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ON THE REPRESENTATION OF NUMERICAL SOLUTIONS USING TAYLOR SERIES APPROXIMATION

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ABSTRACT

In this study, the representation of discretization error using Taylor series in finite difference solutions is investigated as well as the behavior of the exact solutions to the finite difference equations as a function of the grid size and grid refinement factor. The results are compared to the classical Richardson Extrapolation method whereby the numerical solution (or the error) is explicitly expressed as a Taylor series expansion. The exact finite difference solutions are used to demonstrate that oscillatory convergence is a common occurrence. The expansion of the numerical solutions in Taylor series is based on the exact finite difference solutions that are obtained using different discretization schemes. It is shown that in some cases the numerical solution exhibited a singular behavior which can not be remedied easily. Some exact finite difference solutions also exhibited oscillatory behavior which was not due to the use of mixed order terms as is usually believed by the Computational Fluid Dynamics community. Moreover, representation of the numerical solution using Taylor series is not always satisfactory even in case of relatively simple one-dimensional problems.

INTRODUCTION

Grid convergence studies in applications of CFD (Computational Fluid Dynamics) requires estimation of discretization and modeling errors along with associated uncertainty limits on both. This is commonly done using the classical Richardson extrapolation (RE) technique [1-3]. In this approach a minimum of three substantially different grid sets are needed to determine the three unknowns, namely, the apparent order of the scheme, *p*, the value of the independent variable extrapolated to zero mesh size, ϕ_0, and the constant of proportionality in $\phi_0 - \phi_{num} = Ch^p$. Examining the difference between the solutions $E_{12} = \phi_1 - \phi_2$, and $E_{23} = \phi_2 - \phi_3$ on consecutively refined meshes, $h_1 < h_2 < h_3$, respectively, and their ratio denoted by $R = E_{12} / E_{32}$ three possibilities are identified, (1) $0.0 < R < 1.0$, monotonic convergence, (2) $R > 1.0$ monotonic divergence, and (3) $R < 0.0$ oscillatory behavior (undetermined convergence behavior). In the case of oscillatory behavior it is fair to say that some ad hoc criteria is used to determine whether the behavior can be considered a convergent and or divergent case (see for examples [4-7]). In view of the fact that the apparent oscillatory convergence occurs often [5, 8, 9], the present authors find the practice used in the literature unsatisfactory. Hence, in the current study the convergence behaviors of some simple finite difference schemes are examined in the whole spectrum of meshes using exact analytical solutions to the finite difference equations (FDEs). The objective is to investigate mechanisms by which oscillatory behavior can be realized and to determine whether such convergence behavior is acceptable or not.

Another essential assumption used in Richardson extrapolation is that the numerical solution can be expanded into a Taylor expansion having the mesh size as the expansion parameter. To best of our knowledge, this basic assumption in RE has never been questioned or challenged. Since we had the exact numerical solutions to the FDEs it was possible to construct their Taylor series counterparts and examined the behavior of the series approximation versus the exact solutions. This also made it possible to study asymptotic behavior of the numerical solutions in the context of extrapolating them to zero mesh size. The objective here was to see under what conditions Taylor series can be used as a good approximation to the exact finite difference solution.

NOMENCLATURE

a constant
C proportionality constant

E	approximate error
f	function
h	grid size
p	apparent order
x	x-coordinate

Greek symbols

ϕ	scalar
ϕ_0	boundary value of the scalar

Subscripts

num	numerical
1	solution on the fine grid
2	solution on the medium grid
3	solution on the coarse grid

METHODOLOGY

Solutions of governing equations where complicated source terms are applied are commonly found in CFD applications as is the case of the non-linear dissipation rate equation used in the $k-\varepsilon$ turbulence model. The model equation (Eq.(1)) studied in this work can be considered a simplified version of the ε-equation since it is written in one dimension and the temporal and diffusion terms are not considered.

The equation to be solved is

$$\frac{d\phi}{dx} = a_1\phi - a_2\phi^2 \quad (1)$$

where $0 \le x \le 1$ and the equation is subject to the boundary condition

$$\phi(0) = \phi_o \quad (2)$$

The non-linear problem represented by Eq. (1) is one of the two cases considered in this study and the second one is a linear case where $a_2 = 0$.

The exact solution to Eq. (1) is given by

$$\phi = \frac{a_1\phi_o}{a_2\phi_o + (a_1 - a_2\phi_o)\exp(-a_1x)} \quad (3)$$

and for the particular linear case where $a_2 = 0$, the exact solution reduces to

$$\phi = \phi_o \exp(a_1 x) \quad (4)$$

For both cases, the linear and non-linear one dimensional equations, the numerical solutions are obtained using different discretization schemes as well as different grid densities.

RESULTS

Linear case

The first part of this section will focus on the solution of the linear one-dimensional equation where the selected parameter a_1 is set to -25 and $a_2 = 0$.

Discretization of the governing equation (1) using first order forward differencing results in the following exact numerical solution

$$\phi_i = (1 + a_1 h)^i \phi_0 \quad (5)$$

where h is the grid size and ϕ_0 is the boundary value at x=0.

