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ANALYSIS OF COMPACT SCHEMES FOR DIFFUSION TERMS WITH VARIABLE PROPERTIES

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Abstract. *This study presents a numerical investigation on the treatment of diffusive terms with variable properties. A theoretical analysis illustrates the accuracy loss phenomenon related to many known schemes, where spatial resolution tests of fourth order accurate centered schemes. For this formulation, conservative and non-conservative compact finite difference were employed. They are compared to different finite difference methods. These comparisons are based on several criteria: numerical stability of the reference time-marching scheme, spatial error distribution, spatial accuracy order, computational cost and spectral resolution. A new fourth-order formulation is proposed in order to overcome the difficulties associated with different schemes analyzed here.*

Keywords: *spatial resolution, diffusive terms, spectral resolution, compact schemes*

1. INTRODUCTION

Over the past decades, the development of new numerical methods for spatial resolution of the governing equations for transport phenomena concentrated effort in the construction of discrete approximations to their advective terms, giving less attention to the diffusive terms. This is due to the increased complexity of the first compared to the second. An example is in aerospace (Laney, 1998), where the simulation of high-speed compressible flows using the Euler equations to model the propagation of shock waves and expansion, among other phenomena. This paper attempts to fill this gap. It is dedicated to the study of diffusive terms properties containing variables, such as those existing in the Navier-Stokes equations.

Before discussing the numerical treatment of the diffusive terms, we must distinguish between the two approaches most commonly used in fluid mechanics and computational heat transfer. They are the finite difference and finite volume (Lomax *et al.*, 2001). The first approach is based on the use of Taylor series expansions around a discrete point applied directly to the differential form of the governing equations (Tannehill *et al.*, 1997). It has two major advantages, the rigorous mathematical deduction order error and numerical stability of its discrete schemes and also the flexibility in choosing conservative or non-conservative formulations for their schemes. The second approach is based on the integral form of the conservation equations (Versteeg and Malalasekera, 1995).Its formulation intrinsically conservative and its ability to deal with irregular geometries naturally. Because of these differences between the methods of difference and finite volume, the main features of the schemes used to discretize the diffusive terms can vary significantly.

In the study by Zhong (1998), he uses direct numerical simulation to study the phenomenon of laminar-turbulent transition in supersonic boundary layers in the presence of shock waves. It uses a finite difference scheme with high-order temporal and spatial resolution.

In a sequence of papers published by Rango and Zingg (2000), Zingg (2000) e Rango (2001), a comparative analysis of different types of spatial discretization for the Navier-Stokes equations is presented. They use the subsonic and transonic turbulent flow, around airfoils as a problem basis for comparison of the simulations.

The study by Lele (1992) examines compact central finite difference schemes with varying error order. The author emphasizes an analysis of the wave number and phase velocity of these modified schemes, demonstrating that compact schemes are closer to the ideal spectral than explicit schemes for the same number of points in the stencil. Thus, there is significant damage in the numerical stability of these schemes. Formulas for the first and second derivatives are provided, which can be used for diffusive terms.

Shen *et al.* (2007) developed a robust high-order schemes for the equations of compressible Navier-Stokes equations using the finite difference scheme with conservative formulations. Both the diffusive advective terms as are considered in this work.

2. ORDER ANALYSIS

A simple analysis of the different types of discretization utilized for diffusive terms in literature is able to illustrate the main differences between them. This step not just explains the this study, from a purely theoretical point of view, but also indicates behavior what should be expected of each method.

2.1 Finite Difference - Conservative

Two important conclusions can be extracted from Eq. (1). The first is implicit in the consecutive application of operators for internal and external derivatives of diffusive term, since the resultant operator of this application has a large stencil. The second is explicit in the final truncation error whose order is reduced due to this same consecutive application of these operators.

$$\frac{\partial}{\partial x}\left(f\,\frac{\partial g}{\partial x}\right)_i \simeq \frac{\delta_i^n\big(f_i\,\gamma_i^m(g)\big)}{\Delta x^2} + O(\Delta x^{m-1}, \Delta x^n) \tag{1}$$

where m is the truncation order error associated with operator γ_i^m and n is the truncation order associated with operator δ_i^m.

