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# Towards a Variational Complex for the Finite Element Method

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Abstract. Variational and symplectic integrators are now popular for mechanical systems, both because of their good long term stability and qualitative fit. Such integrators mimic or inherit the Lagrangian, respectively Hamiltonian, structure of the continuous model. A variational complex is a theoretical tool for the rigorous study of Lagrangian systems and their conservation laws. This article examines whether a formulation of a variational calculus for finite element methods, for an arbitrary finite element approximation scheme, is possible. The motivation is that this would allow a variational scheme to be written down for a given approximation model. Moreover, the stability and the conservation laws of such integrators could be studied without any need for individual, *ad hoc* arguments. A number of examples are considered, mainly one-dimensional, and conditions for a suitable complex derived.

## 1. Context and background

Variational principles are a central concept in the analysis of physically important models. The basic philosophy we take here is that numerical approximations which seek to mimic the underlying physics should have, of themselves, a variational structure to their formulation and analysis. There are several themes in classical and modern research that inform this article; the variational calculus, geometric integration, algebraic topology, and symbolic analysis. We consider these topics in turn.

**1.1. Variational principles.** The central tool in the mathematical analysis of variational principles is the variational calculus ([**32**, §§4.1, 5.4]). This calculus is also the correct setting for understanding the all-important theorem of Noether, which gives a conservation law for every variational symmetry.

A *variational calculus* is formulated in terms of a "locally exact differential complex". The most famous example of this concept is the grad–curl–div sequence

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This is the final form of the paper.

of operators. Exactness means that if one operator in the sequence sends an expression to zero, then that expression is in the image of the previous operator in the sequence, at least locally. So, if the curl of a vector field is zero, then locally it is the gradient of a function, and so forth. For this standard sequence, the extended sequence grad–curl–div–Euler–Lagrange–Helmholtz is still exact. This extended sequence is known as the *continuous variational complex*. With its attendant concepts and calculations, it answers questions such as,

(1) Is my equation an Euler–Lagrange equation[1], and if so, what is the Lagrangian?
(2) Is a given expression a total divergence, i.e. a conservation law?
(3) What are the conservation laws that arise from the symmetries of the Lagrangian?

It is now recognized that in order to obtain a stable numerical scheme, it is important to mimic this exactness.

> "In many contexts it is not enough that the numerical scheme be close to the original problem in a quantitative sense for it to inherit stability. . . the exactness properties of discrete differential complexes and their relation to differential complexes associated with the PDE are crucial tools in establishing the stability of numerical methods." [**3**]

Since exactness and variational principles are both important, it makes sense to investigate exact variational complexes for discretized systems. Such complexes are known for *difference* systems [**22, 25**]. Although there cannot be a "top down" analogue of the continuous variational complex, as there is no tangent structure on a discrete lattice, the difference variational calculus has theorems which are amazingly analogous to those of the continuous case.

**1.2. Geometric integration.** In recent years the area of numerical differential equations has undergone a quiet revolution called geometric integration [**17, 23, 27, 28**]. This arose from the confluence of two developments. The first is the increased awareness of the importance of geometric features of differential equations, not only symplectic structure, but volume-preservation, first integrals, symmetries, foliations and contact structure. The second development of course has been the exponential growth in computer speed over the last decades. Together these two developments have made geometric integration (the exact preservation of geometric features up to round-off error) both desirable and affordable.

> "The motivation for developing structure preserving algorithms for special classes of problems came independently from such different areas of research as astronomy, molecular dynamics, mechanics, theoretical physics and numerical analysis. . . . It turned out that the preservation of geometric properties of the flow not only produces an improved qualitative behaviour, but also allows for more accurate long-term integration than with general-purpose methods."[**17**]

[1]As the equation is precisely given. For equations only equivalent to an Euler–Lagrange equation, the problem is still open, although some particular cases have been solved [**1, 2, 7, 10, 11, 24**].

**1.3. Numerical analysis and simplicial spaces.** The influence of algebraic topology, in particular classical constructions of simplicial spaces, chains and cochains, boundary and coboundary operators, is of increasing interest to both physicists and numerical analysts [**5, 19, 31, 36, 37**]. The interplay of such notions with physical quantities and systems is increasingly being explored as a way to ensure that the correct geometry of a problem is encoded in the discretization. Indeed, some authors argue that the original models are already discrete, that is, formulated on the level of a small cell. The process of obtaining a continuum limit and then discretizing using an all-purpose numerical integrator is in fact *removing* the all-important geometry. Worse, this process can lead to a proliferation of "models" of the original, of no physical significance.

Just as one has a de Rham sequence for a smooth space which allows one to define and describe global features of gradient flows and conservation laws, so one has a matching simplicial complex for the triangulated space. The de Rham complex of a space captures the same global topological information of an orientable manifold, as the simplicial complex of its triangulation. Most importantly, one has a discrete Stokes' Theorem, allowing conservation laws to be exactly satisfied at the cellular level.

**1.4. Can we use symbolic algebra to study numerical methods?** Symbolic computation has been used with great success in obtaining symmetries and conservation laws of differential systems, and much progress has been made using these and other, strictly algebraic, techniques in on-line symbolic integrators. The potential use of symbolic computation to address the following questions is intriguing, and should lead to increased understanding of discrete systems in general.

- Can one design a numerical method, automatically, to inherit a variational principle and selected conservation laws?
- Can one obtain symmetries and hence conservation laws, automatically, of variational numerical methods?

These questions are beginning to be answered for finite difference models, (see [**22,30**]). In particular, it is necessary to fully understand certain "no go" theorems, such as the Ge and Marsden result that symplecticity and energy can generally not both be conserved [**15**]. Their result holds when energy is the only integral; there is much that needs to be understood.

For 1-D problems, one can design schemes to inherit invariance under a given Lie symmetry group [**33**] although such schemes are necessarily high order for high dimensional groups. The theory of moving frames ([**12, 13, 29**]) will play a central role in any developments concerning the automatic derivation of such schemes for higher dimensional problems.

The computation of conservation laws for variational discrete systems ([**9, 16, 18, 21**]), with and without a discrete version of Noether's theorem, is also increasingly well understood. Even for smooth systems, however, the *efficient* computation of conserved densities is still being studied [**38**]. Meanwhile, the direct computation of symmetries for discrete systems has at least three different underlying philosophies, and hence theories (cf. [**20, 26, 34**]). Note that Noether's theorem can be applied only once you know the symmetries of the Lagrangian.

**1.5. Road map of the article.** In §2 we discuss the relationship between exact differential complexes and the Finite Element (FE) Method. We take as our starting point the article of D. Arnold [**3**], and discuss the relationship in terms of projection maps. In §3 we discuss the continuous variational complex and in particular, we address the question, what is the Euler–Lagrange (EL) operator? This discussion will be pivotal to motivating what follows. In §4 we look at the projections of Lagrangians as they are used in practice, and consider the question, What is the EL operator for an FE method? For one-dimensional problems, this turns out to be easily answered. However, the examples highlight what can go wrong, and in some cases, be fixed. This section concludes with a conjecture as to when a sensible EL system be obtained. In §5 we look at higher dimensional base spaces. Here, the EL operator depends on the mesh. In §6 we give a theoretical treatment of a variational complex for FE approximation schemes. This highlights the important problems still needing to to be addressed, which are summarized in §7.

## 2. Differential complexes and the finite element method

The fundamental differential complex is the de Rham complex, which for a three-dimensional base space is written as:

$$0 \to \mathbb{R} \to \Lambda^0 \xrightarrow{\mathrm{d}} \Lambda^1 \xrightarrow{\mathrm{d}} \Lambda^2 \xrightarrow{\mathrm{d}} \Lambda^3 \to 0. \tag{2.1}$$

The $\binom{3}{p}$-dimensional vector space $\Lambda^p$ is the set of $p$-forms with coefficients being smooth functions in the co-ordinates of the three-dimensional base space (the independent variables). The linear operator d is the exterior derivative, which satisfies $\mathrm{d}^2 = 0$. One can think of $\Lambda^p$, $p > 0$, as being a vector field with $\binom{3}{p}$ components, and d as either the gradient, curl or divergence operator:

$$0 \to \mathbb{R} \to \mathcal{C}^\infty(X) \xrightarrow{\text{grad}} \mathcal{C}^\infty(X)^3 \xrightarrow{\text{curl}} \mathcal{C}^\infty(X)^3 \xrightarrow{\text{Div}} \mathcal{C}^\infty(X) \to 0,$$

but this is to rob the forms of much of their meaning. In the context of this article, a $p$-form is best thought of as the integrand of a $p$-dimensional integral. For example, inherent in the definition of the $\mathrm{d}x_i$, $\mathrm{d}x_i \wedge \mathrm{d}x_j$ and $\mathrm{d}x_i \wedge \mathrm{d}x_j \wedge \mathrm{d}x_k$ are the correct change of variable formulae learned in undergraduate calculus for such integrands ([**6**, p. 199]).

Remark 2.1. The precise correspondence between forms and vector fields or functions depends on the metric. Assuming the Euclidean metric, as we will throughout this article, the correspondence in 3-space is

$$\begin{aligned}
\Lambda^1 &: (f_1, f_2, f_3) \longleftrightarrow f_1\,\mathrm{d}x_1 + f_2\,\mathrm{d}x_2 + f_3\,\mathrm{d}x_3,\\
\Lambda^2 &: (f_1, f_2, f_3) \longleftrightarrow f_1\,\mathrm{d}x_2\mathrm{d}x_3 - f_2\,\mathrm{d}x_1\mathrm{d}x_3 + f_3\,\mathrm{d}x_1\mathrm{d}x_2,\\
\Lambda^3 &: f \qquad\qquad\;\; \longleftrightarrow f\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3 \equiv f\mathrm{d}\mathbf{x}.
\end{aligned}$$

In the following, we will use these interchangeably to ease the exposition.

