Optimized Compact Scheme with High Order of Accuracy Using Maximum Norm

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Abstract
Compact finite difference schemes have high order of accuracy and high numerical resolution. Because of such characteristics, these schemes are suitable for numerical simulation of multi-scale phenomena, like direct numerical simulation, large eddy simulation and computational aeroacoustics. In this paper, we intend to optimize pentadiagonal compact schemes with a seven point stencil, using maximum error norm with different error threshold. The second goal of this paper is to increase the order of accuracy of the optimized schemes, because optimized schemes with higher order of accuracy resolve large scales better than the lower order ones. Finally, by using numerical experiments, we investigate the order of accuracy and numerical resolution of the new optimized compact schemes.

Keywords: Compact finite difference scheme, Optimized scheme, Numerical dispersion, Maximum norm, High resolution, Direct numerical simulation, Computational aeroacoustics.

Introduction

Multi-scale phenomena are common in many physical and engineering fields like aerodynamics and astrophysics. Turbulence is an important of multi-scale phenomena and direct numerical simulation (DNS) and large eddy simulation (LES) are useful tools to study this problem and understand its underlying physical mechanisms. Another example of such phenomena is aerodynamically generated noise and computational aeroacoustics (CAA). Multi-scale phenomena contain a wide range of time- and length-scales and the largest scale can be orders of magnitude larger than the smallest scales, for example in aeroacoustics problems amplitude of acoustic waves are very small in comparison to mean flow and sound intensity can be five or six order of magnitude smaller [18].

To correctly resolve small scales in numerical simulation of multi-scale phenomena, numerical scheme should have high order of accuracy and high numerical resolution. Another issue in numerical simulation of multi-scale phenomena marginally resolved scales because error from such scales may affect whole computation. To resolve these scales more accurately, the numerical resolution at higher wavenumbers should be increased and optimization of numerical error is a useful method to achieve this goal, but it comes at the expense the order of accuracy of the scheme. Compact schemes are popular and widely used high order and high resolution numerical schemes. Application of compact schemes in computational fluid dynamics (CFD) can be traced back to 1970s [1-4]. Lele [8] proposed a series of compact schemes for derivatives, filtering and interpolation and by using Fourier analysis, showed their spectral-like resolution for a certain range of wavenumbers. Lele also proposed equating modified wavenumber and wavenumber at certain wavenumbers as a method to optimize dispersion error of compact schemes. Tam and Webb [9] proposed the dispersion relation preserving (DRP) scheme and they used an integrated error to form a minimization problem to optimize the dispersion error of an explicit finite difference scheme with a seven point stencil. Kim and Lee [10] used DRP idea to a seven point pentadiagonal compact scheme with second and fourth order of accuracy and later they [11] developed a series of optimized boundary stencils for their optimized compact scheme. Zhuang and Chen [15] developed an optimized fourth order upwind DRP scheme for CAA applications. Bogey and Bailly [19] and Tam [18] extended the stencil size of DRP scheme from seven to nine, eleven, thirteen and fifteen points and the increase in the size of stencil resulted in more numerical resolution at higher wavenumbers.

Chu and Fan [13] and Mahesh [14] independently introduced combined compact schemes. This new family of compact schemes compute the first and second derivatives together and has better numerical resolution. Lui and Lele [16] used Lele [] optimization method to develop a sixth order pentadiagonal compact scheme. Ashcroft and Zhang [17] optimized a five point, fourth order prefactored compact scheme with two independent bidiagonal matrices. Jordan [21] introduced a new method for optimization of compact scheme. Instead of using a Fourier analysis this new method uses a composite template and unlike the Fourier transform, this template analysis the resolution of the whole matrix, including the boundary schemes, and gives a sets of pseudo-wavenumbers for each point. Jordan used these sets and a least square optimization to determine the coefficients of the new optimized scheme and later used the same method to optimize a pentadiagonal compact scheme [26].

Kim [20] introduced a new fourth order optimized pentadiagonal compact scheme and used a combination of polynomials and trigonometric series to formulate extrapolation function for optimization of new boundary schemes with better resolution. Later, Kim and Sandberg [27], Haeri and Kim [28] and Turner et al. [33] introduced new methods for optimization of boundary schemes for fourth order optimized pentadiagonal compact schemes and efficient parallel computation using domain decomposition. Liu et al. [22] used a sequential quadratic programming (SQP) to optimize a fourth order pentadiagonal compact scheme and its boundary schemes. Following Holberg [7], Venutelli [24] used minimization of the group velocity error to optimize fourth and sixth order staggered pentadiagonal schemes. Zhou and Zhang [25] introduced an optimized prefactored compact scheme for the second derivative. Yu et al. [31] developed a fifth order optimized version of combined compact scheme [13-14] to solve advection equation.

Recently, Zhang and Yao [29] used simulated annealing algorithm [6] to optimize zeroth order explicit finite difference scheme with a specified error threshold for maximum norm of error. They showed by this new method one can optimize error more flexibly and increase the cutoff wavenumber. Cunha and Redonnet [30] investigated effect of reduced order of accuracy on performance of DRP schemes. They showed the reduction of the order of accuracy may cause error in larger scales and therefore is harmful when such scales are important in final analysis. To solve this problem they proposed the usage of optimized schemes with higher order of accuracy and later, they proposed a new approach for optimization of explicit finite difference schemes and two optimized scheme with sixth and eighth order of accuracy [32].

