensuring stability. The exterior differentiation is inherited by the Whitney complex from the de Rham complex. Moreover, the naturality of the exterior derivative is preserved in this discretization: The commutative property under pullbacks still holds.

4.2.2 Metric-dependent properties

In Whitney complex we have a structure-preserving discretization of the de Rham complex and the associated Hodge theory. In terms of Hodge operators, for an ideal discretization we would have a commutative diagram of the form (Tarhasaari et al., 1999)

$$\begin{array}{ccc}
L^2F^p(\tilde{d}, \Omega) & \xrightarrow{R} & C^p(M, \Omega) \\
\star & \downarrow & \star \\
L^2F^{\ast p}(\tilde{d}, \Omega) & \xrightarrow{R} & C^{\ast p}(M, \Omega).
\end{array}$$

That is, the Hodge operators on differential forms and cochains should commute with the de Rham map. In the case of FEM, one defines the Galerkin-Hodge operator on simplicial $p$-cochains via Whitney map and $\star$ of differential forms by

$$\langle c_1, c_2 \rangle = \int_{\Omega} W(c_1) \wedge \star W(c_2). \tag{23}$$

16
This is a discrete representation of the Hodge operator, separating the metric-dependent properties in FEM from metric-free ones. The non-degeneracy of (23) is inherited from the $L^2$ Hodge inner product. In FEM, it results in an invertible, but not diagonal matrix, and thus, the locality of $\star$ is not strictly preserved: a manifestation of the discrete star localization problem (Kotiuga, 2008). The weak formulation is thus led to dictate the metric and thus the constitutive laws. The discrete problem for finding the array $x$ of degrees of freedom of the problem obtains the matrix form

$$ C^T M C x = v, \quad (24) $$

where the matrix $M$ is an instance of the discrete Hodge operator, the Galerkin-Hodge. It is this Galerkin-Hodge process which allows us to roll the metric through the variational principle down to the discrete level in an essentially functorial manner. Moreover, we see here the connection to naturality related to geometric structure (see subsection 2.3.2) and how and to what extent it manifests itself via the Galerkin-Hodge process on the discrete level. Note also that the metric of the elliptic complex does not have to come from the Riemannian metric of the underlying manifold: Utilization of different metrics is beneficial in tackling e.g. different constitutive laws.

Whitney forms are flat forms arising from one-to-one correspondence with flat norm completed cochain spaces (Whitney, 1957). The exterior derivative of a flat form is flat but the Hodge star of a flat form is not: This is a fundamental restriction in discretization of metric-dependent constitutive laws of continuum physics utilizing Whitney forms. As a concise introduction to such problematics, we refer the reader to (Kangas et al., 2006). For further considerations on flat and sharp norm topologies and developments on the associated problematics, see Jenny Harrison’s works such as (Harrison, 2005), (Harrison, 2012). Nonetheless, Whitney forms with the Galerkin-Hodge inner product and finite element error analysis combine into a canonical procedure for discretizing inner product dependent properties of continuum in a geometrically compatible manner while keeping track of convergence properties with refinements of the simplicial complex. The properties of Whitney forms bring the essentially geometric nature of such a FEM procedure to the forefront (Trevisan and Kettunen, 2004).

### 4.2.3 Topological properties

This point of view emphasizes the attainment of a discrete version of the theory in question in a more general sense than just the particular solution space. For example, the preservation of cohomological properties in this discretization, which is a natural compatibility requirement, can be proven. An isomorphism on cohomology is induced. Note also that in our above example, $\alpha$ is not necessarily a $p$-form, even though $L_\alpha$ is. Hence, strictly speaking, it is not enough to consider merely the discretization of $L^2 F^p(\tilde{\Omega}, \Omega)$, but the whole complex is important.\footnote{Even though the de Rham complex is the canonical example of an elliptic complex, one can consider discretizations of other complexes, too. In (Arnold et al., 2010), for example, the elasticity complex and its FEM discretization are discussed.}

Let us recap the structure we have here in terms of cohomology. The functors $L^2 F^x$ and $W^x$ attach the $L^2$ de Rham complex and the Whitney complex to a manifold. Given a map $f$ between manifolds $\Omega'$ and $\Omega$, we have the induced cochain maps between the corresponding cochain complexes on $\Omega$ and $\Omega'$: $L^2 F^x(f) : L^2 F^x(\Omega) \to L^2 F^x(\Omega')$ and $W^x(f) : W^x(M, \Omega) \to W^x(M', \Omega')$. These in turn induce maps on cohomology via cohomology functors. The cohomology spaces $H_p^x(\Omega)$ (the simplicial cohomology related to
the Whitney complex) and $H^p_{DR}(\Omega)$ (the de Rham cohomology) are isomorphic. Moreover, between the cohomology functors of different degrees, we have the exterior derivatives (coboundaries) inducing natural transformations. So, in terms of cohomology, such a structure-preserving discretization is characterized by two commutative squares

\[
\begin{array}{cccc}
H^p_s(\Omega) & \xrightarrow{H^p_s(f)} & H^p_s(\Omega') & \xrightarrow{H^p_{DR}(f)} & H^p_{DR}(\Omega') \\
\downarrow d & & \downarrow d & & \downarrow d \\
H^{p+1}_s(\Omega) & \xrightarrow{H^{p+1}_s(f)} & H^{p+1}_s(\Omega') & \xrightarrow{H^{p+1}_{DR}(f)} & H^{p+1}_{DR}(\Omega')
\end{array}
\]

for each $p \in \{0, 1, ..., n - 1\}$, where each of the corresponding simplicial and de Rham cohomology groups are isomorphic.

