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RICHARDSON EXTRAPOLATION FOR LINEARLY DEGENERATE DISCONTINUITIES*

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Abstract. In this paper we investigate the use of Richardson extrapolation to estimate the convergence rates for numerical solutions to advection problems involving discontinuities. We use modified equation analysis to describe the expectation of the approach. In general, the results do not agree with a-priori estimates of the convergence rates. However, we identify one particular use case where Richardson extrapolation does yield the proper result. We then demonstrate this result using a number of numerical examples.

Key words. Richardson extrapolation, error estimation, convergence analysis, shock capturing

AMS subject classifications. 65M12, 65M08, 65M06

1. Introduction.

Estimating the error in numerical approximations to solutions of partial differential equations is important for many reasons. In order to be useful, numerical simulations should be accurate in some measurable norm. A particular application could require the absolute error to be less than a certain level. Other applications might use an estimate of the numerical error to help guide decisions about the most cost effective way to spend scarce resources, for example to choose between higher resolution simulation, to include more physical processes into the model, or to produce more samples for a statistical analysis. Still other applications may use estimates of the error directly for uncertainty quantification purposes. There are many approaches to error estimation found in the literature. Intrusive techniques such as adjoint error estimators [1, 2], error transport [3, 4], or finite element residual and recovery methods [5] are extremely powerful. However, because they are intrusive they require access and modification of the source code. This is often not possible for theoretical, practical, or sometimes legal reasons.

Non-intrusive techniques are those that require only the ability to produce multiple simulation results, but do not require modifications of the source code. Error estimation through Richardson extrapolation is one commonly used non-intrusive technique and essentially relies on asymptotic properties of numerical approximation. Asymptotically correct in this context refers to the fact that expending a certain amount more work yields a predictable increase in the accuracy of the result. Richardson extrapolation estimates can be based on varying the order of approximation, varying the resolution of the grid, or a combination of both. For many applications Richardson extrapolation has been shown to yield very good results. However, behavior of Richardson extrapolation error estimates for simulations of solutions with jumps, such as shock and contact waves for fluid mechanics, is known to be problematic [6]. There have been many attempts to introduce richer ansatz to deal with these situations, and they have yielded varying degrees of success. However, there has

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been very little progress on understanding the fundamental sensitivity of Richardson extrapolation error estimates in the presence of jumps.

In this paper, we investigate one particular realization of Richardson extrapolation error estimation for the canonical problem of linear advection with jump initial data. This is a particularly simple model problem with relevance to many complex physical models of fluid flow, plasma physics, and more. We build on the previous work of [7] which analyzed convergence rates for approximations for solutions of linear advection where the exact solution contained jumps. That work used modified equations to argue that the expected rate of convergence for a nominally p^{th} order method in the presence of a linear jump discontinuity is $p/(p+1)$. In the current work we use the structure of the modified equation solutions to discuss the expected behavior of Richardson extrapolation error estimates. We show that under certain conditions one can expect to obtain the $p/(p+1)$ rate. In addition, we show why the method can fail to obtain the correct result if these conditions are not met.

The remainder of this paper is structured as follows. Section 2 discusses some preliminaries, and provides a very brief overview of the Richardson extrapolation technique for error estimation. A simple model problem consisting of linear advection of a discontinuity is presented in Section 3. In Section 4 we apply the technique to approximations generated by a first-order upwind method, and discuss the results. The technique is found to be effective for this case, and an analysis explaining this surprising result is presented. That analysis is extended in Section 5 to discuss the case of high-order linear schemes. This analysis reveals that one particular instantiation of Richardson extrapolation produces the expected convergence rate. Section 7 demonstrates the theory for upwind discretizations of order 2, 4, and 6, as well as the case of a high-resolution nonlinear TVD discretization. Additional details of the inner workings are presented for the second-order case. Conclusions are presented in 8.

2. Preliminaries and Richardson extrapolation for smooth problems. Richardson extrapolation is a commonly used technique for error estimation, and many variations exist. For a good overview of the technique refer to [6]. Here we focus on one particular approach to Richardson extrapolation which uses numerical approximations at three grid resolutions obtained using the same numerical technique. Even within this particular flavor of the approach, there are essentially three possible realizations. In this section we review the approach and present the three choices. In what follows, we consider numerical approximations to the solution of a partial differential equation (PDE) on an infinite domain. Boundary conditions are an important aspect of many numerical simulations, but are not critical to the present discussion. Thus consider the spatial domain $x \in (-\infty, \infty)$, and introduce a spatial discretization with uniform grid spacing h.