In this paper we intend to optimize compact pentadiagonal finite difference schemes by using maximum error norm and increase their order of accuracy to six and eight. In the second section of paper, we introduce the compact pentadiagonal finite difference scheme and analyze its numerical dispersion error by using Fourier analysis. Later we introduce optimization procedure by using maximum error norm and use this procedure to determine the coefficients of the optimized scheme. In the third section we use numerical experiments to assess the order of accuracy and numerical resolution of the optimized schemes.

Numerical Scheme

A compact pentadiagonal scheme with a seven point stencil is a linear combination as,

$$\beta f'_{i-2} + \alpha f'_{i-1} + f'_i + \alpha f'_{i+1} + \beta f'_{i+2} = \frac{a_1}{h}(f_{i+1} - f_{i-1}) + \frac{a_2}{h}(f_{i+2} - f_{i-2}) + \frac{a_3}{h}(f_{i+3} - f_{i-3}). \quad (1)$$

Tridiagonal and explicit approximation can be achieved in Eq. (1) by setting $\beta = 0$ and $\beta = \alpha = 0$ respectively. By matching Taylor series coefficients of different truncation error terms, one can determine the relations between coefficients of Eq. (1) these relations are:

$$2\alpha + 2\beta = 2a_1 + 4a_2 + 6a_3 - 1, \quad (2)$$

$$\alpha + 4\beta = \frac{1}{3}a_1 + \frac{8}{3}a_2 + 9a_3, \quad (3)$$

$$\frac{1}{12}\alpha + \frac{4}{3}\beta = \frac{1}{60}a_1 + \frac{8}{15}a_2 + \frac{81}{20}a_3, \quad (4)$$

$$\frac{1}{360}\alpha + \frac{8}{45}\beta = \frac{1}{2520}a_1 + \frac{16}{315}a_2 + \frac{243}{280}a_3, \quad (5)$$

$$\frac{1}{20160}\alpha + \frac{4}{315}\beta = \frac{1}{181440}a_1 + \frac{8}{2835}a_2 + \frac{243}{2240}a_3. \quad (6)$$

Solving Eqs. (2)-(6) gives a unique set of coefficients for a tenth-order pentadiagonal compact finite difference scheme.

Error analysis by Fourier transformation

Fourier analysis is an effective tool for analyzing and comparing numerical error of different finite difference and its application for such analysis is extensively described in [8]. Fourier analysis is also an effective method to quantify numerical resolution of different numerical schemes and its results can be used for error optimization [8, 9].
Fourier transformation and its inverse have the following form

$$\tilde{f}(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x)\, e^{-Ikx} dx, \quad (7)$$

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{-Ikx} dk. \tag{8}$$

$\tilde{f}(k)$ is the Fourier transformation of $f(x)$, k is the wavenumber and $I = \sqrt{-1}$. By taking Fourier transformation of Eq. (1), modified wavenumber is obtained as

$$w' = 2\frac{a_1 \sin(w) + a_2 \sin(2w) + a_3 \sin(3w)}{1 + 2\alpha \cos(w) + 2\beta \cos(2w)}, \tag{9}$$

where $w = k\Delta x$ and $w' = k'\Delta x$ are scaled wavenumber and scaled modified wavenumber, respectively. To measure the numerical error, $|w' - w|$ and $\frac{|w'-w|}{w}$ can be defined as the absolute and relative measures of error, respectively [8, 29].

Optimization procedure

Although compact schemes have good numerical resolution in low wavenumber range, but their resolution deteriorates as wavenumber increases. One can use an optimization procedure to increase the numerical resolution of the numerical scheme. To achieve this goal, the scaled modified wavenumber should a give a better approximation of scaled wavenumber at high wavenumbers. Tam and Webb suggested using an integrated error to form a minimization problem for dispersion error and solving this problem will lead to reduced dispersion error in the integration range.

Lele [8] proposed an alternative method for optimization of dispersion error. In this method instead of using integrated error, w' sets to be equal to w at certain wavenumbers, this will lead to new equations as

$$2a_1 \sin(w_j) + 2a_2 \sin(2w_j) + 2a_3 \sin(3w_j) - 2\alpha w_j \cos(w_j) - 2\beta w_j \cos(2w_j) = w_j. \tag{10}$$

By solving these new equations, one can determine some or all of coefficients in Eq. (1) and desired goal for optimization can be achieved by try and error. Zhang and Yao [29] used this method and a simulated annealing algorithm [6] to determine the coefficients of the optimized finite difference scheme by the error tolerance threshold, ε, as the maximum norm of the dispersion error.

