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Multidimensional Methods for Hyperbolic Problems

James Hyman*, Mikhail Shashkov, Blair Swartz, and Burton Wendroff

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 numerical solution of multidimensional wave-propagation problems is considerably more complex than solutions for one-dimensional problems, but improving a method's accuracy produces more significant increases in efficiency. This is particularly true for first-order accurate methods. Higher-order methods, which are already comparatively efficient, are especially difficult to construct on irregular meshes. The passive-scalar advection equation provides an ideal vehicle for investigating the relationships between accuracy, efficiency, and physical acceptability for a variety of finite-difference schemes. Development and analysis of methods for this equation provide insight into solving more complicated problems involving material and/or neutron transport. We found that three approaches to two-dimensional upwind differencing led to schemes equivalent to the dimensionally split Lax-Wendroff method. Assuming stability, we were able to prove that both the split-Lax-Wendroff and a new two-dimensional, predictor-corrector scheme yielded second-order convergence on nonuniform tensor-product grids, despite first-order discretization errors for such grids. We were able to prove that in some cases, Roe's upwinding for triangulations (which is locally inconsistent) converges with first-order accuracy. The sensitivity of fourth-order accurate, conservative, mimetic methods to the roughness of nonuniform grid-spacing was explored analytically and numerically in one-dimension and for logically-rectangular two-dimensional grids. We also considered the application of a novel set of unknowns (parameters) towards conservative second-order methods on irregular polyhedral grids. Queried, we noted that convergent, stable, split schemes for ill-posed problems could not exist. This prompted us to reconsider (for hyperbolic operators whose sum is hyperbolic) conditions implying that splitting is stable for the differential operators and for related difference methods.

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1. Background and Research Objectives

The numerical solution of fluid flow and more general wave-propagation problems in two or more space dimensions is clearly computationally more complex than the same type of problem in one dimension. On the other hand, the geometry of several dimensions is so rich that there can occur opportunities for achieving great efficiencies that have no counterpart in one dimension. Here is a simple example of this. Suppose we wish to obtain the solution of some time dependent partial differential equation with mesh size h in each space dimension. Suppose further that we have a variety of first-order methods available, that is to say, the error of each method is proportional to h . For typical wave propagation problems a stability condition will force the time step also to be proportional to h . Then, in two dimensions, the amount of work done to reach some fixed time will be proportional to $1/h^3$, or to $1/h^4$ in three dimensions. Suppose there are two different first-order methods achieving errors C_1h and C_2h , respectively. To obtain equal error from the two methods, mesh sizes h_1 and h_2 will be required, where $C_1h_1 = C_2h_2$. Assuming that both schemes have the same stability condition, then the ratio of the work done by scheme 1, W_1 , to that done by scheme 2, W_2 , is $W_1/W_2 = (h_2/h_1)^n = (C_1/C_2)^n$, $n = 3, 4$. Thus, a first-order method that is twice as accurate as another one can be expected to be 16 times faster in three dimensions.

It should also be pointed out that higher-order schemes, in which the error is proportional to Ch^p for some $p > 1$, are less sensitive to the coefficient C , for in this case $W_1/W_2 = (C_1/C_2)^{n/p}$. Higher-order methods, however, are difficult to formulate on unstructured grids and tend to produce nonphysical oscillations. On rectangular grids, second-order-accurate methods can easily be created using dimensional splitting. This involves executing a sequence of second-order-accurate but lower-dimensional problems in the particular order that is mathematically consistent (to second order) with the evolution of the original multidimensional problem.

Difficulties with dimensional splitting have led to a revival of interest in true multidimensional methods, in particular, upwind methods. These are first-order and, as we have seen above, benefit greatly from reduction of the truncation error. Upwinding intuitively seems like the right thing to do; if disturbances are propagating in a certain direction with a finite speed, then the update of the solution at a point should not depend on data that cannot possibly affect it, namely, downwind data. This is very easy to arrange in one dimension, but quite difficult in two or more dimensions. One of our long-term objectives is to analyze multidimensional upwind schemes, ultimately for the Euler equations and other fluid models on unstructured grids in two and three dimensions, seeking minimal error, maximal time step, physical correctness, robustness and efficiency.

The passive scalar advection equation $u_t + c_x u_x + c_y u_y = 0$ provides a prototype which, in spite of its analytical simplicity, is numerically challenging. In one space dimension advection provides an excellent starting point from which to design methods for more difficult problems. It is not clear whether or not this will be the case for multidimensional flows where there is not a unique set of characteristic directions along which information moves, and this is one of the questions we will consider. On the other hand, it has been observed that many commonly used methods for fluid flows are very inaccurate for simple linear advection; either there is excessive dissipation or there is clipping of extrema, even in one dimension.

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

It appears then that significant savings in computer time can be achieved by searching for optimal schemes among the first-order ones; optimal in the sense of minimum truncation error. However, there are other considerations, for we need to achieve optimality under constraints of maximal time step, robustness to grid distortions, and physical correctness. Issues of computational complexity also become important; strict mathematical optimality may have to be abandoned in order to be efficient on a given machine architecture, especially if it relies on parallelism.

The variety and complexity of simulations currently being done throughout the Laboratory in climate modeling, geophysics, explosives effects, and wave propagation show a definite need for a continued strong effort in research into optimal methods for such problems. This is basically a mathematical and computational endeavor that fits well into the Laboratory's competency in computation, modeling, and mathematics.