The exact numerical solution at x=1 as a function of the grid size is as shown in Figure 1.

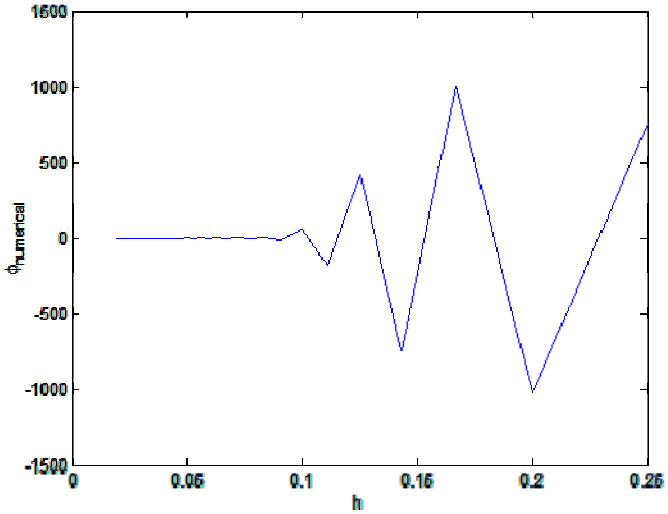


Figure 1 Numerical solution at x=1.0 as a function of the grid size

A naturally occurring oscillatory convergence is observed especially when coarse grids are used i.e. when $1 + a_1 h < 0$. Richardson extrapolation requires at least three sets of grids [10]. Therefore, when performing a grid convergence study, the conclusions arrived at will depend on which grid triplets are used to obtain the numerical solutions. As shown in Figure 2, the conclusions could lead to monotonic convergence, monotonic divergence or oscillatory convergence depending on the selected grids.

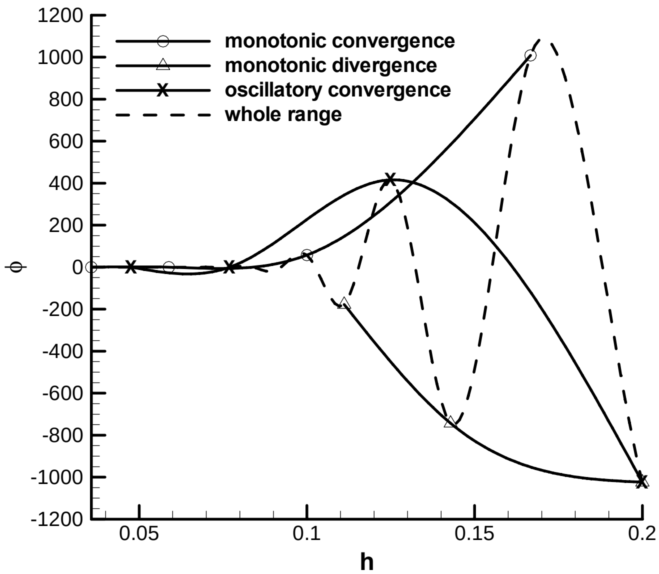


Figure 2 Representation of apparent trends in grid convergence studies depending on the selected grids, $\phi_{exact} = 1.388x10^{-11}$

As mentioned above, oscillatory convergence is observed on coarse grids with about 10 nodes or less. However, with this number of grids, the numerical solutions are not acceptable since they are not close to the exact solution and they are not physical solutions considering that the value at the boundary is 1.0 (ϕ_0) and there is a source term (sink) in the domain, therefore the numerical solution should be between 1.0 and 0.0. The numerical solution using 10 nodes along with the exact solution are shown in Figure 3. Acceptable solutions are obtained when more than 25 nodes are used in the numerical simulations as shown in Figure 4. The challenging problem in grid convergence studies in CFD application is that the exact solution is not known a priori, and the source term can change sign and magnitude almost arbitrarily during the course of iterative solutions.

