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1. INTRODUCTION

The discretization of differential equations is often done on irregular gnds in an attempt to concentrate points where the solution is most rapidly changing. Perhaps the reason is to improve the accuracy of the approximate solution or to illuminate regions where the solution is most interesting. In any case, many authors have noted that the order of the truncation error associated with finite differences defined on irregular gnds is less than those defined on uniform ones. For example, the second-divided difference has truncation error.

$$D_{2}u = \frac{2u(x_{i-1})}{\Delta_{i+12}(\Delta_{i+12} + \Delta_{i-12})} - \frac{2u(x_{i-1})}{\Delta_{i+12}\Delta_{i-12}} + \frac{2u(x_{i-1})}{\Delta_{i-12}(\Delta_{i+12} + \Delta_{i-12})}$$

$$= u''(x_{i}) + \frac{1}{3}(\Delta_{i+12} - \Delta_{i-12})u'''(x_{i}) + O(\Delta^{2}),$$
(1.11)

which is clearly $O(\Delta)$ on an even moderately irregular gnd. Below, we sketch the standard convergence proof for a finite difference approximation.

$$L_{h} v = F_{-}, \tag{1.2}$$

0

to a differential equation (and associated boundary conditions).

$$I.u(x,t) = f$$

The truncation error, this defined by applying the difference operator to the exact solution.

$$L_h u = F + \tau \tag{1}$$

An equation for the error, $e = u - v_0$ is found by subtracting (1.2) from (1.3),

$$L_h(u+v) = L_h e = \tau \tag{1.44}$$

^{*} This work was done under the anapiers of the U.S. Department of Anergy under Continue No. W. (405) I-NG 36:

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$$||L_{\mathbf{A}}^{-1}|| \leq C$$

Thus, if the difference scheme is stable, we get the usual result,

$$||e|| \le C ||t| \tag{1.5}$$

This result gives rise to the rule of thumb t_{id} the approximate solution, v, converges to the exact solution, u, at the same rate that the truncation error converges to zero

Coupling this rule of thumb with (1.1), it is often thought that the accuracy of a finite difference scheme employing the second divided difference must be degraded on an irregular gnd. A number of remedies have been suggested to circumivent this apparent loss of accuracy—use of quasi-regular gnds where the mesh sizes change by $O(\Delta^2)$. Hoffman [11, use of smooth mesh transformations to define a new difference equation on a regular gnd. White [2], solution of the differential equations rewritten as a first order system Keller [3], and use of implicit difference approximations. Doedel [4]

However, in recent work on ordinary differential equations Manteuffel and White [5], Kreiss et al. [6], it has been shown that, in some cases, this apparent loss of accuracy is an artifact of the standard convergence proof and may not actually occur. The following simple example shows how this might happen. The difference equations:

$$v_c = A$$
, $\frac{v_i - v_{i-1}}{4\pi(\Delta_{i+2} + \Delta_{i+2})} + f(x_i) = 0$, $i = 1, 2, ...$ (1.6)

where $\Delta_{i+1} = x_{i+1} - x_i$, are an approximation to

$$u(0) = A$$
, $\frac{du}{dx} + f(x) = 0$ (1.7)

The truncation error is easily seen to be

$$\tau_{i} = -\frac{\Delta_{i+1} - \Delta_{i+1}}{\Delta_{i+1} + \Delta_{i+1}} u'(x_{i}) + O(\Delta t), \qquad (1.8)$$

and, thus, the difference approximation (1.6) is inconsistent with the differential equation (1.7)

However, before we abandon this scheme, let us take a closer look at the error. Recalling (1.4) and rewriting the truncation error, (1.8), ignoring terms which are $O(\Delta)$, we get the following difference equations for the error, \mathcal{E} , caused by the inconsistent term in (1.8).

$$\frac{\mathbf{d}_i - \mathbf{d}_{i-1}}{d\sigma(\Delta_{i+1} + \Delta_{i-1})} = \frac{\mathbf{g}_i - \mathbf{g}_{i-1}}{d\sigma(\Delta_{i+1} + \Delta_{i-1})} = \mathbf{f}_i + O(\Delta_{i-1} + \Delta_{i-1}) \tag{1.9a}$$

where

$$g_{i} = -\frac{1}{2} \Delta_{i+1} u'(x_{i+1})$$
 (1.9b)

$$\ell_1 = R_1 = O(\Delta)$$

Thus, the error, \mathcal{E} , due to the leading order term in (1.8) is really $O(\Delta)$, not O(1) as we might have supposed from the truncation error

