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Original Paper

# New approaches to numerical differentiation for second and third order

Çiğdem Dinçkal[a]

[a]*Faculty of Engineering and Natural Sciences, Ankara Medipol University, Ankara and 06570, Turkey.*

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ABSTRACT

In this article, new numerical methods for calculation of second and third order derivatives are designed by using basic finite difference methods; forward, central and backward finite difference approaches. Those approaches are originally derived from the well-known Taylor series. Main advantage of new numerical formulas (named as Improved Backward Finite Difference Method, Improved Forward Finite Difference Method) is that they produce more accurate numerical results with smaller step size than the well-known backward and forward finite difference methods. For this purpose, some numerical examples are given to compare these new formulas with the traditional finite difference methods; backward and forward. The performance of the new methods in terms of error analysis and elapsed time for both second and third order derivative computations is also presented.

## I. INTRODUCTION

Numerical differentiation is one of the most significant concepts in calculus, which has been everywhere in many fields of applied mathematics and engineering.

There are several methods to treat the numerical differentiation issue. The most widely and commonly preferred method for solving numerical differentiation problems is finite difference method. Since numerical differentiation is an ill-posed problem by means of Hadamard [1-3]. For this reason, Tikhonov regularization method [3] and mollification method [4] have been proposed. Besides, Hanke and Scherzer [5] and Wang et al. [6, 7] have proposed techniques for many ill-posed problems. Nevertheless, most results in literature are sure about f'(x) (first order derivative).

Furthermore, traditional finite difference methods [7-9] are widely used but often face challenges, particularly with ill-posed problems. To address this, the article introduces "Improved Forward Finite Difference" (FFD_improved) and "Improved Backward Finite Difference" (BFD_improved) techniques, which are derived from Taylor series expansions to provide more precise results than standard methods. This is one of the novel sides. There are also some works which employed interpolation methods to compute numerical differentiations [10-13]. Jianping L used Vandermonde determinant for computation of differentiation [14]. Numerical differentiation was performed by use of noisy data in mechanical engineering [15-19]. Yang et al also achieved differentiation by use of higher order spatial discretization method [20].

* Corresponding author. Tel.: 4442010; e-mail: cigdem.dinckal@ankaramedipol.edu.tr

Instead of all these methods in literature, this study presents more straightforward and precise methods with use of basic finite difference methods for second and third order derivative calculations of any functions. The proposed methods for second and third order derivatives are the combinations of Backward with Central Finite Difference and Forward with Central Finite Difference methods.

The article is organized as follows: theoretical background is given in section 2. Proposed methods are given in section 3. Numerical results are presented for comparison purposes in section 4. Finally, results are discussed.

## II. EXPERIMENTAL METHOD / TEORETICAL METHOD

The originating idea of finite difference techniques is based on the well-known Taylor series. The form of the Taylor series by defining a step size $h = x_{i+1} - x_i$ and expressing as [7]

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_{i,})}{2!}h^2 + \frac{f^{(3)}(x_{i,})}{3!}h^3 + \cdots + \frac{f^{(n)}(x_{i,})}{n!}h^n + R_n. \tag{1}$$

Where the remainder term is defined as

$$R_n = \frac{f^{(n+1)}(\varepsilon_1)}{(n+1)!}h^{n+1}. \tag{2}$$

The term in eq (2) corresponds to $O((x_{i+1} - x_i)^{n+1})$ which is $O(h^{n+1})$ called as error. For backward form, Taylor series in eq (1) can be rewritten as

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots \tag{3}$$

One of the ways to approximate the first derivative is to subtract eq (3) from the Taylor series expansion in eq (1) to obtain:

$$f(x_{i+1}) = f(x_{i-1}) + 2f'(x_i)h + \frac{2f^{(3)}(x_i)}{3!}h^3 + \cdots \tag{4}$$

This can be solved for

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{f^{(3)}(x_i)}{3!}h^2 - \cdots \tag{5}$$

Eq (5) can be also expressed as

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2). \tag{6}$$

Error is of the order of $h^2$, even though the forward and backward approximations that are of the order of $h$. Therefore, Taylor series approximations yield the practical information that the centered difference is the most accurate representation of the derivative.

Level of accuracy depends on both decreasing the step size and the number of terms of the Taylor series.