Definition 2.2. Let $X$ be a triangulated space, with the top-dimensional simplices denoted generically by $\tau$. Let $\chi_\tau$ be the characteristic function of $\tau$. A *Finite Element approximation model* $\mathcal{F}_p$ of $\Lambda^p$ is a set of $p$-forms, defined piecewise on the $\tau$,

$$\mathcal{F}_p = \left\{ \sum_{\substack{\tau \\ i_1 < \cdots < i_p}} f_\tau^{i_1\cdots i_p} \chi_\tau\,\mathrm{d}x_{i_1}\cdots\mathrm{d}x_{i_p} \;\middle|\; f_\tau^{i_1\cdots i_p} \colon \tau \to \mathbb{R} \right\}$$

such that:

(1) $\mathcal{F}_p\big|_\tau$ is a finite dimensional real vector space. The coefficients of the basis elements on $\tau$ are called the **shape functions**, or function ansätze of the FE approximation, usually the same for all $\tau$.
(2) The finite number of parameters on which each shape function $f_\tau^{i_1\cdots i_p}$ depends, can be obtained by specified linear functionals, one for each parameter. These functionals are called the **degrees of freedom** or **data** for the FE model.
(3) Each degree of freedom depends, in some sense, on a (sub)simplex of some dimension. Where a sub-simplex is shared by two top-level simplices in the triangulation, we assume the corresponding degrees of freedom for the shape functions in the different simplices agree.

Schemes which do not satisfy the third condition are said to be *non-conforming*. Strictly speaking, it is necessary to assign shared sub-simplices to just one $\tau$ in the sum above, in order to prevent double counting at those points.

Definition 2.3. The **projection map** $\Pi_p\colon \Lambda^p \to \mathcal{F}_p$ is the assignment to a given form, of a form with coefficients in the ansatz of the shape function, with those particular choices of the parameters such that the data of the function and its projection are equal.

Example 2.4. One of the simplest examples of an FE approximation space in 3-space is that of piecewise constant 3-forms. The projection operator from $\Lambda^3$ is:

$$\Pi_3(f\,\mathrm{d}\mathbf{x}) = \sum_\tau \alpha_\tau(f\,\mathrm{d}\mathbf{x})\chi_\tau\,\mathrm{d}\mathbf{x},$$

where

$$\alpha_\tau(f\,\mathrm{d}\mathbf{x}) = \frac{\int_\tau f\,\mathrm{d}\mathbf{x}}{\int_\tau \mathrm{d}\mathbf{x}},$$

that is, the normalized zeroth moment of the 3-form on $\tau$.

Example 2.5. One of the simplest projection operators defined on $\Lambda^0 = \mathcal{C}^\infty$ is the usual piecewise linear interpolant defined by the values of the function at the vertices.

Following the discussion in [**3**], we make the following definition.

Definition 2.6. A **coherent** differential complex $\mathcal{F}^*$ of FE spaces, all relative to the same triangulation of the base space $X$, is defined as a set of choices of FE spaces $\mathcal{F}_i$ and projection maps $\Pi_i$ such that the following diagram *commutes*,

$$\begin{array}{ccccccccccccc}
0 & \to & \mathbb{R} & \to & \Lambda^0 & \xrightarrow{\mathrm{d}} & \Lambda^1 & \xrightarrow{\mathrm{d}} & \Lambda^2 & \xrightarrow{\mathrm{d}} & \Lambda^3 & \to & 0 \\
 & & & & \big\downarrow\Pi_0 & & \big\downarrow\Pi_1 & & \big\downarrow\Pi_2 & & \big\downarrow\Pi_3 & & \\
0 & \to & \mathbb{R} & \to & \mathcal{F}_0 & \xrightarrow{\mathrm{d}} & \mathcal{F}_1 & \xrightarrow{\mathrm{d}} & \mathcal{F}_2 & \xrightarrow{\mathrm{d}} & \mathcal{F}_3 & \to & 0.
\end{array} \tag{2.2}$$

We will motivate this definition at the end of §3.

Remark 2.7. In the literature, the spaces $\mathcal{F}_i$ are denoted as:

$$\mathcal{F}_0 = W_h, \quad \mathcal{F}_1 = Q_h, \quad \mathcal{F}_2 = S_h, \quad \mathcal{F}_3 = V_h,$$

where $h$ is a real parameter indicating the "size" or "diameter" of the triangulation. Here we use an index to denote the dimension of the forms the space includes, for simplicity of the exposition.

Even though the respective projection operators are sometimes referred to as vertex, edge, face etc operators, it is not necessarily the case that the data for these spaces depends respectively only on function values on vertices, edges, faces and so on. It is also important to note that the functions in these spaces are defined piecewise on the top dimensional simplices. The exterior derivative in the lower sequence is usually taken to be defined only in the interior of the top dimensional simplices, because the forms are only piecewise smooth. When trying to prove theorems about such forms rigorously, concerning their local and global properties, the correct algebraic setting involves locally smooth forms together with an object which encodes how the mesh is put together. We will discuss this further in §§5,6. Using weak or distributional derivatives can lead to trouble for the applications in this article, see Example 4.2.

EXAMPLE 2.8 (The zeroth order Raviart and Thomas scheme). Let $\tau$ be a 3-simplex with faces $\sigma_i$, edges $e_i$ and vertices $v_i$. For a $p$-form $\omega$ defined on $\tau$, the projection map takes $\omega$ to the piecewise linear $p$-form with the same zeroth moments on the $p$-dimensional sub-simplices of $\tau$. So, letting $a$ and $b$ be constants, **a**, **b** be constant vector fields, and writing the shape functions as vector fields,

| Space | Dim | Shape | Data |
|---|---|---|---|
| $\mathcal{F}_0$ | 4 | $a+\mathbf{b}\bullet\mathbf{x}$ | $f \mapsto f(v_i)$ |
| $\mathcal{F}_1$ | 6 | $\mathbf{a}+\mathbf{b}\times\mathbf{x}$ | $\omega \mapsto \int_{e_i}\omega$ |
| $\mathcal{F}_2$ | 4 | $\mathbf{a}+b\mathbf{x}$ | $\omega \mapsto \int_{\sigma_i}\omega$ |
| $\mathcal{F}_3$ | 1 | $a$ | $\omega \mapsto \int_{\tau}\omega$ |

where "Dim" denotes the dimension of the space per simplex $\tau$. Stokes' theorem ([**6**, p. 212ff]),

$$\int_{\partial\rho}\omega = \int_{\rho}\mathrm{d}\omega,$$

where $\partial\rho$ is the boundary of the simplex $\rho$, implies that the diagram commutes. For example, if $f \in \Lambda^0 \equiv \mathcal{C}^\infty(X,\mathbb{R})$ and $e$ is the edge running from vertex $v_1$ to $v_2$, then

$$\begin{aligned}\int_e \Pi_Q(\mathrm{d}f) = \int_e \mathrm{d}f = \int_{\partial e} f = f(v_2) - f(v_1)\\ &= (\text{gradient of linear function with values}\\ &\qquad f(v_i) \text{ at } v_i)\cdot(v_2 - v_1)\\ &= \int_e \mathrm{d}\Pi_W(f).\end{aligned}$$

Since forms in the $\mathcal{F}_i$ with equal data are equal, $\Pi_Q(\mathrm{d}f) = \mathrm{d}\Pi_W(f)$.

REMARK 2.9. The **de Rham** map is the pairing,

$$\langle\rho,\omega\rangle \mapsto \int_\rho \omega,$$

where $\rho$ is a $p$-simplex, $\omega \in \Lambda^p$, extended linearly in both arguments. This map is used to show that the global topological information inherent in the de Rham and simplicial cohomology theories is equivalent for orientable manifolds ([**6**, p. 226]). In fact, the coherent FE differential complex given by the zeroth order Raviart and Thomas scheme, and the simplicial complex with real coefficients, are isomorphic.

By commutativity, that is, $\Pi_{p+1}\mathrm{d}(\omega) = \mathrm{d}\Pi_p(\omega)$, and Stokes' Theorem, the choice of data at the $\mathcal{F}_{p+1}$ level dictates to some extent the choice of data at the $\mathcal{F}_p$ level.

EXAMPLE 2.10. Consider the one-dimensional problem,

$$\begin{array}{ccccccccc} 0 & \to & \mathbb{R} & \to & \Lambda^0 & \xrightarrow{\mathrm{d}} & \Lambda^1 & \to & 0 \\ & & & & \big\downarrow \Pi_0 & & \big\downarrow \Pi_1 & & \\ 0 & \to & \mathbb{R} & \to & \mathcal{F}_0 & \xrightarrow{\mathrm{d}} & \mathcal{F}_1 & \to & 0 \end{array}$$

where the projection $\Pi_1$ is to the piecewise constant 1-form

$$\omega\big|_e \mapsto \frac{\int_e \psi_e \omega}{\int_e \psi_e \,\mathrm{d}x}\,\mathrm{d}x$$

and the $\psi_e$ are weight functions. Then since we require that the derivative of a 0-form in $\mathcal{F}_0$ lie in $\mathcal{F}_1$, the elements of $\mathcal{F}_0$ can be at most piecewise linear. Further, the projection map $\Pi_0$ on the edge $e$ needs to involve the moment with respect to the weight function $\mathrm{d}\psi_e/\mathrm{d}x$, as well as the values of the 0-form at the vertices. Indeed, we have that

$$\begin{array}{ccc} u & \to & u_x \,\mathrm{d}x \\ \big\downarrow & & \big\downarrow \\ \sum_e (a_e x + b_e)\chi_e & \to & \sum_e a_e \chi_e \end{array}$$

where

$$a_e = \frac{\int_e \psi_e u_x \,\mathrm{d}x}{\int_e \psi_e \,\mathrm{d}x} = \frac{1}{\int_e \psi_e \,\mathrm{d}x}\left(\psi_e u|_{\partial e} - \int_e \psi_{e,x} u \,\mathrm{d}x\right).$$

The constants $b_e$ are then chosen to make the elements in $\mathcal{F}_0$ piecewise continuous. While we have written the integrations to be over $e$, this is not necessary. There are examples where the intervals of integration for neighboring edges overlap to some small extent.

