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The chain collocation method: A spectrally accurate calculus of forms

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A B S T R A C T

Preserving in the discrete realm the underlying geometric, topological, and algebraic structures at stake in partial differential equations has proven to be a fruitful guiding principle for numerical methods in a variety of fields such as elasticity, electromagnetism, or fluid mechanics. However, structure-preserving methods have traditionally used spaces of piecewise polynomial basis functions for differential forms. Yet, in many problems where solutions are smoothly varying in space, a spectral numerical treatment is called for. In an effort to provide structure-preserving numerical tools with spectral accuracy on logically rectangular grids over periodic or bounded domains, we present a spectral extension of the discrete exterior calculus (DEC), with resulting computational tools extending well-known collocation-based spectral methods. Its efficient implementation using fast Fourier transforms is provided as well.

1. Introduction

Recent years have seen the development of novel discretizations for a wide variety of systems of partial differential equations. In particular, preserving in the discrete realm the underlying geometric, topological, and algebraic structures at stake in differential equations has proven to be a fruitful guiding principle for discretization [1–4]. This geometric approach has led to numerical methods, analyzed in, e.g., [5,3], that inherit a variety of properties from the continuous world, and that surprisingly outperform their known theoretical guarantees [6]. However, geometric discretizations of elasticity, electromagnetism, or fluid mechanics have mostly been demonstrated using spaces of piecewise polynomial differential forms. Many problems where solutions are smoothly varying in space call for a spectral numerical treatment instead, as it produces low-error, exponentially converging approximations by leveraging fast implementations of transforms such as the Fast Fourier Transform. In an effort to provide structure-preserving numerical tools with spectral accuracy on logically rectangular grids over periodic or bounded domains, we present a spectral extension of the discrete exterior calculus described in [7–10]—and point out that the resulting computational tools extends well-known spectral collocation methods.

1.1. Review of previous work

Computational methods preserving geometric structures have become increasingly popular over the past few years, gaining acceptance among both engineers and mathematicians [11]. Computational electromagnetism [7,2], mimetic (or natural) discretizations [12,9], finite-dimensional exterior calculus (including Discrete Exterior Calculus (DEC, [13,8]), and Finite Element Exterior Calculus (FEEC, [1,3])) have all proposed discretizations that preserve vector calculus identities in order to

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improve numerics. In particular, the relevance of exterior calculus (Cartan's calculus of differential forms [14]) and algebraic topology [15] to computations came to light.

Exterior calculus is a concise mathematical formalism to express differential and integral equations on smooth and curved spaces, while revealing the geometric structures at play and clarifying the nature of the physical quantities involved. At the heart of exterior calculus is the notion of differential forms, denoting antisymmetric tensors of arbitrary order. As integration of differential forms is an abstraction of the measurement process, this calculus of forms provides an intrinsic, coordinate-free approach particularly relevant to neatly describe a multitude of physical models making heavy use of line, surface and volume integrals [16–20]. Moreover, physical measurements, such as fluxes, represent local integrations over a small surface of the measuring instrument. Pointwise evaluation of such quantities does not have physical meaning; instead, one should manipulate these quantities only as geometrically-meaningful entities integrated over appropriate submanifolds.

Algebraic topology, specifically the notion of chains and cochains [21,15] has been used to provide a natural discretization of differential forms and to emulate exterior calculus on finite grids: a set of values on vertices, edges, faces, and cells are proper discrete versions of respectively pointwise functions, line integrals, surface integrals, and volume integrals [7]. This point of view is entirely compatible with the treatment of volume integrals in finite volume methods, or scalar functions in finite element methods; however, it also involves the "edge elements" and "facet elements" (as first introduced in computational electromagnetism) as special H_{div} and H_{curl} basis elements [22]. Equipped with such discrete forms of arbitrary degree, Stokes' theorem connecting differentiation and integration is automatically enforced if one thinks of differentiation as the dual of the boundary operator—a particularly simple operator on meshes. With these basic building blocks, important structures and invariants of the continuous setting directly carry over to the discrete world, culminating in a discrete Hodge theory [8,3]. As a consequence, such a discrete exterior calculus has already proven useful in many areas such as electromagnetism [7,2], fluid simulation [4,6], (re)meshing of surfaces [23,24], and graph theory [10] to mention a few. So far, only piecewise polynomial basis functions [1,25] have been employed in these applications, thus limiting their computational efficiency in terms of convergence rates.

1.2. Spectral methods

Spectral methods are a class of spatial discretizations of differential equations widely recognized as crucial in fluid mechanics, electromagnetics and other applications where solutions are expected to be smooth. Central to the efficiency of this large family of numerical methods is the fact that the approximation of a periodic C^∞ function by its trigonometric interpolation over evenly spaced points converges faster than any polynomial order of the step size. This is sometimes referred to as "spectral accuracy" or "super-convergence". In practice, spectral accuracy can be achieved for bounded domains through continuation methods [26] or using Gauss–Lobatto quadrature on Legendre or Chebyshev grids [27]. A larger number of spectral methods have been designed, varying in the mesh they consider (primal grids only, or staggered grids [28]), and the locations at which they enforce partial differential equations (PDE). Be it for Galerkin, Petrov–Galerkin, or collocation-based spectral schemes, it has however been noticed that besides constructing spectrally accurate approximations of the relevant fields and their derivatives involved in a PDE, numerically preserving conservation properties helps in obtaining stable and/or physically adequate results [27]. Yet, numerical schemes are often proven conservative a posteriori, as a formal approach to guarantee conservation properties by design remains elusive.

1.3. Motivations and contributions

Despite an increasingly large body of work on numerical approaches based on exterior calculus, developing a spectrally accurate calculus of discrete forms has received very little attention—with a few recent exceptions [29–32] that we will build upon. We present a discrete exterior calculus of differential forms on periodic or bounded domains, including wedge product, Hodge star, and exterior derivative, all of which converge spectrally under grid refinement while utilizing fast Fourier methods to remain computationally efficient. In order to construct a spectral representation of the operators on differential forms, we expand the conventional tools of spectral methods to give spectrally accurate approximations of fields for which integral values over specified domains are known—a process referred to as histopolation [29,25]. In this paper we construct a histopolation using trigonometric polynomials on periodic domains, and consider the extension to bounded domains using a Chebyshev grid, thereby allowing the use of the fast Fourier transform for efficient calculation.

Our work lays out a set of spectral, structure-preserving computational tools with the following distinguishing features:

- We leverage existing work in algebraic topology to discretize space through *chains* (linear combination of mesh elements) and differential forms through cochains (discrete forms). The resulting discrete de Rham complex, that by construction satisfies Stokes' theorem, offers a consistent, "structure-preserving" manipulation of integrals and differentials which respect important conservation laws. This approach, used mainly so far in non-spectral computations [1], was identified in [30,31] as a significant departure in the construction of conservative schemes from traditional spectral methods, since divergences, gradients, and curls are no longer computed through derivation but directly evaluated via metric-independent exterior derivative without having recourse to approximations—thus exactly enforcing the divergence theorem, Green's theorem, etc.