In this paper, we used Lele's method [8] for optimization of the numerical error. We found try and error is a fast and easy way to optimize the compact finite difference scheme by maximum norm of error and therefore we did not use any other extra algorithm for optimization, like the usage of simulated annealing algorithm by Zhang and Yao [29]. Optimization of numerical comes at expense of the order of accuracy, because equations like Eq. (10) should be used to determine some of coefficients in Eq. (1) instead of using Eqs. (2)-(6). Cunha and Redonnet [30] showed this reduction of the order of accuracy can result in considerable error in lower wavenumber range and therefore optimized schemes with increased order of accuracy may be needed. Table 1 to Table 3 show coefficients of optimized fourth, sixth and eighth order scheme with different error thresholds, and we determined these coefficients by using Eqs. (2)-(5) and Eq. (10).

Table 1 Coeffients of fourth order optimized scheme with different error treshold

	$\varepsilon = 10^{-2}$	$\varepsilon = 10^{-3}$	$\varepsilon = 10^{-4}$
α	0.6082258801733940	0.5799409399256260	0.5562135732927600
β	0.1119841895552910	0.0913025587073633	0.0767799831080962
a_1	0.6226500993288040	0.6488542583945110	0.6691663401223610
a_2	0.2832201917744050	0.2514903896275570	0.2253610769453380
a_3	0.0103731956170232	0.0064694869944544	0.0043683541292728

Table 2 Coeffients of sixth order optimized scheme with different error treshold

	$\varepsilon = 10^{-2}$	$\varepsilon = 10^{-3}$	$\varepsilon = 10^{-4}$
α	0.5763671534480410	0.5538290120198530	0.5365894666122440
β	0.0873786847225768	0.0746214733595378	0.0659778177265754
a_1	0.6523994549163750	0.6717832954024240	0.6847527593400610
a_2	0.2476871227189510	0.2224843288821100	0.2043581271773250
a_3	0.0053240459387800	0.0038995107375816	0.0030327568813695

Table 3 Coeffients of eighth order optimized scheme with different error treshold

	$\varepsilon = 10^{-2}$	$\varepsilon = 10^{-3}$	$\varepsilon = 10^{-4}$
α	0.5367930568824080	0.5241025757235620	0.5157437214861430
β	0.0647172227529633	0.0596410302894250	0.0562974885944574
a_1	0.6868707168185950	0.6942734974945880	0.6991494957997490
a_2	0.2031640938486790	0.1911504383516390	0.1832373896735490
a_3	0.0027704583731389	0.0023897439383735	0.0021389783112510

Figure 1 to Figure 3 shows the absolute error of w' with different error thresholds for fourth, sixth and eighth order optimized schemes, respectively. We also plot the absolute error of w' for the original tenth order compact scheme. By comparing plots in different figures, we can conclude each optimized scheme has better resolution than the original scheme in higher wavenumbers.

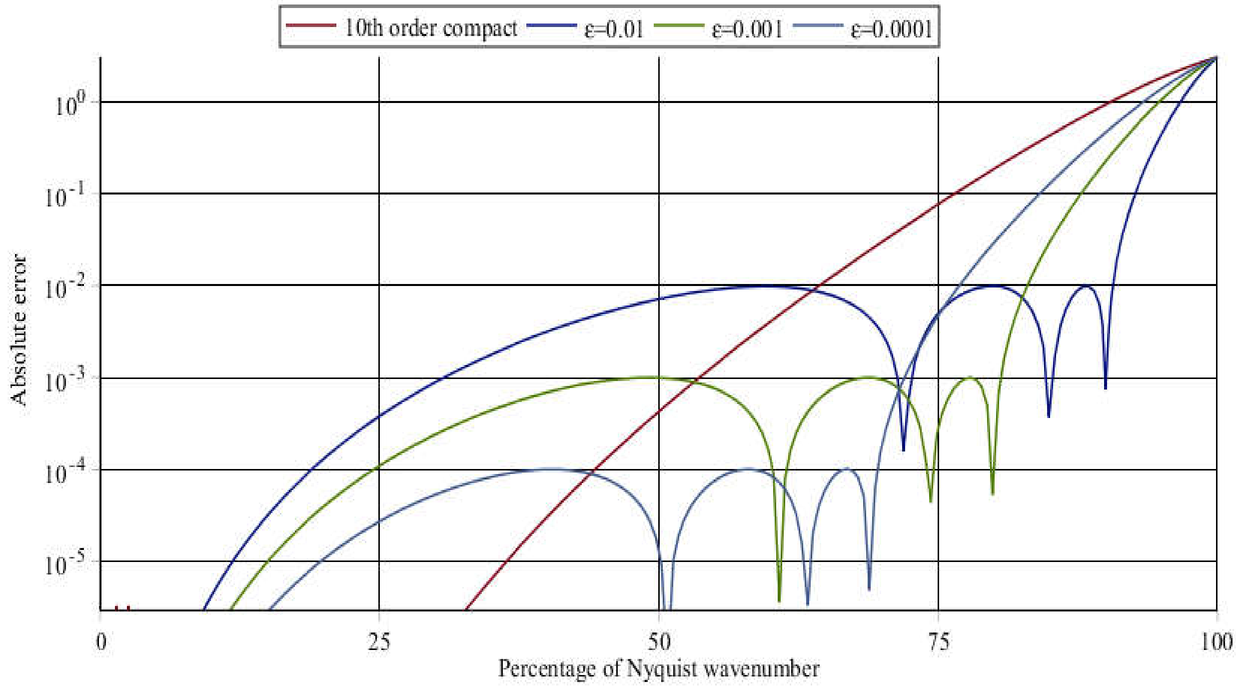

Figure 1 absolute error of w' for optimized fourth order schemes with different error threshold.

