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ABSTRACT

This manuscript is meant to give a short summary of the advantages of high order schemes and suitable test problems which can properly illustrate these advantages.

1 The Advantages of High Order Schemes

The advantages of high order schemes are well-documented in the scientific literature in both the theoretical form and in computational form. It is really the theory that one should focus on since the whole story in its unpolluted form lies there. If one needs computational evidence, then such evidence is copious.

The classic reference is the paper by Kreiss and Oliger [15]. However, here the simplest exposition of the key issues will be given. It is the truncation error of the differentiation operator which holds the key to the advantages of high order schemes when applied to hyperbolic systems. For non-spectral operators, this truncation error has an upper bound of the form, see [9],

$$E = c(\Delta x)^p k^{p+1}, \tag{1}$$

where c is a constant that will depend on the exact scheme in use, Δx denotes the distance between adjacent grid points, p denotes the order of the derivative, and k denotes the Fourier wave number. That is, if one were to differentiate $f(x) = \sin(kx)$ then the truncation error for differentiation is bounded above by the above expression. Now, since,

$$\Delta x = \frac{L}{N}, \tag{2}$$

where L denotes the length of the interval and where N denotes the number of grid points in this interval, we can let $L = 1$, and replace $(\Delta x)^p$ with

$(1/N)^p$. Next, we can now solve equation 1 for N. Beginning with

$$E = (1/N)^p k^{p+1}, \tag{3}$$

where we let $c = 1$ for simplicity, we then get,

$$E^{1/p} = (1/N) k^{(p+1)/p} \tag{4}$$

and

$$(1/N) = \frac{E^{1/p}}{k^{(p+1)/p}}, \tag{5}$$

and finally,

$$N = \frac{k^{(p+1)/p}}{E^{1/p}}. \tag{6}$$

Now, for hyperbolic systems, the floating point operations (flops) scale as,

$$flops = const * O_{time} * O_{space} * N^{d+1}, \tag{7}$$

where d is the dimension of the calculation, O_{time} is the order of the temporal discretization, O_{space} is the order of the spatial discretization, and where *const* is a constant that will depend on the scheme used but will not deviate much from .5. By definition $p = O_{space}$ and for hyperbolic equations $O_{time} = O_{space}$ is roughly the best choice. Into this expression for flops we can substitute the above expression for N to get,

$$flops = const * p^2 * \frac{k^{(d+1)(p+1)/p}}{E^{(d+1)/p}}. \tag{8}$$

Now, let's see what this expression produces for a few values of the parameters. Let $d = 3$ and let's require that the error in the derivative be $E = 10^{-4}$. For a first order scheme, $p = 1$ we see that this expression becomes,

$$flops(p = 1) = 10^8 * k^8, \tag{9}$$

and if we let $p = 4$ we find that the flops scale as,

$$flops(p = 4) = 16 * 10^4 * k^5. \tag{10}$$

Recall, k is the wavenumber. For flows that contain structure, such as turbulent flows or any calculation where, say, vortices are present, there will

be significant energy in the high values of k. Thus, one can see that the rate of growth of the flops is very different. Further, the constant in front of the expression is also very different. This is really the whole story. With a low order scheme, one quickly reaches the limit of the computer. With the high order scheme, one can obtain far more modes before the limit of the computer is reached.

2 Designing Problems to Evaluate Schemes

First and foremost, if one wants conclusive evidence of the differences between schemes, one must design problems that have exact solutions. Without exact solutions one can not have clear evidence of the advantages of high order schemes. It should be noted, that if the flow does not contain structure, then one does not expect to see any advantage of high order schemes. In fact, for problems that are essentially piecewise linear with only a small amount of low order structure in, say, the expansion wave, then one will not see any advantage of high order schemes. This can easily be seen from the derivative. If one differentiates data that essentially lies on a line, then one is wasting flops if the differentiation operator is designed to approximate any polynomial higher than a line.

