Numerically Tracking Contact Discontinuities

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Abstract

We review some of the classic numerical techniques used to analyze contact discontinuities and compare their effectiveness. Several finite difference methods (the Lax-Wendroff method, a Multidimensional Positive Definite Advection Transport Algorithm (MPDATA) method and a MUSCL scheme with an Artificial Compression Method (ACM)) as well as the finite element Streamlined Upwind Petrov-Galerkin (SUPG) method were considered. These methods were applied to solve the 2D advection equation. Based on our results we concluded that the MUSCL scheme produces the sharpest interfaces but can inappropriately steepen the solution. The SUPG method seems to represent a good balance between stability and interface sharpness without any inappropriate steepening. However for solutions with discontinuities the MUSCL scheme is superior. Several of these methods were also used to solve the Sod shock tube problem. In addition a preliminary implementation in a GPU program (CLAMR) is discussed.

1 Introduction

The earthquake and resulting tsunami in Japan caused a release of radioactive material into the pacific ocean. This radioactive waste was carried by the Kuroshio current into the North Pacific current and is making its way to the US coastline. These currents can produce sharp flow discontinuities with the surrounding ocean water. The idea of tracking these flows and accurately resolving the interfaces between the radioactive and non radioactive fluids provides a motivation for resolving contact discontinuities.

Many classic techniques have been developed to analyze contact discontinuities and compare their effectiveness. Several finite difference methods (the Lax-Wendroff method, a Multidimensional Positive Definite Advection Transport Algorithm (MPDATA) method and a Monotone Upwind Scheme for Conservation Laws (MUSCL) with an Artificial Compression Method (ACM)) as well as the finite element Streamlined Upwind Petrov-Galerkin (SUPG) method are considered. These methods were applied to solve the 2D advection equation. Based on these results we were able to conclude that the MUSCL scheme with artificial compression produces the sharpest interfaces but can inappropriately steepen the solution. The SUPG method seems to represent a good balance between stability and interface sharpness without any inappropriate steepening but is a non-conservative method. However, for solutions with discontinuities, the MUSCL scheme is superior. Some of the finite difference methods and a combined finite element/finite difference method (based on the Lax-Wendroff and SUPG method) were also used to solve the Euler equations. Each of these methods is detailed in Section 2 followed by a brief description of the results from the different methods in Section 3. We then discuss the conclusions and future directions we hope to take with the research in Section 4.

2 Discription of Methods

2.1 Lax-Wendroff

The Lax-Wendroff method is a finite difference method designed for hyperbolic PDEs that is second order accurate in both space and time. This scheme can be understood as a two-step method. On the first step the fluxes at a half step in both space and time are calculated. On the second step of the method the half-step fluxes are used to calculate the new value of the conserved variable at each point in the domain. This scheme works well for smooth data but can run into trouble when the solution develops a discontinuity. When this occurs, the solution becomes highly oscillatory around the discontinuity.

It has been shown by numerous authors [4,5] that there is a simple fix for oscillations around discontinuities. First order schemes for hyperbolic PDEs (such as upwind finite differencing) do not lead to oscillations like higher order schemes (Lax-Wendroff). Flux limiters work by interpolating between the flux calculated by a first order scheme and the flux calculated by a higher order scheme. Oscillations near a discontinuity can be eliminated by making the approximation mimic a first order scheme near a steep gradient using a flux limiter and while higher order accuracy is achieved in smoother regions.

It has been mathematically shown that certain formulas for flux limiters in linear PDEs lead to schemes which are monotonicity preserving. This means that if the solution is monotonic at a certain time step it will remain monotonic at the next time step. This property is equivalent to saying that the scheme will not introduce new extrema and that the scheme is Total Variation Diminishing (TVD). We explored several limiters to preserve the monotonicity of our solutions and settled on the Superbee method, which produces the sharpest possible gradients while still being TVD.