By substituting first order derivative in eq (6) into eq (1), centered finite difference (CFD) representation of the second order derivative based on error $O(h^2)$ can be found as

$$f''(x_i) = \frac{f(x_{i+1}) - 2\mathrm{f}(x_i) + f(x_{i-1})}{h^2}. \tag{7}$$

Third order derivative based on error $O(h^2)$:

$$f^{(3)}(x_i) = \frac{f(x_{i+2}) - 2\mathrm{f}(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}. \tag{8}$$

With similar way, first derivative by Forward Finite Difference (FFD) based on O(h) is

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h). \tag{9}$$

Second order derivative by FFD based on $O(h)$ can be written as

$$f''(x_i) = \frac{f(x_{i+2}) - 2\mathrm{f}(x_{i+1}) + f(x_i)}{h^2}. \tag{10}$$

Third order derivative by FFD based on $O(h)$ can be written as

$$f^{(3)}(x_i) = \frac{f(x_{i+3}) - 3\mathrm{f}(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}. \tag{11}$$

Similarly, the first derivative by Backward Finite Difference (BFD) based on O(h) is

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h). \tag{12}$$

Second order derivative by BFD based on $O(h)$ can be written as

$$f''(x_i) = \frac{f(x_i) - 2\mathrm{f}(x_{i-1}) + f(x_{i-2})}{h^2}. \tag{13}$$

Third order derivative by BFD based on O($h$) can be written as

$$f^{(3)}(x_i) = \frac{f(x_i) - 3\mathrm{f}(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}. \tag{14}$$

By employing eq (6) and combining with eq (12), Improved Backward Finite Difference (BFD_improved) for second order derivative computation is

$$f''(x_i) = \frac{f(x_{i+1}) - \mathrm{f}(x_{i-1}) - \mathrm{f(x)} + f(x_{i-2h})}{2h^2}. \tag{15}$$

For third order derivative calculation, with combination of eq (6) and eq (13) the formulation by BFD_improved is

$$f^{(3)}(x_i) = \frac{f(x_{i+1}) - \mathrm{f}(x_{i-1}) - 2\mathrm{f(x)} + 2f(x_{i-2}) - f(x_{i-3})}{2h^3}. \tag{16}$$

Similarly, by using eq (6) and eq (9), Improved Forward Finite Difference (FFD_improved) for second order derivative computation is

$$f''(x_i) = \frac{f(x_{i+2}) - \mathrm{f}(x_{i+1}) - \mathrm{f(x)} + f(x_{i-h})}{2h^2}. \tag{17}$$

For third order derivative calculation, with the combination of eq (6) and eq (10), the formulation by FFD_improved is

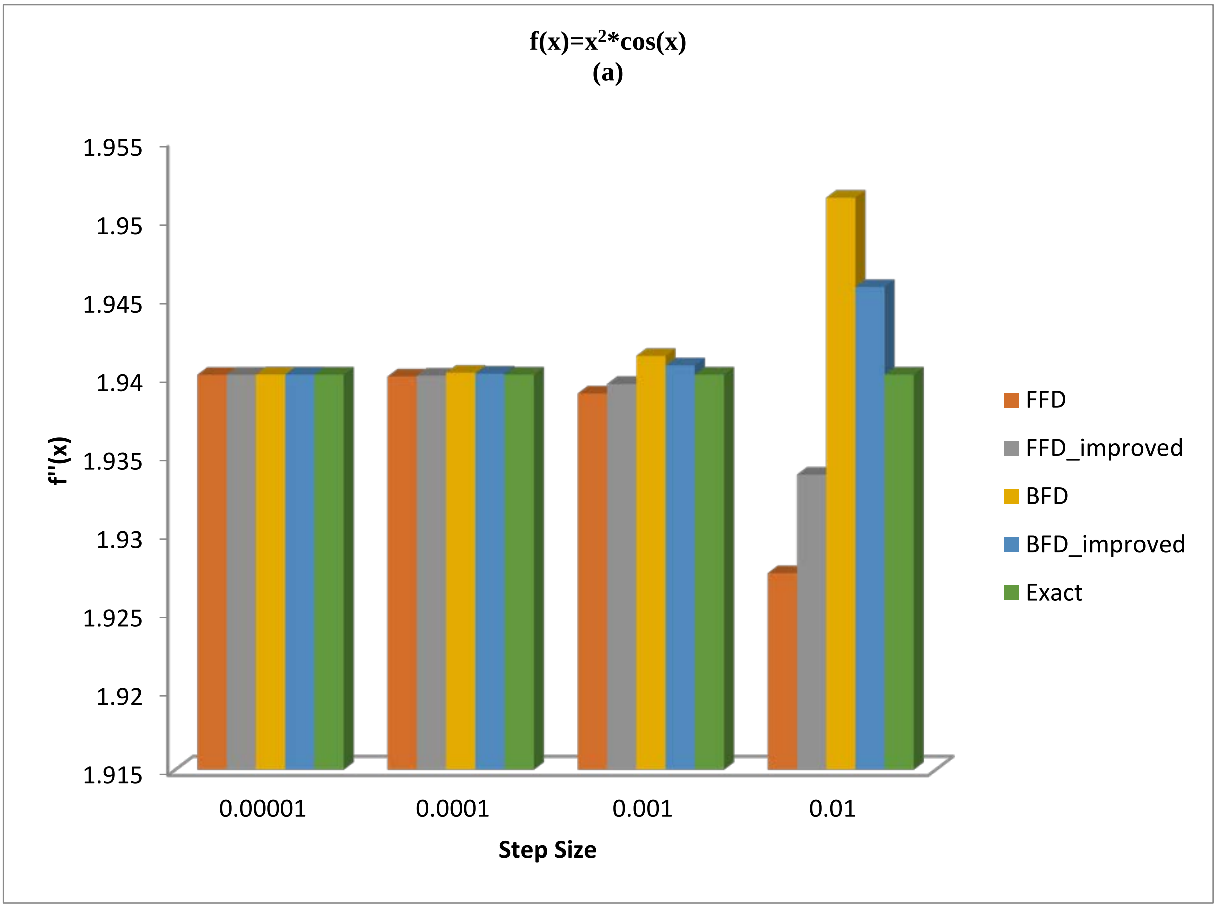
$$f^{(3)}(x_i) = \frac{f(x_{i+3}) - 2\mathrm{f}(x_{i+2}) + 2\mathrm{f(x)} - f(x_{i-1})}{2h^3}. \tag{18}$$