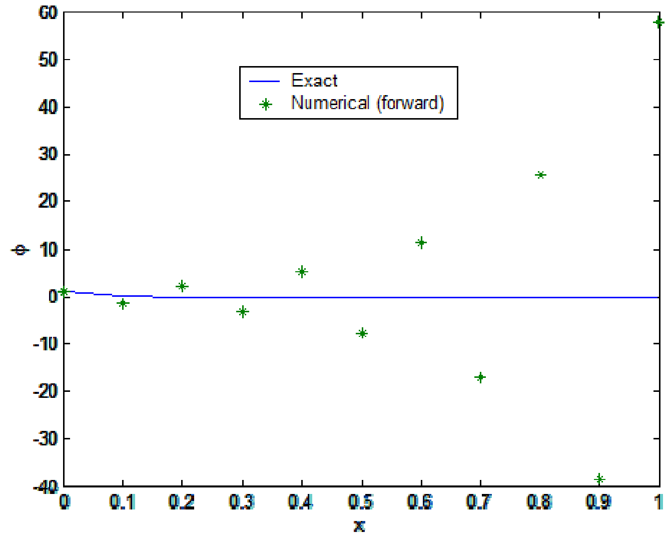


Figure 3 Numerical solution using 10 nodes

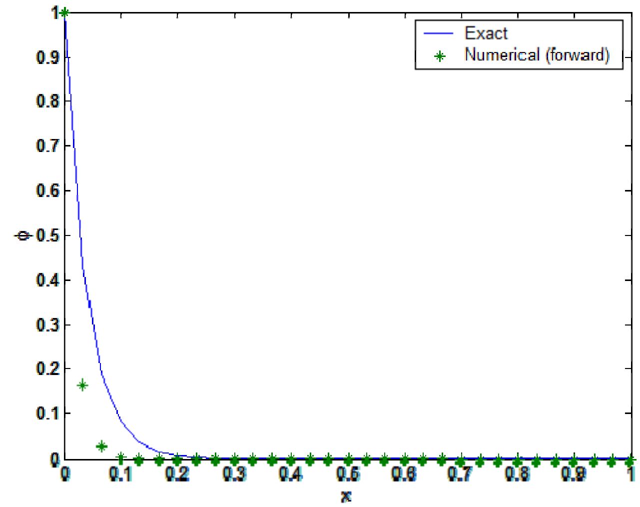


Figure 4 Numerical solution using 30 nodes

Considering numerical solutions with more than 30 grids ($1 + a_1 h > 0$), the oscillations at x=1.0 shown in Figure 1 are no longer apparent as shown in Figure 5. From the same figure, at first glance it could be thought that the numerical solution at that point is diverging as the grid is refined since an asymptotic trend is not observed as is usually expected to determine that a solution is becoming grid independent. However, this is not the case because, in fact, the solution is converging to the exact value ($1.388x10^{-11}$).

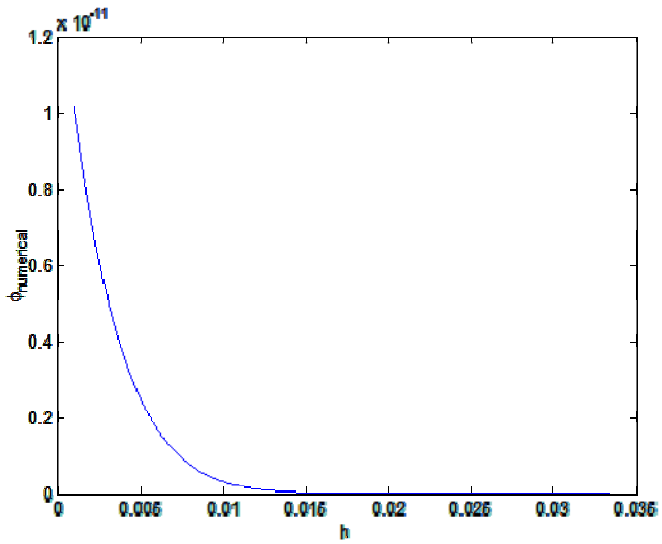
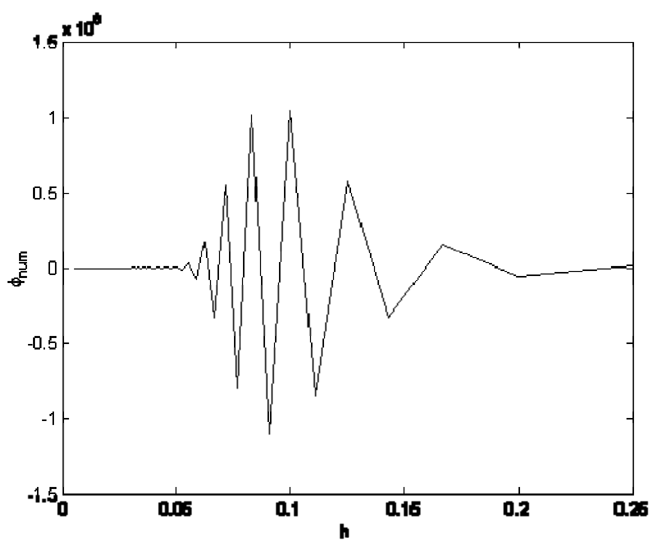
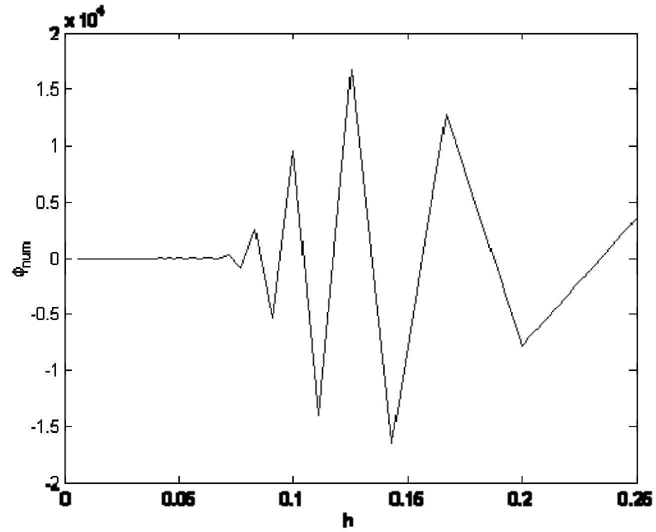


Figure 5 Numerical solution at x=1.0 as a function of the grid size with h_{max}=1/30

As examples of oscillatory behavior when the linear equation is discretized using first order forward differencing schemes for different values of the parameter a_1 in Eq. (1) are shown in Figure 6. As is demonstrated with Figures 1 and 6, the oscillatory convergence is present as long as $1+a_1h<0$.



