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Mimetic Difference Approximations of Partial Differential Equations

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Abstract

This is the final report of a three-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The goal of this research has been to construct local high-order difference approximations of differential operators on nonuniform grids that mimic the symmetry properties of the continuum differential operators. Partial differential equations solved with these mimetic difference approximations automatically satisfy discrete versions of conservation laws and analogies to Stoke's theorem that are true in the continuum and therefore are more likely to produce physically faithful results. These symmetries are easily preserved by local discrete high-order approximations on uniform grids, but are difficult to retain in high-order approximations on nonuniform grids. We also desire the approximations to be local and use only function values at nearby points in the computational grid; these methods are especially efficient on computers with distributed memory. We have derived new mimetic fourth-order local finite-difference discretizations of the divergence, gradient, and Laplacian on nonuniform grids. The discrete divergence is the negative of the adjoint of the discrete gradient, and, consequently, the Laplacian is a symmetric negative operator. The new methods we are deriving are local, accurate, reliable and efficient difference methods that mimic symmetry, conservation, stability, the duality relationships and the identities between the gradient, curl, and divergence operators on nonuniform grids. These methods are especially powerful on coarse nonuniform grids and in calculations where the mesh moves to track interfaces or shocks.

1. Background and Research Objectives

The goal of this research has been to develop more efficient, stable and accurate methods for solving systems of nonlinear partial differential equations (PDEs). The discrete approximation of differential operators is a critical element in any computer simulation based on solving these equations. Most PDEs can be formulated in terms of invariant, first-order differential operators, such as the divergence of vectors and tensors, the gradient of scalars and

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vectors, and curl of vectors. These first-order differential operators are the main objects of vector and tensor analysis and satisfy integral identities that are closely related to the conservation laws of continuum models. We use these coordinate invariant first-order operators to create high-quality finite-difference methods (FDMs) based on discrete analogs of vector and tensor analysis. This effort has resulted in new solution algorithms that mimic the crucial properties, such as conservation laws or symmetries, of the PDEs being solved.

2. Importance to LANL's Science and Technology Base and National R&D Needs

Developing discrete algorithms that capture all the important characteristics of the physical problem is more difficult as mathematical models become more complex to account for additional physical processes and more complex domains or boundary conditions. These mathematical models involve, in an essential role, the numerical solution of systems of nonlinear PDEs. The difficulties will be easier to overcome if we are able to derive new discrete algorithms based on a general approach for solving these PDEs that can be applied to a wide range of physical systems. Experience has confirmed that the best results are usually obtained when the discrete model preserves the fundamental properties of the original continuum model for the underlying physical problem. Robust, realistic algorithms for large-scale simulations are more capable when they are based on solid mathematical theory and when the discrete model maintains many of the important properties of the continuum model. These properties include conservation laws, symmetries in the solution, and the nondivergence of particular vector fields (i.e., they are divergence free).

Our research on mimetic difference approximations has reached a point where we have a complete set of consistent discrete approximations for the gradient, divergence and curl operators on nonuniform grids in one, two and three spatial dimensions. These operators preserve the underlying structure and mimic the integral properties of the differential operators, including the divergence and circulation theorems. This past year we began comparing the new methods with other standard finite difference methods and found that the new algorithms are more effective approaches in solving complex mathematical models in fluid dynamics, combustion and nonlinear optics.

3. Scientific Approach and Accomplishments

We have concentrated on deriving discrete difference methods that automatically preserve crucial properties of differential operators, such as conservation laws, and the identities between the gradient, curl, and divergence operators. The discrete versions of the divergence, gradient, curl, and Laplacian operators should be consistent with each other and satisfy the standard vector identities. For example, in magnetohydrodynamics, taking the divergence of the equation for the magnetic field B reveals that if B is initially divergence free, then it remains so, based on these identities. Numerically, if the identities are not satisfied, the divergence of B will drift during the calculation. Stokes' theorem states that the exterior derivative is the adjoint of the boundary operator with respect to the pairing induced by integration. This operator generates the discrete versions of the divergence, gradient, and curl operators; the discrete vector identities follow automatically from standard geometric identities.

The discrete analogs of integral identities can be used to construct discrete operators satisfying these identities using the support-operator method (SOM). In the SOM, first a discrete approximation is defined for a first-order differential operator, such as the divergence or gradient, that satisfies the appropriate integral identity, such as Stokes' theorem. This initial discrete operator, called the prime operator, then supports the construction of other discrete operators, using discrete formulations of the identities for differential operators. For example, if the initial discretization is defined for the divergence (prime operator), it should satisfy a discrete form of Gauss' theorem. This prime discrete divergence, DIV, is then used to support the derived discrete operator GRAD; GRAD is defined to be the negative adjoint of DIV.