In a more general setting, which will be the template for what follows in the remaining sections, the error equation on an irregular grid might be written as

$$L_h e = \tau_1 + \tau_2 \quad . \tag{1.10}$$

where t₁ is that part of the truncation error explicitly caused by the irregular grid and

$$\tau_1 = O(\Delta^{p-1}), \ \tau_2 = O(\Delta^p)$$

If we can rewrite to in the following way,

$$\mathbf{T}_1 = L_h \mathcal{E} + O(\Delta^p) \quad , \quad \mathcal{E} = O(\Delta^p) \quad , \tag{1.111}$$

as in (1.9a), then (1.10) becomes

$$L_h(e - e) = \tau_2 + O(\Delta^r) \approx \tau_2 \tag{1.12}$$

At this point, the usual convergence proof can be employed to get

$$||e - e|| \le C ||\tau_1||$$

and since both \tilde{c} and $\tilde{\tau}_2$ are $O(\Delta^p)$, we have

$$\|\mathbf{u} - \mathbf{v}\| = O(\Delta^p)$$
.

The key, of course, is being able to satisfy (1.11). In Section 2, we will examine two 'upwind' difference schemes discussed in Pike [7] for approximating the solution of the scalar wave equation on an irregular, but Cartesian product grid. In Section 3, we will illustrate the difficulties that arise from a mesh allowed to move irregularly in time, by approximating the solution of a simple heat equation on such a grid. In Section 4, we will make some brief comments on this work.

2. HYPERBOLIC EQUATIONS ON PRODUCT GRIDS

In this section, we will examine (using hyperbolic equations as a vehicle) the error analysis of difference schemes on product grids. In particular, we will look at (x,t) grids of the form

$$(x_j^k, t_j^k) = (x_j, t^k)$$
 (2.11)

that is, the gnd is a product of two, one dimensional, irregular grids. For a different approach to this problem, see, for example Orszag and Jayne [8] or Chin [9]. Pike [7] has noted that although an upwind difference scheme for

$$c \frac{\partial u}{\partial x} + \frac{\partial u}{\partial t} = 0 \tag{2.21}$$

with first order truncation error is easily found, the scheme is not conservative. He then derives a conservative scheme for (2.2), namely

$$L_{ww} v = c \frac{v_i^k - v_{i-1}^k}{\frac{1}{2}(\Delta_{i+1/2} + \Delta_{i-1/2})} + \frac{v_i^{k+1} - v_i^k}{\Delta T} = 0 , \qquad (2.31)$$

but notes that the truncation error is O(1) on an irregular grid. However, computation with these two schemes leads to the observation that algorithm (2.3) yields solutions "similar in quality to the first-order accurate nonconservative solution." In what follows, we will show that this remark is in fact correct, that algorithm (2.3) is first-order accurate.

Calculating the truncation error for (2.3) yields the error equation.

$$L_{\text{Min}} e = \tau_{\text{Min}} = -c \frac{\Delta_{i-1} - \Delta_i}{\Delta_{i+1} + \Delta_i} u_x(x_i, t^k) + O(\Delta) , \qquad (2.4)$$

where $O(\Delta)$ here refers to terms both in Δx and ΔT . We note that the leading order term in (2.4) is due entirely to the spatial difference in (2.3). In fact, the upwind algorithm (2.3) is precisely the same as (1.6) considered in the introduction, with a time difference replacing $f(x_i)$. Equations (1.9a.b) yield the identity,

$$\tau_{\mu\nu} = e^{-i\frac{\vec{e}_{\perp}^{k} - \vec{e}_{\perp}^{k}}{i_{1}(\Delta_{\perp}, r_{2} + \Delta_{\perp}, r_{2})}} + O(\Delta) \quad . \tag{2.5a}$$

$$\bar{\mathcal{E}}_{i}^{k} = -\frac{1}{2} \Delta_{i+1} u_{i} \left(\lambda_{i+1} u_{i} \left(\lambda_{i+1} u_{i} \right) T^{k} \right) \tag{2.5b}$$