## III. RESULTS AND DISCUSSIONS

A general algorithm with use of various step sizes is generated for application of the proposed methods in Matlab R2022a. Function list for numerical analyses is presented in Table 1. Corresponding numerical results for these functions are displayed in Figures 1-5.

**Table 1.** Examples for several functions

| **Example** | **Function** |
|---|---|
| 1 | $x^2\cos(x)$ |
| 2 | $15^{2x}$ |
| 3 | $x^2 e^{-\frac{x^2}{2}}$ |
| 4 | $12x^4 + 10x^3 + 5x^2 + 3x + 2$ |
| 5 | $\cos(x) e^{(x^2+5x+3)}$ |



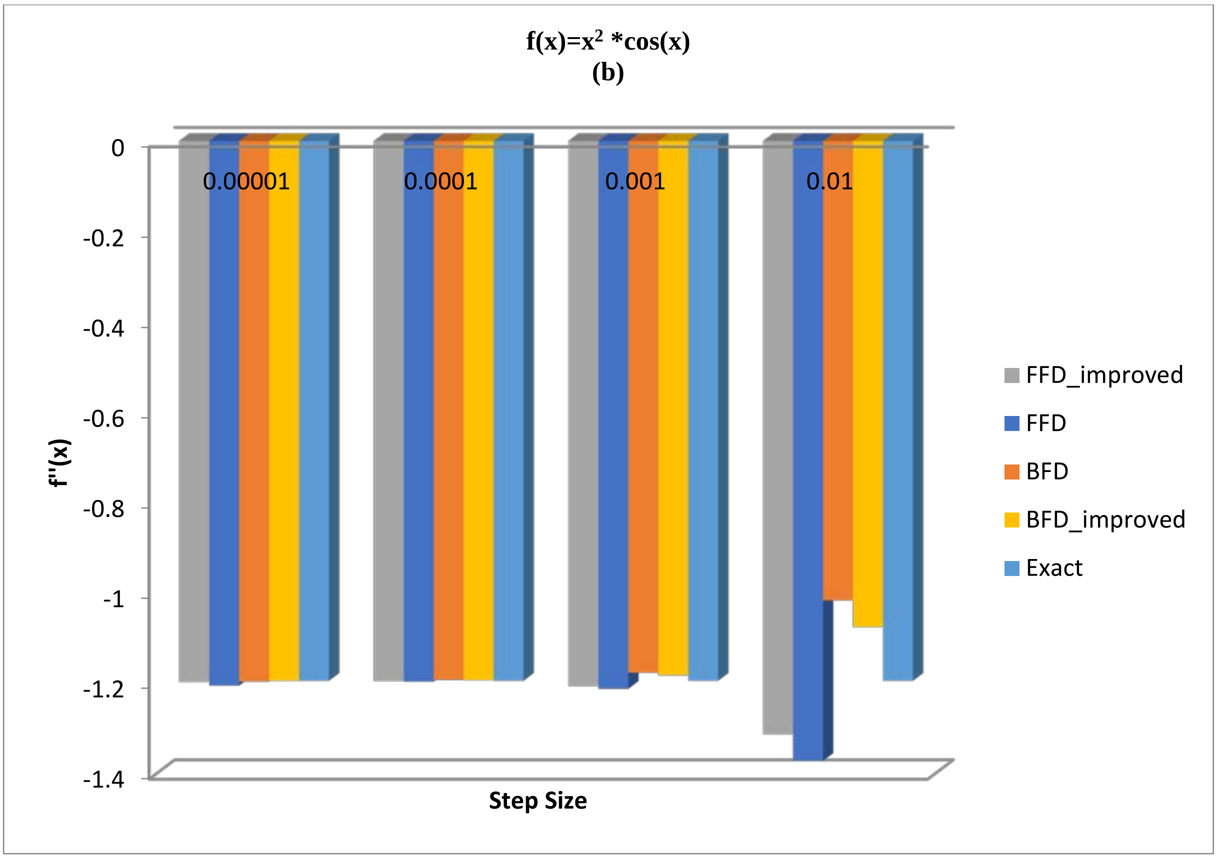
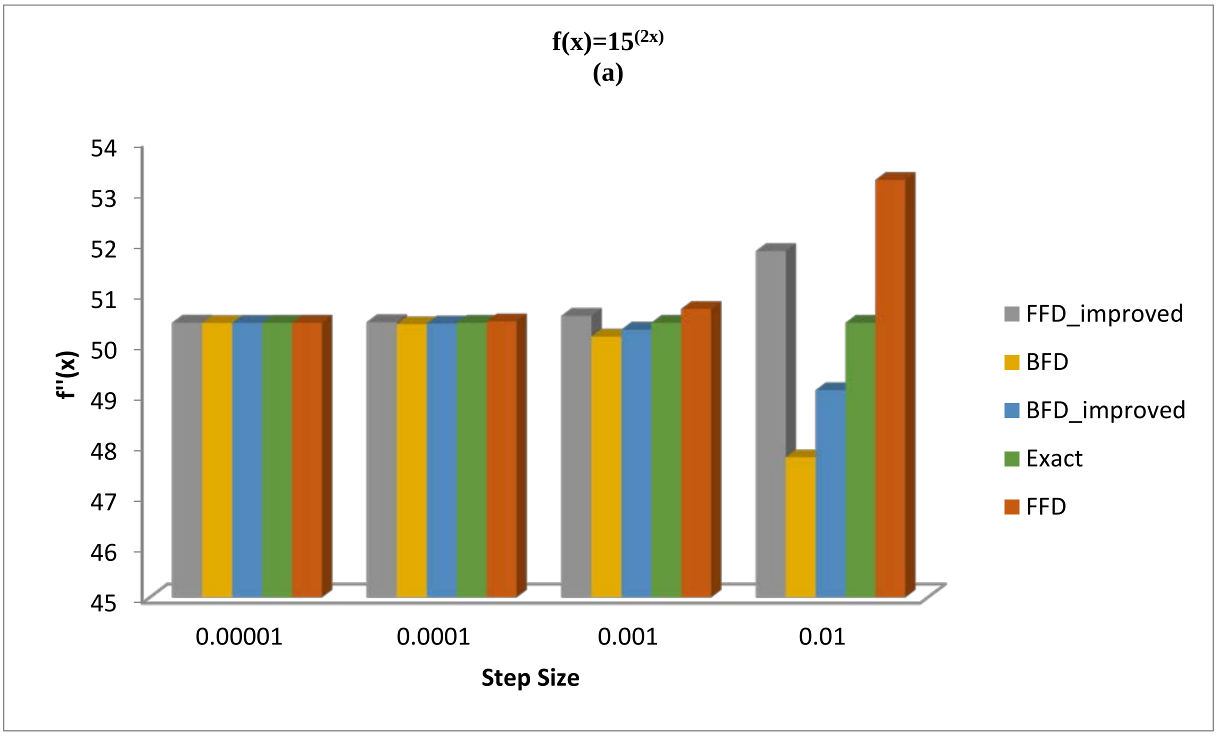




**Figure 1**. Numerical results for **(a)** second order derivative of f(x)=$x^2$cos(x) **(b)** third order derivative of f(x)=$x^2$cos(x)



