ISSN 2176-5480

22nd International Congress of Mechanical Engineering (COBEM 2013)
November 3-7, 2013, Ribeirão Preto, SP, Brazil

ANALYSIS OF THE SPATIAL RESOLUTION OF DIFFUSIVE TERMS

Kledson Flávio Silveira Santiago
Leonardo Santos de Brito Alves
Laboratory of Theoretical and Applied Mechanics (LMTA), Mechanical Engineering Graduate Program (PGMEC), Universidade Federal Fluminense, Rua Passos da Pátria, 156, 24210-240 Niterói, RJ, Brazil
kflavio@id.uff.br, leonardo.alves@mec.uff.br

Abstract. *This study presents an extensive numerical investigation on the treatment of diffusive terms with variable properties. A theoretical analysis illustrates the accuracy loss phenomenon related to many known schemes. Spatial resolution tests are restricted to second order accurate centered schemes. For this formulation, conservative and non-conservative finite difference methods 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 and spectral resolution. A new formulation is proposed in order to overcome the difficulties associated with each studied scheme.*

Keywords: *spatial resolution, diffusive terms, spectral analysis.*

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. He is devoted to the study of properties diffusive terms 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 his ability to handle 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 this study the boundary condition is the shock wave itself to avoid numerical errors caused in the treatment of discontinuity. With respect to diffusive term treatment, the author describes the two formulations traditional finite differences: conservative and non-conservative. The first ensures conservation of diffusive flow, which are conductive and viscous flows in the case of the Navier-Stokes equations. It is obtained essentially by applying a discrete approximation to the first derivative twice. This is easier to implement, but leads to a stencil having a greater number of points. Already the non-conservative formulation expands the diffusive operator, making the second derivative appears explicitly. The discretization of this version takes the fewest points possible in order stencil for a given error. For this reason, the numerical stability of non-conservative formulation is greater than the version conservative, but it does not guarantee preservation of diffusive flow.

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 main focus of these studies are the advective terms, but a new discretization of diffusive terms is also presented. As the authors using finite volumes, the first approximation, related to the first external derivative, is made in relation to the volume faces. The resulting term that includes the multiplication of a internal fluid property and the first derivative is then estimated using information in the centers of the volumes. For this reason, the number of points stencil is smaller than that used in the conservative formulation equivalent of the finite difference scheme, but it is still higher than that used in the formulation of this non-conservative equivalent method. The authors state that the loss of accuracy is not significant, but not have to order error results obtained numerically.

ISSN 2176-5480

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. A number of classical problems in compressible flows are simulated to demonstrate the features of these schemes. The developed schemes are subsequently used for the simulation of fluid-structure problems (Shen *et al.*, 2008), and the treatment of the diffusive terms compared with formulated by Rango and Zingg (2000). One important difference appears in the calculation of the first internal derivative, which uses a formula with higher error order without causing an increase in the number of end points of the stencil. This is done to minimize the problem of loss of order in the discretization of the diffusive terms in the presence of non constants properties, noted by the authors using the scheme proposed by Rango and Zingg (2000). It is worth mentioning that no order calculation error or numerical stability is presented in these studies.

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.

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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

$$\left.\frac{\partial T}{\partial x}\right|_{x=0} = 0 \tag{5}$$

and heat transfer by convection

$$k \left.\frac{\partial T}{\partial x}\right|_{x=L} + h\,T(x=L,t) = h\,T_L \tag{6}$$

with a prescribed temperature is constant and chosen as an initial condition,

$$T(x, t=0) = T_0 \tag{7}$$

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. (8).

$$k(x) \quad = \quad \frac{(k_{max} + k_{min})}{2} + \left[\frac{(k_{max} - k_{min})}{2}\right] \tanh[\theta(x + 1/2)] \tag{8}$$

On the other hand the temperature function has the form of Eq. (9).

$$\begin{aligned} T^*(x) \quad &= \quad T_L \left(\frac{1}{2}\tanh\left(\theta\left(\frac{x}{L} - \frac{1}{2}\right)\right) + \frac{1}{2}\right)\left(\sin\left(\frac{ax}{L}\right) + \cos\left(\frac{ax}{L}\right)\right) \\ &+ \quad T_R \cos\left(\frac{x}{L}\right)\left(\frac{1}{2} - \frac{1}{2}\tanh\left(\theta\left(\frac{x}{L} - \frac{1}{2}\right)\right)\right) \end{aligned} \tag{9}$$

The source term which needs to be introduced in Eq. (4) to generate the Eq. (9) is obtained from a steady-flow, thus

$$q = -\frac{\partial}{\partial x}\left(k \frac{\partial T^*}{\partial x}\right) \tag{10}$$

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.