Consider a set of numerical approximations given by $u_{h_M}(x,t) \approx u_e(x,t)$ where $u_e(x,t)$ is the exact solution, and h_M indicates the size of the mesh. We consider performing an estimate at some time $t = t_f$, and whenever the time argument is not included, it is assumed to imply $t = t_f$ (i.e. $u(x) = u(x, t_f)$). Let an estimated convergence rate be denoted by $\mathcal{R}\left(u_{h_1}, u_{h_2}, u_{h_3}\right)$ where the various u_{h_M} are numerical approximations obtained using grid spacing h_M, and $\mathcal{R}\left(u_1, u_2, u_3\right) = \sigma$ is the solution of the scalar equation $f(\sigma; u_1, u_2, u_3) = 0$, where

$$f(\sigma; u_1, u_2, u_3) = \frac{||u_{h_1}(x) - u_{h_2}(x)||}{||u_{h_2}(x) - u_{h_3}(x)||} - \frac{|h_1^\sigma - h_2^\sigma|}{|h_2^\sigma - h_3^\sigma|}. \tag{2.1}$$

For the purposed of the remainder of this paper we will assume that $||\cdot||$ indicates a discrete approximation to the L_1 norm. This is the norm which is most often considered when discussing hyperbolic equations with discontinuities. For a given set of three numerical approximations, there are essentially three distinct ways that the estimate can be computed $\mathcal{R}\left(u_{h_1}, u_{h_3}, u_{h_2}\right)$, $\mathcal{R}\left(u_{h_1}, u_{h_2}, u_{h_3}\right)$, and $\mathcal{R}\left(u_{h_2}, u_{h_1}, u_{h_3}\right)$. As shown below, this distinction is irrelevant for smooth problems. However, it will become important for solutions with discontinuities. For smooth problems, the basic assumption underlying the approach is that a given numerical approximation $u_{h_M}(x,t)$ is related to the exact solution $u_e(x,t)$ as

$$u_{h_M}(x,t) = u_e(x,t) + c(x,t)h_M^p$$

where p is the formal order of accuracy of the approximation, and $c(x,t)$ is an order one function which is independent of the mesh parameters. For any two resolutions, the difference between approximations is

$$\begin{aligned} u_{h_1}(x) - u_{h_2}(x) &= u_e(x) + c(x)h_1^p - u_e(x) + c(x)h_2^p \\ &= c(x)\left(h_1^p - h_2^p\right). \end{aligned}$$

For any three resolutions then we find that

$$\begin{aligned} \frac{||u_{h_1}(x) - u_{h_2}(x)||}{||u_{h_2}(x) - u_{h_3}(x)||} &= \frac{||c(x)\left(h_1^p - h_2^p\right)||}{||c(x)\left(h_2^p - h_3^p\right)||} \\ &= \frac{||c(x)||\,|h_1^p - h_2^p|}{||c(x)||\,|h_2^p - h_3^p|} \\ &= \frac{|h_1^p - h_2^p|}{|h_2^p - h_3^p|}. \end{aligned} \tag{2.2}$$

Assuming $h_1 \neq h_2 \neq h_3$, Equation (2.2) and its counterparts can easily be used to show that $\mathcal{R}\left(u_{h_1}, u_{h_3}, u_{h_2}\right) = \mathcal{R}\left(u_{h_1}, u_{h_2}, u_{h_3}\right) = \mathcal{R}\left(u_{h_2}, u_{h_1}, u_{h_3}\right) = p$. Note that in principle one can then use the computed convergence rate σ in order to estimate the exact solution and obtain field estimates of the error. Such an approach is presented in detail in [8] and [9]. Also note that there is the possibility multiple roots in (2.1), but this situation is easily recognized in practice and so we do not discuss this further.

3. A model problem with discontinuity. We now seek to understand the nature of Richardson extrapolation error estimation for problems with discontinuities or other self similar behavior. As a model, consider the one dimensional linear advection equation

$$\frac{\partial}{\partial t}u(x,t) + a\frac{\partial}{\partial x}u(x,t) = 0 \tag{3.1}$$

with constant advection velocity $a > 0$. A canonical model problem with discontinuity can be defined using the initial conditions

$$u(x,0) = \begin{cases} u_L & \text{for} \quad x < 0 \\ u_R & \text{for} \quad x \geq 0. \end{cases} \tag{3.2}$$

The method of characteristics is used to define the exact solution for all $t > 0$ as $u(x,t) = u(x - at, 0)$, which applies also to discontinuous solution profiles using the notion of weak solutions [10, 11].

4. First Order Upwind Discretization. As an introductory example, consider the first-order accurate explicit upwind scheme

$$u_i^{n+1} = u_i^n - \lambda \left[u_i^n - u_{i-1}^n \right] \tag{4.1}$$

where u_i^n is a numerical approximation to $u(x_i, t^n)$ and the so called CFL number is $\lambda = \frac{a\Delta t}{h}$. The computational domain $[x_L, x_R]$ is a truncation of the infinite domain, and has been discretized with $x_i = x_L + ih$ where $h = (x_R - x_L)/(N-1)$ and N an integer. Similarly, time has been discretized as $t_n = n\Delta t$ with initial conditions $u(x, 0)$ being given at $t = 0$. Numerical stability is obtained for $\lambda \leq 1$.