EXAMPLE 2.11. Suppose the data for the projection map for $\Lambda^p$ includes the first degree moments on the $p$-simplex $\sigma$. Let $x$ denote a generic co-ordinate on $X$. Then since we have the identity

$$\int_\sigma x\mathrm{d}\omega = \int_\sigma \big(\mathrm{d}(x\omega) - \mathrm{d}x \wedge \omega\big) = \int_{\partial\sigma} x\omega - \int_\sigma \mathrm{d}x \wedge \omega$$

the data for $\Lambda^{p-1}$ will involve the first order moments on the $p-1$ simplices, as well as the quantities $\int_\sigma \mathrm{d}x \wedge \omega$, which are the zeroth moments of the components of the form on $p$-dimensional simplices. One sees this in the data for the first order Raviart and Thomas scheme, where the shape functions are piecewise quadratic [**3**].

THEOREM 2.12. *The de Rham complex, restricted to a top-level simplex, is* exact*, that is,*

$$\ker \mathrm{d}\big|_{\Lambda^p} = \operatorname{im} \mathrm{d}\big|_{\Lambda^{p-1}}. \tag{2.3}$$

This result is known as Poincaré's Lemma and is proved ([**6**, p. 224]) by producing a sequence of maps $h_p \colon \Lambda^p \to \Lambda^{p-1}$, such that

$$\mathrm{d}h_p + h_{p+1}\mathrm{d} = \mathrm{id}\big|_{\Lambda^p}.$$

The maps $h_p$ are called *homotopy maps*. For then, if $\mathrm{d}\omega = 0$, we have $(\mathrm{d}h_p + h_{p+1}\mathrm{d})\omega = \mathrm{d}h_p\omega = \omega$. This shows that $\ker \mathrm{d} \subseteq \operatorname{im} \mathrm{d}$ while $\mathrm{d}^2 = 0$ shows the converse. In fact, whenever the base space $X$ is diffeomorphic to the unit sphere, then the de Rham sequence on $X$ is exact.

THEOREM 2.13. *Let a coherent FE differential complex $\mathcal{F}^*$ be given, so that the diagram* (2.2) *commutes. If the upper sequence in* (2.2) *is exact, then so is the lower sequence;*

$$\ker \mathrm{d}\big|_{\mathcal{F}_p} = \operatorname{im} \mathrm{d}\big|_{\mathcal{F}_{p-1}}.$$

PROOF. For both upper and lower sequences we have that $\mathrm{d}^2 = 0$, so we need only produce homotopy operators for the lower sequence. If the homotopy operators for the upper sequence are $h_i$, then the homotopy operators for the lower sequence are $\Pi_i h_{i+1} \colon \mathcal{F}^{p+1} \to \mathcal{F}^p$, where we are using implicitly that $\mathcal{F}^p \subset \Lambda^p$ on every simplex. For

$$\begin{aligned}(\mathrm{d}\Pi_{i-1}h_i + \Pi_i h_{i+1}\,\mathrm{d})\omega &= \Pi_i(\mathrm{d}h_i + h_{i+1}\mathrm{d})\omega \\ &= \Pi_i\omega \\ &= \omega, \quad \text{as } \omega \in \mathcal{F}_i.\end{aligned}$$

□

When designing coherent FE differential complexes, the fact that they consist of finite dimensional vector spaces means that the following useful theorem applies:

THEOREM 2.14. *If $\mathcal{F}^*$ is an exact complex, then* $\sum(-1)^n \dim(\mathcal{F}_n) = 0$.

Note that $\mathbb{R} \equiv \mathcal{F}_{-1}$ is included in this sum. Putting the above results together, we have that the alternating sum of the dimensions of the function spaces on each $\tau$ add to zero. Thus for the zeroth order Raviart and Thomas scheme, we have indeed that $1 - 4 + 6 - 4 + 1 = 0$. The theorem can be used to check that the correct amount of data at each level has been obtained. Of course, the converse is not true!

## 3. The variational complex for smooth forms

The variational complex is a theoretical tool for studying Lagrangian systems and their conservation laws. A detailed discussion with proofs can be found in Olver's text [**32**]. We define the basic objects for later reference, and consider in some depth the derivation of the continuous Euler–Lagrange operator. This is the map we wish to develop in the context of a FE approximation scheme, as a first step in asking whether a full variational complex for a given FE scheme exists.

The first half of the variational complex is similar to the de Rham complex, but with one major difference. The coefficient functions in $\Lambda^p$ are now functions not just of the independent variables, but of the dependent variables and their derivatives. We assume that these functions are smooth functions with a finite number of arguments, but we do not specify any bounds in the degree of the derivatives. Moreover, the exterior derivative is taken to be a *total* exterior derivative, which we now denote by D. So, for example, we have

$$\mathrm{D}(yu_x\,\mathrm{d}x) = (yu_{xy} + u_x)\,\mathrm{d}y \wedge \mathrm{d}x + yu_{xz}\,\mathrm{d}z \wedge \mathrm{d}x.$$

DEFINITION 3.1. Forms in the dependent variables and their derivatives, regarded as separate indeterminants, are known as *vertical* forms. The space of vertical $p$-forms is denoted by $\widehat{\Lambda}^p$. The vertical derivative $\widehat{\mathrm{d}}\colon \widehat{\Lambda}^p \to \widehat{\Lambda}^{p+1}$ operates in the natural way, but treats the independent variables as constants, for example,

$$\widehat{\mathrm{d}}\big((uu_x + 3xu_{xx})\mathrm{d}u\big) = u\,\mathrm{d}u_x \wedge \mathrm{d}u + 3\,\mathrm{d}u_{xx} \wedge \mathrm{d}u.$$

THEOREM 3.2. [**32**, §5.4, p. 344] *The vertical complex*

$$\widehat{\Lambda}^0 \xrightarrow{\widehat{\mathrm{d}}} \widehat{\Lambda}^1 \xrightarrow{\widehat{\mathrm{d}}} \widehat{\Lambda}^2 \xrightarrow{\widehat{\mathrm{d}}} \cdots \tag{3.1}$$

*is exact.*

The second half of the variational complex are the vertical forms multiplied by the volume form on the base space, but with the "twist" that forms are defined only up to total divergence.

DEFINITION 3.3. Let the total derivative with respect to the independent variable $x_j$, denoted by $\mathrm{D}_j$, act linearly on the space of vertical forms, together with $\mathrm{D}_j(\omega\wedge\eta) = \mathrm{D}_j(\omega)\wedge\eta+\omega\wedge\mathrm{D}_j(\eta)$ and $\mathrm{D}_j\widehat{\mathrm{d}} = \widehat{\mathrm{d}}\mathrm{D}_j$. Then, for example, $\mathrm{D}_j\,\mathrm{d}u = \mathrm{d}u_{x_j}$, $\mathrm{D}_j\,\mathrm{d}x_k = 0$, and $\mathrm{D}_j(x_j\,\mathrm{d}u_{x_k}) = \mathrm{d}u_{x_k} + x_j\,\mathrm{d}u_{x_k x_j}$.

DEFINITION 3.4. We say two vertical forms on an $n$-dimensional base space are equivalent if they differ by a total divergence, that is,

$$\omega \sim \eta \iff \omega - \eta = \mathrm{D}_1\zeta_1 + \cdots + \mathrm{D}_n\zeta_n. \tag{3.2}$$

The space of equivalence classes is the space of functional $p$-forms,

$$\Lambda^p_* = \widehat{\Lambda}^p/\mathrm{Div}(\widehat{\Lambda}^p)^n.$$

All elements of $\Lambda^1_*$ on a one-dimensional base space can be represented as $f(x, u, u_x, \dots)\,\mathrm{d}u \wedge \mathrm{d}x$. For example,

$$xu_{xx}\,\mathrm{d}u_x = \mathrm{D}(xu_{xx}\,\mathrm{d}u) - \mathrm{D}(xu_{xx})\,\mathrm{d}u$$

and similarly for all $f\,\mathrm{d}u_{x\cdots x}$; note that $\mathrm{D}(\mathrm{d}u) = \mathrm{d}u_x$ etc. and $\mathrm{D}(\mathrm{d}x) = 0$.

THEOREM 3.5. *The vertical derivative* $\widehat{\mathrm{d}}$ *is well defined on equivalence classes, and hence induces a map, the* variational derivative*,*

$$\delta\colon \Lambda^p_* \to \Lambda^{p+1}_*.$$

The variational complex in 3-space is written as

$$0 \to \mathbb{R} \to \Lambda^0 \xrightarrow{\mathrm{D}} \Lambda^1 \xrightarrow{\mathrm{D}} \Lambda^2 \xrightarrow{\mathrm{D}} \Lambda^3 \xrightarrow{\mathrm{E}} \Lambda^1_* \xrightarrow{\delta} \Lambda^2_* \xrightarrow{\delta} \cdots \tag{3.3}$$

where E is the Euler–Lagrange operator. The main theorem regarding this complex is the following.

THEOREM 3.6 ([**32**, §5.4]). *If the base space is diffeomorphic to* $\mathbb{R}^3$ *then the complex* (3.3) *is exact.*

This means that an expression is precisely an Euler–Lagrange (EL) system if and only if the Helmholtz operator sends it to zero (it may be that a system is only equivalent to an EL system, in which case the test fails). An expression is precisely a total divergence if and only if the Euler–Lagrange operator sends it to zero. Moreover, there are operators called homotopy operators which allow you to answer questions such as, "if my system is an EL system, what is the Lagrangian?" and "if my system is a total divergence, what is it the divergence of?" Finally, the calculations and proofs for Noether's theorem are best given in the language of the variational complex.