4.2.4 Brief summary and outlook

When discretizing, Whitney forms are a very effective bridge to the cochain perspective in the context of naturality associated with differentiable structure, as well as from the perspective of essential topological properties. When it comes to naturality associated with geometric structure, we rely on the Galerkin-Hodge process, and in particular, on the Galerkin-Hodge inner product (23) to induce an inner product on cochains. Moreover, naturality should provide us with ideas to extend these concepts to a Galerkin-based discussion of connections and curvature, relevant for e.g. generalizations of electromagnetism such as the Yang-Mills theory (Garrity, 2015).

5 FEM versus cochain methods

We have now seen the fundamental ideas behind FEM. One starts from the point of view of differential forms and differential equations, and through a discretization of the elliptic complex arising from piecewise smooth $L^2$ differential forms and the weak exterior derivatives, one obtains a discrete, finite formulation suitable for computers.

But what about cochain methods? For example in CM, one starts from cochains, the macroscopic counterpart of differential forms, formulates the defining properties of physical quantities in terms of them, and representing the equations in a cochain complex arising from a cellular mesh complex, obtains a discrete formulation.

Hence, let us scrutinize the diagram

\[
\begin{array}{cccc}
\text{Cochains} & \xrightarrow{\text{Limit process}} & \xrightarrow{\text{Integration}} & \text{Differential forms} \\
\downarrow \text{Discretization} & & & \downarrow \text{Discretization} \\
\text{Discrete formulation} & & & \text{Discrete formulation}
\end{array}
\]

again. As we have seen, there is a bijective way to travel from cochains to differential forms and vice versa, via limit process and integration, respectively. However, what is probably not as evident, is the interpretation that even in cochain methods, we discretize, as we hint in the above diagram.
5.1 Cochain methods: Discretization

We can view cochain methods on a compact $\Omega$, such as CM, starting with chain and cochain complexes $C_x(\Omega)$ and $C^x(\Omega)$. Taking the complexes of e.g. all cellular chains and cochains on $\Omega$, these complexes consist of infinite-dimensional spaces, giving rise to infinite-dimensional cochain complexes. In physics, we want to express the defining properties as universal laws: It is necessary that an equation holds for all $p$-chains. We might have an equation of the form

$$\Psi(\partial \Gamma) = 0, \quad \forall \Gamma \in C_p(\Omega),$$

(25)

where $\Psi$ is a $(p-1)$-cochain and $\Gamma$ is a $p$-chain. For example, Gauss’s law for magnetic field is of this form: The magnetic flux through the boundary of any volume is zero. Obviously, requiring the defining properties of a physical theory to hold for all chains in the complex gives rise to an infinite number of equations. Again, note that this is absolutely necessary: the essence of a law of nature is manifest in the universal quantifier $\forall$. Hence, to obtain a finite formulation, one needs to discretize the complexes. The discretization is achieved by forming a cellular mesh complex $M$ (and its dual) into $\Omega$, that gives rise to the finite-dimensional subcomplexes $C^x(M,\Omega)$ and $C^x(M,\Omega)$. This is the meshing process required by cochain methods. Thus, we observe the following:

**Remark 1** While in FEM, one discretizes the differential equations that govern physics by restricting the spaces of basis and test functions to finite-dimensional ones, in cochain methods one discretizes the corresponding algebraic equations by restricting the spaces of (co-)chains for which the equations are required to hold to finite-dimensional ones.

As an example, let us consider the complex $C^x(\Omega)$ of square-summable cochains and its subcomplex $C^x(M,\Omega)$ in particular. Clearly, for each $p$, $C^p(M,\Omega) \subset C^p(\Omega)$ and $dC^p(M,\Omega) \subset C^{p+1}(M,\Omega$) hold. Hence, $C^x(M,\Omega)$ is a subcomplex of $C^x(\Omega)$. Thus, in an abstract sense, this discretization is exactly the same process as in FEM. Note also again that $C^x(M,\Omega)$ arising from a simplicial $M$ is isomorphic to the Whitney complex $W^x(M,\Omega)$, widely utilized in FEM, further highlighting the similarity of these methods. Comparing, for example, CM and FEM, the stiffness matrices of these methods coincide when simplicial (primal) complexes and linear interpolation are used (Tonti, 2001).

Let us recap the above into a single remark.

**Remark 2** Cochain methods and FEM both rely on first giving a mathematical representation of physical phenomena in a cochain complex consisting of infinite-dimensional spaces and then discretizing the complex to obtain a finite formulation. Concretely, this discretization means finding a finite subcomplex of the infinite-dimensional complex.