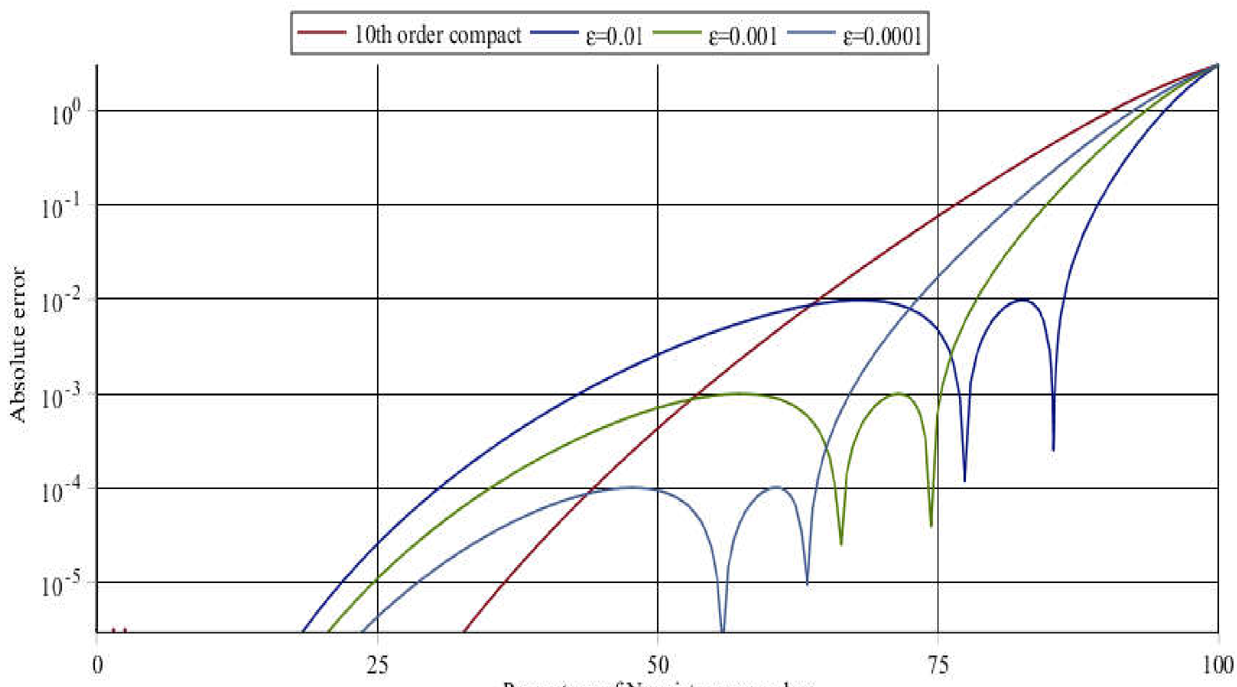

Figure 2 absolute error of w' for optimized sixth order schemes with different error threshold.