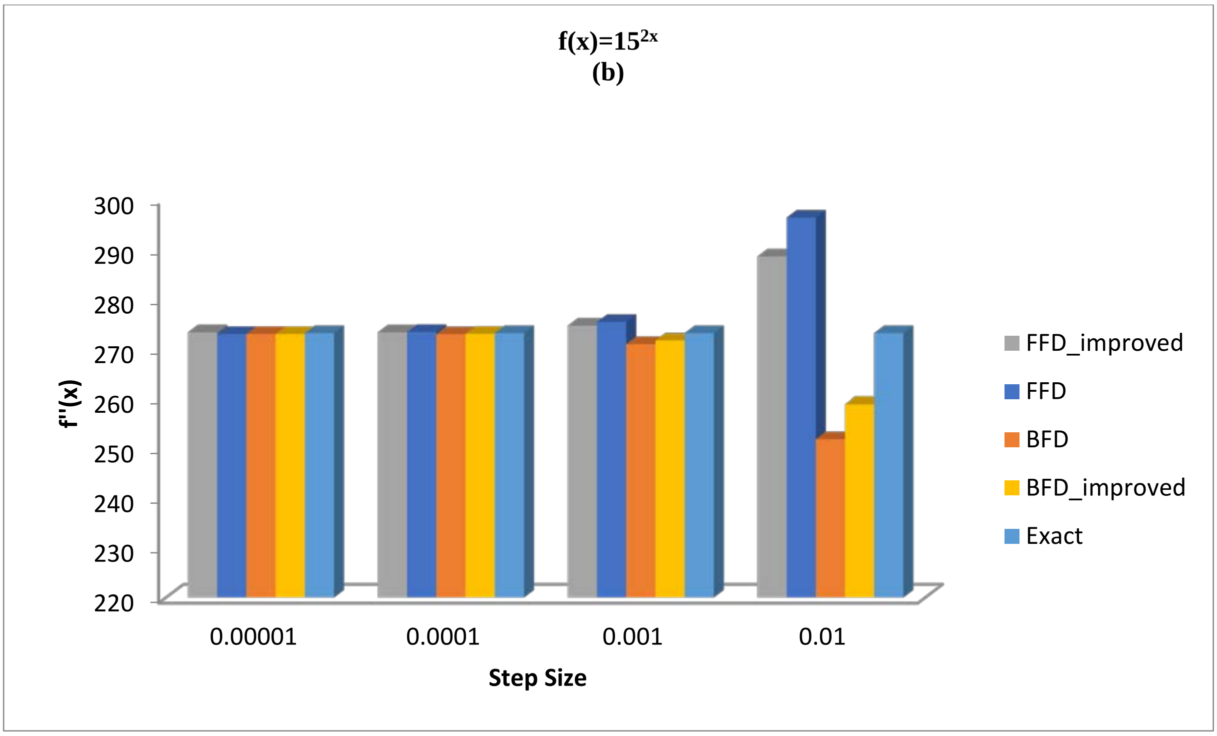
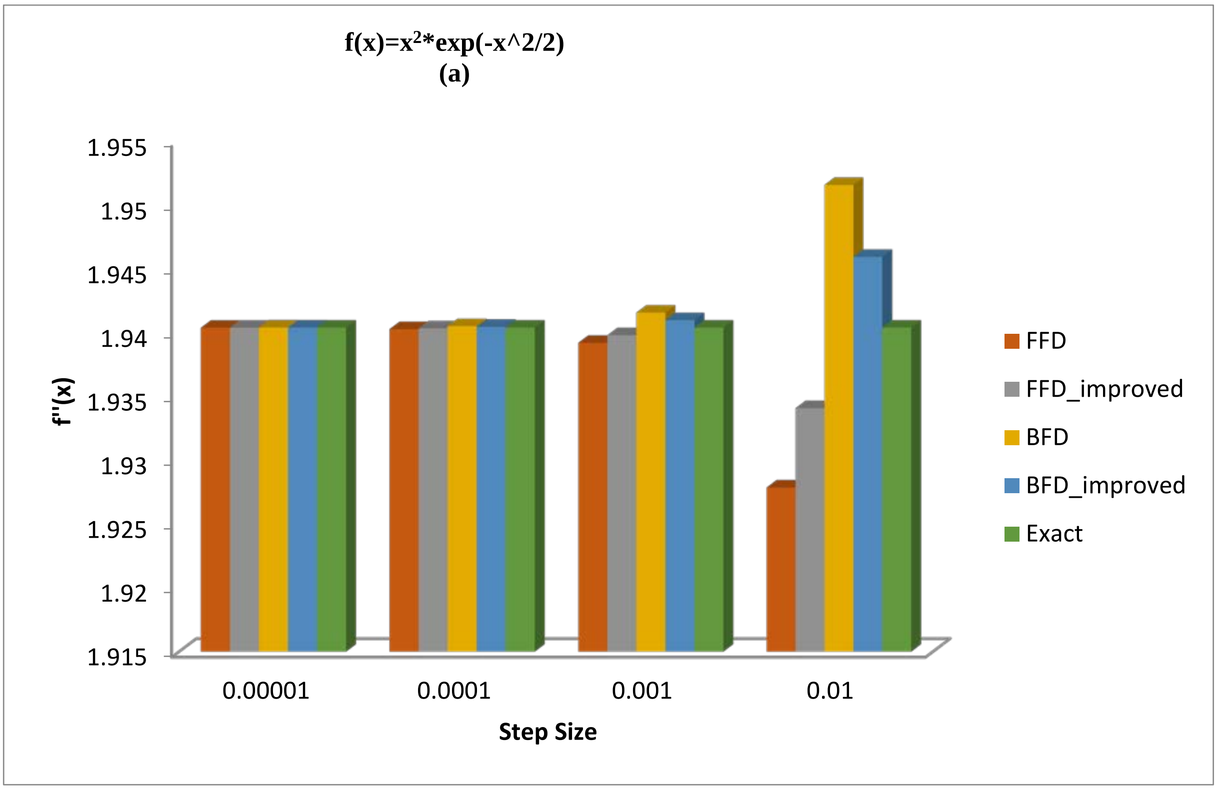