The smooth Euler–Lagrange operator on $\Lambda^3$ is obtained in a two step process. First take the vertical exterior derivative, $\widehat{\mathrm{d}}$, and then take the projection $\pi$ onto an equivalence class. For example, for the one-dimensional, degree 2 Lagrangian, $L = L(x, u, u_x, u_{xx})$,

$$\begin{aligned}\widehat{\mathrm{d}}L\,\mathrm{d}x &= \left(\frac{\partial L}{\partial u}\,\mathrm{d}u + \frac{\partial L}{\partial u_x}\,\mathrm{d}u_x + \frac{\partial L}{\partial u_{xx}}\,\mathrm{d}u_{xx}\right)\wedge \mathrm{d}x\\ &= \left(\frac{\partial L}{\partial u} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial L}{\partial u_x} + \frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{\partial L}{\partial u_{xx}}\right)\mathrm{d}u\wedge \mathrm{d}x + \mathrm{D}(A)\wedge \mathrm{d}x\end{aligned}$$

where

$$A = \left(\frac{\partial L}{\partial u_x} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial L}{\partial u_{xx}}\right)\mathrm{d}u + \frac{\partial L}{\partial u_{xx}}\,\mathrm{d}u_x$$

and then

$$\mathrm{E}(L) = \pi\circ\widehat{\mathrm{d}}(L\,\mathrm{d}x) = \left(\frac{\partial L}{\partial u} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial L}{\partial u_x} + \frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{\partial L}{\partial u_{xx}}\right)\mathrm{d}u\wedge \mathrm{d}x,$$

where $\pi(\omega) = \omega/\sim$, and $\omega\sim\psi \iff \omega - \psi = Dh$. The equivalence class of $\omega$ is written as $\int_X \omega$. Since by Stokes' Theorem we have

$$\int_X \mathrm{Div}h = \int_{\partial X} h,$$

the equivalence class can be thought of as "throwing away the boundary terms".

So the smooth Euler–Lagrange operator is the variational extremum for interior variations.

Important Remark 3.7. The motivation for studying coherent FE approximation schemes is that variational problems benefit from their use. This is shown in some detail by Arnold [**3**]. In 3-space, Lagrangians are 3-forms, which are made up of products of 0, 1, 2 and 3-forms. Arnold shows that provided the approximations of the components of a Lagrangian lie in the relevant FE approximation space of a *coherent* complex of such spaces, then the numerical approximation obtained will be stable; the exactness of a coherent complex implies that the functional analytic requirements of Brezzi's theorem, [**4**], for stability of mixed element schemes, will hold. The benefit of using a coherent scheme is that exactness is a relatively simple algebraic property, both to verify and to design.

## 4. Lagrangians and Euler–Lagrange equations for finite element schemes—the one-dimensional case

Comparing the complexes (2.2) and (3.3), the question, "Can we obtain a projection of the smooth variational complex to a Finite Element sequence and hence obtain similar or analogous results?" is a natural one. However, investigating the "top down" approach leads one to suspect that the answer is "no". First of all, for a wide range of projection operators,

$$\Pi(fg)\neq\Pi(f)\Pi(g),\quad \Pi(u_x)\neq\Pi(u)_x.$$

The left hand sides are how a "top down" version of a complex would project a Lagrangian. But the right hand sides are how a Lagrangian is projected in practice. Then, there is the problem of what is the meaning of the 100th derivative of a piecewise linear (quadratic, cubic…) approximation of $u$? Recall that there is no bound on the degree of differentiation in the arguments of Lagrangians. Finally, insisting on a commutative diagram leads quickly to strange looking results. For example, for the one-dimensional linear interpolation scheme, one obtains (using calculations that are explained in the sequel), that the projection of $\int 1\,\mathrm{d}u \wedge \mathrm{d}x$ must be $\sum \frac{1}{2}(x_{n+1} - x_n)\,\mathrm{d}u_n$.

On the other hand, finite element methods for variational problems are textbook material ([**8, 14**]). Hence the line of attack we take is to look at textbook examples using the mindset/technology/terminology of formal variational processes, and induce what the full analogue of the Finite Element variational complex should be.

In this section, we look at one-dimensional problems for simplicity. Hence, Lagrangians are 1-forms and the grid is a partition on $\mathbb{R}$. In the next section we will consider higher dimensional problems.

EXAMPLE 4.1. Take the Lagrangian $L[u] = (u_x^2 + 2u)\,\mathrm{d}x$ which has the Euler–Lagrange equation,

$$\mathrm{E}(L) = \left(\frac{\partial}{\partial u} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial}{\partial u_x}\right)(L) = -2(u_{xx} - 1).$$

The standard triangulation of $\mathbb{R}$ has vertices $x_n$ and edges $e_n = (x_n, x_{n+1})$. The standard interpolation scheme with data $u_n = u(x_n)$ has projection operator

$$\begin{aligned} \Pi(u)|_{e_n} &= x \mapsto \frac{u_{n+1} - u_n}{x_{n+1} - x_n}\, x + \frac{u_n x_{n+1} - u_{n+1} x_n}{x_{n+1} - x_n} \\ &= u^{e_n}, \\ \Pi(u) &= \sum u^{e_n} \chi_{e_n}, \end{aligned} \tag{4.1}$$

where $\chi_A$ is the characteristic function for the set $A$.

The discrete Lagrangian is $\big(\Pi(u)_x^2 - 2\Pi(u)\big)\,\mathrm{d}x$ and hence

$$\mathcal{L}[u] = \int [\Pi(u)_x^2 - 2\Pi(u)]\,\mathrm{d}x = \sum_n \int_{e_n} \big((u^{e_n})_x^2 - 2u^{e_n}\big)\,\mathrm{d}x.$$

Performing the integrations yields

$$\mathcal{L}[u] = \sum_n \frac{(u_{n+1} - u_n)^2}{x_{n+1} - x_n} + (u_n x_{n+1} - u_{n+1} x_n) + (u_{n+1} x_{n+1} - u_n x_n).$$

The final group of terms telescopes and hence is in fact a boundary term, and ends by being discarded in the projection to the equivalence class.

Calculating the obvious analogue of the vertical derivative of $\mathcal{L}[u]$ yields

$$\sum_n \left(2\frac{u_{n+1} - u_n}{x_{n+1} - x_n} - x_n\right)\mathrm{d}u_{n+1} + \left(-2\frac{u_{n+1} - u_n}{x_{n+1} - x_n} + x_{n+1}\right)\mathrm{d}u_n. \tag{4.2}$$

Using the identity

$$\sum a_n \mathrm{d}u_{n+1} = \sum a_{n-1}\mathrm{d}u_n + \text{boundary terms} \tag{4.3}$$

yields the variational derivative, modulo boundary terms, of $\mathcal{L}[u]$ to be

$$\sum_n \left(2\frac{u_n - u_{n-1}}{x_n - x_{n-1}} - x_{n-1} - 2\frac{u_{n+1} - u_n}{x_{n+1} - x_n} + x_{n+1}\right)\mathrm{d}u_n.$$

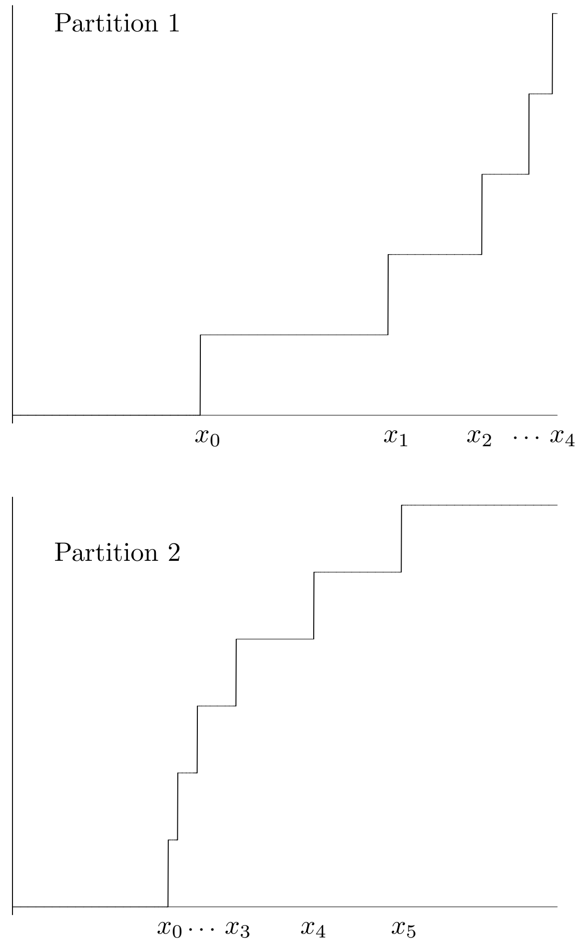


FIGURE 1. The solution to $\alpha_{n+1} - \alpha_n = \kappa \in \mathbb{R}$ for two different partitions.

Since each variation $\mathrm{d}u_n$ is independent, each coefficient must be zero (at least in the function space $\ell_2$), and this then yields the discrete Euler–Lagrange equation. Integrating twice gives

$$u_n = \tfrac{1}{2}x_n^2 + \kappa x_n + \left(u_0 - \tfrac{1}{2}x_0^2 - \kappa x_0\right)$$

which is the exact solution at each node.

Not all choices of Finite Element are suited to variational methods. We look now at two examples to show the problems that can occur. The first example shows that having too few degrees of freedom can lead to problems. We then show how the problem can be addressed.