4.1. Richardson extrapolation error estimation. One can perform an estimate of the convergence rate using Richardson extrapolation and simply ignore the fact that the assumptions underlying the approach are not strictly valid for cases with discontinuities. We set $a = 1$, choose a computational domain with $[x_L, x_R] = [-\pi, \pi]$, integrate to a time $t_f = 2$, and use $\lambda = 0.6$. These choices are made to ensure that the discontinuity never lies on a cell boundary which can be problematic if finite-precision arithmetic leads to a jump in the initial discontinuity location during the refinement process. A series of approximations is generated using a uniform refinement process with a ratio $0 \geq r < 1$ (i.e. $h_2 = rh_1$ and $h_3 = r^2 h_1$), and starts with 51201 points in the domain (i.e. $h_1 = \frac{2\pi}{51200}$). Table 4.1 shows the results using the three basic variants of Richardson extrapolation, and various choices of the uniform refinement ration r. The table makes clear that the estimated convergence rate is 0.5 for any choice, which agrees exactly with the expected convergence rate for a first-order scheme with a linear jump [7].

r	$\mathcal{R}\left(u_{h_1}, u_{rh_1}, u_{r^2h_1}\right)$	$\mathcal{R}\left(u_{h_1}, u_{r^2h_1}, u_{rh_1}\right)$	$\mathcal{R}\left(u_{rh_1}, u_{h_1}, u_{r^2h_1}\right)$
$\frac{1}{2}$	0.50	0.50	0.50
$\frac{2}{5}$	0.50	0.50	0.50
$\frac{1}{3}$	0.50	0.50	0.50
$\frac{2}{7}$	0.50	0.50	0.50
$\frac{1}{4}$	0.50	0.50	0.50

TABLE 4.1

Estimated convergence rates for the first-order upwind scheme for a solution with a discontinuity. The base resolution uses 51201 *points, and uniform refinement is carried out using a ratio of* r*. Results using the three independent variants of Richardson extrapolation are presented in the various columns.*

4.2. Explanation of the result. The fact that Richardson extrapolation seems to work, in terms of convergence rate estimates, for the first order upwind scheme even with a discontinuous solution is surprising. In order to understand this result we extend the analysis in [7]. The approach makes use of modified equation for a more complete understanding of the behavior. The modified equation is a continuous PDE whose solution describes the approximate behavior of the well resolved components of the discrete solutions, and is derived by substituting continuous functions $U(x, t)$ into the discrete equation (4.1) by setting $u_i^n = U(x_i, t^n)$, and expanding all terms in Taylor series about the point $(x, t) = (x_i, t^n)$. For the first-order upwind scheme the result is

$$\frac{\partial}{\partial t}U(x,t) + a\frac{\partial}{\partial x}U(x,t) - \frac{ah}{2}(1-\lambda)\frac{\partial^2}{\partial x^2}U(x,t) + \cdots = 0. \qquad (4.2)$$

Truncating Equation (4.2) yields the advection-diffusion equation

$$\frac{\partial}{\partial t}U(x,t) + a\frac{\partial}{\partial x}U(x,t) - \nu\frac{\partial^2}{\partial x^2}U(x,t) = 0 \qquad (4.3)$$

where $\nu = \frac{ah(1-\lambda)}{2}$. For discontinuous initial data (3.2), $U(x,0) = u_L$ for $x < 0$ and $U(x,0) = u_R$ for $x \geq 0$. The analytic solution to (4.3) for $t > 0$ is then found to be

$$U(x,t) = \frac{u_L + u_R}{2} + \frac{u_R - u_L}{2}\operatorname{erf}\left(\frac{x - at}{\sqrt{4\nu t}}\right) \qquad (4.4)$$

where $\operatorname{erf}(\zeta)$ is the error function

$$\operatorname{erf}(\zeta) = \frac{2}{\pi}\int_0^\zeta e^{-\chi^2}d\chi.$$

For additional details on this derivation refer to [7].

The analysis to follow assumes the use of the L_1 norm and sets $z = x - at_f$, $\delta_1 = \sqrt{4\nu_1 t_f}$ and $\delta_2 = \sqrt{4\nu_2 t_f}$. Furthermore, assume $h_1 > h_2$. As in [7], assume that the solution to the modified equation is an accurate approximation to the numerical solution so $u_h(x,t) = U(x,t)$. Following a similar line of reasoning as in Section 2 gives