2.2 Finite Difference - Non-Conservative

As opposed to Eq. (1), the below formula does not have increased stencil, since no consecutive applications of an operator. However, we also observed a reduction order in truncation error in Eq. (2), which now appears on a larger scale. It is clearly associated with approximations product for derivatives. Moreover, this order reduction is only in areas where the properties are not constant. This analysis indicates that errors introduced by this approximation if both derivatives are higher.

$$\left\{\frac{\partial f}{\partial x}\,\frac{\partial g}{\partial x} + f\,\frac{\partial^2 g}{\partial x^2}\right\}_i \simeq \frac{\gamma_i^m(f)\,\delta_i^n(g)}{\Delta x^2} + f_i\,\frac{\epsilon_i^o(g)}{\Delta x^2} + O(\Delta x^{m-1},\, \Delta x^{n-1},\, \Delta x^o) \tag{2}$$

where O is the truncation order associated with the operator for the second derivative.

2.3 Finite Volume

Equation (3) shows that the formulation generated by Finite Volume Scheme combines the problems found in the two previous formulations generated by Finite Difference Scheme. Both the consecutive application of algebraic operators as the multiplication of approaches, now appearing as a function times derivative instead of derivative times derived, are found. As a result, there is a major decrease in the order of final approach.

$$\left.\frac{\partial h}{\partial x}\right|_i \simeq \frac{\bar{\gamma}_i^m\big(\phi_i^n(f)\,\gamma_i^o(g)\big)}{\Delta x^2} + O(\Delta x^{n-2},\, \Delta x^{o-1},\, \Delta x^m) \tag{3}$$

where n is the order of the truncation error associated with the operator to function.

3. MATHEMATICAL MODEL

3.1 Heat Equation

A comparative analysis of the different methodologies used for the diffusive term of the Navier-Stokes equations can be made if we consider a simple test problem but which still contains this term. The equation that models the one-dimensional transient heat conduction with variable thermal conductivity, given by

$$\rho\,C_P\,\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) + q \tag{4}$$

where ρC_p is the heat capacity at constant pressure and q is a source term. The boundary conditions chosen for this problem are thermal insulation $\frac{\partial T}{\partial x}\big|_{x=0} = 0$ and heat transfer by convection $k\,\frac{\partial T}{\partial x}\big|_{x=L} + h\,T(x = L, t) = h\,T_L$ with a prescribed temperature is constant and chosen as an initial condition, $T(x, t = 0) = T_0$, where L is the length, h the coefficient of heat transfer by convection and T_L the temperature of the external fluid.

3.2 Manufactured Solution

It was originally developed by Roache (1998) and can be used to verify numerical schemes for the equations of computational fluid dynamics (Roy *et al.*, 2004) and its boundary conditions (Bond *et al.*, 2005). This construction approach, the solution is assumed to satisfy a partial differential equation of interest. The main idea of the method of manufactured solution is simply to produce an exact solution without being interested in the physical reality of the problem (Roy, 2005).

This method can be used both to avoid the exponential growth of the solution with time as to avoid confusion between physical and numerical instabilities (Salari and Knupp, 2000).

The decrease in order discretization of diffusive terms is due to the product of derivatives from the property and the potential.

Thus, we use the method of the manufactured solution to induce large gradients in both the thermal conductivity and in temperature. The function chosen in the thermal conductivity is in the form of Eq. (5).

$$k(x) = \frac{(k_{max}+k_{min})}{2} + \left[\frac{(k_{max}-k_{min})}{2}\right]\tanh[\theta(x+1/2)] \tag{5}$$

On the other hand the temperature function has the form of Eq. (6).

$$\begin{aligned} T^*(x) &= T_L\left(\frac{1}{2}\tanh\left(\theta\left(\frac{x}{L}-\frac{1}{2}\right)\right)+\frac{1}{2}\right)\left(\sin\left(\frac{ax}{L}\right)+\cos\left(\frac{ax}{L}\right)\right) \\ &+ T_R\cos\left(\frac{x}{L}\right)\left(\frac{1}{2}-\frac{1}{2}\tanh\left(\theta\left(\frac{x}{L}-\frac{1}{2}\right)\right)\right) \end{aligned} \tag{6}$$

The source term which needs to be introduced in Eq. (4) to generate the Eq. (6) is obtained from a steady-flow, thus

$$q = -\frac{\partial}{\partial x}\left(k\,\frac{\partial T^*}{\partial x}\right) \tag{7}$$

4. NUMERICAL METHODS

4.1 Temporal Discretization

The objective of this paper is to evaluate the performance of schemes for spatial resolution of diffusive terms, which can be largely done only with the analysis of steady-flow equations. We chose the explicit Euler method, since it is conditionally stable to heat diffusion problems. As its implicit version is unconditionally stable, it does not allow an assessment of numerical stability.