EXAMPLE 4.2. Consider the projection to piecewise constant functions,

$$\Pi(u) = \sum_n \alpha_n \chi_{e_n},$$

where

$$\alpha_n = \frac{1}{x_{n+1} - x_n} \int_{x_n}^{x_{n+1}} u \,\mathrm{d}x.$$

For $L[u] = \frac{1}{2}u_x^2 \,\mathrm{d}x$ we have $\Pi(u)_x = \sum(\alpha_n - \alpha_{n-1})\delta(x - x_n)$ taking the weak or distributional meaning of the derivative, and thus

$$\frac{1}{2}\int u_x^2 \,\mathrm{d}x \mapsto \frac{1}{2}\sum_n (\alpha_n - \alpha_{n-1})^2.$$

The weak derivative is needed to avoid a null discrete Lagrangian[2]. The variational derivative of the discrete Lagrangian with respect to the moments $\alpha$ is

$$\sum_n (\alpha_n - \alpha_{n-1})(\mathrm{d}\alpha_n - \mathrm{d}\alpha_{n-1}). \tag{4.4}$$

Equation (4.4) is equivalent to $\sum_n (2\alpha_n - \alpha_{n-1} - \alpha_{n+1})\mathrm{d}\alpha_n$, modulo boundary terms. The discrete Euler–Lagrange equation is then $2\alpha_n - \alpha_{n-1} - \alpha_{n+1} = 0$ or $\alpha_{n+1} - \alpha_n = \kappa$, $\kappa \in \mathbb{R}$.

Figure 1 shows the solution to this equation for two different partitions. By changing the partition, we can make the piecewise constant function $\alpha$ resemble a wide variety of functions! Note that $\alpha_n$ is the average value of $u$ in $[x_n, x_{n+1}]$ and so the graph of $\alpha$ resembles that of $u$ in some sense. The correct answer to the continuous Euler–Lagrange problem is $u(x) = ax + b$ for constants $a$ and $b$. This has zeroth moments

$$\alpha_n = \frac{1}{x_{n+1} - x_n} \int_{x_n}^{x_{n+1}} (ax + b) \,\mathrm{d}x = \frac{1}{2}a(x_{n+1} + x_n) + b$$

and thus $\alpha_{n+1} - \alpha_n = \frac{1}{2}a(x_{n+2} - x_n)$. This is constant only for the regular partition, so that the discrete EL equation is correct only in that case.

This approximation scheme yields even worse problems for other Lagrangians, including unsolvable EL equations such as $1/\alpha_n = 0$!

By taking a piecewise linear approximation for a degree 1 Lagrangian, we avoid the need for a distributional or weak derivative. This can be achieved, still using the zeroth moments $\alpha_n$ and $\alpha_{n+1}$ for $u$, on $(x_n, x_{n+1})$ and $(x_{n+1}, x_{n+2})$ respectively, to create a piecewise linear approximation for $u$ on $(x_n, x_{n+2})$. This yields

$$\Pi(u)_n = x \mapsto A_n x + B_n \tag{4.5}$$

where

$$\begin{aligned} A_n &= 2\left(\frac{\alpha_n - \alpha_{n+1}}{x_n - x_{n+2}}\right), \\ B_n &= \left(\frac{x_{n+1} + x_{n+2}}{x_{n+2} - x_n}\right)\alpha_n - \left(\frac{x_{n+1} + x_n}{x_{n+2} - x_n}\right)\alpha_{n+1}. \end{aligned} \tag{4.6}$$

Hence we get a piecewise linear approximation on the partition

$$\cdots x_{n-4},\ x_{n-2},\ x_n,\ x_{n+2},\ x_{n+4}, \cdots .$$

Doing the same calculations as before, the resulting EL equation "integrates" to

$$\frac{\alpha_n - \alpha_{n+1}}{x_n - x_{n+2}} = \kappa, \quad \kappa \in \mathbb{R}$$

[2]We note that products of such derivatives is problematic and the conditions we specify in the sequel will in fact avoid them.

which is correct.

This and other examples lead one to the conclusion that there must be at least as many data per top-level simplex as the order of the Euler–Lagrange equation, that is, double the order of the Lagrangian.

Unfortunately, this condition is still insufficient for success, as the next example shows.

EXAMPLE 4.3. Suppose we take in each edge $e_n = [x_n, x_{n+1})$ the piecewise linear approximation

$$\Pi(u)\big|_{e_n} = x \mapsto u_n + u_n'(x - x_n)$$

constructed from the data

$$u_n = u(x_n), \qquad \alpha_n = \frac{1}{x_{n+1} - x_n} \int_{x_n}^{x_{n+1}} u \,\mathrm{d}x.$$

Then

$$u_n' = 2\frac{\alpha_n - u_n}{x_{n+1} + x_n}.$$

Substituting this into any first order Lagrangian and taking the variational derivatives, one for the moments $u_n$ and one of the moments $\alpha_n$, leads to two Euler–Lagrange equations in two unknowns; $u_n$ and $\alpha_n$. No recurrence relation is obtained, there is no one "solution" to the global problem depending on two constants of integration linking all the moments; in short, the result is nonsense. The problem is that the degrees of freedom in the one edge are unrelated, they are not shifts of each other in some sense.

In Examples 4.2 and 4.3, approximation schemes were given for functions, that is, for $\Lambda^0$, without any reference to what the approximation might be for $\Lambda^1$ that would be coherent with it, in the sense of Definition 2.6. When trying to ponder what these might be, it seems that in fact there isn't one! For example, using the zeroth moment for $\Lambda^0$ presupposes that the first degree moment is used for $\Lambda^1$. This in turn implies that not only $u(x_n)$ but $u(x_{n+1})$ is needed in the approximations of functions in each edge. This would then lead to the discrete Euler–Lagrange equations being recurrence relations of the correct order.

The improved approximation scheme in Example 4.2, given in Eqs: (4.5) and (4.6), does in fact form part of a coherent scheme. The projection of the 1-form $u(x)\,\mathrm{d}x$ is to the piecewise constant 1-form with the value

$$\int_{x_n}^{x_{n+2}} u(x)\psi_n(x)\,\mathrm{d}x,$$

where

$$\psi_n(x) = \begin{cases} \frac{2(x-x_n)}{(x_{n+2}-x_n)(x_{n+1}-x_n)}, & x_n < x < x_{n+1}, \\[2ex] \dfrac{2(x_{n+2}-x)}{(x_{n+2}-x_n)(x_{n+2}-x_{n+1})}, & x_{n+1} < x < x_{n+2} \end{cases}$$

in the interval $(x_n, x_{n+2})$.

CONJECTURE 4.4. Suppose that a one-dimensional Lagrangian of order $m$ is given together with a coherent Finite Element differential complex, and that at least twice as many degrees of freedom are involved in the projected Lagrangian as the order of the Lagrangian. Then the Euler–Lagrange system is a recurrence system whose solution depends on $2m$ constants and converges to the solution of the continuous Euler–Lagrange equations in some well defined sense.

Our final example in this section shows that Noether's Theorem can be applied, at least where the group acts on the dependent variables. This takes advantage of the fact that the theorem is known for Lagrangian difference systems (cf. [**18, 22**]), and the clear analogy of these to the discrete EL equations obtained here. We show only a simple case.

EXAMPLE 4.5. Consider the scaling invariant Lagrangian,

$$L[u] = \frac{1}{2}\left(\frac{u_x}{u}\right)^2 \mathrm{d}x.$$

Using the standard piecewise linear interpolation, we have

$$\int L[u]\,\mathrm{d}x \mapsto \sum_n L_n = \sum_n \frac{(u_{n+1}-u_n)^2}{2u_{n+1}u_n(x_{n+1}-x_n)}.$$

Now the discrete EL equation is

$$\mathrm{E}(L) = \partial_{u_n} L_n + S^{-1}\partial_{u_{n+1}} L_n, \tag{4.7}$$

where $S$ is the shift map, $x_n \mapsto x_{n+1}$, $u_n \mapsto u_{n+1}$. The scaling symmetry $u \mapsto \mu u$ "translates" to the discrete Lagrangian as:

$$(u_n\partial_{u_n} + u_{n+1}\partial_{u_{n+1}})L_n = 0 \tag{4.8}$$

which can be checked directly. This last is by analogy with the characteristic form of the variational symmetry. Now, (4.7) and (4.8) together give a first integral of the EL equation:

$$u_n\partial_{u_n} L_n = \kappa, \quad \kappa \in \mathbb{R}.$$

This yields

$$\left(\frac{u_{n+1}}{u_n}\right)^2 - \kappa(x_{n+1}-x_n)\left(\frac{u_{n+1}}{u_n}\right) - 1 = 0$$

or

$$u_{n+1} = H_n u_n, \quad H_n \sim \big(\mp 1 + \tfrac{1}{2}\kappa(x_{n+1}-x_n)\big).$$

If $(x_{n+1}-x_n) \sim x/n$ this integrates to

$$u_n = \left(1 + \frac{\kappa x}{2n}\right)^n u_0 \sim u_0 \exp(\kappa x/2)$$

which is the correct result.

## 5. Higher dimensional calculations

The question, "what is the Euler–Lagrange operator for a Lagrangian defined on a mesh" comes down to the question, "which forms have integrals depending only on their boundary values?" Inside a simplex, such forms are, of course, a total divergence. But piecewise projected forms are not necessarily smooth across the boundaries of a simplex. For forms defined piecewise on a mesh, the analogue of a divergence is known as a "coboundary of a cochain". We next explain this concept.

While we restrict ourselves to the two-dimensional case for the sake of a simple exposition, the definitions and arguments are all adaptable to higher dimensions. We take a two-dimensional mesh to be a triangulation with vertices $v$, oriented edges $e$ and oriented faces $\sigma$.