$$\begin{aligned}
||u_{h_1}(x) - u_{h_2}(x)|| &= \left|\left|\frac{u_L + u_R}{2} + \frac{u_R - u_L}{2}\operatorname{erf}\left(\frac{z}{\delta_1}\right) - \frac{u_L + u_R}{2} - \frac{u_R - u_L}{2}\operatorname{erf}\left(\frac{z}{\delta_2}\right)\right|\right| \\
&= \int_{-\infty}^{\infty}\left|\frac{u_R - u_L}{2}\left(\operatorname{erf}\left(\frac{z}{\delta_1}\right) - \operatorname{erf}\left(\frac{z}{\delta_2}\right)\right)\right| dz \\
&= |u_R - u_L|\left(\int_0^\infty - \operatorname{erf}\left(\frac{z}{\delta_1}\right) + \operatorname{erf}\left(\frac{z}{\delta_2}\right) dz\right) \\
&= \frac{2\sqrt{at_f}\,|u_R - u_L|}{\sqrt{\pi}}\left(\sqrt{\nu_1} - \sqrt{\nu_2}\right) \\
&= \sqrt{\frac{at_f(1-\lambda)}{2\pi}}\,|u_R - u_L|\left(\sqrt{h_1} - \sqrt{h_2}\right).
\end{aligned}$$

Therefore, under the assumption that the three numerical approximations have been obtained using the same CFL λ, the factor of $\sqrt{\frac{at_f(1-\lambda)}{2\pi}}\,|u_R - u_L|$ will appear in both the numerator and denominator when the ratio of the norms of differences is taken. As a result

$$\frac{||u_{h_1}(x) - u_{h_3}(x)||}{||u_{h_2}(x) - u_{h_3}(x)||} = \frac{\left|\sqrt{h_1} - \sqrt{h_3}\right|}{\left|\sqrt{h_2} - \sqrt{h_3}\right|},$$

and it is easy to verify that all three approaches to Richardson extrapolation will yield convergence at the expected rate of 0.5.

Remark: Although the results presented in Table 4.1 use simulations with uniform refinement, this is not critical in the analysis for this case. In fact, it is primarily the monotone nature of the similarity solution which is responsible for the robust nature of the estimates. Uniform refinement was used in order to match the analysis for high-order schemes below, where uniform refinement is important.

5. Arbitrary Order Linear Scheme. In general, robust results like those represented in Table 4.1 are not expected. In this section we analyze why this is the case and determine a particular strategy which yields accurate estimates even in the presence of discontinuities (or other self-similar features). We restrict our attention to noncompressive stable p^{th} order schemes for advection with modified equations of the form

$$\frac{\partial}{\partial t}U(x,t) + a\frac{\partial}{\partial x}U(x,t) - \eta_h \frac{\partial^{p+1}}{\partial x^{p+1}}U(x,t) + \cdots = 0 \tag{5.1}$$

where $\eta_h = \tilde{\eta} h^p$ and $\tilde{\eta}$ is a constant depending on the CFL λ. Following the analysis in [7], a simple change of variables is performed to translate into a frame of reference traveling with the wave

$$z = x - at$$
$$\tau = t.$$

After dropping the higher order terms, (5.1) becomes

$$\frac{\partial}{\partial \tau}U(z,\tau) - \kappa_h \frac{\partial^{p+1}}{\partial z^{p+1}}U(z,\tau) = 0 \tag{5.2}$$

where κ_h is either plus or minus η_h depending on the value of p. Similarity solutions can be sought with similarity variable

$$\xi_h = \frac{z}{\sqrt[p+1]{\kappa_h t_f}}. \tag{5.3}$$

We again assume that the solution of the modified equation is an accurate representation of the numerical approximation and set $u_h = U$. For jump initial condition (3.2) the solution can then be written in the general form

$$u_h(\xi_h) = \frac{u_L + u_R}{2} + \frac{u_R - u_L}{2}S(\xi_h). \tag{5.4}$$

where S is an approximation to the jump from -1 to 1 (similar to an error function but perhaps with more complex behavior). In general, S will take the form of generalized hypergeometric functions which oscillate on one or both sides of the discontinuity. In a Richardson style error estimate, norms of the difference between two solutions will be used, and so we write

$$\begin{aligned}
||u_{h_1}(x) - u_{h_2}(x)|| &= \left|\left| \frac{u_L + u_R}{2} + \frac{u_R - u_L}{2}S(\xi_{h_1}) - \frac{u_L + u_R}{2} - \frac{u_R - u_L}{2}S(\xi_{h_2}) \right|\right| \\
&= \frac{|u_R - u_L|}{2} \int_{-\infty}^{\infty} \left| S\left(\frac{z}{\sqrt[p+1]{\kappa_{h_1} t_f}}\right) - S\left(\frac{z}{\sqrt[p+1]{\kappa_{h_2} t_f}}\right) \right| dz
\end{aligned}$$

Making the change of variables to

$$\chi = \frac{z}{\sqrt[p+1]{\kappa_{h_1} t_f}} \tag{5.5}$$

gives

$$||u_{h_1}(x) - u_{h_2}(x)|| = |u_R - u_L| \sqrt[p+1]{\kappa_{h_1} t_f} \int_{-\infty}^{\infty} \left| S(\chi) - S\left(\chi \sqrt[p+1]{\frac{h_1}{h_2}}\right) \right| d\chi. \tag{5.6}$$