In this framework, both FEM and cochain methods are discretization methods: Both can be seen as techniques for finding a finite-dimensional subcomplex of an infinite-dimensional complex. The requirement that algebraic cochain equations hold for all chains of type and dimension in question renders the spaces of an algebraic formulation of physics infinite-dimensional. Hence, via this interpretation, such a formulation is no more inherently discrete than one utilizing differential equations. These two are two different paths to a discrete formulation of physics but they are based on a discretization of exactly the same type. Problematics related to directly discrete methods is thus related to the fact that classical cochain constructions presuppose a continuum; but one can argue that one does not want to approximate continuum physics without assuming that a continuum limit exists.14

14There has, however, been interest in schemes that formally build upon an inherently discrete space.
5.2 On the discrete Hodge

For representing constitutive relations, cochain methods typically rely on dual complexes of so-called outer oriented chains and twisted cochains.\(^{15}\) We will not dwell on this issue too much here. Nonetheless, the fundamental issue of the local nature of constitutive laws and that of discrete Hodge operator and how such should be defined, underlie this connection (Auchmann and Kurz, 2006; Hiptmair, 2001b; Kangas et al., 2011, 2007; Tarhasaari et al., 1999; Kotiuga, 2008). Another way to introduce the discrete Hodge is to express the Poincaré duality using a commutative cup product on cochains and define the Hodge by combining it with an inner product to avoid the dual mesh construction (Wilson, 2007).

On the matrix level, cochain methods tend to end up in a similar place as FEM: An equation of the form

\[
C^T H C x = v, \tag{26}
\]

where \(H\) is a realization of the discrete Hodge, is formed. As we mentioned, utilizing the same simplicial complex, the implied system matrix is the same in e.g. CM and FEM. However, the discrete Hodge is not the same. The essential difference in FEM and various cochain method discretizations is thus in the instantiation of the discrete Hodge – the way metric properties and constitutive laws are incorporated into the discretization. As discussed in (Tarhasaari et al., 1999), equations of the form (24) and (26) give rise to a circuit interpretation: The numerical approaches have similar structure to that of circuit equations arising from circuit theory. There, the role of discrete Hodge is played by the impedance, which connects chains to cochains. This also raises further questions on the category theoretical interpretation of discretizations and coupled discrete problems, e.g. via a monoidal categorical framework for circuit theory (Baez and Fong, 2015).\(^{16}\)

5.3 Final remarks

From this perspective, a numerical method based on an algebraic formulation of physics is not free of the questions and compatibility issues related to the differences of the continuous and the discrete, some of which we have touched upon in this paper. Error analysis is essential, and e.g. naturality should play a similar role in the discrete descriptions as it does in the continuum descriptions. Even though there are different and differently motivated ways to approach cochain methods, such as e.g. those of Wilson and Harrison (see (Wilson, 2007), (Harrison, 2005)), it all boils down to, in some sense, functorially preserving the continuum properties. Utilizing Whitney forms and the Galerkin-Hodge process, this is especially evident and natural.

Notably, in (Mansfield and Hydon, 2008), a cohomology theory of so-called difference forms was constructed, aiming to provide a discrete space foundation for finite difference methods on a lattice variety. They do not assume the existence of a continuum limit, while providing some analogies with de Rham complex. However, there are open problems related to such a construction. For example, the theory cannot handle local refinements of the mesh nor is the functoriality of the theory or independence of a covering of the space shown.

\(^{15}\)Some physical quantities (cochains) are naturally associated with an inner orientation of the geometric entity they are related to, while some (twisted cochains) require to be interpreted on outer oriented chains. Hence, in the primal-dual complex pair, we associate an outer oriented \(n - p\)-cell of the dual complex \(\bar{M}\) to each inner oriented \(p\)-cell of the primal complex \(M\). Formally, in such a complex pair, a dual cell of a \(p\)-cell is such that its cofaces are the dual cells of the boundary of the \(p\)-cell. The outer orientation of the dual complex is induced by the inner orientation of the primal one. For example, the positive crossing direction of a 2-cell of the dual complex on 3-dimensional \(\Omega\), or a 1-cell on 2-dimensional \(\Omega\), is induced by the inner orientation of a 1-cell piercing it.

\(^{16}\)For monoidal categories, see e.g. (Baez and Stay, 2011) and (Coecke and Paquette, 2011).
6 Categories, homotopy, and data structures for discrete solvers

On the basis of the discussion we have presented, it is clear that categorical notions are effective and ubiquitous when articulating concepts essential for discrete descriptions of continuum physics. In terms of CEM, algebraic topology, as the study of functors from topological to algebraic categories and natural transformations between such functors, forms the cornerstone of how circuit theory connects to field theory. In particular, (co)homology functors and natural transformations play a key role in translating ideas from differential forms and partial differential equations into discrete cochains and complexes, which form data structures for numerical solution methods.

In this section, we consider the functorial relation between abstract simplicial complexes and their geometric realizations and make a few remarks on how higher-category theory and homotopy theory interface with modelling software design in computational physics of continuum. Finally, based on the discussion, we identify opportunities to utilize such concepts in computational physics.

6.1 On the relation between abstract simplicial complexes and their geometric realizations

In both finite element analysis and the study of manifolds, the notion of a simplicial complex has long been used as a basic data structure enabling one to model spaces without making implicit geometrical or topological assumptions. Even though in numerical methods we tend to play with the geometrical realization of a simplicial complex, there is a rich, purely algebraic structure in data structures built from simplicial complexes, which points to more systematic use of category theory and homotopy theory in practice.