In this scheme, the approximation of the temporal derivative of the temperature is given by:

$$\frac{\partial T}{\partial t} \simeq \frac{\Delta T}{\Delta t} + O(\Delta t) \tag{8}$$

where $\Delta T = T^{n+1} - T^n$.

4.2 Spatial Discretization

4.2.1 Compact Schemes

Conservative Formulation

From Eq. (4), it is possible to develop a compact non-conservative formulation. Setting the heat flow by conduction can reach the diffusive flow and apply compact scheme at the exterior derivative and then the internal derivative. Using a fourth order classical Padé compact scheme for first derivatives of temperature (Lele, 1992). We have

$$\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{i-1} + 4\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{i} + \left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{i+1} = \frac{3(T_{i+1}-T_{i-1})}{\Delta x} \tag{9}$$

Non-Conservative Formulation

Likewise, it is possible to develop a compact non-conservative formulation of the problem being studied. Using a fourth order classical Padé compact scheme for first (shown above) and second derivatives of temperature. For second derivative we have

$$\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{i-1} + 10\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{i} + \left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{i+1} = \frac{12(T_{i+1}-2T_iT_{i-1})}{\Delta x^2} \tag{10}$$

4.2.2 Finite Difference Schemes

Non-Conservative Formulation

Again, from Eq. (4), it is possible to develop a non-conservative formulation of the problem being studied. Using fourth order central scheme (CDS) at the first and second derivatives of the temperature.

$$\begin{aligned}\Delta T &= \frac{\Delta t}{\rho C_p}\left(\frac{k_{i-2}^n - 8k_{i-1}^n + 8k_{i+1}^n - k_{i+2}^n}{12\Delta x}\right)\left(\frac{T_{i-2}^n - 8T_{i-1}^n + 8T_{i+1}^n - T_{i+2}^n}{12\Delta x}\right) \\ &+ \frac{k_i^n \Delta t}{\rho C_p}\left(\frac{-T_{i-2}^n + 16T_{i-1}^n - 30T_i^n + 16T_{i+1}^n - T_{i+2}^n}{12\Delta x^2}\right) + \frac{q_i^n \Delta t}{\rho C_p}\end{aligned} \tag{11}$$

where $\Delta T = (T^{n+1} - T^n)$.

Conservative Formulation

Likewise, it is also possible to derive the conservative formulation of the problem being studied. Setting the heat flow by conduction can reach the diffusive flow and apply CDS at the exterior derivative and then the internal derivative.

$$\begin{aligned}\left.\frac{\mathrm{d}E}{\mathrm{d}x}\right|_i &= \frac{E_{i-2}^n - 8E_i^n - 1 + 8E_{i+1}^n - E_{i+2}^n}{12\Delta x} \\ &= \frac{\left(\left(k\frac{\mathrm{d}T}{\mathrm{d}x}\right)_{i-2}^n - 8\left(k\frac{\mathrm{d}T}{\mathrm{d}x}\right)_{i-1}^n + 8\left(k\frac{\mathrm{d}T}{\mathrm{d}x}\right)_{i+1}^n - \left(k\frac{\mathrm{d}T}{\mathrm{d}x}\right)_{i+2}^n\right)}{12\Delta x} \\ &= \frac{(k_{i-2}(T_{i-4}^n - 8T_{i-3}^n + 8T_{i-1}^n - T_i^n) - 8k_{i-1}(T_{i-3}^n - 8T_{i-2}^n + 8T_i^n - T_{i+1}^n)}{244\Delta x^2} \\ &+ \frac{8k_{i+1}^n(T_{i-1}^n - 8T_i^n + 8T_{i+2}^n - T_{i+3}^n) - k_{i+2}^n(T_i^n - 8T_{i+1}^n + 8T_{i+3}^n - T_{i+4}^n)}{244\Delta x^2}\end{aligned} \tag{12}$$

where E is the heat flow.