2.1 The Role of AMR

Adaptive Mesh Refinement schemes can reduce work in a computation when the flow variables contain structure that is localized in a small fraction of the computational domain throughout the duration of the computation. If a significant fraction of the domain is filled with structure, then it is not cost effective for adaptive gridding and a uniform grid calculation is preferable. AMR can be a good approach when this criteria is met. Exact estimates of what constitutes a small fraction of the domain for various orders of AMR is discussed in [14].

2.2 The Value of Convergence Tests

Numerical calculations are discrete versions of continuous systems. As the number of degrees of freedom increases, this discrete version must approach

the continuous system it is intended to model. A poorly designed scheme, however, might diverge, or even worse, it might converge to the wrong answer. Thus, a first necessary, though not sufficient condition, is that a numerical calculation converge. Of course, in general we will not have an exact solution, but at least the distance between solutions should decrease as the grid is refined:

$$|solution(N) - solution(2N)| > |solution(2N) - solution(4N)|, \qquad (11)$$

where $solution(N)$ denotes the values of one of the flow variables when there are N grid points in the domain, and $|f|$ denotes a suitable distance measure.

If the calculation converges, then one accepts the calculation at the finest grid point density as the "solution". Without convergence there is no clear concept of what the "solution" is and the calculation does not yield reliable information.

2.3 Suitable Test Problems

Here we outline test problems that will yield conclusive information on the value of high order schemes. First of all, for non-linear hyperbolic systems, the derivative is the key numerical operation.

2.3.1 Linear Convection

So, in order to isolate this operation we first suggest,

$$U_t = U_x, \qquad (12)$$

with periodic boundary conditions and with a given single mode as the initial condition:

$$U(x, 0) = \sin(kx). \qquad (13)$$

This equation is simple and perfect for seeing the value of high order schemes. However, some might insist it is of no value because it is not non-linear. But, if one writes the Euler equations in characteristic variables, and one looks at the local linearization of this system, then along each eigenvector of the linearized system, one obtains linear convection. Hence, this simple equation is an essential and *necessary* first test problem. If one's scheme does not perform well on this problem, then there is no need to go further.

2.3.2 Burgers' Equation

Ok, then the second suggestion is Burgers' equation,

$$U_t = (U^2)_x + \epsilon U_{xx}, \tag{14}$$

with period boundary conditions and an initial condition that is a sine wave shifted up in order to produce a moving shock,

$$U(x, 0) = 1/3 + 2/3 * \sin(x). \tag{15}$$

This equation has an exact solution and one can even obtain a shock by setting $\epsilon = 0$. The two equations alone are sufficient to obtain conclusive evidence of the value of high order schemes. Once one starts testing schemes on calculations that do not have exact solutions, then it becomes very difficult to understand what is numerically produced and what is physical.

2.3.3 RM and RT calculations

This is not the regime to test schemes. In other words, the physics is too complicated for one to be able to draw any conclusions about the scheme itself. As stated above, one needs calculations that have exact solutions if one wants to separate the physics from the numerics. RM and RT calculations should be done only *after* one has a clear understand of the numerical issues.

However, if one does attempt to evaluate schemes using these physical setups one should do the following in order to show the advantage of high order schemes. First, the interface between the materials should have many modes on it and not just one. With a single mode the small structure is limited to a small fraction of the domain and does not clearly show the advantage of high order schemes. Second, the calculation should be run for a long time until the domain is almost full. A principle advantage of high order schemes comes with long-time integration as showed by Kreiss and Oliger cited above. Third, the calculation should be physically symmetric. It will be very difficult to decipher numerical artifacts from physical ones, but loss of symmetry will be one clear sign that a scheme has broken down. Finally, convergence tests *must* be done. This final point can not be over emphasized.

3 Conclusion

This document is intended to give a guide to the value of high order schemes and how to clearly show this value. As with physical experiments, if the experiment is not clearly thought out then one will never be able to isolate the phenomenon of interest. Certainly this is true of laser experiments and also of numerical experiments.

In the bibliography many references have been given that illucidate high order schemes.

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