**Figure 2.** Numerical results for **(a)** second order derivative of f(x)= $15^{2x}$ **(b)** third order derivative of f(x)= $15^{2x}$



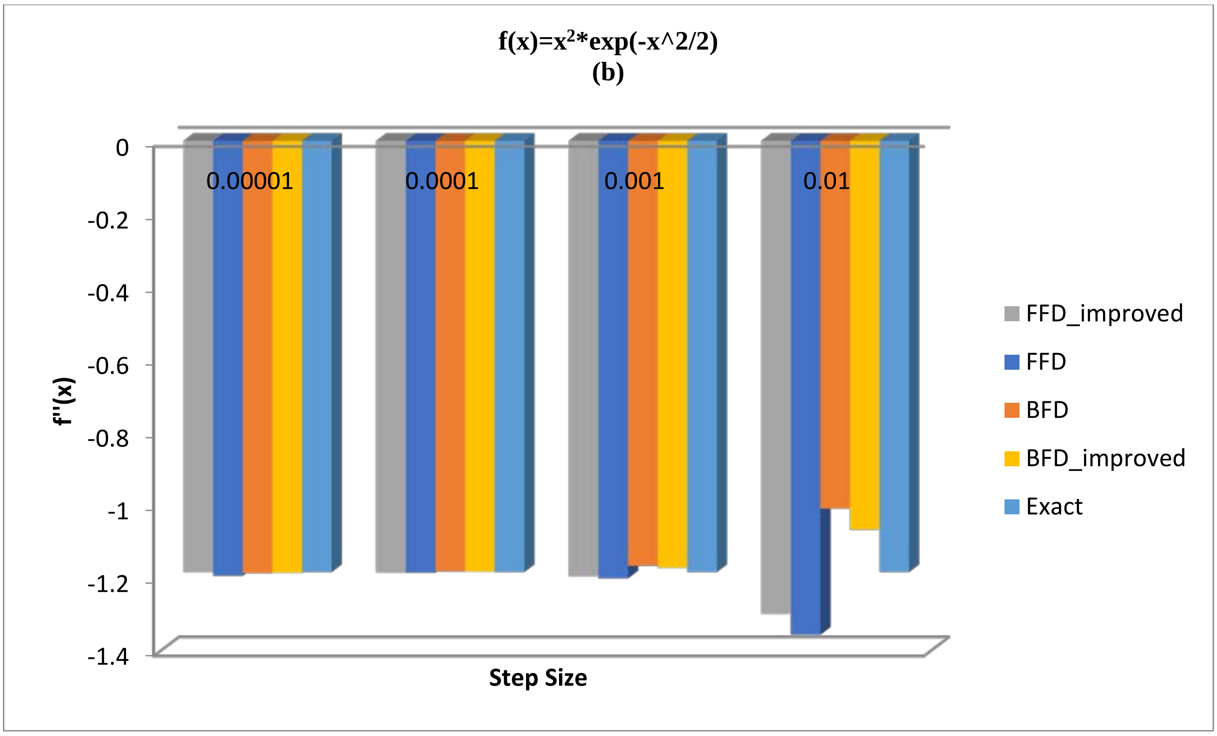
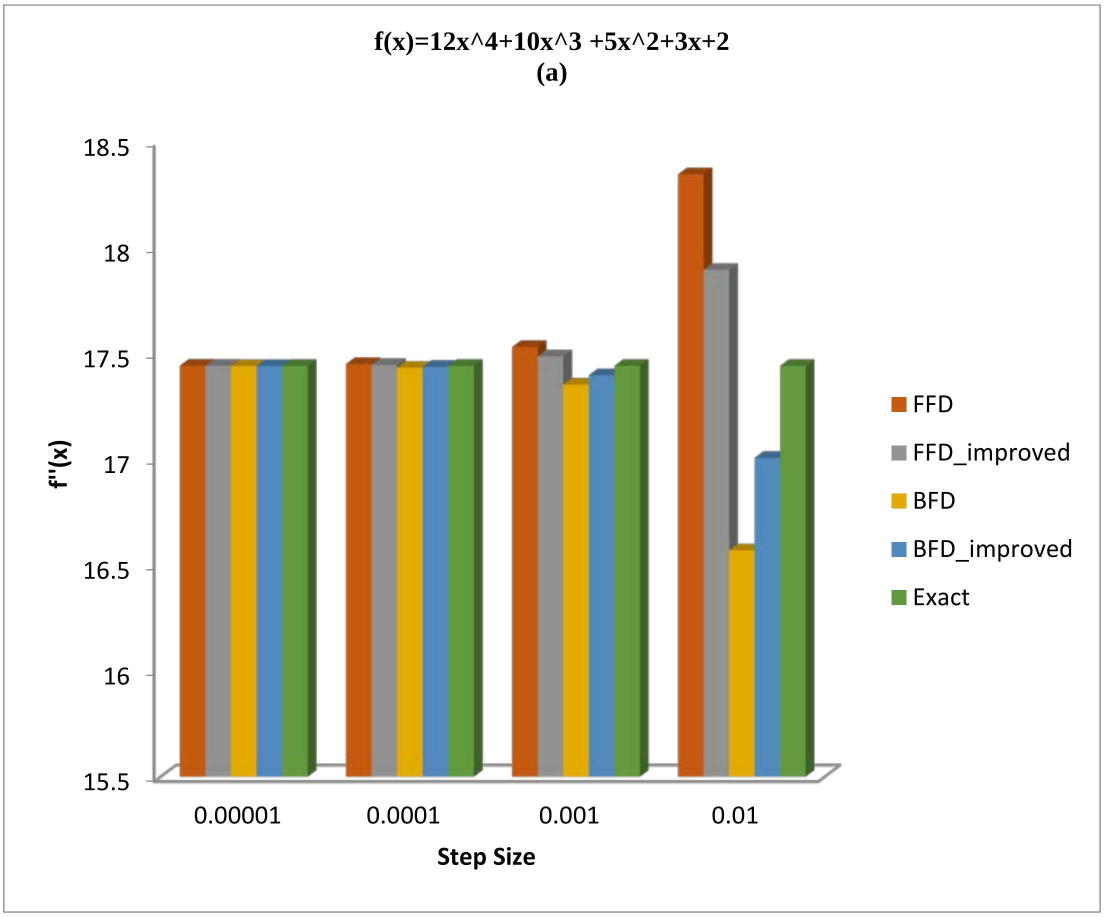