4.2.3 Finite Volume Schemes

Traditional Finite Volume Formulation: One of the fourth order central schemes used in these paper is the traditional conservative finite volume scheme, which uses fourth order in both the function and derivative. Thus, the scheme takes the following form:

$$\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{i-\frac{1}{2}}^n = \frac{T_{i-2}^n - 27T_{i-1}^n + 27T_i^n - T_{i+1}^n}{24\Delta x} \tag{13}$$

New Finite Volume Formulation - 4(2): This new formulation increases for sixth order only the internal derivative. Thus, the scheme to the diffusive term takes the following form

$$\begin{aligned}\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_i^n &= ((k_{i-3}^n - 9k_{i-2}^n - 9k_{i-1}^n + k_i^n) \\ &\cdot (9T_{i-4}^n - 125T_{i-3}^n + 2250T_{i-2}^n - 2250T_{i-1}^n + 125T_i^n - 9T_{i+1}^n) \\ &- 27(k_{i-2}^n - 9k_{i-1}^n - 9k_i^n + k_{i+1}^n) \\ &\cdot (9T_{i-3}^n - 125T_{i-2}^n + 2250T_{i-1}^n - 2250T_i^n + 125T_{i+1}^n - 9T_{i+2}^n) \\ &+ 27(k_{i-1}^n - 9k_i^n - 9k_{i+1}^n + k_{i+2}^n) \\ &\cdot (9T_{i-2}^n - 125T_{i-1}^n + 2250T_i^n - 2250T_{i+1}^n + 125T_{i+2}^n - 9T_{i+3}^n) \\ &+ (k_i^n - 9k_{i+1}^n - 9k_{i+2}^n + k_{i+3}^n) \\ &\cdot (-9T_{i-1}^n + 125T_i^n - 2250T_{i+1}^n + 2250T_{i+2}^n - 125T_{i+3}^n + 9T_{i+4}^n))/737280\Delta x^2\end{aligned} \tag{14}$$

New Finite Volume Formulation - 4(3): The next new formulation increases to sixth order function only. Thus, the scheme to the diffusive term takes the following form

$$\begin{aligned}\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_i^n &= ((3k_{i-4}^n - 25k_{i-3}^n + 150k_{i-2}^n + 150k_{i-1}^n - 25k_i^n + 3k_{i+1}^n) \\ &\cdot (T_{i-3}^n - 27T_{i-2}^n + 27T_{i-1}^n - T_i^n) \\ &- 27(3k_{i-3}^n - 25k_{i-2}^n + 150k_{i-1}^n + 150k_i^n - 25k_{i+1}^n + 3k_{i+2}^n)\end{aligned}$$

$$
\begin{aligned}
\cdot &\quad (T^n_{i-2} - 27T^n_{i-1} + 27T^n_i - T^n_{i+1}) \\
+ &\quad 27(3k^n_{i-2} - 25k^n_{i-1} + 150k^n_i + 150k^n_{i+1} - 25k^n_{i+2} + 3k^n_{i+3}) \\
\cdot &\quad (T^n_{i-1} - 27T^n_i + 27T^n_{i+1} - T^n_{i+2}) \\
- &\quad (3k^n_{i-1} - 25k^n_i + 150k^n_{i+1} + 150k^n_{i+2} - 25k^n_{i+3} + 3k^n_{i+4}) \\
\cdot &\quad (T^n_i - 27T^n_{i+1} + 27T^n_{i+2} - T^n_{i+3}))/147456\Delta x^2
\end{aligned} \tag{15}
$$

New Finite Volume Formulation - 4(4): And the last new formulation increases to sixth order both function and first internal derivative. Thus, the scheme to the diffusive term takes the following form

$$
\begin{aligned}
\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|^n_i &= ((3k^n_{i-4} - 25k^n_{i-3} + 150k^n_{i-2} + 150k^n_{i-1} - 25k^n_i + 3k^n_{i+1}) \\
\cdot &\quad (-9T^n_{i-4} + 125T^n_{i-3} - 2250T^n_{i-2} + 2250T^n_{i-1} - 125T^n_i + 9T^n_{i+1}) \\
+ &\quad 27(3k^n_{i-3} - 25k^n_{i-2} + 150k^n_{i-1} + 150k^n_i - 25k^n_{i+1} + 3k^n_{i+2}) \\
\cdot &\quad (9T^n_{i-3} - 125T^n_{i-2} + 2250T^n_{i-1} - 2250T^n_i + 125T^n_{i+1} - 9T^n_{i+2}) \\
+ &\quad 27(3k^n_{i-2} - 25k^n_{i-1} + 150k^n_i + 150k^n_{i+1} - 25k^n_{i+2} + 3k^n_{i+3}) \\
\cdot &\quad (-9T^n_{i-2} + 125T^n_{i-1} - 2250T^n_i + 2250T^n_{i+1} - 125T^n_{i+2} + 9T^n_{i+3}) \\
+ &\quad (3k^n_{i-1} - 25k^n_i + 150k^n_{i+1} + 150k^n_{i+2} - 25k^n_{i+3} + 3k^n_{i+4}) \\
\cdot &\quad (9T^n_{i-1} - 125T^n_i + 2250T^n_{i+1} - 2250T^n_{i+2} + 125T^n_{i+3} - 9T^n_{i+4}))/11796480\Delta x^2
\end{aligned} \tag{16}
$$