Now take the ratio of such norms to arrive at

$$\frac{||u_{h_1}(x) - u_{h_2}(x)||}{||u_{h_2}(x) - u_{h_3}(x)||} = \left(\frac{h_1}{h_2}\right)^{\frac{p}{p+1}} \frac{\int_{-\infty}^{\infty} \left|S(\chi) - S\left(\chi \sqrt[p+1]{\frac{h_1}{h_2}}\right)\right| d\chi}{\int_{-\infty}^{\infty} \left|S(\chi) - S\left(\chi \sqrt[p+1]{\frac{h_2}{h_3}}\right)\right| d\chi}. \tag{5.7}$$

In general therefore, the Richardson estimate will depend on the ratio of integrals of scaled similarity functions

$$\frac{\int_{-\infty}^{\infty} \left|S(\chi) - S\left(\chi \sqrt[p+1]{\frac{h_1}{h_2}}\right)\right| d\chi}{\int_{-\infty}^{\infty} \left|S(\chi) - S\left(\chi \sqrt[p+1]{\frac{h_2}{h_3}}\right)\right| d\chi}. \tag{5.8}$$

The function S can be an extremely complex object, and so computing this ratio in closed form is in general impractical. In fact, the definition of S is often found to make this ratio difficult to even estimate numerically due to ill-conditioning and finite precision arithmetic. However, for the case of uniform refinement when $h_3 = rh_2 = r^2h_1$, this ratio is simply unity. Therefore, for this special case, the estimated convergence rate will be given by $\mathcal{R}(u_{h_1}, u_{rh_1}, u_{r^2h_1}) = \frac{p}{p+1}$. This is the expected convergence rate as discussed in [7]. Notice that such cancelation requires both uniform refinement, and that the estimate be performed using differences of successive refinement. Other choices will in general not yield the rate $\frac{p}{p+1}$.

6. Second Order Linear Scheme. In order to demonstrate the implications of the analysis in Section 5, consider the linear second-order upwind method

$$u_i^{n+1} = u_i^n - \lambda \left[\left(u_i^n + \frac{1}{4}(1-\lambda)(u_{i+1}^n - u_{i-1}^n) \right) - \left(u_{i-1}^n + \frac{1}{4}(1-\lambda)(u_i^n - u_{i-2}^n) \right) \right]. \tag{6.1}$$

This is simply a second order unlimited Godunov method. As before, one can perform an estimate of the convergence rate using Richardson extrapolation. Again we set $a = 1$, choose a computational domain with $[x_L, x_R] = [-\pi, \pi]$, integrate to a time $t_f = 2$, and use $\lambda = 0.6$. The series of approximations is generated using a uniform refinement process with a ratio $0 \geq r < 1$ (i.e. $h_2 = rh_1$ and $h_3 = r^2h_1$), and starts with 51201 points in the domain (i.e. $h_1 = \frac{2\pi}{51200}$). Table 6.1 shows the results

r	$\mathcal{R}\left(u_{h_1}, u_{rh_1}, u_{r^2h_1}\right)$	$\mathcal{R}\left(u_{h_1}, u_{r^2h_1}, u_{rh_1}\right)$	$\mathcal{R}\left(u_{rh_1}, u_{h_1}, u_{r^2h_1}\right)$
$\frac{1}{2}$	0.67	0.14	1.63
$\frac{2}{5}$	0.67	0.22	1.73
$\frac{1}{3}$	0.71	0.38	1.69
$\frac{2}{7}$	0.67	0.41	1.49
$\frac{1}{4}$	0.67	0.47	1.35

TABLE 6.1

Estimated convergence rates for the second-order upwind scheme for a solution with a discontinuity. The base resolution uses 51201 *points, and uniform refinement is carried out using a ration of* r*. Results using the three independent variants of Richardson extrapolation are presented in the various columns.*

using the three basic variants of Richardson extrapolation, and various choices of the

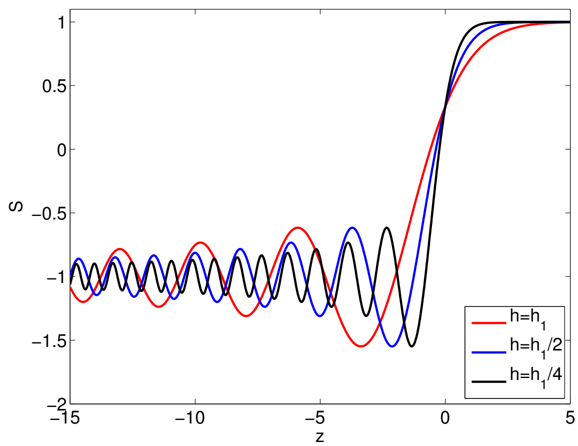

FIG. 6.1. *Similarity jumps for the unlimited second order scheme in the frame of reference moving with the discontinuity.*

uniform refinement ratio r. The table shows that the expected rate of 2/3 is obtained as advertised when using the appropriate approach. Also shown in the table are the type of results that can be experienced if other approaches are used.