**Figure 3.** Numerical results for **(a)** second order derivative of f(x)= $x^2e^{-\frac{x^2}{2}}$ **(b)** third order derivative of f(x)= $x^2e^{-\frac{x^2}{2}}$



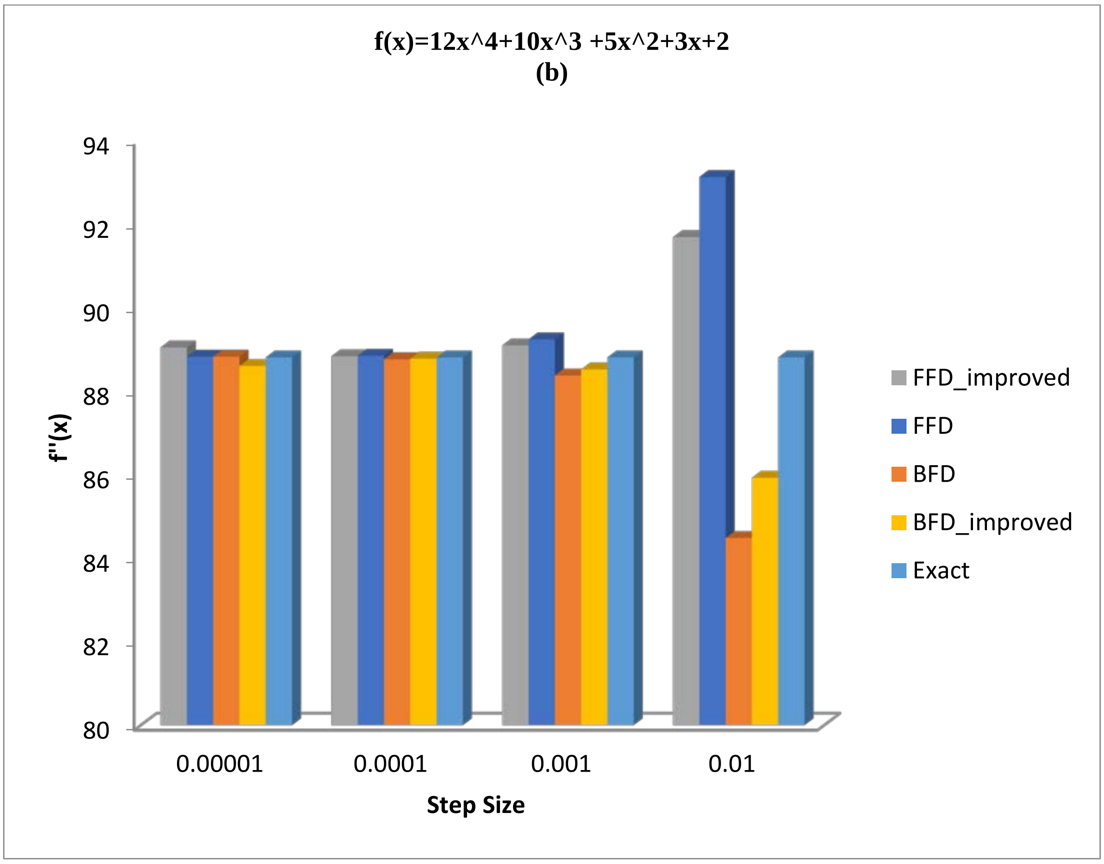