5. RESULTS

Following are results for finite difference schemes, finite volume schemes, spectral analysis and computational cost. Noting that the graphs of finite difference schemes, the results dimensionless. It can be seen in the compact scheme, conservative and non-conservative, that the method is unstable (Fig. 1 and Fig. 2). It is not possible to make a conclusive analysis of order for greater θ. The oscillation that one perceives in the conservative finite difference scheme (Fig. 3) happens because decouples points peers and odd points. It is also observed that it is not possible to make a conclusive analysis of order, because as is noted in Fig. 3, the method is very unstable, causing even for larger values of θ, oscillation in the solution. In finite volume conservative scheme, we noted in Fig. 4 further loss of order in the variable property region to $\theta = 90$. The results of the first new finite volume formulation of fourth order, SA 4(2), show in Fig. 5 that there is an apparent loss order when $\theta = 80$, but in the variable property region there is a greater loss to $\theta = 60$. For new finite volume formulation of fourth order SA 4(3), we noted in Fig. 6 a slight loss of order, and for $\theta = 90$ we lose accuracy in the calculation of order. Now, we have new finite volume formulation of fourth order SA 4(4). In which we clearly see that the order remains more stable in virtually every field, oscillating and losing order in the region where the property varies. We can see this loss of order in Fig. 7 for $\theta = 60$.

Fig. 8 shows a comparison for various schemes. Where we can see that comparing the non-conservative schemes with the finite difference conservative schemes, we see the curve of the wave number of the finite difference scheme far below the non-conservative. We see also that the compact schemes don't have a good approach for the curve K^2. When we look at the new finite difference schemes, we note that two are equivalent which provides best result, ie, best approached the curve K^2

Finally, Fig. 9 shows the analysis of computational time where we can see a big difference especially among compact schemes and new finite volume formulations in terms of maximum error and runtime. The new finite volume formulations are even better than all the other schemes in this analysis.

6. CONCLUSIONS

After studying the results, we note that the conservative method of finite differences can be clearly ruled out, due to its high sensitivity in the calculation of numerical order and error analysis, which considerably increases the region of higher gradient, and instability in solution and worse results in the spectral analysis.

The compact schemes have not had satisfactory results in computational cost analysis and spectral analysis being worse than most of the schemes.

The new finite volumes formulations showed some stability in the calculation of numerical order, except for some cases in the region variable property. However the new finite volume formulation SA 4(4) presented better stability in this region. The new finite volume formulations SA 4(2) and SA 4(4) presented best modified wave numbers. Furthermore the new finite volume formulation presented best computational cost than the other schemes.

We conclude that after all this study, the new finite volume formulation 4(4) proposed in this paper, which was, in general, showed better results.

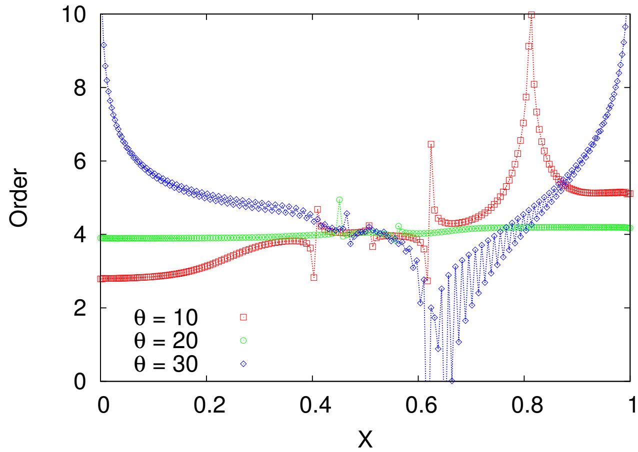

Figure 1. Numerical Order. Compact Conservative Formulation.