(a)



(b)

Figure 6 Numerical solution at x=1.0 as a function of the grid size when (a) a_1=-50 and (b) a_1=-35

On the other hand, when using first order backward discretization of the governing equation, the exact finite difference solution of the governing equation takes the following form

$$\phi_i = \frac{\phi_0}{(1-a_1h)^i} \tag{6}$$

The use of backward discretization does not show oscillatory convergence at x=1.0 even with coarse grids as shown in Figure 7.

The exact finite difference solution shown in Eq. (6) potentially shows two problems. The most important one is that the solution is singular when $a_1h=1$ (if $a_1 = \text{constant}$) which can happen depending on the selected grid in relation with the magnitude of the source term which might vary with space in actual CFD applications. As an example, in Figure 8 the relative true error is plotted at the center point of the domain as a function of the grid size h for several values of the parameter a_1. As it can be seen, the singularity occurs at different grid size h depending on the magnitude of the parameter a_1. In general, a_1 changes values in space, hence it can be expected that in different regions of the computational domain the singular behavior will occur at different grid resolutions.

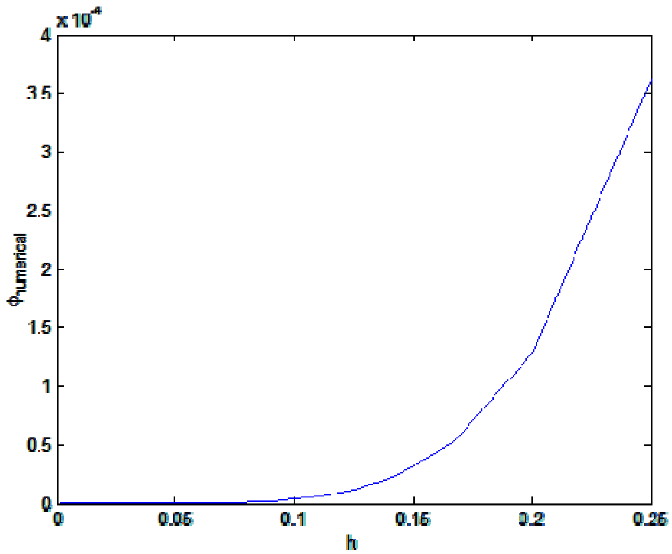


Figure 7 Numerical solution at x=1.0 as a function of the grid size using 1st. order backward differencing

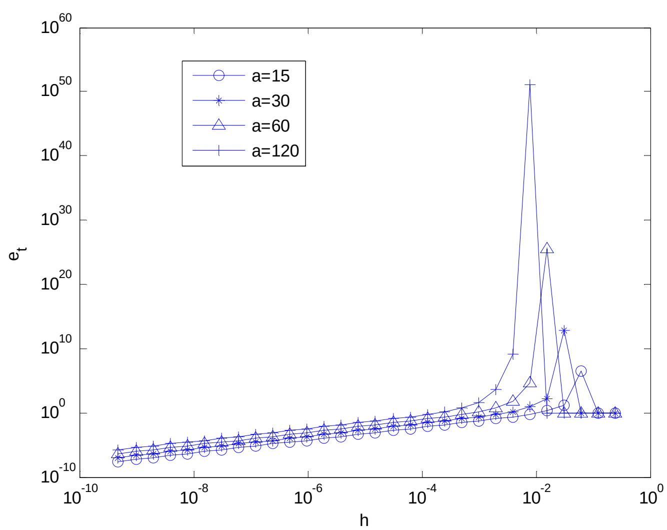


Figure 8 Relative true errors in the center point of the computational domain as a function of the grid size for several values of the parameter a_1 in Eq. (6)

This problem can not be remedied in any way because it is a consequence of the nature of numerical methods, and presumably any finite difference solution scheme should reproduce the exact behavior of that scheme. The origin of the singularity is not due to the discretization of the governing equation using mixed order terms as is usually believed by the CFD community. One might think that changing to backward differencing may solve the problem, but then similar problems occur for $a_1 > 0$.

The other problem arises when the grid size approaches zero, which produces a numerical solution of 1 over the whole domain. The singularity occurs when $h \approx 0.05$ (for $a_1 = 2.5$) which is a reasonable grid size. The problem of the numerical solution approaching unity happens when the grid size is less than 10^{-16} (out of the double precision range). However, this is unlikely to happen in practical application of CFD since using such a grid resolution, especially in three-dimensional simulations, is impractical at present.