We also note that, because we are on a product gnd where each spatial mesh is the same.

$$\frac{|\vec{c}_{i}^{k+1} - \vec{c}_{i}^{k}|}{\Delta T} = -\frac{1}{2} |\Delta_{i+1/2}| \frac{|u_{x}(x_{i+1/2}, t^{k+1}) - u_{x}(x_{i+1/2}, t^{k})|}{\Delta T}| = O(\Delta)$$
 (2.6)

provided the solution is sufficiently smooth. Combining (2.5a) and (2.6), we can rewrite the error equation (2.4) as in (1.12). That is,

$$L_{un}(e - \mathcal{E}) = O(\Delta) . \tag{2.7}$$

where \mathcal{E} is defined in (2.5b) and is clearly $O(\Delta)$

Thus, we have shown that if the solution of (2.2) is sufficiently smooth and if the difference scheme (2.3) is stable, then

$$v_i^k = u\left(x_i\,d^k\right) + \frac{1}{2}\,\Delta_{i+i_2}u_i\left(x_{i+i_2},t^k\right) + O\left(\Delta\right)$$

That is, in spite of the zero order (inconsistent) truncation error, the approximate solutions, v_i^k , are first order accurate.

Let's briefly consider the solution of the nonlinear wave equation,

$$\frac{\partial f(u)}{\partial x} + \frac{\partial u}{\partial t} + 0$$
.

via the upwind difference scheme,

$$N_{\text{ath}}(v) = \frac{f(v_i^k) - f(v_{i-1}^k)}{\frac{1}{2}(\Delta_i \omega_2 + \Delta_{i-1} \omega_2)} + \frac{v_i^{k+1} - v_i^k}{\Delta T} = 0.$$
 (2.8)

The truncation error is derived as before by replacing v_i^k with $u(x_i, t^k)$,

$$N_{uw}(u) = -\frac{\frac{1}{2}\Delta_{1+\frac{1}{2}} - \frac{1}{2}\Delta_{1-\frac{1}{2}}}{\frac{1}{2}(\Delta_{1+\frac{1}{2}} + \Delta_{1-\frac{1}{2}})} \frac{\partial u_{1}^{k}}{\partial z} \frac{\partial f(u_{1}^{k})}{\partial u} + O(\Delta) .$$

However, just as in the linear case, the leading order term in the truncation error can be readily incorporated into the nonlinear operator,

$$N_{\rm int}(\bar{u}) = O(\Delta) \quad . \tag{2.92}$$

where

$$u_i^k = u_i^k + \frac{1}{2} \Delta_{i+1} + \frac{\partial u_{i+1}^{k}}{\partial x} = \frac{\partial u_{i+1}^{k}}{\partial x}$$
 (2.45)

Now, combining (2.8) with the modified truncation error expression (2.9a,b) will yield sharp error estimates for the nonlinear problem.

3 PARABOLIC EQUATIONS ON NONPRODUCT GRIDS

In this section, we will be primarily concerned with the solution of the inhomogeneous heat equation in one-spatial dimension,

$$\frac{\partial u}{\partial t} - \kappa \frac{\partial^2 u}{\partial x^2} = f(x,t) . \tag{3.1}$$

The additional complexity will come from allowing the spatial grid points to move in time. We note in passing that if the mesh trajectories are smooth functions of t, then we can transform to a new coordinate system and derive difference schemes in the new coordinates on a product grid. Thus, we will allow the mesh motion to be irregular.

In Maliteuffel and White [5], it was shown that the truncation error for the second-divided difference (sec. (1-1)), can be written as

$$D_2 u_i = u_i'' + D_2 g_i + O(\Delta^2)$$

where $g_i = \frac{1}{6} \sum_{l=1}^{4} \Delta_i^{3/4} u'''(x_{l-1/2}) = O(\Delta^2)$. With this in hand, let's look for a moment at a Crank

Nicholson type scheme defined on a product grid,

$$L_{CK}v = \frac{v_i^k - v_i^{k-1}}{\Delta T} - \kappa \frac{1}{2} [D_2 v_i^k + D_2 v_i^{k-1}] = f$$
 (5.3)