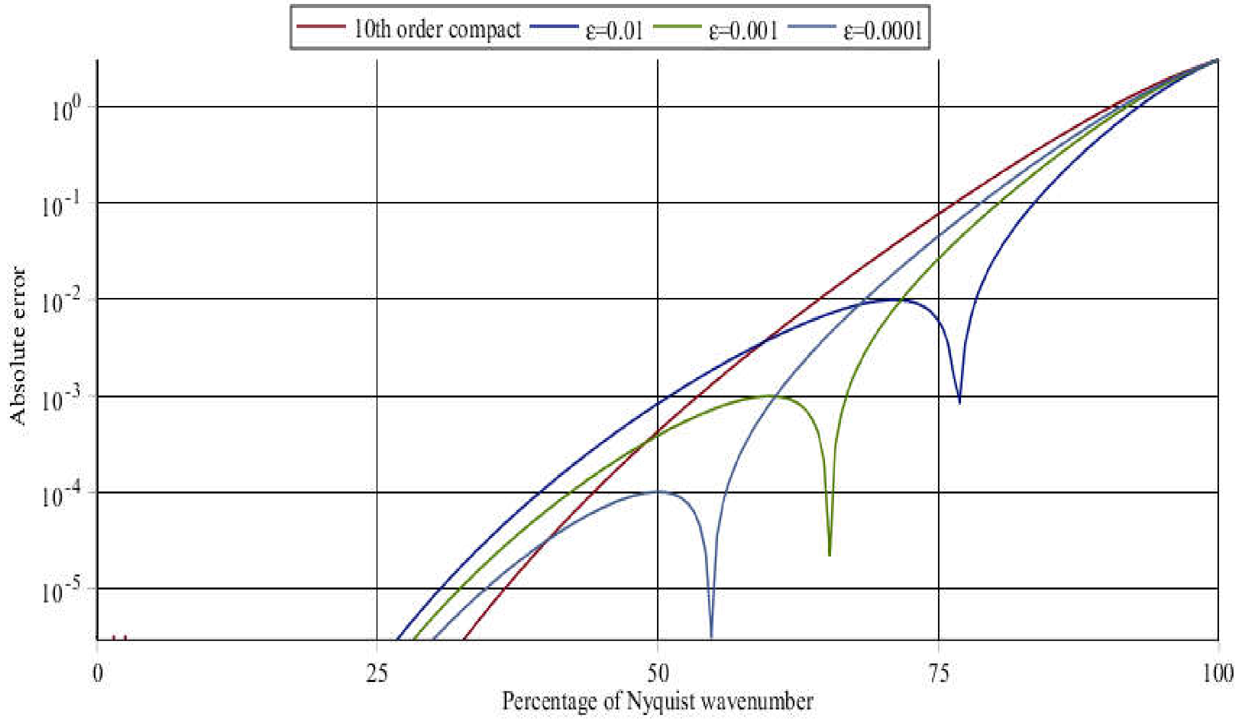

Figure 3 absolute error of w' for optimized eighth order schemes with different error threshold.

Numerical results

In this section we use numerical experiments to test the order of accuracy. To achieve this goal, we numerically solve a wave equation as

$$\frac{\partial u}{\partial t}+\frac{\partial u}{\partial x}=0, \qquad -1\leq x\leq 1. \tag{11}$$

The boundary conditions of this equation are periodic, and its initial condition is

$$u(t=0)=\sin(2\pi x), \tag{12}$$

which leads to an exact solution as

$$u(t)=\sin(2\pi(x-t)). \tag{13}$$

We use a forth order ten stage strong stability preserving (SSP) Runge-Kutta method [23] for time integration. The CFL number of fourth, sixth and eighth order schemes are 0.4, 0.05 and 0.01, respectively. The reason behind CFL number reduction for sixth and eighth order schemes is to reduce the effect time discretization error.

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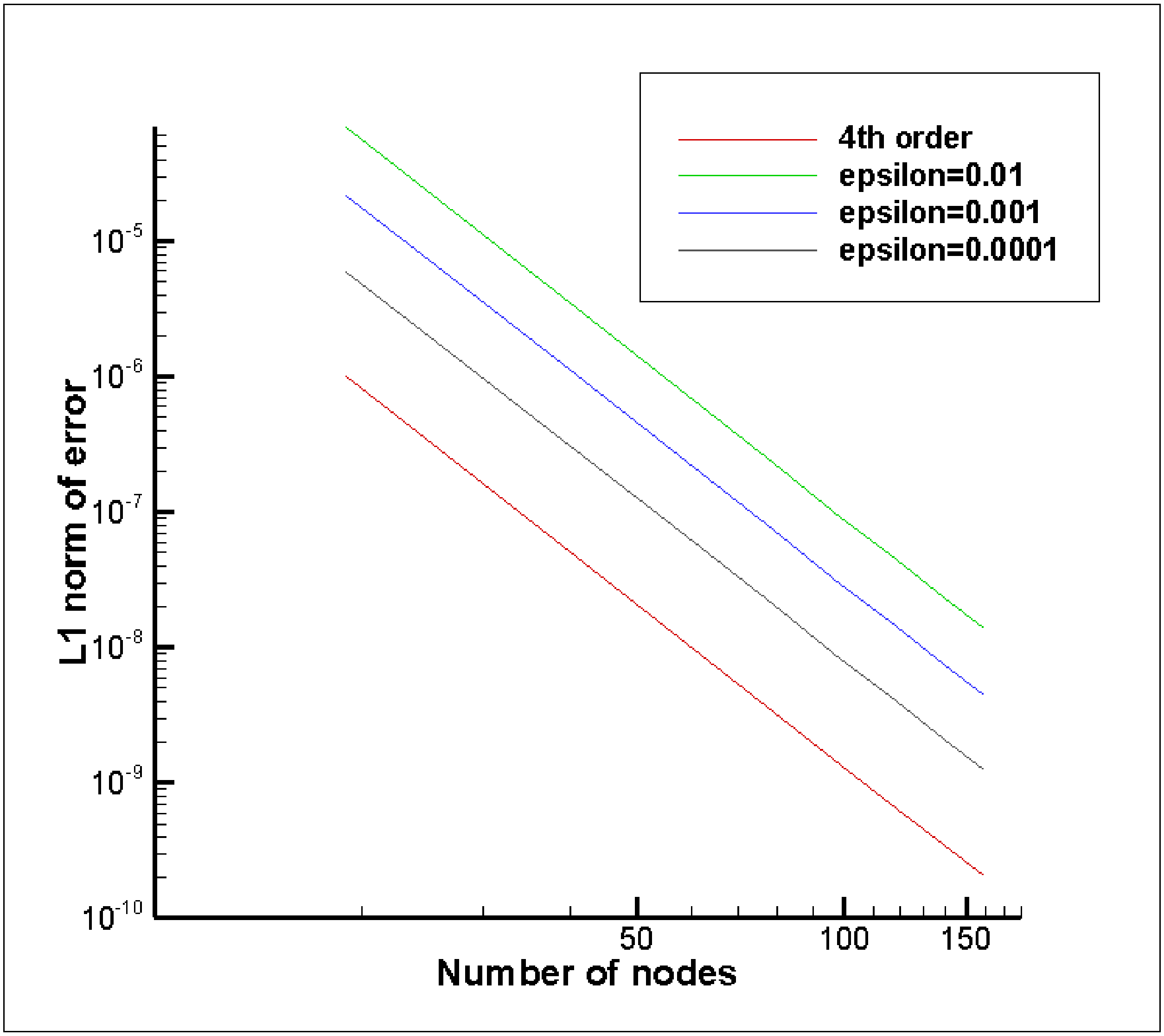

Figure 4 Convergence of L1 norm of error for fourth order optimized schemes with different error thresholds.