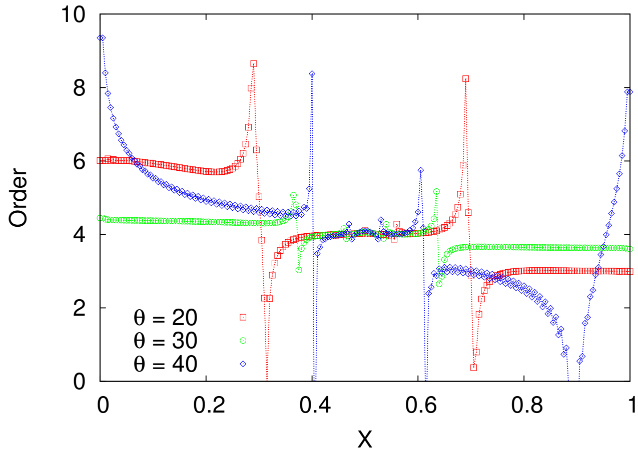

Figure 2. Numerical Order. Compact Non-Conservative Formulation.

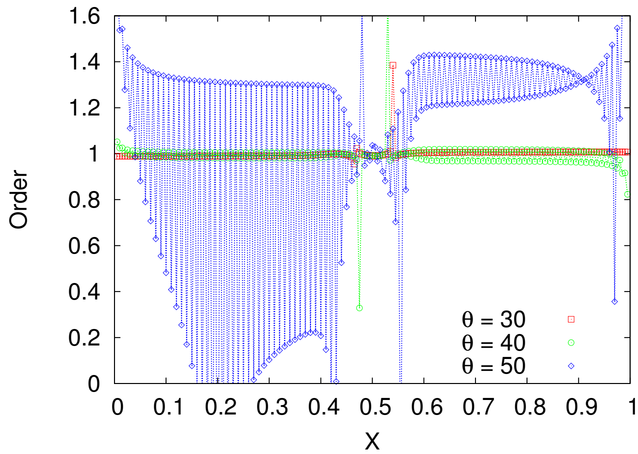

Figure 3. Numerical Order. Finite Difference Formulation.

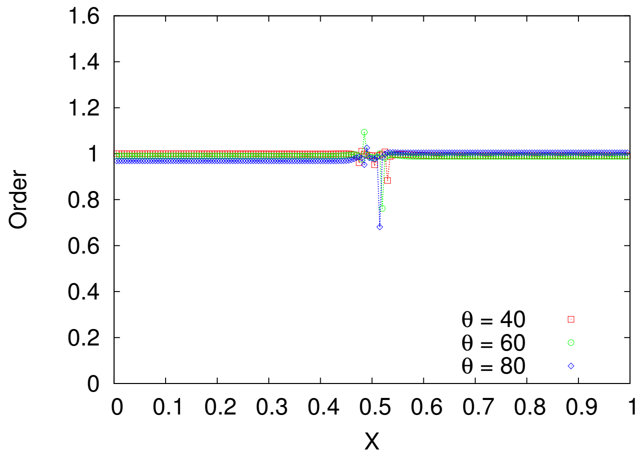

Figure 4. Numerical Order. Finite Volume Formulation.

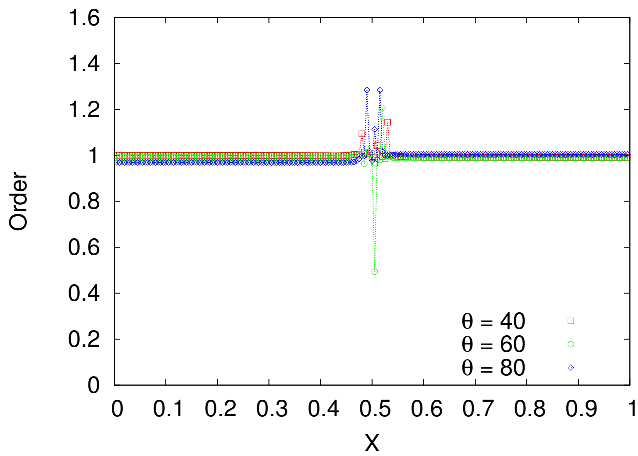

Figure 5. Numerical Order. New Finite Difference Formulation - 4(2).