The comparison of the numerical solutions using 1st. order forward and backward differencing is shown in Figure 9 where in both cases the computational domain was discretized using 10 nodes.

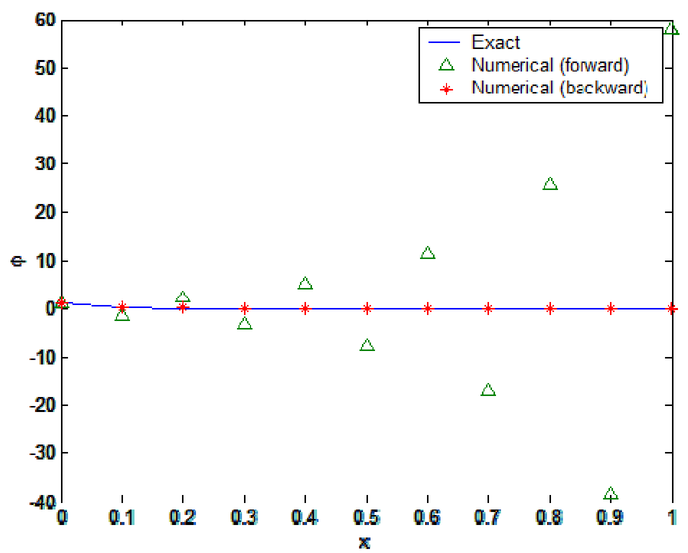


Figure 9 Comparison of numerical solutions using 10 nodes along with forward and backward differencing

In fact, the numerical solution using backward differencing with 10 nodes is more accurate than the numerical solution with 30 grids using forward differencing as can be observed by comparing Figure 4 and Figure 10, where the numerical solution with 10 nodes using backward differencing is shown.

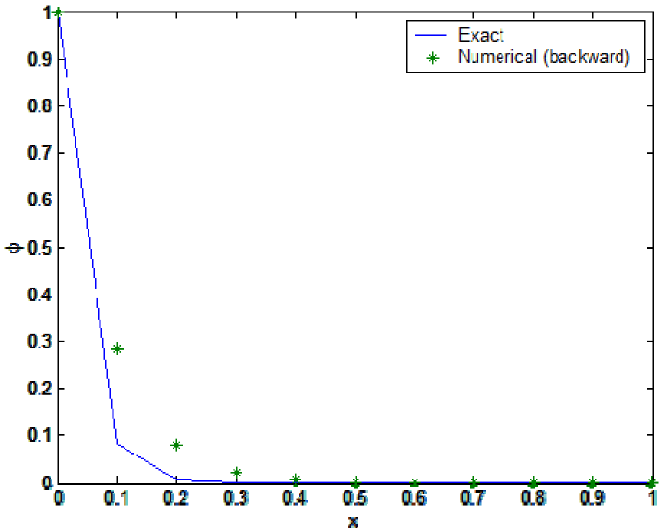


Figure 10 Numerical solution using backward differencing with 10 nodes

Non-linear case

For the non-linear case, the parameters a_1 and a_2 were set as 14.5 and 0.0127, respectively.

By using first order forward differencing to discretize the governing equation, the numerical solution takes the form

$$\phi_i = (1 + a_1 h)\phi_{i-1} - a_2 h \phi_{i-1}^2 \qquad (7)$$

The solution at x=1.0 with different grid resolutions is shown in Figure 11. In this case, the problem illustrated in Figure 8 manifests itself somewhat smoothly. The solution seems to diverge first, but then it starts converging to the right value as *h* tends toward zero.

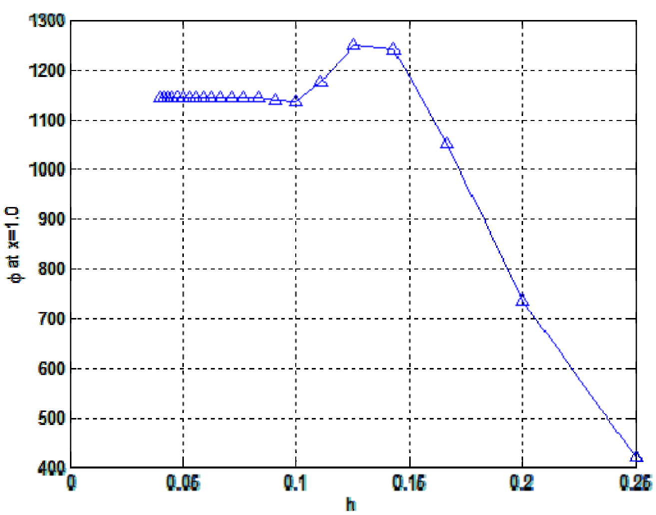
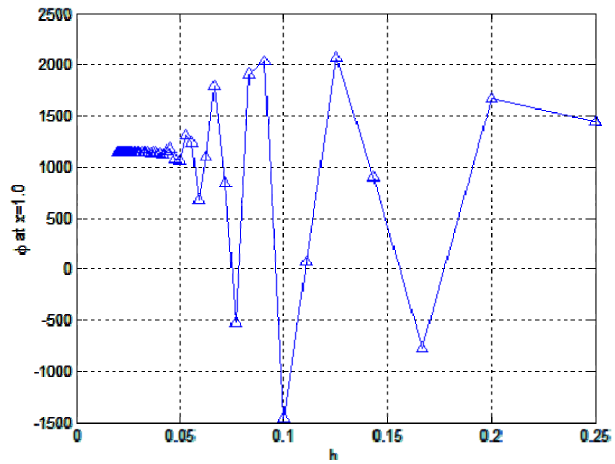