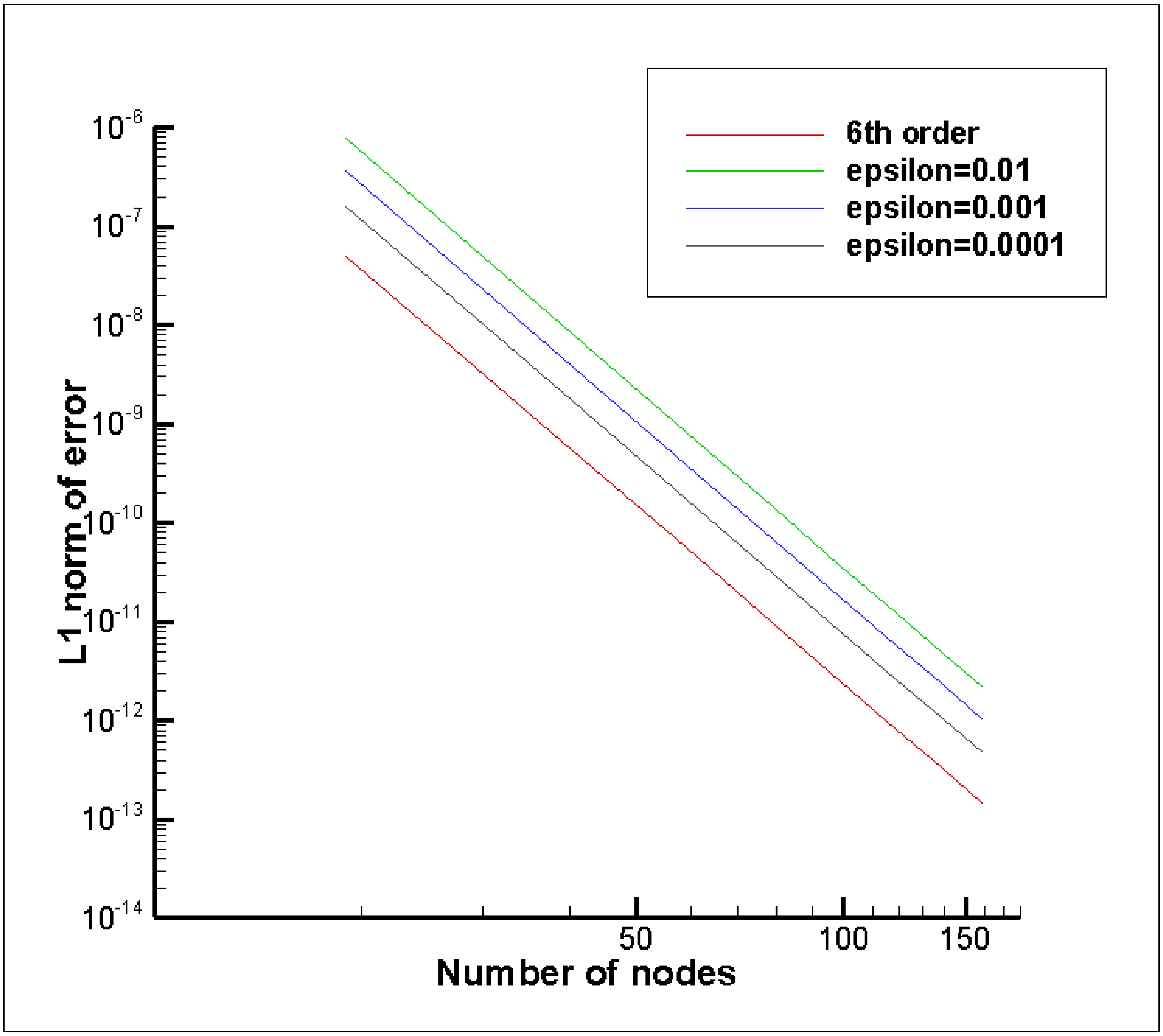

Figure 5 Convergence of L1 norm of error for sixth order optimized schemes with different error thresholds.

