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Discrete calculus methods for diffusion

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Abstract

A general methodology for the solution of partial differential equations is described in which the discretization of the calculus is exact and all approximation occurs as an interpolation problem on the material constitutive equations. The fact that the calculus is exact gives these methods the ability to capture the physics of PDE systems well. The construction of both node and cell based methods of first and second-order are described for the problem of unsteady heat conduction – though the method is applicable to any PDE system. The performance of these new methods are compared to classic solution methods on unstructured 2D and 3D meshes for a variety of simple and complex test cases.

Keywords: Discrete calculus; Staggered mesh; Face/edge elements; Unstructured; Finite volume; Finite element

1. Introduction

This paper is dedicated to Pieter Wesseling. It bears his hallmark at many levels. Philosophically, it is a paper about the intimate connection between physics and mathematics. Prof. Wesseling, an Aerospace Engineer turned Mathematician has always produced papers that are always keenly aware of the connection. Topically, it is a paper about staggered mesh methods – one of many areas in which Pieter and his coworkers are prolific (see the references in [1,2]). And in particular, the paper addresses fundamental questions about how to apply staggered mesh methods to compressible flow problems – an area Pieter is particularly interested in [3–6].

Staggered mesh methods have traditionally been applied to incompressible flows. The lack of pressure modes is particularly attractive in that application. There is therefore considerable literature addressing the issue of how to discretize the momentum equations with structured [7], curvilinear [8,9], and unstructured staggered mesh methods [10–14,30,31]. However, in the context of compressible flow there arises the additional issue of how to discretize the density and energy equations.

The discrete differential operators in incompressible staggered mesh methods have very unique and attractive mathematical properties that allow the discrete equations to physically mimic their continuous counterparts. This not only leads to a lack of pressure modes, but kinetic energy and vorticity conservation statements

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[15,16], maximum principles and many other attractive properties [17]. If we wish the compressible discretization to also have these sorts of attractive physical properties (like entropy increase), then presumably the scalar equations (density and energy) must also be discretized appropriately.

Until recently, it was not clear to the authors what criteria should be used to judge if a scalar transport equation was discretized 'appropriately'. We believe this dilemma is addressed by the Discrete Calculus approach presented in this paper. In order to carefully explain the Discrete Calculus approach, this paper actually only focuses on the unsteady diffusion equation (not the advection–diffusion equation). The diffusion term contains sufficient complexity to present the fundamental ideas of the Discrete Calculus approach. Due to space limitations, the issues concerning advection must be addressed in a subsequent paper.

The premise of this paper is that numerical methods that capture the physics of the equations well have an associated exact Discrete Calculus. The fact that PDE's can always be discretized exactly is demonstrated in the Section 2. To make the presentation clear and concrete the paper focuses on the diffusion (or heat) equation. However, we emphasize from the outset that the basic ideas presented are generally applicable to almost any PDE system. The paper is really an introduction to the Discrete Calculus method. The fact that the diffusion equation is simple and has analogs in many fields of application should make the paper, and hence this method, available to a broad audience.

Two different node-centered Discrete Calculus methods are derived in detail (Section 3). The paper then shows how these ideas can be applied to cell-based discretizations and how they differ from traditional finite volume and discrete Galerkin methods (Section 4). Section 5 then compares these four Discrete Calculus methods to some classic finite volume methods for the diffusion equation on a variety of test problems.

2. Exact discretization

Discretization takes a continuous PDE equation with essentially an infinite number of equations and unknowns (at least one for every point in space) and reduces it to a finite system of algebraic equations and unknowns. It is frequently assumed that the act of discretizing a PDE must involve approximation or the introduction of some sort of error. This is not the case [18]. *Solving* a PDE system numerically does indeed require approximation, but it is possible to separate the process of discretization and approximation and when this is done discretization can be performed exactly. One premise of this paper is that exact discretization is highly advantageous and leads to methods that have very interesting mathematical and physical properties.

Exact discretizations ultimately require approximation because the discretization is not closed. There are more discrete unknowns than algebraic equations. Closure of the system requires the coupling of some of the discrete unknowns. This coupling process is an interpolation problem where all the numerical approximation and errors are introduced. It is often characterized by a transfer of information from one mesh to a different (dual) mesh, and it invariably involves a material constitutive relation.

The profound benefits of separating the discretization process (where the continuous PDE system is made finite) from the approximation process (where the finite system becomes solvable) will become very clear as we proceed. Nevertheless, we describe the key ideas abstractly here to preview what will be seen in the paper. It will be seen that the closure (and therefore approximation) of the exact finite equation system always occurs in the material constitutive relations embedded in the PDE. These constitutive relations are actually physical approximations of bulk material behavior. They are not exact to begin with. This approach therefore places all numerical errors/approximation in the already physically approximate material relations. The physics of a PDE (such as conservation, and wave propagation) never depend on the details of the material. This approach will therefore always capture the physics of the PDE exactly by placing all numerical approximation or errors in the material properties.

To make the presentation of the Discrete Calculus method concrete we will use a simple equation that is common to many fields of engineering and science – the heat equation.

$$\frac{\mathrm{d}(\rho CT)}{\mathrm{d}t} = \nabla \cdot k\nabla T \tag{1}$$