Figure 11 Convergence of the numerical solution using forward differencing as a function of the grid size at x=1.0 where $\phi_{exact} = 1144$

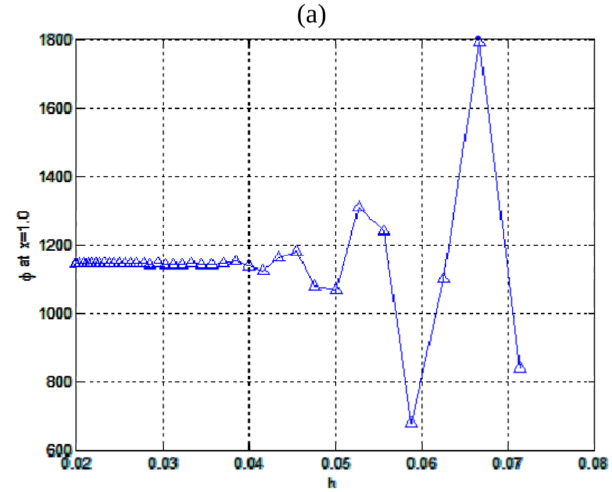
Using central differencing, the discretized equation takes the following form

$$\phi_{i+1} = \phi_{i-1} + 2a_1 h \phi_i - 2a_2 h \phi_i^2 \qquad (8)$$

The convergence behavior of the numerical solution at x=1.0 is highly oscillatory (see Figure 12) where numerical solutions with *h>0.072* do not show acceptable solutions since negative values are obtained at that location.



(a)



(b)

Figure 12 Convergence of the numerical solution using central differencing as a function of the grid size at x=1.0 where $\phi_{exact} = 1144$ **(a)** h_{max}**=0.25 and (b)** h_{max}**=1/13**

Judging from Figures 11 and 12, depending on the selected grids to study grid convergence, it could be concluded that monotonic convergence, oscillatory convergence or monotonic divergence is occurring in the numerical solutions.

Although the convergence is more stable using first order forward differencing, the numerical solutions using this discretization scheme are not as accurate when compared with central differencing discretization as shown in Figure 13, where the numerical solutions obtained from both schemes are presented with *h=0.04*. Discretization with 2nd order forward differencing did not provide acceptable solutions since the scheme showed instabilities that led to divergence.

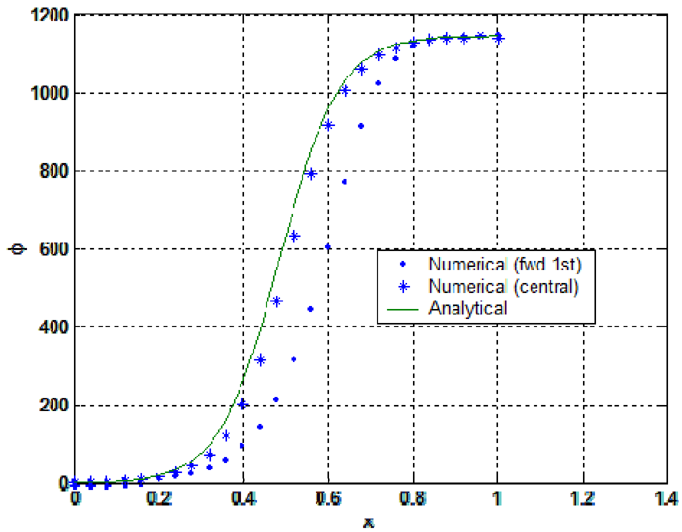
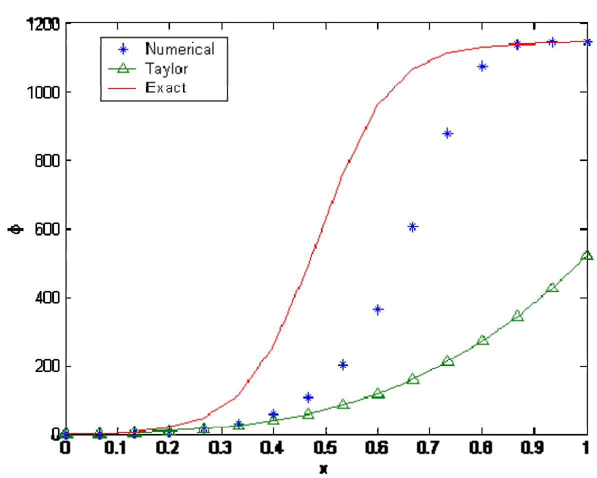