6.1. A closer look at this case. In order to more clearly explain what is going on we present additional details for this case. As discussed above in Section 5, the crux of the matter centers around the similarity solution S. For this second-order scheme, the solution can be found as

$$u_h(\xi_h) = \frac{1}{3} - \frac{\xi_h \left(\xi_h \sqrt{3}\left(\Gamma\left(\frac{2}{3}\right)\right)^2 \, {}_1F_2\left(\frac{2}{3}; \frac{4}{3}, \frac{5}{3}; \frac{\xi_h^3}{27}\right) - 4\pi \, {}_1F_2\left(\frac{1}{3}; \frac{2}{3}, \frac{4}{3}; \frac{\xi_h^3}{27}\right)\right)}{6\Gamma\left(\frac{2}{3}\right)\pi} \tag{6.2}$$

where Γ is the Euler Gamma function, and ${}_1F_2$ is a generalized hypergeometric function. Figure 6.1 shows similarity solutions in the reference frame moving with the discontinuity at three resolutions. The grid spacing is essentially a parameter, and so we have chosen a normalization $h_1 = 1$. Solutions with two grid doublings are also shown. Following the analysis in Section 5, differences of the three solutions will be taken. Figure 6.2 shows the three sets of differences which are produced for the three variants of the Richardson extrapolation error estimate. All three plots show the very complex character of the function whose absolute integral is taken. The key observation of this paper is presented in Figure 6.3 where the spatial variable is scaled to the common reference variable χ, as suggested in (5.5). For the case of uniform refinement when the differences are made as suggested, the integrals in the numerator and denominator of (5.8) are identical, and the estimate follows. In this case the method essentially avoids the need to calculate the actual integral and relies on the fact that the ratio is known a-priori for any similarity function.

7. Additional demonstration of the theory. In order to further demonstrate the validity of the theory we have just described, we perform a series of tests for linear schemes of increasing order, as well as a high-resolution nonlinear TVD scheme. The linear schemes we investigate here are upwind biased single step schemes (i.e. in advancing from t^n to t^{n+1} they use data from t^n only) that are high-order accurate

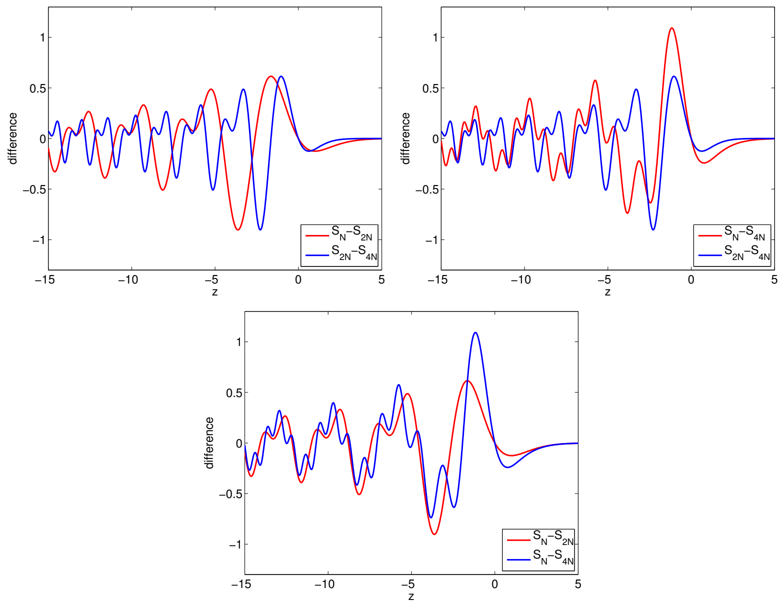

FIG. 6.2. *Differences of similarity jumps in the frame of reference moving with the discontinuity.*

in space and time. Derivation of these schemes follows standard procedures using a Cauchy-Kowalewski process, sometimes called the Lax-Wendroff procedure [12]. Further details on these derivations can be found in [13, 14, 15]. The nonlinear TVD discretization is of the high-resolution Godunov type described in [16, 17].

7.1. Fourth-Order Linear Scheme. Consider the linear fourth-order upwind method

$$u_i^{n+1} = u_i^n + \sum_{s=-3}^{2} C_{4+s}^{(4)} u_{i+s}^n \tag{7.1}$$

where $C^{(4)}$ is a vector of stencil coefficients given by

$$C^{(4)} = \frac{\lambda}{144} \begin{bmatrix} 5 - 8\lambda^2 + 3\lambda^3 \\ -37 - 6\lambda + 52\lambda^2 - 9\lambda^3 \\ 146 + 96\lambda - 104\lambda^2 + 6\lambda^3 \\ -50 - 180\lambda + 80\lambda^2 + 6\lambda^3 \\ -71 + 96\lambda - 16\lambda^2 - 9\lambda^3 \\ 7 - 6\lambda - 4\lambda^2 + 3\lambda^3 \end{bmatrix}.$$

Table 7.1 shows results using the three basic variants of Richardson extrapolation, and various choices of the uniform refinement ration r using (7.1). The first column shows remarkable agreement between the estimated convergence rate and the expected rate of $\frac{p}{p+1} = 0.8$. The other two columns indicate that results which are difficult to interpret can be obtained for other procedures.