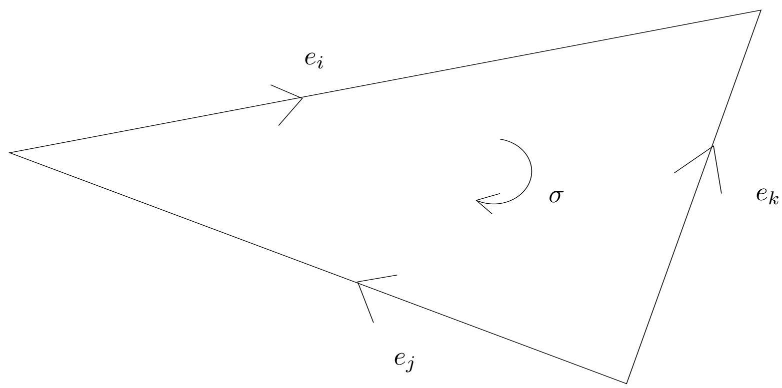


FIGURE 2. A 2-simplex and its boundary.

DEFINITION 5.1. For any set $S$, let $\langle S\rangle_R$ denote the linear space with elements of $S$ considered as a basis, and with coefficients in a ring $R$. We define *cochains* as follows:

- 0 cochains are linear maps $\langle\{v_i\}\rangle_R \to R$,
- 1 cochains are linear maps $\langle\{e_i\}\rangle_R \to R$,
- 2 cochains are linear maps $\langle\{\sigma_i\}\rangle_R \to R$.

The set of $p$-cochains will be denoted by $\mathcal{C}^p$. The ring $R$ will be $\mathbb{R}$ at first, but will be extended later on.

DEFINITION 5.2. Given the 1-cochain $F\colon \langle\{e_i\}\rangle_R \to R$, define the *coboundary* of $F$ to be the 2-cochain $\delta F\colon \langle\{\sigma_i\}\rangle_R \to R$ by $\delta(F)(\sigma) = F(\partial\sigma)$ where $\partial\sigma$ is the sum of edges constituting the boundary of the face. We note that edges are signed in this sum according to whether their orientation matches that induced on the boundary by the orientation of the face. The map $\delta$ is then extended linearly to act on the space of 1-cochains, and is called the *coboundary operator*.

EXAMPLE 5.3. For $\sigma$ as in Figure 2, the coboundary map is $(\delta F)(\sigma) = F(e_i + e_j - e_k) = F(e_i) + F(e_j) - F(e_k)$.

If you are using an interpolation scheme, all the data lie on the vertices. The set of faces is then a set of ordered triples of indices and the set of edges is a set of ordered pairs of indices; see Figure 3. The ordering gives the orientation. The coboundary of a map $F$ on the face $(ijk)$ is easily seen to be

$$(\delta F)(ikj) = F(kj) + F(ji) + F(ik).$$

That is, coboundaries are cyclic sums on edges.

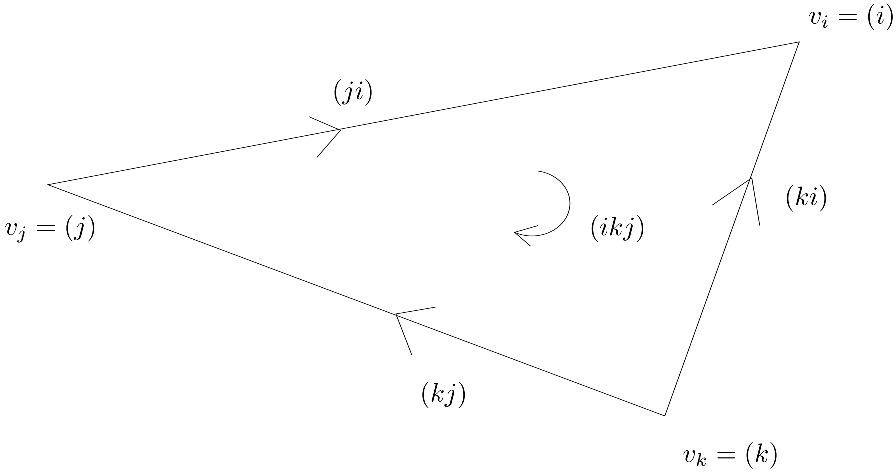


FIGURE 3. A 2-simplex and its sub-simplices labelled in ordered index notation.

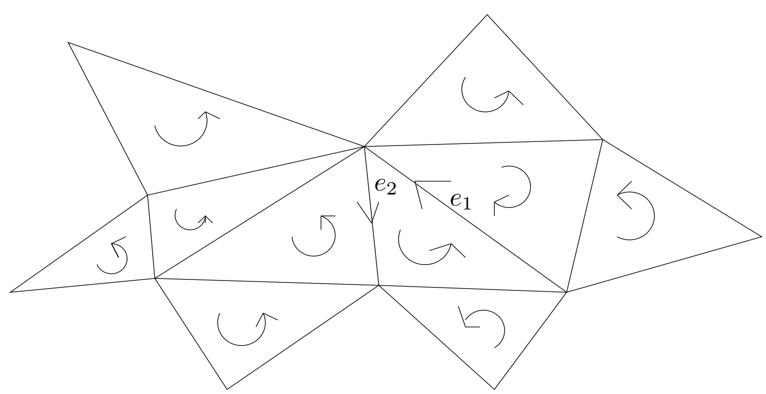


FIGURE 4. A mesh showing faces with their orientations. When integrating a coboundary, the sums over all the internal edges, for example $e_1$ and $e_2$, will cancel.

DEFINITION 5.4. For a $p$-cochain $F$, and a $p$-surface $Y$ composed of $p$-simplices $\rho_i$, $i = 1, \ldots, N$, define the integral of $F$ over $Y$ as

$$\int_Y F = \sum_{k=1}^{N} (-1)^{[\rho_k, Y]} F(\rho_k),$$

where

$[\rho_k, Y] = 0$ if the orientation of $\rho_k$ matches that induced by $Y$,

$[\rho_k, Y] = 1$ otherwise.

Theorem 5.5 (Discrete Stokes' Theorem). *If the dimension of $X$ is $n$ and $F$ is an $(n-1)$-cochain, then*

$$\int_X \delta(F) = \int_{\partial X} F.$$

*Indeed, we have that*

$$\int_X \delta(F) := \sum_\tau (-1)^{[\tau,X]} \delta F(\tau) = \sum_{\sigma\in\partial X} (-1)^{[\sigma,X]} F(\sigma) =: \int_{\partial X} F.$$

For in the left hand sum, every internal edge will appear twice, with opposite signs, leaving only the sum over the external edges; see Figure 4. In fact, there is a version of the discrete Stokes' Theorem valid at every dimension, not just the top one (and with the same proof) but a proper discussion of this topic requires a knowledge of the Poincaré duality between homology and cohomology of a triangulation.

The astute reader will have noticed that coboundaries of 1-cochains derive from maps on edges, while coherent FE complexes have all forms defined throughout. By using the de Rham map defined in Remark 2.9, the two concepts can be "married" as follows.

Definition 5.6. Let $\omega \in \Lambda^p$, and let the $p$-simplices be denoted as $\sigma$. Define the $\mathbb{R}$-valued p-cochain $\boldsymbol{\omega}$, induced by $\omega$, by

$$\boldsymbol{\omega}\colon \langle\{\sigma\}\rangle_{\mathbb{R}} \to \mathbb{R}, \quad \sum a_i\sigma_i \mapsto \sum a_i \int_{\sigma_i} \omega.$$

We will also denote $\boldsymbol{\omega}$ by $\int \omega$, and write

$$\int : \Lambda^p \to \mathcal{C}^p.$$

The map $\int$ is well-defined on $\mathcal{F}^n$ where $n$ is the dimension of the base space $X$. Piecewise defined $n$-forms whose global integrals depend only on their boundary values are those whose induced cochains are coboundaries; $\boldsymbol{\omega} = \delta\boldsymbol{\eta}$. For then we have that

$$\int_X \omega = \int_X \boldsymbol{\omega} = \int_X \delta\boldsymbol{\eta} = \int_{\partial X} \boldsymbol{\eta}, \tag{5.1}$$

where $\int_X \omega$ is the standard integral from calculus, and $\int_X \boldsymbol{\omega}$ is given in Definition 5.4.

The fact that the forms in $\mathcal{F}^n$ are not smooth, and indeed may not even be defined on internal faces, means that globally, the smooth Stokes' Theorem does not hold, and we are forced to use the discrete version on the induced forms.

We are interested in the case where we have a Lagrangian depending on arbitrary functions and their derivatives. This projects to an FE Lagrangian depending on arbitrary, or unevaluated, degrees of freedom. For these forms, the above arguments all go through, but now the coefficients are functions of these unevaluated degrees of freedom; note that the degrees of freedom are labelled by the (sub)simplices of the mesh.

In the $n$-dimensional case where the $n$-form is a Lagrangian density, the projection of $\int_X L[u]\,\mathrm{d}\mathbf{x}$ used in practice is

$$\sum_\tau (-1)^{|\tau|} \int_\tau \Pi(L[u]\,\mathrm{d}\mathbf{x}), \tag{5.2}$$

where $|\tau| = 0$ if $\tau$ has the anti-clockwise orientation, and $|\tau| = 1$ for the reverse orientation. We thus take the induced $n$-cochain of $\Pi(L[u]\,\mathrm{d}\mathbf{x})$ to be

$$\tau \mapsto \int_\tau \Pi(L[u]\,\mathrm{d}\mathbf{x}).$$

In order to prove, rigorously, theorems concerning exactness and to obtain (eventually) formulae for conservation laws, it is helpful to introduce the following algebraic device to ease the notation. We first define a particular cochain which is reminiscent of the characteristic function of a simplex and plays a similar role.