Everything in (3.3) is centered about $\frac{1}{2}(t^k + t^{k-1})$, so the only terms in the truncation error which are not $O(\Delta^2)$ are those associated with the irregular x-grid. Recalling (3.2), we have

$$\frac{u_i^k - u_i^{k-1}}{\Delta T} - \kappa \cdot \frac{1}{2} \left[D_2(u_i^k - g_i^k) + D_2(u_i^{k-1} - g_i^{k-1}) \right] = f + O(\Delta^2)$$
 (5.4)

Because the x-grid does not change in time, the t-difference just passes through the grid information, yielding

$$\frac{g_i^k - g_i^{k-1}}{\Delta T} = \frac{1}{6} \sum_{l=1}^{i} \Delta_{l-l/2}^{3} \left[\frac{u_{xxx}(x_{l-l/2}, t^k) - u_{xxx}(x_{l-l/2}, t^{k-1})}{\Delta T} \right]$$

and if u(x,r) is sufficiently smooth then

$$\frac{g_i^k - g_i^{k-1}}{\Delta T} = O(\Delta^2) \tag{3.5}$$

With (3.5) in hand,

$$L_{CN}(u_t^k - g_t^k) = f + O(\Delta^2) . {3.6}$$

Once again, employing (3.3) and (3.6), the standard convergence proof will yield a sharp error estimate for (3.3) defined on a product grid.

Unfortunately, when the x-grid is allowed to move, (3.5) is no longer true unless some restrictions are placed on the mesh movement. Recalling the definition of g_i and for simplicity assuming that $u_{xxx}(x_i t) = 6$, we have

$$\frac{g_{i}^{k} - g_{i}^{k-1}}{\Delta T} = \sum_{l=1}^{i} \left[\frac{(\Delta_{l-l/2}^{k})^{3} - (\Delta_{i-l/2}^{k-1})^{3}}{\Delta T} \right]$$
(3.7)

In order for the argument to work as before, we need to show that this time difference is $O(\Delta^2)$. A sufficient condition is

$$\frac{\Delta x_{i+1_2}^k - \Delta x_{i+1_2}^{k-1}}{\Delta T} = O(\Delta T) . {(3.8)}$$

which is roughly equivalent to saying that x, lies in the dotted, funnel-shaped region in Figure 3.1.

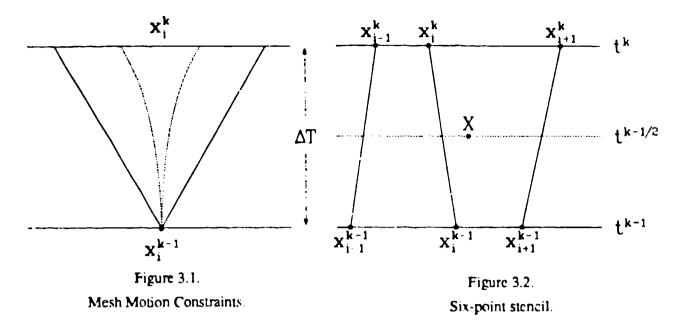
In Levermore, Manteuffel, and White [10], it is shown that Crank-Nicholson-like schemes can be derived which retain their second-order accuracy on meshes with the property that

$$\mathbf{x}_{i}^{k} = \mathbf{x}_{i}^{k-1} + O\left(\Delta T\right) \tag{3.9}$$

This condition requires that x_i^k approach x_i^{k-1} in the V-shaped region in Figure 3.1, is less restrictive than (3.8), and more reasonable.

A family of difference schemes depending on the point, (X, t^{k+l_2}) , at which the function, f(x, t), is evaluated, is considered in Levermore et al. [10]. The stelled of interest for the (i, k)-th equation is shown in Figure 3.2.

We will compare the computational order of convergence of one of these schemes $(X = \frac{1}{2}(x_i^{k+1} + x_i^k))$ which has first-order truncation error with another scheme whose truncation error happens to be $O(\Delta^2)$.