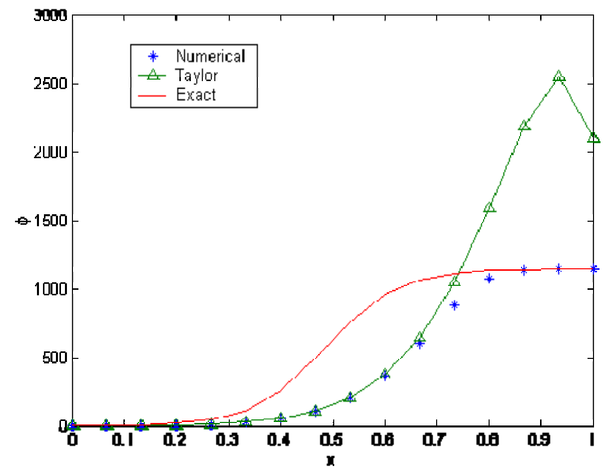
Figure 13 Numerical solutions using 1st order forward and central differencing to discretize the first derivative (h=0.04)

Taylor series approximation

In this section, the representation of the numerical solution using Taylor series is evaluated. The comparison of the numerical solution and the Taylor series representation of the numerical solution for the non-linear equation is presented in Figure 14. In Figure 14(a) 3 terms were considered in the Taylor series and the solution using 10 terms is presented in Figure 14(b). The domain was discretized using 15 interior nodes in both cases. It's apparent that, the Taylor series representation of the numerical solution is not satisfactory even with 10 terms.



(a)



(b)

Figure 14 Taylor series representation of the numerical solution using first order forward differencing in the non-linear equation with (a) 3 terms and (b) 10 terms in the Taylor series

The derived equation for the Taylor series at *x*=1.0 using first order forward differencing to discretize the non-linear equation is

$$f = 1 + \frac{21731}{100}h + \frac{2.064x10^{8}}{9375}h^{2} + \frac{1.033x10^{14}}{7.5x10^{7}}h^{3} + \frac{3.76x10^{18}}{6.328x10^{10}}h^{4} + \frac{1.41x10^{24}}{7.593x10^{14}}h^{5} + ... \quad (9)$$

Application of the Taylor series approximation to the linear case where $a_2 = 0$ is also performed. The Taylor series approximation of the numerical solution along with the exact and numerical solutions using first order forward discretization where $a_1 = -25$ are shown in Figure 15.

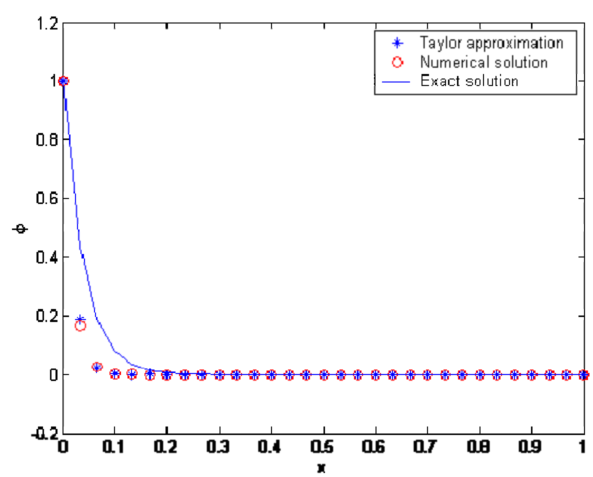
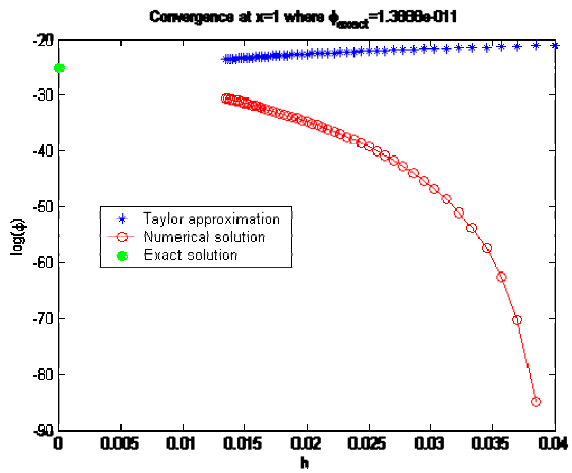
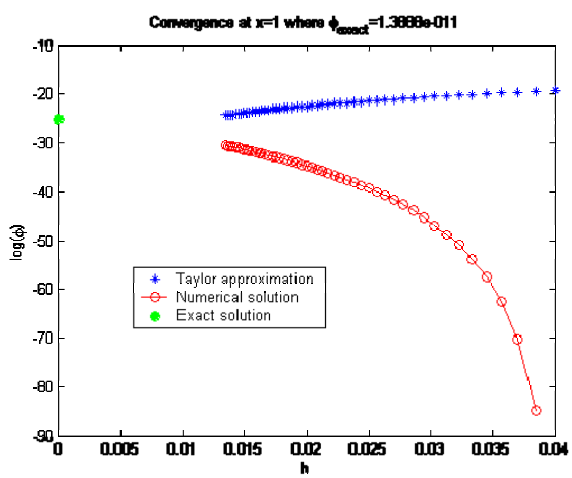


