Journal of Computational Physics 359 (2018) 45–76

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Formulation and computation of dynamic, interface-compatible Whitney complexes in three dimensions

Richard M.J. Kramer, Christopher M. Siefert*, Thomas E. Voth, Pavel B. Bochev

Sandia National Laboratories [1], *Albuquerque, NM, United States*

ARTICLE INFO

Article history:
Received 30 January 2017
Received in revised form 4 October 2017
Accepted 25 December 2017
Available online 2 January 2018

Keywords:
Material interface
De Rham complex
Compatible discretizations
Algebraic constraints
Conformal mesh decomposition

ABSTRACT

A discrete De Rham complex enables compatible, structure-preserving discretizations for a broad range of partial differential equations problems. Such discretizations can correctly reproduce the physics of interface problems, provided the grid conforms to the interface. However, large deformations, complex geometries, and evolving interfaces makes generation of such grids difficult. We develop and demonstrate two formally equivalent approaches that, for a given background mesh, dynamically construct an interface-conforming discrete De Rham complex. Both approaches start by dividing cut elements into interface-conforming subelements but differ in how they build the finite element basis on these subelements. The first approach discards the existing non-conforming basis of the parent element and replaces it by a dynamic set of degrees of freedom of the same kind. The second approach defines the interface-conforming degrees of freedom on the subelements as superpositions of the basis functions of the parent element. These approaches generalize the Conformal Decomposition Finite Element Method (CDFEM) and the extended finite element method with algebraic constraints (XFEM-AC), respectively, across the De Rham complex.

1. Introduction

The De Rham differential complex encodes the mathematical structure of a large class of partial differential equations (PDEs). It is now well understood that compatible discretizations for such PDEs require approximation of the De Rham complex by a collection of interconnected discrete spaces that form its discrete analog [1,2]. This implies defining discrete spaces and operators that provide a discrete vector-calculus structure supporting discrete versions of fundamental vector calculus results such as the Hodge decomposition, the Stokes' theorem and the Divergence theorem; see, e.g., [3]. The resulting compatible spatial discretization then preserves key aspects of the mathematical structures that govern the well-posedness of the PDE [4–6]. Such discretizations not only give rise to stable and accurate numerical methods, but also tend to produce physically meaningful approximate solutions free of spurious modes.

The Whitney complex [7], which is defined on simplicial mesh partitions, is perhaps the earliest example of a discrete De Rham complex. Its role for the stable and accurate discretization of the Maxwell's equations was first elucidated by

* Corresponding author.
E-mail address: csiefer@sandia.gov (C.M. Siefert).

[1] Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

https://doi.org/10.1016/j.jcp.2017.12.037
0021-9991/

Bossavit [8]. Subsequently, these ideas have been applied to develop an extensive collection of discrete vector calculus structures in multiple discretization contexts, including finite differences [2,9], finite volumes [10–13], *hp* finite elements [14], and spectral elements [15,16].

Many important physical problems, such as two-phase flows, thermal conduction or electromagnetic diffusion across two different materials, and linear elasticity with discontinuous Poisson ratios, involve material discontinuities across interfaces embedded in the model domain. One important aspect of compatible discretization methods for such problems is their ability to capture the correct physical behavior of the exact solutions across the material interfaces, *provided the mesh is body fitted*, i.e., aligned with the interface. Then, compatible discretizations preserve properties such as continuity of tangential components of electric fields between two different conductors and continuity of normal heat fluxes on the interface between two different heat conducting materials. These properties are critical in simulation of electromagnetic phenomena, for example, which requires the accurate resolution of surface effects, as current tends to concentrate near material interfaces.

However, generation of body-fitted grids can be difficult or and/or prohibitively expensive if the interface has complex geometry, is evolving in time, or the material domain undergoes large deformations. This presents a significant challenge for the implementation and use of compatible discretization methods in many practically important simulation scenarios. Yet, simply ignoring the lack of mesh conformity to the interface is not an option. Besides the incorrect physical behavior of the numerical solutions, methods that proceed along this path also tend to lose accuracy; see e.g., [17], thereby reducing both the physical fidelity and the computational efficiency of the simulations.

The field of interface-capturing finite element methods has primarily dealt with standard nodal C^0 finite element spaces. These methods include the eXtended Finite Element Method (XFEM), e.g., [18–22], the Conformal Decomposition Finite Element Method (CDFEM), e.g., [23], the Interface-enriched Generalized Finite Element Method (IGFEM), e.g., [24,25], and the Hierarchical Interface-enriched Finite Element Method (HIFEM), e.g., [26]. To the best of our knowledge, this work is the first attempt to address construction of a complete finite element De Rham complex in the presence of material discontinuities. In particular, in this paper we develop two complementary approaches for tetrahedral mesh partitions that dynamically construct an interface-compatible discrete Whitney complex on a mesh that is not required to conform to the interface.

Remark 1.1. We call an element conforming to an interface if it has a k-dimensional entity, $k = 0, 1, 2$, whose vertices all belong to the interface. Note that this does not require the entity itself to be contained in the interface, except when $k = 0$ and the entity reduces to a single vertex. This definition is equivalent to a piecewise linear approximation of the true interface. Such an approximation is acceptable because our focus is on the Whitney complex, which is the lowest order De Rham complex on simplices. In this case the error made in the approximation of the interface does not exceed the discretization error of the finite element spaces in the complex.

Both approaches start by decomposing elements cut by the interface into subelements that conform to the material boundary and then dynamically introduce new basis functions for these subelements. The principal difference between them is in the manner in which this basis update is performed.

In the first approach the basis functions on every cut element are replaced by basis functions of the same kind on each one of its subelements, thereby creating a conforming finite element space defined on a body-fitted mesh. This space can then be used in a standard finite element workflow with the caveat that it contains dynamic global degrees of freedom, i.e., any change in the interface can potentially trigger renumbering of the global degrees of freedom. This approach extends the Conformal Decomposition Finite Element Method (CDFEM) [23] to all spaces in the De Rham complex.

The second approach does not discard the basis functions on the cut elements but instead multiplies them by the indicator functions of their subelements to obtain an enriched set[2] of basis functions. The latter is discontinuous and therefore non-conforming with respect to the spaces in the De Rham complex. To restore conformity, we constrain the enriched basis by suitable algebraic conditions that enforce the appropriate inter-element continuity for each Whitney space. This effectively expresses the *constrained, interface-conforming* enriched basis on the subelements entirely in terms of the existing *non interface-conforming* basis on their parent cut elements. As a result, any given Whitney element basis can be adapted to an evolving interface without changing the mesh topology, but at the cost of constructing the constraints to enforce conformity.

This approach draws upon the ideas of the algebraically constrained extended finite element method (XFEM-AC) [27,28] and expands its scope to include the entire De Rham complex. Among the principal challenges here are to ensure that the constrained, interface-conforming, enriched Whitney bases continue to provide an exact sequence, which is a key requirement for the existence of discrete vector calculus properties. An equally important challenge is to guarantee the stability of the resulting XFEM-AC Whitney spaces. As in our previous work we accomplish this by showing the equivalence between the interface-conforming Whitney spaces obtained by the XFEM-AC and CDFEM approaches. As a result, although XFEM-AC involves constraints, its stability does not require verification of an inf-sup condition.

This should be contrasted with traditional ways of enforcing conformity in Heaviside-enriched nodal finite elements, which depend on either Lagrange multipliers or penalty terms for this purpose. Stability of these formulations can be tied

[2] This process is often referred to in the literature as “Heaviside enrichment”.