First, let us consider abstract simplicial complexes and their geometric realizations in a very concrete sense in terms of finite element data structures. Given a triangulated \( n \)-dimensional manifold \( \Omega \) (with boundary) embedded in \( \mathbb{R}^n \), we can define two data structures, together characterizing the geometric realization of the arising simplicial complex (Gross and Kotiuga, 2004). Namely, these are the lists of globally numbered vertices of the simplicial complex and their Cartesian coordinates in \( n \)-tuples \( x_i \),

\[
\{1, \ldots, m_0\}, \quad \{x_1, \ldots, x_{m_0}\}, \tag{27}
\]

and the list of \( n \)-simplices given in terms of the global node numbering of the vertices

\[
\{s_1, \ldots, s_{m_n}\}, \tag{28}
\]

with each \( s_i \) being a list of the \( n + 1 \) vertices of the simplex. Indeed, (27) and (28) capture the essence of the geometric realization of the simplicial complex. From this data, an abstract simplicial complex may be extracted. This consists of the array (28) and an array of plus and minus ones, obtained by computing the oriented volume of each \( n \)-simplex \( \text{Vol}(s_i) \) using the Cartesian coordinates in the second array of (27) and dividing the result by its absolute value, yielding either +1 or −1:

\[
\{\text{Vol}(s_1)/|\text{Vol}(s_1)|, \ldots, \text{Vol}(s_{m_n})/|\text{Vol}(s_{m_n})|\}. \tag{29}
\]

In this process, we “forget” the geometric information present in the geometric realization and, in fact, transfer from the category of geometric realizations of abstract simplicial complexes and simplicial maps between such realizations, \( \text{SGeom} \), to the category of abstract simplicial complexes and simplicial maps, \( \text{S} \). That is, we have a forgetful functor

\[
\text{Abstr} : \text{SGeom} \to \text{S}, \tag{30}
\]
that takes the geometric realization to the underlying abstract simplicial complex with the operation on morphisms defined in an obvious way, i.e. simplicial maps in \( \text{SGeom} \) are taken to simplicial maps in \( \text{S} \). Functoriality of such a construction, i.e. preservation of identities and composition, is evident.

Now, having a clear distinction between an abstract simplicial complex and its geometric realization in terms of concrete finite element data structures, it is clear that many important topological computations can be done in the abstract simplicial complex without resorting to floating point arithmetic at all. We simply utilize the forgetful functor (30) to obtain the abstract simplicial complex from its geometric realization, compute, and “pull back” the results to the geometric realization.

### 6.2 Higher-categories and simplicial sets

Even though the expressiveness of category theory suggests its utilization in modelling software design and development, category theory is arguably difficult as it allows and demands one to shift perspectives so often. Functors between categories can be morphisms in another category, as can natural transformations between functors. Moreover, we can, and sometimes have to, shift to a higher-categorical viewpoint and view morphisms between morphisms or morphisms between morphisms between morphisms (Baez and Dolan, 1998).

But indeed, this property embodies the power of category theory in discerning structures. And this is at the heart of programming too: Category theory is about structure and programming is about structure. For articulating e.g. functoriality, naturality or chain homotopies and related mathematics of discrete solvers efficiently in software, such shifts of perspective are crucial. If the framework in which we are programming supports this, all the better. This points to the direction of type-theoretic accounts of programming, which are in close relationship with category theory, such as Hazelnut (Omar et al., 2017).

Higher-categorical thinking is manifest in simplicial sets as a combinatorial abstraction of space, which in some sense, generalize directed multigraphs to higher dimensions. Indeed, information about directions in a complex is essential for e.g. finite element computations through the concept of orientation. Moreover, we can view simplicial sets as generalizations of simplicial complexes. For expositions of the rich theory arising from such objects, the reader is referred to e.g. (Goerss and Jardine, 1999) and (Riehl, 2014). Also, the review on (Goerss and Jardine, 1999) by Brayton Gray can be used as an introduction (Gray, 1999). The following short exposition is mainly based on these references.

A simplicial set, or a semi-simplicial complex, first introduced in (Eilenberg and Zilber, 1950), is an algebraic model of a topological space that is reasonably nice: It is a contravariant functor \( X : \Delta \to \text{Set} \) from the simplex category \( \Delta \) to the category of sets. A Simplex category consists of non-empty totally ordered sets as objects and order-preserving functions as morphisms. Hence, simplicial sets are presheaves on \( \Delta \) by definition. With natural transformations between such functors as morphisms, simplicial sets form a category, typically denoted as \( \text{sSet} \). Then there exists a geometric realization functor, which takes simplicial sets to topological spaces, CW complexes in particular (Milnor, 1957). Indeed, again, this kind of a geometric realization is tied with the concept of mesh in numerical methods.