Definition 5.7. Let the cochain which takes the value 1 on the simplex $\sigma$ and zero elsewhere be called $\boldsymbol{\chi}_\sigma$. Then the set of $p$-cochains with real coefficients is $\mathcal{C}^p(\mathbb{R}) = \langle \boldsymbol{\chi}_\sigma \mid \sigma \in X^p\rangle_{\mathbb{R}}$, where we use $X^p$ to denote the set of $p^{\text{th}}$ simplices in the triangulation. Changing the coefficients to $R$, where $R$ is to be specified, we have

$$\mathcal{C}^p(R) \cong R \otimes \mathcal{C}^p(\mathbb{R}),$$

where $\otimes$ is the tensor product[3]. Then for example, the 0-cochain which takes the value $a_n$ at $x_n$ is written as $\sum a_n \otimes \boldsymbol{\chi}_{x_n}$ or more simply as $\sum a_n \boldsymbol{\chi}_{x_n}$, while the integral over $X$ is then the signed sum of the coefficients, $\int_X \sum_\tau a_\tau([u]) \otimes \boldsymbol{\chi}_\tau = \sum_\tau (-1)^{[\tau,X]} a_\tau([u])$. The tensor notation gives explicitly the value of a cochain on each simplex in the form of a sum. This will enable us to write down the variational derivative of an induced cochain in the next section.

Note that the induced cochain of $\chi_\tau \mathrm{d}\mathbf{x}$, where $\chi_\tau$ is the characteristic function for $\tau$, is $(\int_\tau \mathrm{d}\mathbf{x}) \otimes \boldsymbol{\chi}_\tau$.

The simplicial theory of cochains and coboundaries is attractive. It allows us to use results and intuition from classical work on triangulations in algebraic topology, and it generalizes to $n$ dimensions. However, using it to obtain closed form expressions for the EL equations defined on an arbitrary mesh seems difficult. Much better is to use the coboundary operator in matrix form, and to take advantage of the well-developed theory concerning the incidence matrices of meshes. This is a development for the future.

For regular meshes, it is simple to obtain a closed form expression for the EL equations. Collate triangles into a regular "square" lattice, for example, as 1, 2 or 3 in Figure 5. Since

$$\sum_{\text{triangles}} = \sum_{\text{squares}}$$

the boundary terms are then of the form

$$\sum (\mathrm{Shift}_1 - id)(\cdots) + (\mathrm{Shift}_2 - id)(\cdots).$$

This can be used in the same way as the identity (4.3) was used in the one-dimensional case. Euler–Lagrange equations then become difference systems, and can be studied using methods for those [**22**]. In particular, Noether's theorem is known for such systems (see references listed in §1.4).

[3] If $V$ and $W$ are real vector spaces of dimension $n$ and $m$ and with bases $v_i$ and $w_j$ respectively, then $V \otimes W$ is a real vector space of dimension $nm$ and basis $v_i \otimes w_j$, satisfying $c(v \otimes w) = (cv) \otimes w = v \otimes (cw)$ for $c$ a constant. In physics texts the symbol $\otimes$ is usually omitted in expressions of elements.

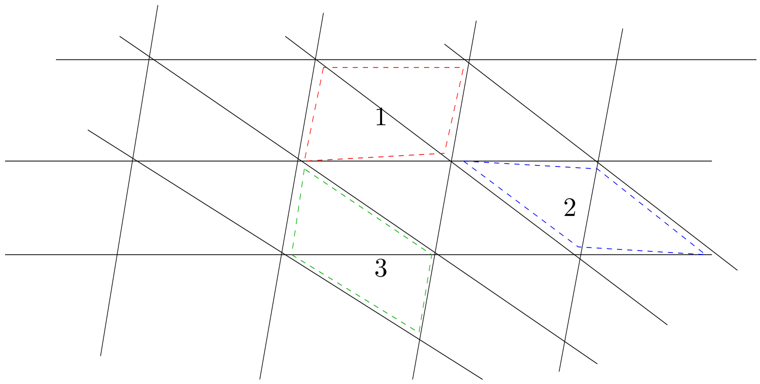


FIGURE 5. In a regular mesh, triangles can be collated into "squares".

## 6. A variational complex for coherent finite element schemes

We can now put together an FE variational complex, based on a coherent FE approximation scheme, which incorporates how the calculations are naturally done. But first, we look more closely at the algebraic structure of the de Rham complex, to motivate the construction of the complex we eventually study in Theorem 6.12.

The de Rham complex $\Lambda^*$, (2.1), is a *graded algebra* ([**6**, p. 197]). This means that forms can be added, multiplied by constants, and multiplied together, in this case using the wedge product;

$$\wedge \colon \Lambda^p \times \Lambda^q \to \Lambda^{p+q}, \quad (\alpha, \beta) \mapsto \alpha \wedge \beta.$$

The degree of the form gives the grading. Finally, the de Rham complex is a *differential graded algebra* since it is closed under the exterior derivative (i.e. the operator sends the set of all forms to itself). In addition, there is a metric dependent Hodge star operator, $*$, which sends, in $n$-space, $p$-forms to $(n-p)$-forms.

Lagrangians for physical problems in 3 dimensions are 3-forms which are composed of products of 0, 1, 2 and 3-forms. For example, $(u_x^2 + u_y^2 + u_z^2)\,\mathrm{d}\mathbf{x}$ is in fact $(*\mathrm{d}u) \wedge \mathrm{d}u$, and since $u \in \Lambda^0$, $\mathrm{d}u \in \Lambda^1$ and $*\mathrm{d}u \in \Lambda^2$, we have $(*\mathrm{d}u) \wedge \mathrm{d}u \in \Lambda^3$. A potential function $V(u)$ in a Lagrangian is in fact a three-form $*V(u) = V(u)\mathrm{d}\mu$, where $\mathrm{d}\mu$ is the volume form for the given metric. It can be seen that the construction of Lagrangians takes advantage of the differential graded algebra structure of $\Lambda^*$. Moreover, these 3-forms have the dependent variables and their derivatives appearing explicitly in the coefficient functions. One way to think of this is that the dependent variables are "unevaluated". And indeed when solving the EL equations, we regard them as variables to be determined.

On the other hand, a coherent FE complex is not an algebra, because the wedge product of elements in $\mathcal{F}^*$ need not be in $\mathcal{F}^*$. Looking at the discrete Lagrangians derived in §3, we see that in fact they are not in $\mathcal{F}^3$ as it stands, but in a larger space, the 3-forms in the algebra that $\mathcal{F}^*$ generates. Moreover, just as in the continuous case, we need the degrees of freedom to be unevaluated, so that we may speak of forms with coefficients that depend on arbitrary dependent variables and their derivatives. Such coefficient functions take the form, in the simplest one-dimensional case,

$$f\big(x, \Pi(u), \big(\Pi(u)\big)_x, \big(\Pi(u)\big)_{xx}, \dots\big),$$

where all such coefficients are smooth functions of a *finite* number of arguments.

DEFINITION 6.1. For $\mathcal{F}^*$ be a coherent FE approximation complex, let $\widetilde{\mathcal{F}}^*$ denote the algebra generated by $\mathcal{F}^*$.

THEOREM 6.2. *The algebra $\widetilde{\mathcal{F}}^*$ is a differential graded algebra. Moreover,*

$$0 \to \mathbb{R} \to \widetilde{\mathcal{F}}^0 \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}^1 \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}^2 \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}^3 \xrightarrow{\mathrm{d}} \cdots \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}^n \tag{6.1}$$

*is exact in every $n$-dimensional simplex.*

PROOF. Elements of $\widetilde{\mathcal{F}}^*$ can be written as *finite* sums and wedge products of elements in $\mathcal{F}^*$. Since the exterior derivative operator d is linear and an antiderivation, that is, obeys the product rule (up to signs), and $\mathcal{F}^*$ is closed under d, then so will $\widetilde{\mathcal{F}}^*$ be closed. Local exactness of (6.1) follows using the same homotopy maps as in the proof as the continuous case, but where instead of $u$, $v$, ... appearing in the coefficients, we have $\Pi(u)$, $\Pi(v)$, ... appearing. The homotopy operators $H$ in the continuous case are maps which satisfy $\mathrm{id} = H\mathrm{d} + \mathrm{d}H$ for every specialization of every unevaluated dependent variable, and this is precisely what we need for the present result (see the discussion in [**32**, p. 343]). Finally, we note that the top-dimensional simplices satisfy the domain requirements for the continuous theorem to hold. □

REMARK 6.3. The Hodge star operator also does not map $\mathcal{F}^*$ to itself and therefore needs to be modified. A first attempt might be to use $\Pi \circ *$, but this fails to satisfy the other properties of the star operator, such as being its own inverse (up to a sign). A better idea, propounded by several authors ([**31, 37**]) is that the discrete Hodge operator is defined in terms of a bilinear mapping between the mesh and its Poincaré dual. A full analogy of the variational complex involving these concepts is an important development for the future.

The second ingredient in a variational complex is the vertical complex (3.1), consisting of forms in the dependent variables. In our case, these dependent variables will be the unevaluated degrees of freedom in the approximation scheme. The exterior derivative of a Lagrangian with respect to the degrees of freedom in the model is a vertical form; for example (4.2) in Example 4.1, or (4.4) in Example 4.2.

In order to fix the notation, we will denote all the degrees of freedom by $\alpha^j_\sigma$ where $\sigma$ is a simplex, and $j$ being the labelling on the different degrees of freedom per simplex.