3. Scientific Approach and Results

An investigation of the relation among various upwind schemes for scalar advection in two dimensions has been carried out. The particular types of methods involve either interpolation, upwind transport and projection of a piecewise linear distribution, or reduction of truncation error. It was found, surprisingly, that these three are equivalent to the split-dimension Lax-Wendroff method.

The phenomenon of supra-convergence concerns the apparent loss of accuracy, due to a change in the order of truncation error, in going from uniform to nonuniform non-smooth grids. Both the dimensionally split Lax-Wendroff scheme and a new multi-dimensional predictor-corrector scheme are proven to be supraconvergent in [5]. That is, if one assumes

stability, then they maintain second-order accuracy in computing approximate solutions, even on very rough grids. Roe's upwind scheme [1] for triangular grids is locally inconsistent but is shown in [2] to be first-order accurate in some cases.

The sensitivity of high-order methods to the degree of smoothness of a nonuniform grid is explored for the example of fourth-order methods [7,8]. To do this, conservative fourth-order-accurate approximations to the divergence and gradient are constructed that are adjoint to each other—for nonuniform grids in one dimension and for logically rectangular grids in two dimensions—by combining the technique of "support operators" with mapping methods. Fourth-order accuracy is confirmed for smooth logically rectangular grids in certain steady state and evolutionary contexts. In one dimension, the schemes maintain second-order accuracy even for rough, random grid perturbations. Moreover, they yield more accurate results than the usual second-order method for the same amount of computational work. But the effect of the size of random perturbations to the logically rectangular grid does not correlate appropriately with the order of the truncation error as it did in one dimension; so this alone seems an inappropriate characterization of the quality of two dimensional grids.

The requirements of conservation and second-order accuracy for irregular, polygonal/polyhedral cells pose particular difficulties. Conservation here seems simplest in the context of schemes based on finite volumes, i.e., using cell-integrals of various terms of the differential equation. A novel set of unknowns (rather than cell-means or vertex values) now leads to conservation in certain contexts. The unknowns associated with a function defined on a polyhedron in n dimensions that is bounded by m edges/faces consists of the m edge/face-integrals of the function. With these, the cell-integral of (say) the directional derivative $c \cdot \text{grad } u$ (c some constant vector) is simply the sum over the cell boundary of the product of each edge/face integral with the corresponding (piecewise constant) normal component of c . This is exact, by the divergence theorem, for an arbitrary function u —and so, in particular, for quadratic functions. Specific choices for c now express the cell-mean of the gradient—and so a second-order accurate approximation for $\text{grad } u$ at the cell's centroid—as a combination of the m edge/face integrals of u (and as cannot be done for triangles or quadrilaterals using the m values of u at the vertices instead). Moreover, curved edges/faces can be treated for curvatures small compared to the spatial mesh size using a locally averaged unit normal.

We approximate the cell-mean of u_t using some combination of its edge/face integrals that is exact for linear functions only, so the function's value at the cell's centroid will suffice. For this its values at, say, $n+1$ edge/face centroids in general position will suffice. But each of the last is the mean value over the corresponding edge/face. At this point a scheme with second-order truncation error for the cell-mean of the equation $u_t + c \cdot \text{grad } u = 0$ is in hand. Application of the trapezoidal rule in time (Crank-Nicholson) would insure conservation, and

the resulting method reduces to the box scheme for a single space dimension. For $n > 1$ dimensions, unfortunately, since we have defined only one equation for each of the F cells of a tessellation, we do not yet have enough equations for the $E=m$ unknowns. [To see this in, e.g., two dimensions, and with V the number of vertices, the Euler characteristic says we need $E - F = V - 1$ additional equations (less boundary conditions)]. The accuracy of the gradient approximation at cell centroids, though, allows its easy second-order accurate global approximation. These observations provide a basis for multidimensional difference schemes that is new to us.

An approach that is different in spirit from domain-of-dependence schemes and domain-of-influence methods is centered differencing: simply replace derivatives by differences in a consistent way. The box scheme is an example: given unknowns at the vertices of a special rectangular grid, replace derivatives by differences of averages of vertex values over appropriate faces of the space-time box. There is one important difference between the box scheme and the others. The box scheme is known to be unconditionally stable in one dimension [3] and appears to be so in two dimensions. Numerical examples involve an initial cone on a coarse, very nonuniform, rectangular grid (diagonals are added for the piecewise linear scheme). The shape of the cone after advection up the diagonal of a square domain by the piecewise linear and box schemes was computed. The piecewise linear scheme took 120 time steps to reach the same time level that the box scheme reached in 20 steps. The box scheme shows a sharper profile but has oscillations and does not maintain positivity. It is conservative and second-order accurate on arbitrary rectangular grids, while the piecewise linear method is neither conservative nor consistent in general. On the other hand, the box method is basically implicit, and it is only the special nature of the scalar advection equation and its boundary conditions that make it appear as an explicit procedure.

The connection between the notion of a well-posed initial value problem and a stable difference scheme is well-known, at least for constant coefficient differential equations. What about an ill-posed problem? Can there exist a stable convergent scheme for such? No, for the exact solution at convergence must then depend continuously on the initial data; i.e., the problem must be well-posed. Nevertheless, a recent query proposing the contrary prompted us to explore once again the conditions, on hyperbolic operators whose sum is hyperbolic, which imply that (exact) splitting is stable—and the associated consequences this can have for related difference methods [4].

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