Quasi-categories i.e. \( \infty \)-categories i.e. weak Kan complexes are essential in higher-category theory, their link to engineering and modelling software being, again, algebraic topology. In a quasi-category, we have morphisms between objects, morphisms between

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17http://hazel.org/

18More generally, given a category \( \text{C} \), a simplicial object is a contravariant functor \( X : \Delta \to \text{C} \).
morphisms (i.e. 2-morphisms) et cetera. However, in essence, composition is defined up to homotopy. A quasi-category is a simplicial set that satisfies the so-called weak Kan-condition (Riehl, 2014). It follows that $k$-morphisms that are eligible as composition of two given morphisms are related by an invertible $k + 1$-morphism i.e. a $k + 1$-simplex for each $k \geq 2$: This allows one to introduce the notion of homotopy between such morphisms, and composition is defined up to homotopy. To elaborate a bit, a horn $\Lambda_p[k]$ of a $k$-simplex is the union of all its faces disregarding the $p$th one. If $p = 0$ or $p = k$ a horn is an outer horn, otherwise it is an inner horn. Then, the weak Kan-condition may be stated so that all inner horns have fillers, which means that given the inclusions of the horn $\Lambda_p[k]$ to the $k$-simplex $\Delta_k$ and simplicial set $X$, and the obvious maps from these objects to the one element set 1, there exists a morphism (a filler) from $\Delta_k$ to $X$ making the diagram

\[
\begin{array}{ccc}
\Lambda_p[k] & \rightarrow & \Delta_k \\
\downarrow & & \downarrow \\
X & \rightarrow & 1
\end{array}
\]

commute. In this sense, the inner horns can be extended to simplices. These fillers, which are unique up to homotopy, are then thought of as the composites of the $k - 1$-simplices making up the horn. If all horns have fillers, a quasi-category (a weak Kan complex) becomes a Kan complex. The space of fillers of a horn in a quasi-category is a contractible Kan complex – this is the “up to homotopy” statement of composition in a quasi-category. This yields a clear connection to ordinary categories: Replacing the 1-simplices of a quasi-category with their homotopy classes gives us a category, the homotopy category associated to the quasi-category.

6.3 Identifying opportunities

Here, we identify three application areas of abstract simplicial complexes, simplicial sets and homotopy theory, interfacing computational physics and modelling software.

6.3.1 Topological computations

Already in Kotiuga’s early work on computing cuts for magnetic fields using harmonic maps into the circle, albeit not explicitly using such terms, there is a clear distinction between an abstract simplicial complex attached to the finite element mesh and its geometric realization (Kotiuga, 1989b). Moreover, a simplicial set, as a generalization of simplicial complex relates a finite element mesh to higher-categorical interpretations. Hence, there is an intimate relationship between higher-category theory, homotopy theory and data structures for numerical methods for computational physics of continuum. This points to utilization of this rich algebraic structure and categorical notions in discrete solver software. Weak homotopy relations in finite element meshes are indeed already utilized in e.g. simplifying homology computations in engineering applications (Pellikka, 2011). However, a more systematic use of categorical notions in such contexts is yet to be seen. Given the success of simplicial complexes and Whitney forms in numerical methods, and their intimate relation to homotopy theory and higher-category theory, the technology transfer of these ideas to programming numerical methods for computational physics seems inevitable.
6.3.2 Combinatorial cochain algebras

Homotopy theory and higher-categorical notions are tied to FEM and cochain methods also via the work of D. Sullivan and S. O. Wilson. For example, the combinatorial analogue of the exterior product of differential forms, the cup product of cochains defined in a simplicial complex via \( \tau_1 \cup \tau_2 = R(W_{\tau_1} \wedge W_{\tau_2}) \), is a product in a \( C_\infty \)-algebra, which is (an almost) commutative ring with commutativity relaxed up to higher homotopy. Wilson shows in (Wilson, 2007), that in the continuum limit, all the higher homotopies converge to zero and the algebra converges to the commutative and associative algebra of differential forms given by the exterior product. However, again, in the discrete side, we are bound to work \textit{up to homotopy}. For the local construction of \( \infty \)-structures used, see e.g. the appendix to (Tradler and Zeinalian, 2006) by D. Sullivan.

6.3.3 Homotopy type theory and computation

Looking further forward, computational interpretations of homotopy type theory (HTT) (Univalent Foundations Program, 2013) could be of interest in the context of computational physics. An extension of the Martin-Löf type theory (MLTT) (Martin-Löf, 1984), HTT stems from the idea of a correspondence between homotopy theory and higher-category theory. In essence, in HTT, types are interpreted as homotopy types of abstract homotopy theory. MLTT is the theory behind e.g. the common proof assistants Agda\(^\text{19}\) (Norell, 2007) and Coq\(^\text{20}\), and indeed, Vladimir Voevodsky’s motivation to develop HTT arose from the need for computer-assisted proofs. However, the basic formalism suggests that it lends itself to higher-categorical thinking ubiquitous in algebraic topology, and hence, in discrete solvers of continuum physics. The computational interpretation of HTT as a programming language is, however, still an open question. For some recent related developments, see e.g. (Angiuli \textit{et al.}, 2014), (Angiuli \textit{et al.}, 2017), (Shulman, 2014).

6.4 Final remarks

In terms of software design, to benefit from category theory, programming numerical methods should manifest itself in designing and programming the appropriate category theoretical concepts. A programming language or approach that makes categorical notions transparent, would surely help in articulating and concretizing such abstractions. Functional programming, being an instance of categorical thinking, could be a starting point (Milewski, 2017), (Omar \textit{et al.}, 2017). The other side of the coin is the semantics of computation: Monoidal categories and higher-categories provide robust models of computation and logic (Baez and Stay, 2011), (Stay and Meredith, 2015). Thus, category theory serves as a language for articulating semantics and syntax in computation.