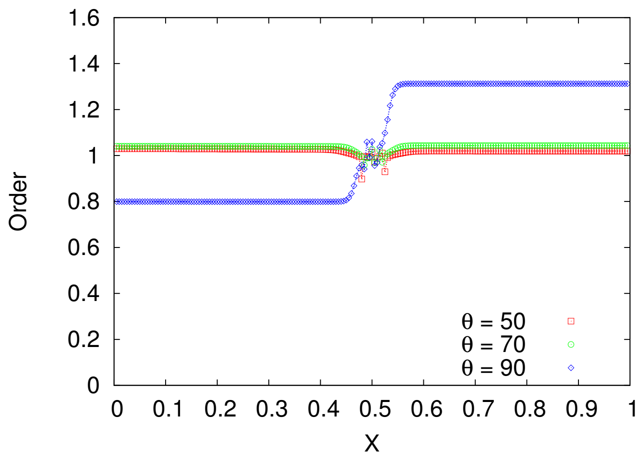

Figure 6. Numerical Order. New Finite Difference Formulation - 4(3).

7. ACKNOWLEDGEMENTS

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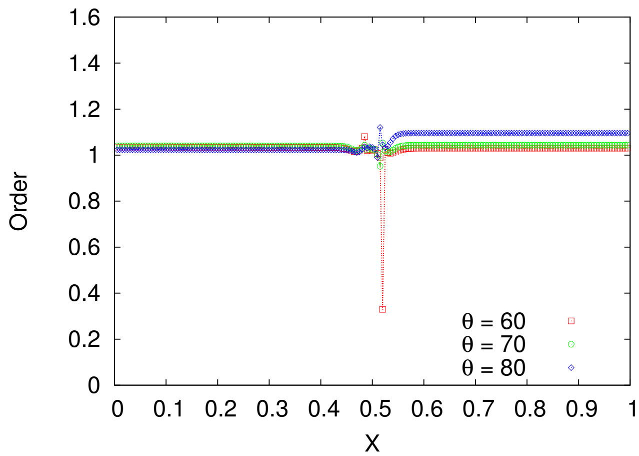

Figure 7. Numerical Order. New Finite Difference Formulation - 4(4).

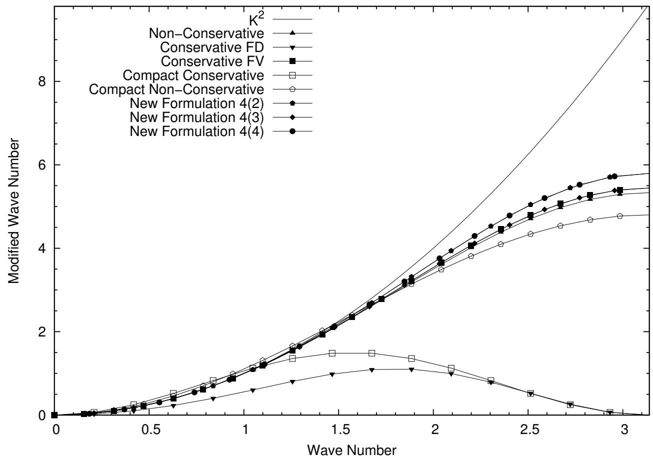

Figure 8. Modified wave number described as wave number, for second derivative.

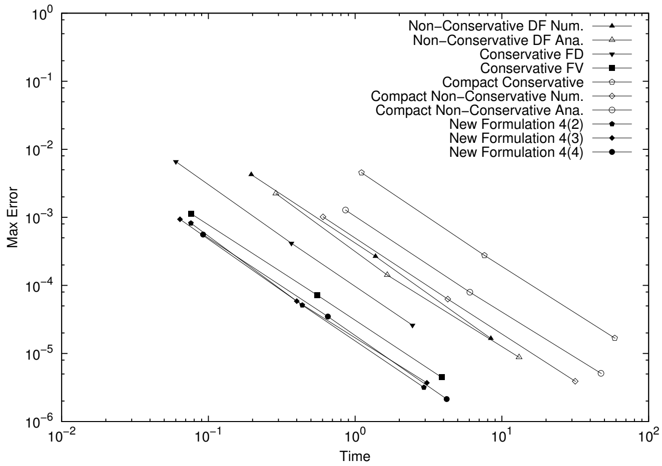

Figure 9. Computational cost for all schemes.

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