The SOM FDMs are based on fundamental mathematical principles that correspond to basic physical principles, and these FDMs provide accurate, robust, and stable approximations to differential operators on nonuniform structured and unstructured grids. Because the new FDMs mimic the invariant properties of continuum differential operators, they require fewer points to obtain the same accuracy when compared with many traditional methods. They also lead to a deeper understanding of FDMs and of which physical laws are captured by an FDM.

These methods are especially effective on coarse grids and in calculations where the mesh moves to track interfaces or shocks. We have developed some effective conservative, fourth-order accurate approximations to nonlinear systems of hyperbolic equations being solved on nonuniform grids. These approximations maintain their accuracy on moving, tensor-product grids with random spacing in one, two and three dimensions. We have

compared the second- and fourth-order SOM FDMs with traditional FDMs in solving conservation laws on extremely rough grids and demonstrated the advantages of the SOM approach.

Mimetic difference operators, which preserve (mimic) the properties of the differential operators, can also be investigated using functional analysis. This approach has been successfully applied to the study of problems in mathematical physics. For example, the method of orthogonal projections forms a considerable part of the theory of generalized solutions, and Weil's theorem on orthogonal decomposition plays a fundamental role in solving the Navier-Stokes equations. The difference version of Weil's theorem, for square grids in 2-D, can be used to construct high-quality FDMs for these equations.

Applying the algebraic topology to construct the discrete analog of the metric conjugacy operator * on non-orthogonal, non-smooth, logically rectangular grids requires establishing a complex set of definitions and mathematical tools. Moreover, this approach is natural for a specific discretization of the vector field and cannot be easily used for many widely used discretizations, including the usual nodal discretization of the Cartesian components of a vector.

The language and tools of advanced calculus are more widely known and used for formulating the theorems and concepts of vector and tensor analysis than is the language of algebraic topology. This is especially true among researchers in the field of scientific computing, solving systems of PDEs. Because this applied numerical community is our primary audience, we formulate our discrete vector and tensor analysis without using the language of algebraic topology.

Using the language of advanced calculus, we constructed different discrete representations of scalar, vector, and tensor functions on logically rectangular grids and defined projection operators between different spaces that preserve some important properties of the functions. We also defined the discrete analog of the line integral, the potential vector, the flux of the vector through a surface, and the circulation of a vector along a contour and construct discrete analogs for the gradient of scalar functions and investigate discrete analogs for directional derivatives. The natural discrete analogs of the divergence, gradient, and curl operators are based on coordinate invariant definitions and interpret these formulas in terms of curvilinear coordinates, such as length of elements of coordinate lines, areas of elements of coordinate surfaces, and elementary volumes. We then define a discrete analog of the

divergence operator based on Gauss' theorem and use Stokes' theorem to define a discrete curl. We prove discrete versions of the standard theorems of vector analysis, including a discrete Gauss' theorem: the discrete analog of the theorem that $\operatorname{div} \mathbf{A} = 0$ if and only if $\mathbf{A} = \operatorname{curl} \mathbf{B}$, and $\operatorname{curl} \mathbf{A} = 0$ if and only if $\mathbf{A} = \operatorname{grad} \varphi$; the discrete analog of the theorem that if $\mathbf{A} = \operatorname{grad} \varphi$, then line integral does not depend on path; and, if line integral of some vector function is equal to zero for any closed path, then this vector is the gradient of some scalar function.

The new discrete approximations of the divergence, gradient, and curl using discrete analogs of the integral identities are satisfied by the differential operators. These new discrete operators are adjoint to the previously derived natural discrete operators defined using "natural" coordinate-invariant definitions, such as Gauss' theorem for the divergence. The natural operators cannot be combined to construct discrete analogs of the second-order operators **div**, **grad**, **grad div**, and **curl curl** because of incompatibilities in domains and in the ranges of values for the operators. The same is true for the adjoint operators. However, the adjoint operators have complementary domains and ranges of values, and the combined set of natural and adjoint operators allow a consistent formulation for all of the compound discrete operators.

Publications

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6. Hyman, J. and Shashkov, M., "Adjoint Operators for the Natural Discrete Divergence, Gradient, and Curl," Los Alamos National Laboratory document (submitted to Applied Numerical Mathematics).
7. Hyman, J. and Shashkov, M., "Support-Operators Method and High Order Finite-Difference Schemes in One Dimension," Los Alamos National Laboratory document (in preparation).