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

$$\frac{\partial T}{\partial t} \simeq \frac{\Delta T}{\Delta t} + O(\Delta t) \tag{11}$$

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

4.2 Spatial Discretization

4.2.1 Finite Difference Schemes

Non-Conservative Formulation

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

$$\Delta T = \frac{\Delta t}{\rho C_p} \left.\frac{\partial k}{\partial x}\right|_i^n \left(\frac{T_{i+1}^n - T_{i-1}^n}{2\Delta x}\right) + \frac{k_i^n \Delta t}{\rho C_p} \left(\frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}\right) + \frac{q_i^n \Delta t}{\rho C_p} \tag{12}$$

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

Conservative Formulation

From Eq. (4), 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 to obtain

$$\left.\frac{\partial E}{\partial x}\right|_i^n = \frac{(k_{i+1}^n(T_{i+2}^n - T_i^n) - k_{i-1}^n(T_i^n - T_{i-2}^n))}{4\Delta x^2} \tag{13}$$

where E is the heat flow.

4.2.2 Finite Volume Schemes

Traditional Finite Volume Formulation

One of the second order central schemes used in these paper is the traditional conservative finite volume scheme, which uses second order in both the function and derivative. Thus, the scheme to the diffusive term takes the following form:

$$\left.\frac{\partial T}{\partial x}\right|_i^n = \frac{(T_{i-1}^n - T_i^n)(k_{i-1}^n + k_i^n) + (T_{i+1}^n - T_i^n)(k_i^n + k_{i+1})}{2\Delta x^2} \tag{14}$$

New Finite Volume Formulation - 0

This new formulation increases for fourth order only the internal derivative. Thus, the scheme to the diffusive term takes the following form

$$\begin{aligned}\left.\frac{\partial T}{\partial x}\right|_i^n &= \frac{-(k_{i-1}^n + k_i^n)(T_{i-2}^n - 27T_{i-1}^n + 27T_i^n - T_{i+1}^n)}{48\Delta x^2} \\ &+ \frac{(k_i^n + k_{i+1}^n)(T_{i-1}^n - 27T_i^n + 27T_{i+1}^n - T_{i+2}^n)}{48\Delta x^2}\end{aligned} \tag{15}$$

New Finite Volume Formulation - 1

The next new formulation increases to fourth order function only. Thus, the scheme to the diffusive term takes the following form

$$\begin{aligned}\left.\frac{\partial T}{\partial x}\right|_i^n &= \frac{(k_{i-2}^n - 9k_{i-1}^n - 9k_i^n + k_{i+1}^n)(T_i^n - T_{i-1}^n)}{16\Delta x^2} \\ &+ \frac{(k_{i-1}^n - 9k_i^n - 9k_{i+1}^n + k_{i+2}^n)(T_i^n - T_{i+1}^n)}{16\Delta x^2}\end{aligned} \tag{16}$$

New Finite Volume Formulation - 2

And the last new formulation increases to fourth order both function and first internal derivative. Thus, the scheme to the diffusive term takes the following form

$$\begin{aligned}\left.\frac{\partial T}{\partial x}\right|_i^n &= \frac{(k_{i-2}^n - 9k_{i-1}^n - 9k_i^n + k_{i+1}^n)(T_{i-2}^n - 27T_{i-1}^n + 27T_i^n - T_{i+1}^n)}{384\Delta x^2} \\ &- \frac{(k_{i-1}^n - 9k_i^n - 9k_{i+1}^n + k_{i+2}^n)(T_{i-1}^n - 27T_i^n + 27T_{i+1}^n - T_{i+2}^n)}{384\Delta x^2}\end{aligned} \tag{17}$$

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5. RESULTS

Following are results for finite difference schemes, finite volume schemes and spectral analysis. Noting that the graphs of finite difference schemes, the results dimensionless.

5.1 Finite Difference Schemes

First of all, we present the results of numerical order methods for second order of analytical and numerical non-conservative schemes.

Tables 1 and 2 show clearly derived growth with θ increasing. Using the analytical result for $\partial k/\partial x$, there is no variation order for all θ. However, when the numerical result for $\partial k/\partial x$ is used, it is possible to observe a loss of order more significant from $\theta = 40$. This demonstrates that the derivative product of the property and the potential is primarily responsible for the loss of order in evaluating the diffusive term when these derivatives become significant.