Figure 15 Taylor series representation of the numerical solution using first order forward differencing in the linear equation with 3 terms in the Taylor series

The domain was discretized using 30 interior nodes. A good agreement with the Taylor series can be observed. However, if the convergence at x=1.0 is observed in more detail, it can clearly be seen that the Taylor series is not a good representation of the numerical solution when relatively coarse grids are used, irrespective of whether 3 or 5 terms are considered in the Taylor series (see Figure 16). For the linear case with $a_1 = -25$, at least 30 interior points are needed to obtain an acceptable solution.



(a)



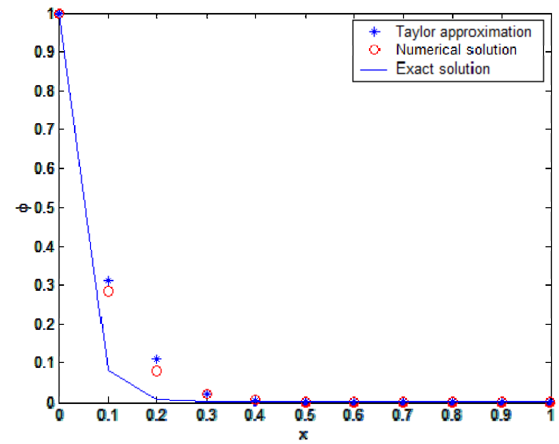
(b)

Figure 16 Convergence at *x*=1.0 using Taylor series representation of the numerical solution using first order forward differencing in the linear equation with (a) 3 terms and (b) 5 terms in the Taylor series

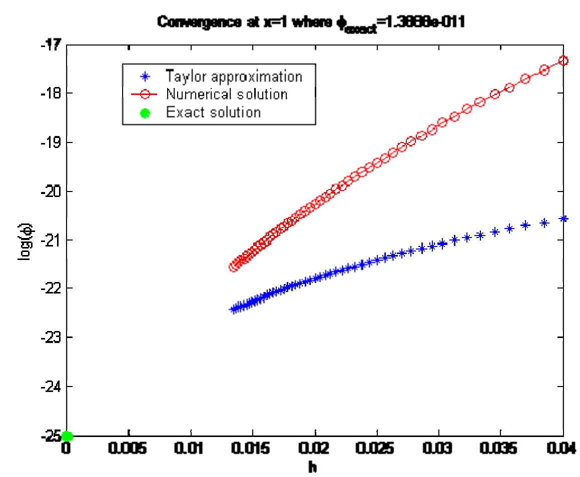
The derived equation for the Taylor series at *x*=1.0 using first order forward differencing to discretize the linear equation is

$$f = \exp(-25)\left[1 - \frac{625}{2}h + \frac{1.047x10^{6}}{24}h^{2} - \frac{1.71x10^{8}}{48}h^{3} + \frac{2.133x10^{11}}{1152}h^{4} + \ldots\ldots\right] \quad (10)$$

Representation of the numerical solution using the Taylor series when the linear equation is discretized using backward differencing is well behaved as shown in Figure 17.



(a)



(b)

Figure 17 Representation of the numerical solution using Taylor series with 3 terms using backward differencing in the linear equation (a) solution in the domain and (b) convergence at x=1.0

CONCLUSIONS

The method of the exact finite difference solution was applied to linear and non-linear one-dimensional governing equations. Different discretization schemes were used on both equations.

In the linear equation case, if the source term is negative $(a_1 < 0)$ and a first order discretization scheme is used, the exact finite difference solutions show an oscillatory behavior. With first order backward discretization, the numerical solution will have a singularity when $a_1 h = 1$. The use of backward discretization offers more accurate solutions when compared with forward discretization, which amounts to upwinding in this case. However, this is not a satisfactory remedy since in practical CFD applications the sign of the source term can change independent of the velocity.

Oscillatory behavior in the solution of the non-linear equation was observed on coarse grids when 2nd order forward difference is used as the discretization scheme. Divergence problems were observed with 2nd order forward discretization.

The representation of the numerical solution using the Taylor series is not satisfactory when a first order forward discretization scheme is used in the non-linear equation case even when ten terms are included in the Taylor series. In the linear equation case, using first order forward difference discretization offers a good representation with Taylor series although the convergence with coarse grids is not well represented when compared with the numerical solution. The use of backward discretization provides a good representation of the numerical solution with Taylor series.

This study elucidated some essential facts concerning the grid convergence studies practiced in literature, which are generally based on Richardson extrapolation.

(1) Depending on the sign and magnitude of the source term, the numerical solution may exhibit oscillatory behavior.

(2) Some discretization schemes exhibit singular behavior which may occur at different grid resolutions or at different location in the domain when non-uniform grid distributions are used

(3) When (1) or (2) occurs, Taylor series representation, hence the Richardson extrapolation becomes problematic.

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