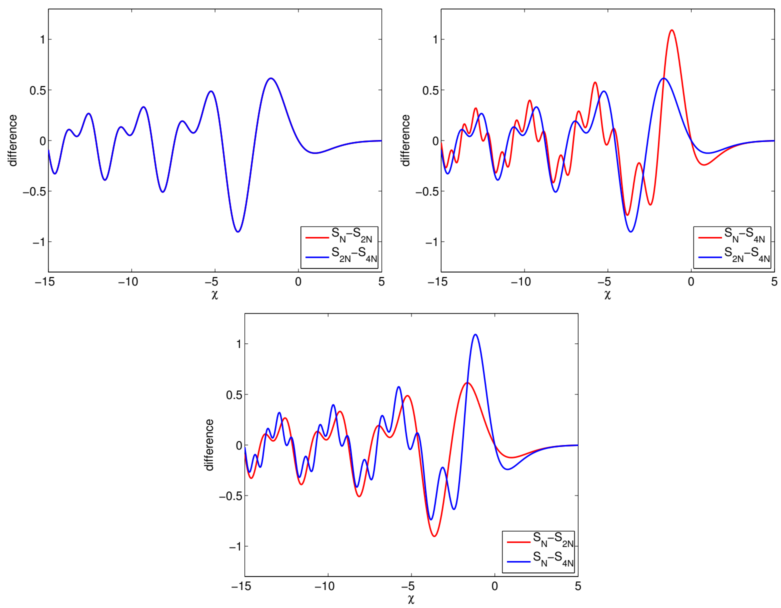

FIG. 6.3. *Differences of similarity jumps in the common scaled reference frame χ (see Equation (5.5) for details). Note that $S_N - S_{2N}$ is nearly identical to $S_2N - S_{4N}$ in the upper left plot and is therefore not visible.*

r	$\mathcal{R}\left(u_{h_1}, u_{rh_1}, u_{r^2h_1}\right)$	$\mathcal{R}\left(u_{h_1}, u_{r^2h_1}, u_{rh_1}\right)$	$\mathcal{R}\left(u_{rh_1}, u_{h_1}, u_{r^2h_1}\right)$
$\frac{1}{2}$	0.86	0.23	2.32
$\frac{2}{5}$	0.83	0.41	2.10
$\frac{1}{3}$	0.83	0.53	1.91
$\frac{2}{7}$	0.84	0.73	1.60
$\frac{1}{4}$	0.85	0.65	1.34

TABLE 7.1

Estimated convergence rates for the fourth-order upwind scheme for a solution with a discontinuity. The base resolution uses 51201 *points, and uniform refinement is carried out using a ratio of r. Results using the three independent variants of Richardson extrapolation are presented in the various columns.*

7.2. Sixth-Order Linear Scheme. Consider the linear sixth-order upwind method

$$u_i^{n+1} = u_i^n + \sum_{s=-4}^{3} C_{5+s}^{(6)} u_{i+s}^n \tag{7.2}$$

where $C^{(6)}$ is a vector of stencil coefficients given by

$$C^{(6)} = \frac{\lambda}{4320}\begin{bmatrix} -31 + 43\lambda^2 - 15\lambda^4 + 3\lambda^5 \\ 289 + 24\lambda - 391\lambda^2 - 30\lambda^3 + 123\lambda^4 - 15\lambda^5 \\ -1299 - 324\lambda + 1623\lambda^2 + 360\lambda^3 - 387\lambda^4 + 27\lambda^5 \\ 4325 + 3240\lambda - 2675\lambda^2 - 1170\lambda^3 + 615\lambda^4 - 15\lambda^5 \\ -1085 - 5880\lambda + 1505\lambda^2 + 1680\lambda^3 - 525\lambda^4 - 15\lambda^5 \\ -2589 + 3240\lambda + 267\lambda^2 - 1170\lambda^3 + 225\lambda^4 + 27\lambda^5 \\ 431 - 324\lambda - 419\lambda^2 + 360\lambda^3 - 33\lambda^4 - 15\lambda^5 \\ -41 + 24\lambda + 47\lambda^2 - 30\lambda^3 - 3\lambda^4 + 3\lambda^5 \end{bmatrix}.$$

Table 7.2 shows results using the three basic variants of Richardson extrapolation, and various choices of the uniform refinement ration r using (7.2). The first column again shows remarkable agreement between the estimated convergence rate and the expected rate of $\frac{p}{p+1} = 0.86$. The other two columns indicate that results which are difficult to interpret can be obtained for other procedures.