There may be much more to say, but the raised questions cannot be fully answered within the scope of this paper: This calls for further research. The basic question is: How to translate the category theoretical thinking into code in a way that reflects it?

7 From “missed opportunities” to forward-looking research problems

The revealed structural similarities and “missed opportunities” frame forward-looking research problems (RP). Structure-preservation is the essence of a proper discretization and

\(^{19}\text{http://wiki.portal.chalmers.se/agda/}\)

\(^{20}\text{https://coq.inria.fr/}\)
at the core of functoriality. Thus, category theory, as a unifying language between computer science, algebraic topology and differential geometry, let alone other areas of mathematics and science, holds promise for the future of computational physics of continuum. Let us end this paper with a few relevant research problems raised by our discussion, in relation to programming discrete solvers. With each RP, we associate the most relevant sections of this paper. Details related to the RPs go beyond this paper, but we give some relevant references.

**RP 1 (Categories and data structures for discrete solvers)** The rich algebraic structure of abstract simplicial complexes, separate from its geometrical realization, points to richer use of category theory in practice of programming modelling software. Utilizing functors from the category of abstract simplicial complexes to categories of algebraic topology, computations can be done without recourse to floating point arithmetic. (Section 6)

**RP 2 (Whitney forms in a general category theoretical framework)** The Eilenberg-Steenrod axioms yield means of dealing with essential topological aspects of physics on a level separate from any cochain realization (Eilenberg and Steenrod, 1952). André Weil’s reaction to this led to the birth of Whitney forms (Weil, 1952). Given the connection of Whitney forms and cochains to rational homotopy theory (Sullivan, 1970), (Wilson, 2007), the axiomatics and the importance of chain homotopy in this context suggest a niche for a categorical interpretation. In particular, to provide a framework for the Whitney and de Rham maps, one should consider e.g. functors between exterior algebra bundles, cochain complexes and manifolds. (Sections 2, 3, 6)

**RP 3 (Galerkin FEM and cochains: functoriality)** The success of Whitney form Galerkin discretizations and cochain methods in CEM and continuum physics in general arises from their geometrical essence. This essence can be articulated via naturality, and often, via elliptic complexes. (Note: This is instead of utilizing more general Hilbert complexes (Arnold et al., 2010). See our discussion of elliptic and Fredholm complexes in section 2.) A central question is, how to articulate the discretization process fully functorially. Moreover, what do we ultimately mean by, or what comprises, a (structure-preserving) discretization? After all, we are searching for finite formulations of physics. (Sections 2, 3, 4, 5)

**RP 4 (Discretizing contractions and Lie derivatives)** Weil’s concept of “spaces of infinitely near points” (Weil, 1953) has led to that of Weil bundles, which lend themselves to a characterization of all product-preserving functors on manifolds (Kolar et al., 1993). Inspired by the theory of jets, Weil bundles provide an algebraic framework for prolongations of manifolds within the context of naturality. This points to their utilization in the context of discretizations related to vector fields understood as infinitesimal diffeomorphisms, adducing their connection to flows and Lie derivatives and the duality between extrusion of a manifold and contraction with a vector field, as discussed by Bossavit in (Bossavit, 2003). (Sections 2, 4)

**RP 5 (Discrete natural operations in elasticity and fluids)** The Euler equations of fluid dynamics involve the naturality of the de Rham complex, while elasticity and the viscosity term of the Navier-Stokes’ equations involve invariance under structure-preserving isometries. Naturality unifies and ties categorical notions to discretizations of such equations via Andre Weil’s 1953 paper (Weil, 1953) and the modern setting exemplified by (Kolar et al., 1993), which captures the seemingly different aspects of naturality under the same structure. (Sections 2, 4)
RP 6 (Natural differential operators in multiphysics) As a parallel to RP 5, the different notions of naturality related to e.g. MHD, plasmas and superconductivity should be studied. These involve geometric free boundary problems associated with them. These in turn relate to near force-free magnetic fields, having possible implications for e.g. fusion research. (Sections 2, 4)

RP 7 (Higher-categories, type theory, and discrete solvers) There is an intimate relationship between homotopy theory and higher-category theory (Riehl, 2014). In particular, there is a connection to homology computation (Kotiuga, 1989b), (Pellikka, 2011) and combinatorial cochain algebras (Wilson, 2007). This is further tied to computational interpretations through homotopy type theory and type theory in general (Univalent Foundations Program, 2013), (Angiuli et al., 2014), (Angiuli et al., 2017), (Shulman, 2014) and functional programming (Milewski, 2017). This is a vast, unexplored world in terms of computational physics software. (Section 6)

All of the identified “missed opportunities” above are manifestations of the possibilities of category theory as a link between modelling tool development and computational physics. Category theory brings synthesis to the field, which derives from a large and scattered set of fields of science and mathematics, helping us identify and formulate research questions.

8 Summary and conclusions

Having identified several concepts in modern mathematics as missed opportunities in computational physics, we shall finally summarize the key ideas presented in this paper.

8.1 Cochain methods and FEM

Formulating physics in a discrete, finite manner is necessary for computer simulations of natural phenomena. Computers are finite by nature, and discretizations are needed to perform simulations with finite amount of information and in finite time. In this sense, convergence properties aside, infinite-dimensional function spaces and functional analysis are not fit for computer simulations.