2.2 MPDATA

Developed by Smolarkiewicz beginning in the early 1980s [6–8], the MPDATA algorithm is a finite-difference approximation for the advective terms in the fluid equations. A donor-cell approximation to the equation is defined in terms of the local Courant number. The resulting equation is a first order upwind finite difference scheme, which is very diffusive.

By analyzing the approximation from the first step using a modified equation analysis, it can be seen that a diffusive convective flux term is added to the model equation. This erroneous diffusion damps out nonphysical oscillations but also overly smears the solution over time.

As an example, the pure advection equation,

$$\frac{\partial \Psi}{\partial t} = -\frac{\partial}{\partial x}(u\Psi)$$

becomes,

$$\frac{\partial \Psi}{\partial t} = -\frac{\partial}{\partial x}(u\Psi) - \frac{\partial}{\partial x}\left(-K\frac{\partial \Psi}{\partial x}\right)$$

using an upstream approximation. The added dissipation error, $\frac{\partial}{\partial x}\left(K\frac{\partial \Psi}{\partial x}\right)$, is then subtracted out of the solution using an antidiffusive velocity to cancel the additional convective flux.

2.3 MUSCL with ACM

The MUSCL that we used is a modified Osher-Chakravarthy scheme [10], which is a second order TVD approximation to the scalar conservation laws. The modifications produce a third order accurate MUSCL solver [9]. The method is upwind biased and uses a minmod function to avoid numerical oscillations in the solution.

Hartens ACM [1] was initially intended to be used to sharpen contact discontinuities for first order accurate schemes. However, this technique has been extended to higher order methods such as Essentially Non-Oscillatory (ENO) schemes [3], MUSCL [9] and RAGE [2], which is widely used at LANL. This slope modification method relies on a switch to increase or decrease the slope of a function near a discontinuity. For the purposes of this presentation, the advection equation is solved using a MUSCL scheme with ACM.

2.4 SUPG

In the finite element method a set of trial functions are assumed to represent the solution of a differential equation over a region. These trial functions have certain degrees of freedom that must be solved for. The differential equation is multiplied by test functions and then integrated over the region that the differential equation is to be solved on. This generally yields algebraic equations for the degrees of freedom. In Galerkin approaches, the test functions are assumed to be the same as the trial functions. However, when sharp gradients are present CG methods produce highly oscillatory solutions. This can be helped by introducing the more general Petrov-Galerkin (PG) approach in which the test functions can be different from the trial functions. The streamline upwind Petrov-Galerkin (SUPG) approach chooses a specific set of test functions which can be shown to significantly reduce oscillations in the solution. For the 2D advection equation these test functions are the same as the trial functions with two additional terms:

$$W = N + \frac{\alpha h}{2}\left(\frac{u}{\sqrt{u^2+v^2}}\frac{\partial N}{\partial x} + \frac{v}{\sqrt{u^2+v^2}}\frac{\partial N}{\partial y}\right) \tag{1}$$

Where W is test function, N is one of the trial functions, α is an arbitrary parameter usually taken to be 1 for pure advection, h is a 1D length of an element, and u-v are the velocity in the x-y direction, respectively

3 Results

4 Conclusions and Future Directions

From the above diagrams it is apparent that the MUSCL scheme was most effective at preventing diffusion of material interfaces. However, the MUSCL is the most expensive scheme and also unnaturally sharpens normally smooth waves as is evident from the evolution of the initially Gaussian distribution. The SUPG scheme gradually diffuses the solution while the Lax-Wendroff TVD and the MPDATA schemes are overly dissipative. The choice of method is therefore problem specific and most production scale codes should have the option to switch between algorithms. Several of these schemes have been implemented in a Euler equation solver for further testing and stability analysis. Additionally, we are in the process of applying the ACM to a threaded GPU shallow water equation solver. A mixed finite element/finite difference approach for the Euler equations was unsuccessful and thus a full finite element approach is planned.

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