DEFINITION 6.4. We first define vertical forms on a top-dimensional simplex, which is a form in the $\{\mathrm{d}\alpha^j_\sigma\}$, that is, a *finite* sum

$$\sum_{j_1<j_2<\cdots<j_p} f^{k_1\cdots k_p}_{j_1\cdots j_p}\,\mathrm{d}\alpha^{k_1}_{j_1}\dots\mathrm{d}\alpha^{k_p}_{j_p},$$

where the coefficients $f$ are smooth functions with a *finite* number of arguments, in the $\alpha^j_\sigma$ and the mesh variables. The space of such $p$-forms is denoted $\mathcal{V}^p$. The exterior derivative $\widehat{\mathrm{d}}\colon \mathcal{V}^p \to \mathcal{V}^{p+1}$ operates in the natural way, but treats any mesh variables (the "independent variables") as constants; for example,

$$\begin{aligned}\widehat{\mathrm{d}}[(x_n\alpha_n^{j-1}\alpha_n^j)^2\,\mathrm{d}\alpha_n^j] &= 2(x_n\alpha_n^{j-1}\alpha_n^j)(x_n\alpha_n^{j-1}\,\mathrm{d}\alpha_n^j + x_n\alpha_n^j\,\mathrm{d}\alpha_n^{j-1})\wedge \mathrm{d}\alpha_n^j\\ &= 2x_n^2\alpha_n^{j-1}(\alpha_n^j)^2\,\mathrm{d}\alpha_n^{j-1}\wedge\mathrm{d}\alpha_n^j,\end{aligned}$$

since $(\mathrm{d}\alpha_n^j)^2 = 0$.

Definition 6.5. Globally, the vertical $p$-forms are obtained by taking a copy of $\mathcal{V}$ for each simplex, and composing the tensor product, $\widehat{\mathcal{F}}^p = \mathcal{V}^p \otimes \mathcal{C}^n$, where $n$ is the dimension of the base space. Then the vertical derivative is given by

$$\widehat{\mathrm{d}}(v\otimes\boldsymbol{\omega}) = (\widehat{\mathrm{d}}v)\otimes\boldsymbol{\omega}.$$

In other words, global vertical forms are $n$-cochains with coefficients in $\mathcal{V}$.

Theorem 6.6. *The complex*

$$\widehat{\mathcal{F}}^0 \xrightarrow{\widehat{\mathrm{d}}} \widehat{\mathcal{F}}^1 \xrightarrow{\widehat{\mathrm{d}}} \widehat{\mathcal{F}}^2 \xrightarrow{\widehat{\mathrm{d}}} \widehat{\mathcal{F}}^3 \xrightarrow{\widehat{\mathrm{d}}} \cdots \tag{6.2}$$

*is exact in every top-dimensional simplex.*

The proof of this theorem is the same as for the corresponding smooth vertical complex ([**32**, p. 344]), since the cochain part of the expressions are unaffected by the vertical derivative operator.

The next step is to consider equivalence classes of vertical forms, where equivalence is up to forms whose integrals depend only on their boundary values. To do this, we use the induced action of the coboundary operator discussed in the previous section, but on the spaces $\widehat{\mathcal{F}}^p$.

Example 6.7. Let us look at the simplest $1-\mathrm{d}$ case, using the new notation we are developing. Using the standard interpolation approximation given in Eq. (4.1), the projection of $\frac{1}{2}u_x^2\,\mathrm{d}x$ is

$$\sum_n \frac{1}{2}\left(\frac{u_{n+1}-u_n}{x_{n+1}-x_n}\right)^2 \chi_{e_n}\,\mathrm{d}x$$

and the induced cochain is

$$\boldsymbol{\omega} = \sum_n \frac{1}{2}\frac{(u_{n+1}-u_n)^2}{x_{n+1}-x_n}\otimes\boldsymbol{\chi}_{e_n},$$

where we have used the fact that the induced cochain of $\chi_{e_n}\,\mathrm{d}x$ is $(x_{n+1}-x_n)\boldsymbol{\chi}_{e_n}$ (see Definition 5.7). Then (omitting the $\otimes$ symbol)

$$\widehat{\mathrm{d}}\boldsymbol{\omega} = \sum_n\left(\frac{u_{n+1}-u_n}{x_{n+1}-x_n}\right)(\mathrm{d}u_{n+1}-\mathrm{d}u_n)\boldsymbol{\chi}_{e_n}.$$

Definition 6.8. Two vertical forms are said to be *equivalent* if their induced cochains differ by a coboundary. We write the equivalence class of a form $\omega$ as $\pi(\omega)$. The space of equivalence classes is the space of Finite Element *functional p-forms* (compare Definition 3.4),

$$\mathcal{F}_*^p = \widehat{\mathcal{F}}^p/\delta(\mathcal{V}^p\otimes\mathcal{C}^{n-1}).$$

Remark 6.9. Our notation follows that of the smooth case as given by Olver [**32**]. There, the de Rham complex was denoted by $\Lambda^*$, the vertical complex by $\widehat{\Lambda}^*$ and the complex of functional forms by $\Lambda^*_*$. Since $\Lambda^*$ is an algebra, there is no need to introduce $\widetilde{\Lambda}^*$.

Example 6.5 (cont.). An arbitrary 0-cochain is $\boldsymbol{\eta} = \sum a_n \boldsymbol{\chi}_{x_n}$ and its coboundary is $\delta\boldsymbol{\eta} = \sum a_n \delta\boldsymbol{\chi}_{x_n}$. Now $\delta\boldsymbol{\chi}_{x_n} = \boldsymbol{\chi}_{e_n} - \boldsymbol{\chi}_{e_{n+1}}$ if $x_n$ is an internal vertex. It is not hard to see that

$$\delta\boldsymbol{\eta} = \sum_n (a_{n+1} - a_n)\boldsymbol{\chi}_{e_n}.$$

To obtain $\pi\widehat{\mathrm{d}}\boldsymbol{\omega}$, we can add whatever coboundary we like—the point is to find a good coboundary to obtain the most useful representative of the vertical derivative. So, if we add the coboundary of

$$\boldsymbol{\eta} = -\sum_n \left(\frac{u_{n+1} - u_n}{x_{n+1} - x_n}\right) \mathrm{d}u_n \boldsymbol{\chi}_{x_n},$$

we will get that

$$\pi\widehat{\mathrm{d}}\boldsymbol{\omega} \sim -\sum_n \left(\frac{u_{n+1} - u_n}{x_{n+1} - x_n} - \frac{u_n - u_{n-1}}{x_n - x_{n-1}}\right) \mathrm{d}u_n \boldsymbol{\chi}_{e_n}.$$

Despite the abstraction of "equivalence relations", the operations we perform are all those occurring naturally in practical problems.

Theorem 6.10. *The vertical exterior derivative is well defined on equivalence classes, that is, if* $\omega_1 \sim \omega_2$ *then* $\widehat{\mathrm{d}}\omega_1 \sim \widehat{\mathrm{d}}\omega_2$. *Thus* $\widehat{\mathrm{d}}$ *induces a map* $\mathrm{d}^* \colon \mathcal{F}^p_* \to \mathcal{F}^{p+1}_*$ *which satisfies* $(\mathrm{d}^*)^2 = 0$ *and* $\pi \circ \widehat{\mathrm{d}} = \mathrm{d}^* \circ \pi$.

Definition 6.11. The Euler–Lagrange operator for a coherent FE approximation scheme is

$$\mathcal{E}L = \pi \circ \widehat{\mathrm{d}} \circ \int.$$

Recall that the map $\int$ takes a form to its induced cochain (Definition 5.6).

Theorem 6.12. *The Finite Element variational complex, shown here for a three-dimensional base space,*

$$0 \to \mathbb{R} \to \widetilde{\mathcal{F}}_0 \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}_1 \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}_2 \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}_3 \xrightarrow{\mathcal{E}L} \mathcal{F}^1_* \xrightarrow{\mathrm{d}^*} \mathcal{F}^2_* \xrightarrow{\mathrm{d}^*} \cdots \tag{6.3}$$

*is locally exact.*

Proof. It suffices to show that the following diagram commutes, and the bottom row is exact. The result then follows from standard algebraic arguments (see for example [**22**, §4.1]).

$$\begin{array}{ccccccccc}
 & \xrightarrow{\mathrm{d}} & \widetilde{\mathcal{F}}^3 & \xrightarrow{\widehat{\mathrm{d}}\circ\int} & \widehat{\mathcal{F}}^1 & \xrightarrow{\widehat{\mathrm{d}}} & \widehat{\mathcal{F}}^2 & \xrightarrow{\widehat{\mathrm{d}}} & \cdots \\
 & & \downarrow \pi\circ\int & & \downarrow \pi & & \downarrow \pi & & \\
0 & \to & \mathcal{F}^0_* & \xrightarrow{\mathrm{d}^*} & \mathcal{F}^1_* & \xrightarrow{\mathrm{d}^*} & \mathcal{F}^2_* & \xrightarrow{\mathrm{d}^*} & \cdots
\end{array}$$

That the diagram commutes follows from Theorem 6.10. That the bottom row is exact to the right of $\mathcal{F}^0_*$ onwards, follows from the fact that it is a projection of an exact sequence, (6.2). Thus we need only show exactness at $\mathcal{F}^0_*$. In other words, we need only show that $\mathrm{d}^*\big|_{\mathcal{F}^0_*}$ is an injection. This follows firstly from the fact that any function which maps to zero under the vertical derivative must involve only the independent variables, and is therefore locally a divergence. Secondly, any cochain mapping to a coboundary under the vertical derivative is already a coboundary. □

## 7. Discussion and open problems

In this article, we have laid the foundation for a rigorous analogue of the variational complex for Finite Element schemes. In order for this to be of practical benefit in the design and analysis of schemes that inherit both a variational structure and specified conservation laws, the following open problems and questions need to be addressed.

(1) Incorporate the Poincaré dual mesh model of the Hodge star operator.
(2) Develop a computationally useful notion of the EL equations in terms of the incidence matrix of the mesh.
(3) Derive formulae for discrete Noether's theorem relative to a given mesh.

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