Table 1. Average and minimum error order. Analytical formulation.

NON-CONSERVATIVE ANALYTICAL		
Values of θ	**Minimum Order**	**Average Order**
10	1.97566	1.99991
20	1.99523	2.0027
30	1.99737	2.00629
40	1.99889	2.01142
50	2.00452	2.01995
60	2.03583	2.04693

Table 2. Average and minimum error order. Numerical formulation.

NON-CONSERVATIVE NUMERICAL		
Values of θ	**Minimum Order**	**Average Order**
10	1.9945	1.99697
20	1.98401	1.98804
30	1.96724	1.97305
40	1.94532	1.95209
50	1.91584	1.92586
60	1.88857	1.90021

5.1.1 Conservative Formulation

The results presented below are for the conservative finite difference schemes.

The oscillation that one perceives in the conservative finite difference scheme 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. 1, the method is very unstable, causing even for larger values of θ, oscillation in the solution.

5.2 Finite Volume Schemes

Traditional Finite Volume Formulation

Continuing, results are presented for the finite volume conservative scheme. Where noted in Fig. 2 further loss of order and oscillation in the variable property region to $\theta = 50$.

New Finite Volume Formulation - 0

The following results first new finite volume formulation. We can see in Fig 3, there is a loss of order greater when $\theta = 50$, mainly in the variable property region.

New Finite Volume Formulation - 1

The following results second new finite volume formulation in Fig 4. Where we can see that for $\theta = 40$ there is a loss in variable property region and also for $\theta = 90$ but for that value of θ observed a loss of order in the first half of the domain.

New Finite Volume Formulation - 2

The following results third new finite volume formulation. As in the previous formulation, we also observed in Fig 5

ISSN 2176-5480

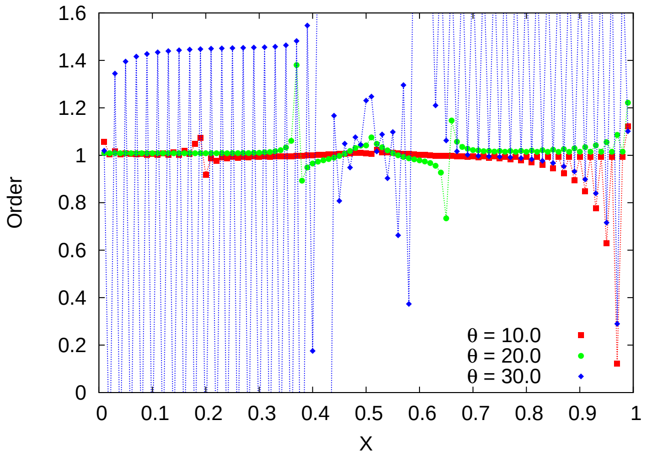

Figure 1. Numerical Order. Finite Difference Formulation.

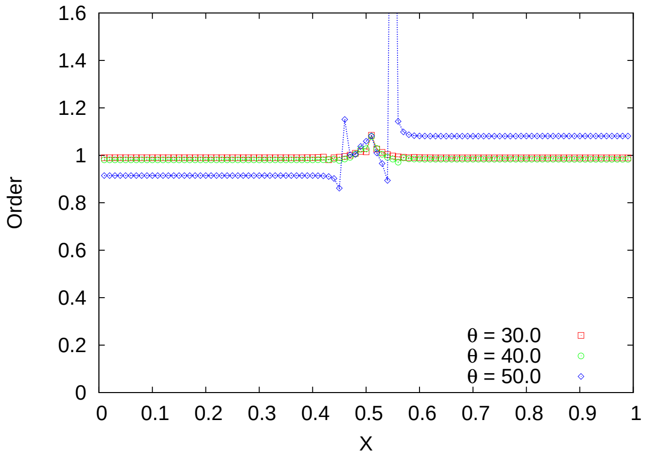

Figure 2. Numerical Order. Finite Volume Formulation.

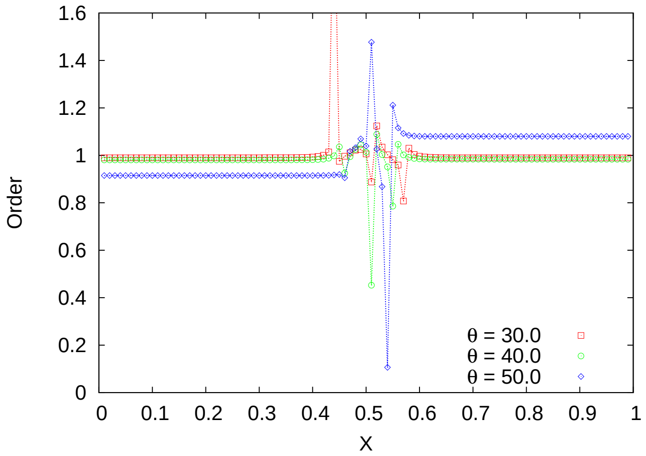

Figure 3. Numerical Order. New Finite Difference Formulation - 0.

loss order for the same values of θ, being larger in this formulation in the region where the property changes.

