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A compatible and conservative spectral element method on unstructured grids

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ABSTRACT

We derive a formulation of the spectral element method which is *compatible* on very general unstructured three-dimensional grids. Here compatible means that the method retains discrete analogs of several key properties of the divergence, gradient and curl operators: the divergence and gradient are anti-adjoints (the negative transpose) of each other, the curl is self-adjoint and annihilates the gradient operator, and the divergence annihilates the curl. The adjoint relations hold globally, and at the element level with the inclusion of a natural discrete element boundary flux term.

We then discretize the shallow-water equations on the sphere using the cubed–sphere grid and show that compatibility allows us to locally conserve mass, energy and potential vorticity. Conservation is obtained without requiring the equations to be in conservation form. The conservation is exact assuming exact time integration.

1. Introduction

The modern form of the spectral finite-element method (henceforth referred to as SEM) dates to [1], which was based on [2]. It can be formulated as a conventional continuous Galerkin polynomial-based finite-element method. The key difference is that the inner product uses an inexact Gauss–Lobatto quadrature. When combined with a nodal basis that interpolates the quadrature nodes, one obtains a diagonal mass matrix. This is a very efficient way to obtain a high-order explicit method on unstructured grids for time-dependent equations. Because of this, the SEM has been used extensively in geophysical applications including global atmospheric circulation modeling [3–9], ocean modeling [10–12] and planetary scale seismology [13,14].

It has been recently discovered that the continuous Galerkin finite-element method is locally conservative [15]. Here we generalize this result to the inexact-integration case of the SEM, where we also obtain a stronger form of local conservation. Local conservation is a statement about the discrete divergence operator. Here we further generalize these results to show that the SEM is *compatible* (also called *mimetic* or the *support operator* method). Compatible discretizations are those that mimic key vector-calculus properties of the divergence, gradient and curl operators [16–22]. Compatible discretizations

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can be formulated for finite-difference, finite-volume and finite-element methods and are considered in a common framework in [23]. They are closely related to discretizations which preserve the properties of the Hamiltonian structure of the continuum equations [24–26].

There is no formal definition of a compatible numerical method. Here we show that the compatible properties of the SEM include:

- A divergence theorem: the discrete divergence and gradient operators are anti-adjoints (adjoints with a negative sign) with respect to the SEM inner product.
- A Stokes theorem: the discrete curl operator is self-adjoint with respect to the SEM inner product.
- The discrete gradient operator is annihilated by the discrete curl operator.
- The discrete curl operator is annihilated by the discrete divergence operator.

The divergence/gradient global adjoint relationship is usually obtained in the SEM by defining a weak-gradient operator as the adjoint of the divergence operator. What is shown here is that merely straightforwardly discretizing gradient and divergence leads to matrices whose adjoint relation implies a discrete statement of the divergence theorem. That these adjoint relations hold globally is shown by first showing that the SEM has discrete divergence and Stokes theorems which hold at the element level. In the continuum, the divergence theorem applied to a volume consisting of a single element includes a boundary term: the integral of a flux term over the surface of the element. The SEM divergence theorem includes a discrete analog of this boundary term. Because the SEM basis functions are globally continuous, the discrete flux will be equal and opposite as computed by adjacent elements, providing local conservation. This element boundary term is similar to the element boundary term that is explicitly included in discontinuous Galerkin (DG) methods. But in a continuous Galerkin method like the SEM, this boundary term is never computed as part of a numerical implementation. A similar concept applies to the SEM curl operator and associated Stokes theorem.

The global divergence/gradient adjoint relationship ensures a symmetric discrete Laplacian, which is of great benefit to iterative solvers. In Cartesian coordinates, the elemental version of this identity can be inferred from Eqs. F.54 and F.55 in [Appendix F [27]]. The fact that this elemental divergence theorem applies to unstructured grids in curvilinear coordinates is not generally known (as with the discrete local version of Stokes theorem). This is evidenced by the fact that the SEM has never been considered a locally conservative method, and local conservation is equivalent to having a discrete divergence theorem. To the best of our knowledge, the annihilator properties of the SEM described here are also previously unknown.

In the case of energy conservation, compatible methods are of interest because they allow conservation without utilizing a total-energy equation [17,28]. In atmospheric modeling, an early use of this property in one dimension dates to [29]. Energy is conserved by the careful mimicking of the energy balance in the original equation: the conversion between kinetic and internal energy terms will exactly balance and the advection operator will not dissipate any kinetic energy. Kinetic-energy dissipation, if needed, must be explicitly added in a compatible method via the introduction of limiters, hyper-viscosity or large-eddy-simulation based approaches.

To verify our results, we use the SEM to discretize the shallow-water equations in curvilinear coordinates on the surface of the sphere and show the method conserves mass, energy and potential vorticity.

2. Spectral-element discretization

We now give a summary of the SEM, using the traditional finite-element inner-product formulation with globally defined continuous basis functions [30,31]. This formulation allows for a clearer illustration of the numerical properties of the method, while the more standard matrix–vector formulation [32,33] is useful for efficient numerical implementations. We present many details which are needed later to show precisely that the method is compatible. We consider only periodic domains, such as the surface of the sphere, so that we may ignore the boundary terms and simplify the exposition.

2.1. Discrete spaces for the SEM

We first define the discrete space used by the SEM. Let x^α and $\vec{x} = \sum_{\alpha=1}^{3} x^\alpha \vec{e}_\alpha$ be the Cartesian coordinates and position vector of a point in the reference cube $[-1,1]^3$ and let r^α and $\vec{r}$ be the (possibly curvilinear) coordinates and position vector of a point in the computational domain, denoted by Ω. We denote the space of polynomials up to degree d in $[-1,1]^3$ by

$$\mathcal{P}_d := \operatorname*{span}_{i,j,k=0}^{d} (x^1)^i (x^2)^j (x^3)^k = \operatorname*{span}_{\vec{i}\in\mathbb{I}} \phi_{\vec{i}}(\vec{x}),$$

where $\mathbb{I} := \{0,\ldots,d\}^3$ contains all the degrees and $\phi_{\vec{i}}(\vec{x}) = \prod_{\alpha=1}^{3} \varphi_{i^\alpha}(x^\alpha), i^\alpha = 0,\ldots,d$, are the cardinal functions, namely polynomials that interpolate the 3D degree-d Gauss–Lobatto-Legendre (GLL) nodes $\vec{\xi}_{\vec{i}} := \sum_\alpha \xi_{i^\alpha} \vec{e}_\alpha$. The cardinal-function expansion coefficients of a function g are its GLL nodal values, so we have