r	$\mathcal{R}\left(u_{h_1}, u_{rh_1}, u_{r^2h_1}\right)$	$\mathcal{R}\left(u_{h_1}, u_{r^2h_1}, u_{rh_1}\right)$	$\mathcal{R}\left(u_{rh_1}, u_{h_1}, u_{r^2h_1}\right)$
$\frac{1}{2}$	0.90	0.16	2.95
$\frac{2}{5}$	0.90	0.47	2.35
$\frac{1}{3}$	0.88	0.60	1.93
$\frac{2}{7}$	0.88	0.78	1.20
$\frac{1}{4}$	0.90	0.83	1.24

TABLE 7.2

Estimated convergence rates for the sixth-order upwind scheme for a solution with a discontinuity. The base resolution uses 51201 *points, and uniform refinement is carried out using a ratio of r. Results using the three independent variants of Richardson extrapolation are presented in the various columns.*

7.3. Second Order Nonlinear Scheme. Finally, we consider a high-resolution TVD limited scheme. The scheme is a second-order MUSCLE type scheme using a MinMod limiter applied to the slopes. The scheme can be written

$$u_i^{n+1} = u_i^n - \lambda\left[\left(u_i^n + \frac{1}{2}(1-\lambda)\alpha\right) - \left(u_{i-1}^n + \frac{1}{2}(1-\lambda)\beta\right)\right]. \tag{7.3}$$

where

$$\alpha = \mathrm{MinMod}(u_{i+1}^n - u_i^n, u_i^n - u_{i-1}^n),$$

$$\beta = \mathrm{MinMod}(u_i^n - u_{i-1}^n, u_{i-1}^n - u_{i-2}^n),$$

and

$$\mathrm{MinMod}(b,c) = \begin{cases} b & \text{if} \quad |b| < |c| \text{ and } bc > 0 \\ c & \text{if} \quad |b| \geq |c| \text{ and } bc > 0 \\ 0 & \text{if} \quad bc \leq 0. \end{cases}$$

Note that this is nothing more than a high-resolution Godunov method (see [16, 17] for details). Table 7.3 shows the results for the three variants of Richardson extrapolation convergence estimation. The results in [7] established that although this scheme is nonlinear, the modified equation has solutions of the form (5.4). Therefore, the analysis still applies to this case, and the method is expected to yield accurate estimates of the convergence rates for uniform refinement case $\mathcal{R}\left(u_{h_1}, u_{rh_1}, u_{r^2h_1}\right)$. The

r	$\mathcal{R}\left(u_{h_1}, u_{rh_1}, u_{r^2h_1}\right)$	$\mathcal{R}\left(u_{h_1}, u_{r^2h_1}, u_{rh_1}\right)$	$\mathcal{R}\left(u_{rh_1}, u_{h_1}, u_{r^2h_1}\right)$
$\frac{1}{2}$	0.48	0.48	0.48
$\frac{2}{5}$	0.55	0.55	0.56
$\frac{1}{3}$	0.57	0.57	0.57
$\frac{2}{7}$	0.57	0.57	0.57
$\frac{1}{4}$	0.60	0.59	0.60

TABLE 7.3

Estimated convergence rates for the high-resolution TVD scheme for a solution with a discontinuity. The base resolution uses 51201 *points, and uniform refinement is carried out using a ratio of* r. *Results using the three independent variants of Richardson extrapolation are presented in the various columns.*

results in Table 7.3 show this to be true, but interestingly the other two estimates, $\mathcal{R}\left(u_{h_1}, u_{r^2h_1}, u_{rh_1}\right)$ and $\mathcal{R}\left(u_{rh_1}, u_{h_1}, u_{r^2h_1}\right)$, also appear accurate. This is not in contradiction with the theory which says that the estimate $\mathcal{R}\left(u_{h_1}, u_{rh_1}, u_{r^2h_1}\right)$ will be accurate but not that the others will be inaccurate. In fact this is a similar result to those results for the first-order scheme in Table 4.1. As was the case for the first-order discretization, this fortuitous behavior can be traced to the monotonicity of the approximations.

8. Conclusions. We have provided an in depth investigation of Richardson extrapolation error estimation for linear advection of a discontinuity. The analysis uses the solution to the modified equation to elucidate the difficulty found in practice. However, the analysis also reveals one particular realization of the technique that reproduces the a-priori convergence rates even in the presence of a discontinuity or other similarity type behavior. The key elements are found to be the use of uniform refinement, and that the comparisons inherent in the Richardson estimator be performed in one specific manner. This result was demonstrated for a number of discretizations ranging in order from first-order to sixth-order. In addition, results were also presented for a high-resolution TVD scheme.

Future work will include investigating the techniques discussed here for nonlinear equations (such as the Euler equations), as well as the extension to higher spatial dimension. Other interesting avenues for future investigation are looking into similarity behavior of differing degrees of smoothness, as well parabolic problems or dispersive wave propagation.

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