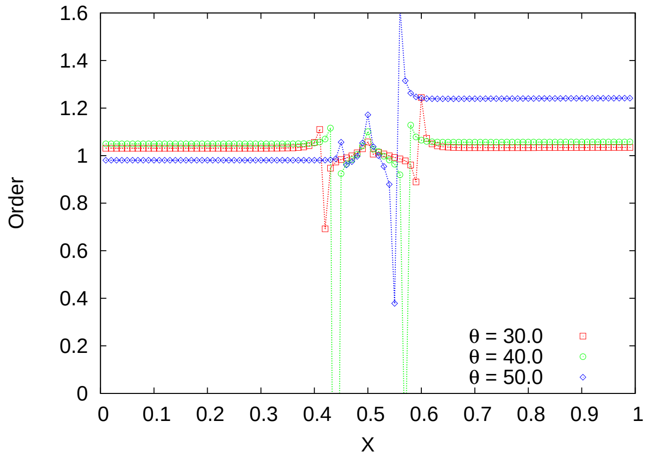

Figure 4. Numerical Order. New Finite Difference Formulation - 1.

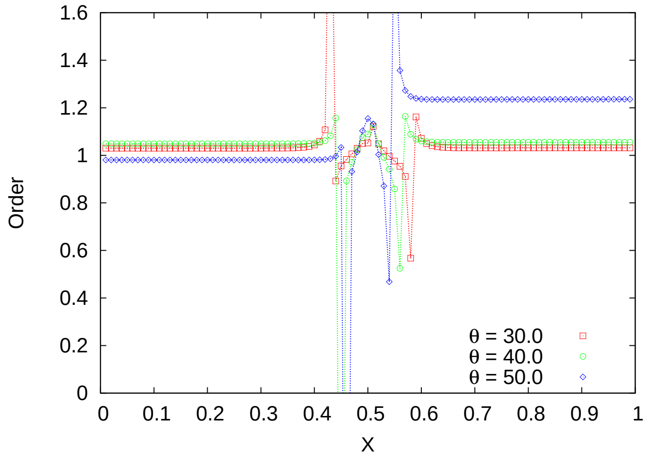

Figure 5. Numerical Order. New Finite Difference Formulation - 2.

5.3 Spectral Analysis

Figure 6 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. When we look at the new finite difference schemes, we note that they are equivalent, except for the first, which provides best result, ie, best approached the curve K^2

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 new finite volumes formulations showed some stability in the calculation of numerical order, except for some cases in the region variable property. Furthermore, the new finite volume formulation - 1 presented better modified wave numbers. We conclude that after all this study, the new finite volume formulation - 1 proposed in this paper, which was, in general, showed better results. For a continuation of this study, we will analyze the computational cost and an extension to fourth order analysis.

7. ACKNOWLEDGEMENTS

The authors would like to acknowledge the financial support of CAPES/Brazil and Universidade Federal Fluminense.

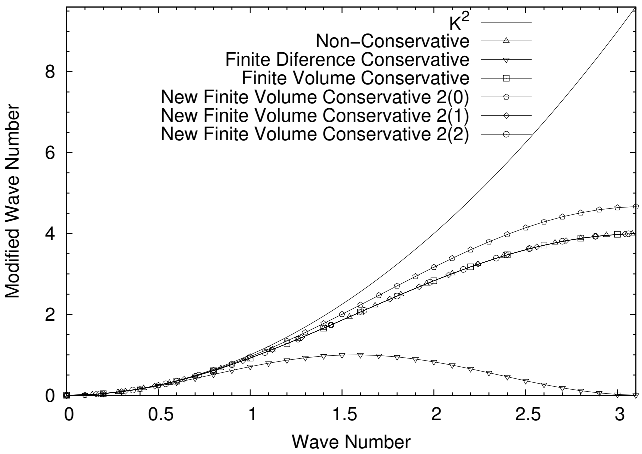

Figure 6. Modified wave number described as wave number, for second derivative

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