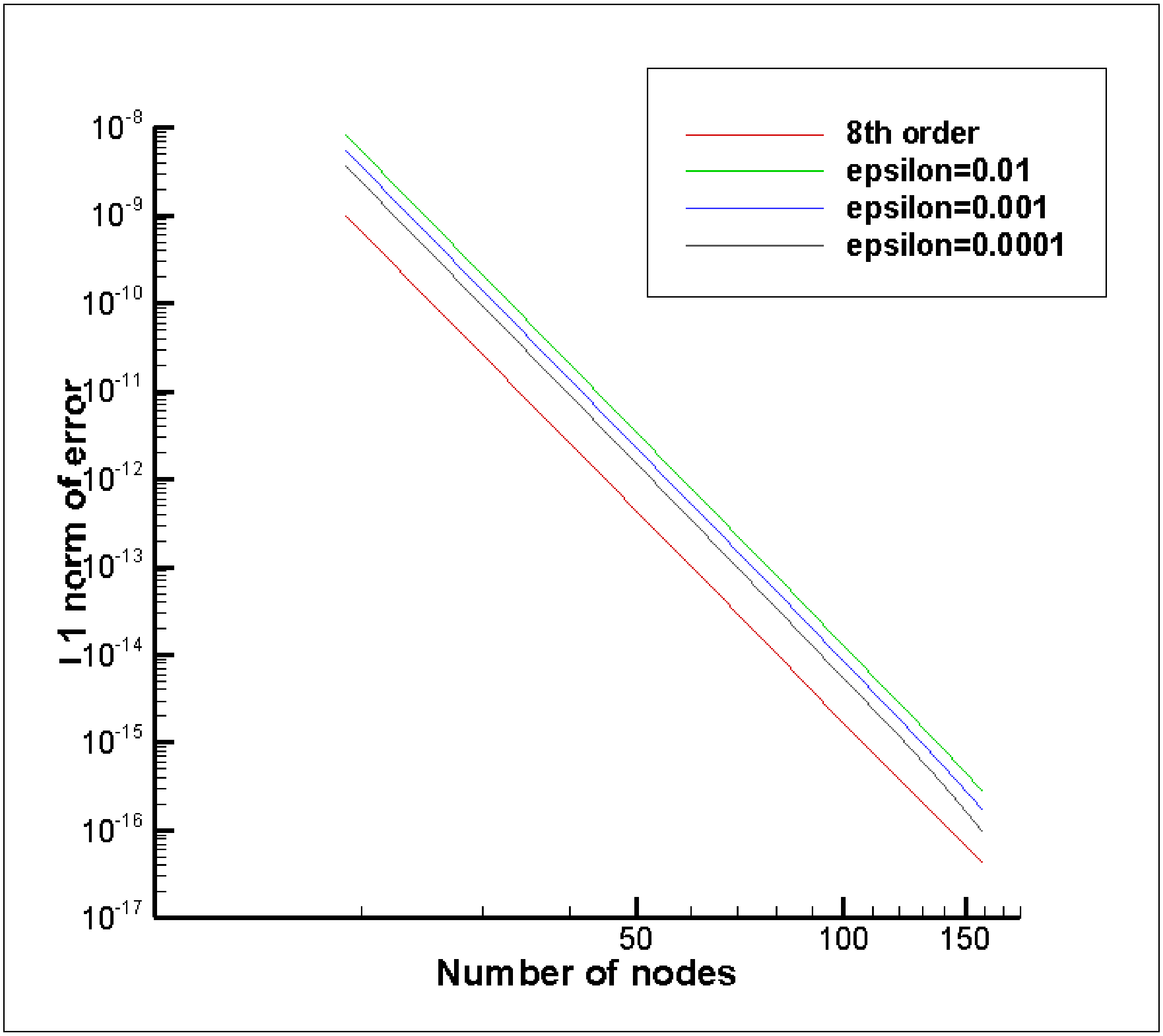

Figure 6 Convergence of L1 norm of error for eighth order optimized schemes with different error thresholds.

Figure 4 to Figure 6 show results of convergence test by solving Eq. (11) for optimized fourth, sixth and eighth order schemes by different error threshold. By considering these plots, we can say all of optimized schemes achieved their nominal order of accuracy and in group of optimized schemes with same order of accuracy, schemes with smaller error threshold have lower error.

Conclusion

In this paper we optimized compact pentadiagonal finite difference schemes by using maximum error norm and different error thresholds. The optimized schemes have fourth, sixth and eighth order of accuracy. We used numerical experiments to investigate the order of accuracy and numerical resolution of optimized schemes. Based upon results of these experiments we can say all schemes achieved their designed order of accuracy and schemes with smaller error threshold have better numerical resolution and lower error in convergence tests.

References

[1] Hirsh, R. S. (1975). Higher order accurate difference solutions of fluid mechanics problems by a compact differencing technique. *Journal of computational physics*, **19**(1), 90-109.

[2] Adam, Y. (1975). A hermitian finite difference method for the solution of parabolic equations. *Computers & Mathematics with Applications*, **1**(3-4), 393-406.

[3] Adam, Y. (1977). Highly accurate compact implicit methods and boundary conditions. *Journal of Computational Physics*, **24**(1), 10-22.

[4] Rubin, S. G., & Khosla, P. K. (1977). Polynomial interpolation methods for viscous flow calculations. *Journal of Computational Physics*, **24**(3), 217-244.

[5] Vichnevetsky, R., & Bowles, J. B. (1982). *Fourier analysis of numerical approximations of hyperbolic equations*. Society for Industrial and Applied Mathematics.

[6] Kirkpatrick, S., Gelatt, C. D., & Vecchi, M. P. (1983). Optimization by simulated annealing. *Science*, **220**(4598), 671-680.