The traditional approach, utilized in e.g. FEM, is to discretize the differential equations, which in their strong form are required to hold pointwise in space. Another approach, is to start from macroscopic quantities represented by cochains. Even though a one-to-one correspondence can be observed between simplicial cochains and differential forms on a triangulated Riemannian manifold, these are, in some sense, fundamentally different points of view.

In continuum physics, the notion of cochain methods being directly discrete is questionable: Traditional (co)chain constructions presuppose a continuum, and laws of physics expressed in terms of cochains should hold for all chains, giving rise to infinite-dimensional spaces yet to be discretized (see section 5). Despite taking a seemingly different path to a discrete formulation from e.g. FEM (see section 4), essentially, cochain methods require a discretization, too. Via interpreting the methods in the common framework of complexes of cochains (see section 2), the discretization present in both abstracts to finding a finite-dimensional subcomplex of an infinite-dimensional complex: A structural similarity underlies them.

Hence, whether one starts from a differential or algebraic description of physics of continuum, one is required to transfer from a continuum description to a discrete description
to obtain a finite formulation suitable for computer simulations. In this sense, one is bound
to consider similar questions of compatibility and structure-preservation for discretizations
of an algebraic formulation as of a differential one: It all boils down to mimicking the
continuum as functorially as possible.

8.2 Functoriality, naturality and complexes

Geometric methods have arguably been the most successful ones in computational physics
of continuum, yielding structure-preserving discretizations. A highly practical setting for
geometric methods is that of a natural elliptic complex (see section 2). Elliptic complexes
arise naturally in computational physics of continuum in compact domains, give rise to
a rich, general Hodge theory and allow us to formulate computations in terms of the
symbol sequence, consisting of finite-dimensional spaces and matrices. With well-posed
boundary conditions, this becomes a Fredholm complex. Moreover, regarding programming
modelling software, such a cochain complex gives rise to natural data structures for discrete
solvers. From the point of view of an engineer programming such software, a general Hilbert
complex is often fruitless. Furthermore, in the discrete setting, the functorial relationship
between abstract simplicial complexes and their geometric realizations on a Riemannian
manifold enable computations without recourse to floating-point arithmetic for some phases
of the computational process (see section 6).

In this paper, we have discussed cochain methods on a general level and the finite
element method with discretizations of geometric essence more carefully. Evidently, the
essentially category theoretical concept of naturality comes up at different levels of ab-
straction when discussing computational physics of continuum, and aspects of naturality
shall be preserved in a discretization. This is the essence of geometric methods: Geometric
means natural in this context. A very comprehensive treatment of this viewpoint beyond
the scope of this paper can be found in (Kolar et al., 1993). There exist different types of
naturality related to different mathematical structures, and they are important in different
settings (see section 2). However, a unification through category theory is possible.

Coming from continuum, one wants to map the metric aspects of the problem in a func-
torial manner to the discrete setting. The Galerkin-Hodge process with Whitney forms
presents itself as a canonical way to achieve these goals (see section 4 and section 5).
Throughout, we have emphasized the functorial nature behind structure-preserving dis-
cretizations, and especially, albeit without explicitly defining such a functor, the functorial
nature of the Galerkin-Hodge process as well as the role of naturality. At the same time,
this functoriality brings the formally similar structures and final goals of the Whitney
form FEM approach and cochain method approach to the forefront. In the context of
discretizations, Whitney’s interpolation formula is uniquely characterized as the structure-
preserving discretization of natural differential operators on a manifold, compatible with
the structure of the complex arising from the triangulation.

8.3 Closing words

Looking at computational physics from an electrical engineering perspective suggests view-
ing several concepts of modern mathematics, not so well-established in computational
physics literature, as “missed opportunities” in the field. These connect through category
theory to form a set of research problems we suggest to pursue (see section 7). Observing
the categorical structures and structural similarities in discrete solvers yields us tools for
abstract and effective communication between scientists, engineers and computers. We see
this as an opportunity.
Acknowledgment

This research was supported by The Academy of Finland project [287027]. A significant part of the research leading to this paper was conducted during Valtteri Lahtinen’s (V.L.) research visit at the ECE department of Boston University (BU). V.L. would like to thank his colleagues at BU for their hospitality during his stay. Moreover, the authors would like to thank Alain Bossavit, André Nicolet and Jim Stasheff for their comments and criticism concerning the manuscript.

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Appendix: Briefly on category theory

This brief appendix provides a quick reference for some of the most basic category theoretical notions.

A.1 Standard category theory

A category formalizes the idea of a cluster of objects and arrows going between them in a compatible manner.

Definition 1 A category $\mathbf{C}$ is a quadruple $(\text{obj}_C, \text{hom}_C, \text{id}, \circ)$, which consists of

- $\text{obj}_C$, a class of objects of $\mathbf{C}$,
- for each pair $(A, B)$ of objects a set $\text{hom}_C(A, B)$ of morphisms or arrows from $A$ to $B$,
- For each object $A$, the identity morphism $\text{id}_A \in \text{hom}_C(A, A)$,
- composition $\circ$, which for each $f \in \text{hom}_C(A, B)$ and for each $g \in \text{hom}_C(B, C)$ associates a morphism $g \circ f \in \text{hom}_C(A, C)$,

such that

- the composition $\circ$ is associative, i.e. $(f \circ g) \circ h = f \circ (g \circ h)$
- for each $f \in \text{hom}_C(A, B)$, $\text{id}_B \circ f = f \circ \text{id}_A = f$,
- The sets of morphisms $\text{hom}_C(A, B)$ are pairwise disjoint.