The easiest way to display the difference scheme is as a first-order system, employing the definition,

$$w_{i+l_2}^k = \frac{v_{i+1}^k - v_i^k}{\Delta_{i+l_2}^k} \tag{3.10a}$$

With (3.10a) in hand, the approximation to (3.1) is given by

$$\frac{v_{1}^{k} - v_{1}^{k-1}}{\Delta T} - \kappa \left\{ \frac{w_{1+l/2}^{k} - w_{1-l/2}^{k}}{\Delta_{l+l/2}^{k} + \Delta_{1-l/2}^{k}} + \frac{w_{1+l/2}^{k-1} - w_{1-l/2}^{k-1}}{\Delta_{1+l/2}^{k-1} + \Delta_{1-l/2}^{k-1}} \right\}
+ \frac{x_{1}^{k} - x_{1}^{k-1}}{\Delta T} \left\{ \frac{(x_{1-l/2}^{k} - X) w_{1+l/2}^{k} - (x_{1+l/2}^{k} - X) w_{1-l/2}^{k}}{\Delta_{1+l/2}^{k} + \Delta_{1-l/2}^{k}} + \frac{(x_{1-l/2}^{k-1} - X) w_{1+l/2}^{k-1} - (x_{1+l/2}^{k-1} - X) w_{1-l/2}^{k-1}}{\Delta_{1+l/2}^{k-1} + \Delta_{1-l/2}^{k-1}} \right\} = f(X, t^{k+l/2}) .$$
(3.10b)

where
$$X = \frac{1}{2} (x_i^k + x_i^{k-1})$$
 and $x_{i+2}^{k-1} = \frac{1}{2} (x_{i+1}^{k-1} + x_i^{k-1})$.

In the following two figures, we display the results of approximating an equation of the form (3.1) on a sequence of irregular grids. Each point shows the maximum error versus maximum mesh size on a different mesh. Each mesh had a uniform t-rash ($\Delta T = \text{constant} = \frac{1}{N}$) and N x-grid points chosen to satisfy (3.9). That is, given a grid point, x_i^{k-1} , at t^{k-1} , the new grid point, x_i^k , was chosen at random in the allowable interval (see V-shaped region in Figure 3.1). Once all grid points at t^k were chosen, they were sorted to prevent grid lines from crossing.

Figure 3.3 shows the accuracy of the scheme given by (3.10a,b), whose truncation error is $O(\Delta)$. The least-squares fit to this scattered data (slope of line, 2.713) indicates that the approximate solutions are $O(\Delta^2)$. For comparison, in Figure 3.4, we show the accuracy of a difference scheme which has $O(\Delta^2)$ truncation error. There is no qualitative difference between these two figures, which lends credence to the claim that, although the truncation error of (3.10a,b) is $O(\Delta)$, the approximate solutions retain $O(\Delta^2)$ accuracy even on an irregular, nonproduct grid.

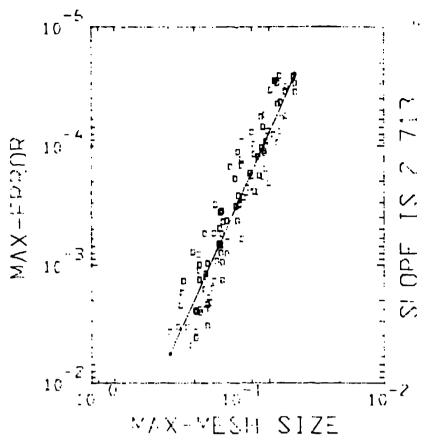
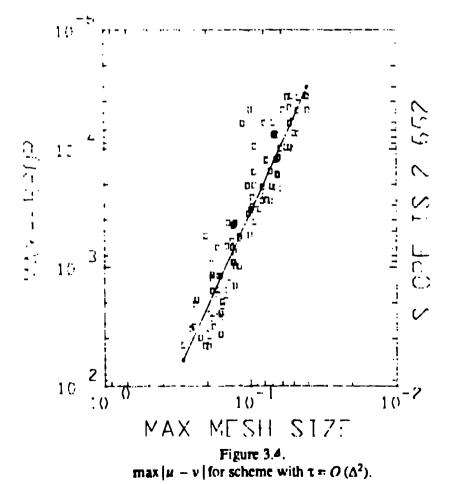


Figure 3.3. $\max |u - v|$ for scheme with $\tau = O(\Delta)$.



4. REMARKS

The truncation error associated with a finite difference scheme is often of lower order on an irregular grid than on a uniform (or smoothly varying) one. This fact gives rise to the feeling that the accuracy of the discrete solutions are likewise degraded. Fortunately, this is not always true. In fact, many schemes retain the same rate of convergence as on a uniform grid. Unfortunately, this is not always true either, as seen in Kreiss et al. [6] for the Numerov scheme.