[7] Holberg, O. (1987). Computational aspects of the choice of operator and sampling interval for numerical differentiation in large-scale simulation of wave phenomena. *Geophysical prospecting*, **35**(6), 629-655.

[8] Lele, S. K. (1992). Compact finite difference schemes with spectral-like resolution. *Journal of computational physics*, **103**(1), 16-42.

[9] Tam, C. K., & Webb, J. C. (1993). Dispersion-relation-preserving finite difference schemes for computational acoustics. *Journal of computational physics*, **107**(2), 262-281.

[10] Kim, J. W., & Lee, D. J. (1996). Optimized compact finite difference schemes with maximum resolution. *AIAA journal*, **34**(5), 887-893.

[11] Kim, J. W., & Lee, D. J. (1997). Implementation of boundary conditions for optimized high-order compact schemes. *Journal of Computational Acoustics*, **5**(02), 177-191.

[12] Baeder, L. T. T. J. D. (1997). Uniformly accurate compact difference schemes. *AIAA paper* 1997-2093.

[13] Chu, P. C., & Fan, C. (1998). A three-point combined compact difference scheme. *Journal of Computational Physics*, **140**(2), 370-399.

[14] Mahesh, K. (1998). A family of high order finite difference schemes with good spectral resolution. *Journal of Computational Physics*, **145**(1), 332-358.

[15] Zhuang, M., & Chen, R. F. (1998). Optimized upwind dispersion-relation-preserving finite difference scheme for computational aeroacoustics. *AIAA journal*, *36*(11), 2146-2148.

[16] Lui, C., & Lele, S. (2001). Direct numerical simulation of spatially developing, compressible, turbulent mixing layers. In *39th Aerospace Sciences Meeting and Exhibit* (p. 291).

[17] Ashcroft, G., & Zhang, X. (2003). Optimized prefactored compact schemes. *Journal of computational physics*, **190**(2), 459-477.

[18] Tam, C. K. (2004). Computational aeroacoustics: an overview of computational challenges and applications. *International Journal of Computational Fluid Dynamics*, **18**(6), 547-567.

[19] Bogey, C., & Bailly, C. (2004). A family of low dispersive and low dissipative explicit schemes for flow and noise computations. *Journal of Computational physics*, **194**(1), 194-214.

[20] Kim, J. W. (2007). Optimised boundary compact finite difference schemes for computational aeroacoustics. *Journal of Computational Physics*, **225**(1), 995-1019.

[21] Jordan, S. A. (2007). The spatial resolution properties of composite compact finite differencing. *Journal of Computational Physics*, **221**(2), 558-576.

[22] Liu, Z., Huang, Q., Zhao, Z., & Yuan, J. (2008). Optimized compact finite difference schemes with high accuracy and maximum resolution. *International journal of aeroacoustics*, **7**(2), 123-146.

[23] KETCHESON, D.I. (2008). HIGHLY EFFICIENT STRONG STABILITY-PRESERVING RUNGE–KUTTA METHODS WITH LOW-STORAGE IMPLEMENTATIONS. *SIAM Journal of Scientific Computation*, **30**(4), 2113–2136.

[24] Venutelli, M. (2011). Holberg's optimisation for high-order compact finite difference staggered schemes. *International Journal of Computational Fluid Dynamics*, **25**(5), 287-296.

[25] Zhou, H., & Zhang, G. (2011). Prefactored optimized compact finite-difference schemes for second spatial derivatives. *Geophysics*, **76**(5), WB87-WB95.

[26] Jordan, S. A. (2011). Optimization, resolution and application of composite compact finite difference templates. *Applied Numerical Mathematics*, **61**(1), 108-130.

[27] Kim, J. W., & Sandberg, R. D. (2012). Efficient parallel computing with a compact finite difference scheme. *Computers & Fluids*, **58**, 70-87.

[28] Haeri, S., & Kim, J. W. (2013). Implementation of genetic algorithm for the optimization of boundary characteristics of compact finite difference schemes, *Submitted to Computer Methods in Applied Mathematics and Engineering*.

[29] Zhang, J. H., & Yao, Z. X. (2013). Optimized explicit finite-difference schemes for spatial derivatives using maximum norm. *Journal of Computational Physics*, **250**, 511-526.

[30] Cunha, G., & Redonnet, S. (2014). On the effective accuracy of spectral-like optimized finite-difference schemes for computational aeroacoustics. *Journal of Computational Physics*, **263**, 222-232.

[31] Yu, C. H., Wang, D., He, Z., & Pähtz, T. (2015). An optimized dispersion–relation-preserving combined compact difference scheme to solve advection equations. *Journal of Computational Physics*, **300**, 92-115.

[32] Cunha, G., & Redonnet, S. (2015). A novel optimization technique for explicit finite-difference schemes with application to AeroAcoustics. *International Journal for Numerical Methods in Fluids*, **78**(4), 189-216.

[33] Turner, J. M., Haeri, S., & Kim, J. W. (2016). Improving the boundary efficiency of a compact finite difference scheme through optimising its composite template. *Computers & Fluids*, **138**, 9-25.