Objects $A$ and $B$ are isomorphic if there exist morphisms $f : A \to B$ and $g : B \to A$ such that $g \circ f = \text{id}_A$ and $f \circ g = \text{id}_B$. The morphism $f$ is an isomorphism.

A category, as defined above, is called locally small as the hom-set of morphisms between a pair of objects is indeed a set. In general, this could be a proper class. If also the class of objects is a mere set, the category is small.

Definition 2 A functor $F$ from a category $\mathbf{C}_1$ to a category $\mathbf{C}_2$, denoted $F : \mathbf{C}_1 \to \mathbf{C}_2$, is a map associating

- to each object $A \in \text{Obj}(\mathbf{C}_1)$ an object $F(A) \in \text{Obj}(\mathbf{C}_2)$,
- to each morphism $f \in \text{hom}_{\mathbf{C}_1}(A, B)$ a morphism $F(f) \in \text{hom}_{\mathbf{C}_2}(F(A), F(B))$,

such that $F$ preserves identities and composition, i.e.,

- for each $A \in \text{Obj}(\mathbf{C}_1)$, $F(\text{id}_A) = \text{id}_{F(A)}$,
- whenever $g \circ f$ is defined, $F(g \circ f) = F(g) \circ F(f)$.

Two functors $F_1 : \mathbf{C}_1 \to \mathbf{C}_2$ and $F_2 : \mathbf{C}_2 \to \mathbf{C}_3$ give rise to the composite functor $F_2 \circ F_1 : \mathbf{C}_1 \to \mathbf{C}_3$. This maps each $A \in \text{Obj}(\mathbf{C}_1)$ to $F_2(F_1(A)) \in \text{Obj}(\mathbf{C}_3)$ and each $f \in \text{hom}_{\mathbf{C}_1}(A, B)$ to $F_2(F_1(f)) \in \text{hom}_{\mathbf{C}_3}(F_2(F_1(A)), F_2(F_1(B)))$. An identity functor $\text{Id}_\mathbf{C} : \mathbf{C} \to \mathbf{C}$ maps each object and morphism to itself. Hence, (small) categories and functors form a category.

Moreover, there are arrows between functors. These are called natural transformations.
Definition 3 Given two functors $F, G : C_1 \to C_2$, a natural transformation $\eta$ from $F$ to $G$ is a mapping assigning to each $A \in \text{Obj}(C_1)$ a morphism $\eta_A : F(A) \to G(A)$ such that for each $f \in \text{hom}_{C_1}(A, B)$ the diagram

$$
\begin{array}{c}
F(A) \xrightarrow{\eta_A} G(A) \\
F(f) \downarrow \quad \downarrow G(f) \\
F(B) \xrightarrow{\eta_B} G(B)
\end{array}
$$

commutes The morphisms $\eta_A$ are called components of $\eta$.

A natural isomorphism is a natural transformation whose all components are isomorphisms.

Covariance and contravariance. The opposite category $C^{\text{op}}$ of a category $C$ is obtained by reversing all the arrows in $C$. Then, having a functor $F : C_1 \to C_2$ and a functor $F' : C_1^{\text{op}} \to C_2$, we say that $F$ is a covariant functor from $C_1$ to $C_2$ and $F'$ is a contravariant functor from $C_1$ to $C_2$. That is, a contravariant functor from $C_1$ to $C_2$ is in fact a covariant functor from $C_1^{\text{op}}$ to $C_2$. In particular, contravariant functors to $\text{Set}$ are called presheaves.

Note that the use of the terms covariant and contravariant in category theory can seem contradictory to that of traditional tensor analysis books. In the case of differential forms, maps of manifolds and induced morphisms on tangent bundles involve covariant functors, while the induced maps on the cotangent bundles and associated exterior algebra bundles are then contravariant. So, in terms of category theory, differential forms behave contravariantly and vector fields behave covariantly.

A.2 Note on higher-categories

Categorifying categories iteratively, one obtains $n$-categories, or even $\infty$-categories: One has not only morphisms between objects, but 2-morphisms between morphisms et cetera. A typical example of a 2-category is the category of categories, with functors between categories as 1-morphisms and natural transformations between functors as 2-morphisms. Note how this is essential e.g. in the cases of Eilenberg-Steenrod axioms and Whitney forms and thus relates directly to computational physics. In a 2-category, between each pair of objects $A$ and $B$, there is a category of morphisms between them, the category of functors between categories $A$ and $B$ with natural transformations as morphisms.

Composing $n$-morphisms, in general, one imposes e.g. units and associativity only up to equivalence, and one has many ways of composing two given morphisms. Then, there are certain coherence laws that should be satisfied. This kind of construction yields a deep relationship between higher-category theory and homotopy theory.

The rich theory and the multitude of emerging subtleties of higher-categories are beyond the scope of the current appendix. Hence, for introduction and further references, we point the reader to e.g. (Baez and Dolan, 1998) and (Riehl, 2014).