Throughout this work, we have made several assuraptions. First, we relied on smooth exact solutions, so the efficacy of these results for problems with shocks or contact discontinuities is in question. Second, throughout, we assumed that the difference schemes examined were stable in the usual sense. This is often very difficult to prove for irregular grids. Third, we have ignored boundary conditions altogether, assuming that they can be approximated appropriately.

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NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS ON IRREGULAR GRIDS*

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1. INTRODUCTION

The discretization of differential equations is often done on irregular grids in an attempt to concentrate points where the solution is most rapidly changing. Perhaps the reason is to improve the accuracy of the approximate solution or to illuminate regions where the solution is most interesting. In any case, many authors have noted that the order of the truncation error associated with finite differences defined on irregular grids is less than those defined on uniform ones. For example, the second-divided difference has truncation error.

$$D_{2}u = \frac{2u(x_{i+1})}{\Delta_{i} + i_{2}(\Delta_{i} + i_{2} + \Delta_{i} - i_{2})} - \frac{2u(x_{i})}{\Delta_{i} + i_{2}\Delta_{i} - i_{2}} + \frac{2u(x_{i-1})}{\Delta_{i} - i_{2}(\Delta_{i} + i_{2} + \Delta_{i} - i_{2})}$$

$$= u''(x_{i}) + \frac{1}{3}(\Delta_{i} + i_{2} - \Delta_{i} - i_{2})u'''(x_{i}) + O(\Delta^{2}).$$
(1.1)

which is clearly $O(\Delta)$ on an even moderately irregular grid. Below, we sketc't the standard convergence proof for a finite difference approximation,

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to a differential equation (and associated boundary conditions).

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The truncation error, τ_i is defined by applying the difference operator to the exact solution,

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An equation for the error, e = u - v, is found by subtracting (1.2) from (1.3),

$$L_h(\mu - \nu) = L_h e = \tau . \tag{1.4}$$

^{*}This work was done under the auspices of the U.S. Department of Energy under Contract No. W-7405-ENG-36

Stability of the difference scheme implies that the inverse of the difference operator (matrix), L_h , is bounded independent of the mesh size; that is,

$$||L_{\bullet}^{-1}|| \leq C .$$

Thus, if the difference scheme is stable, we get the usual result,

$$||e|| \le C ||\mathbf{t}|| \tag{1.5}$$

This result gives rise to the rule of thumb that the approximate solution, v, converges to the exact solution, u, at the same rate that the truncation error converges to zero.

Coupling this rule of thumb with (1.1), it is often thought that the accuracy of a finite difference scheme employing the second divided difference must be degraded on an irregular grid. A number of remedies have been suggested to circumvent this apparent loss of accuracy: use of quasi-regular grids where the mesh sizes change by $O(\Delta^2)$, Hoffman [1]; use of smooth mesh transformations to define a new difference equation on a regular grid, White [2]; solution of the differential equations rewritten as a first-order system Keller [3]; and use of implicit difference approximations, Doedel [4].

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$$\tau_i = -\frac{\Delta_{i+1/2} - \Delta_{i-1/2}}{\Delta_{i+1/2} + \Delta_{i-1/2}} u'(x_i) + O(\Delta) , \qquad (1.8)$$

and, thus, the difference approximation (1.6) is <u>inconsistent</u> with the differential equation (1.7).

However, before we abandon this scheme, let us take a closer look at the error. Recalling (1.4) and rewriting the truncation error, (1.8), ignoring terms which are $O(\Delta)$, we get the following difference equations for the error, \mathcal{E} , caused by the inconsistent term in (1.8),

$$\frac{\mathcal{E}_{i} - \mathcal{E}_{i-1}}{\frac{1}{2}(\Delta_{i+2} + \Delta_{i-2})} = \frac{g_{i} - g_{i-1}}{\frac{1}{2}(\Delta_{i+2} + \Delta_{i-2})} = \tau_{i} + O(\Delta) , \quad i = 1, 2, \dots,$$
(1.9a)

where

$$\mathbf{g}_i = -\frac{1}{2} \Delta_{i+1} \mu \qquad \mu_{A} \tag{1.9b}$$