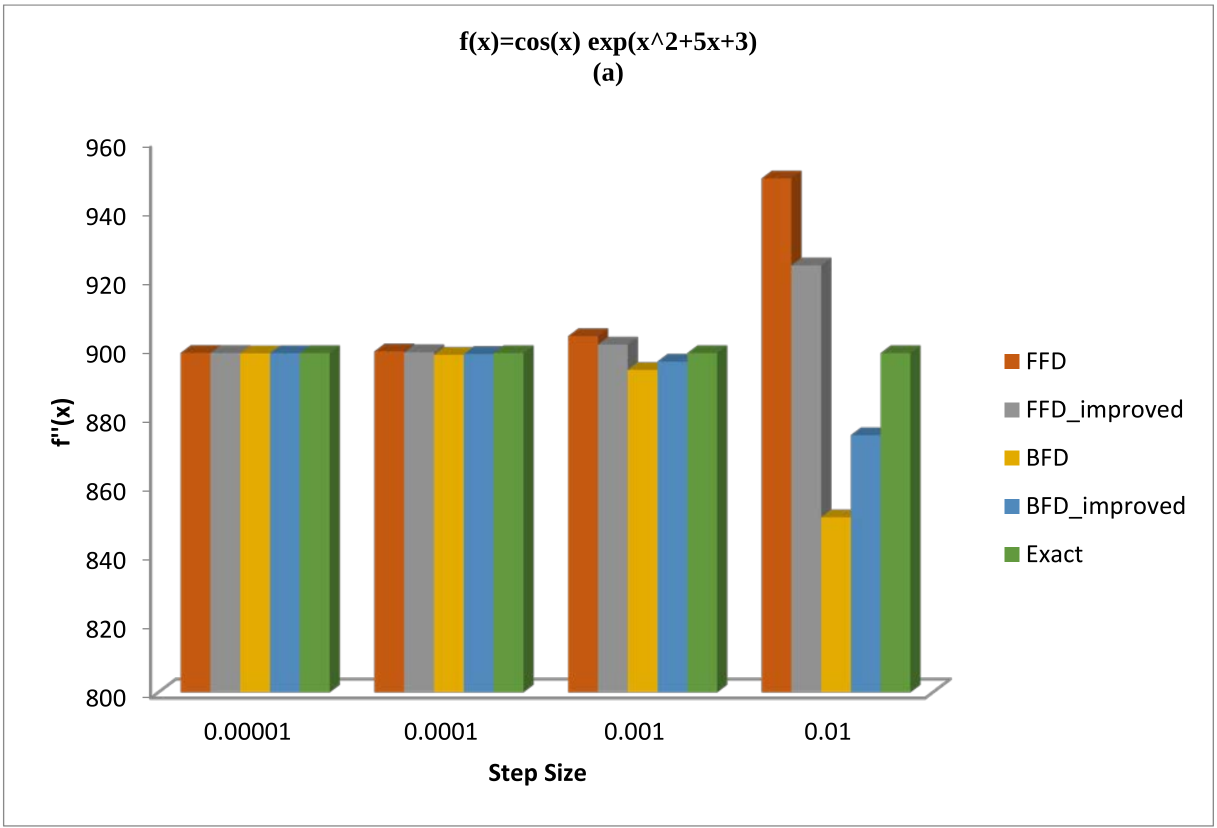




**Figure 4.** Numerical results for **(a)**second order derivative of f(x)= $12x^4 + 10x^3 + 5x^2 + 3x + 2$ **(b)** third order derivative of f(x)=$12x^4 + 10x^3 + 5x^2 + 3x + 2$



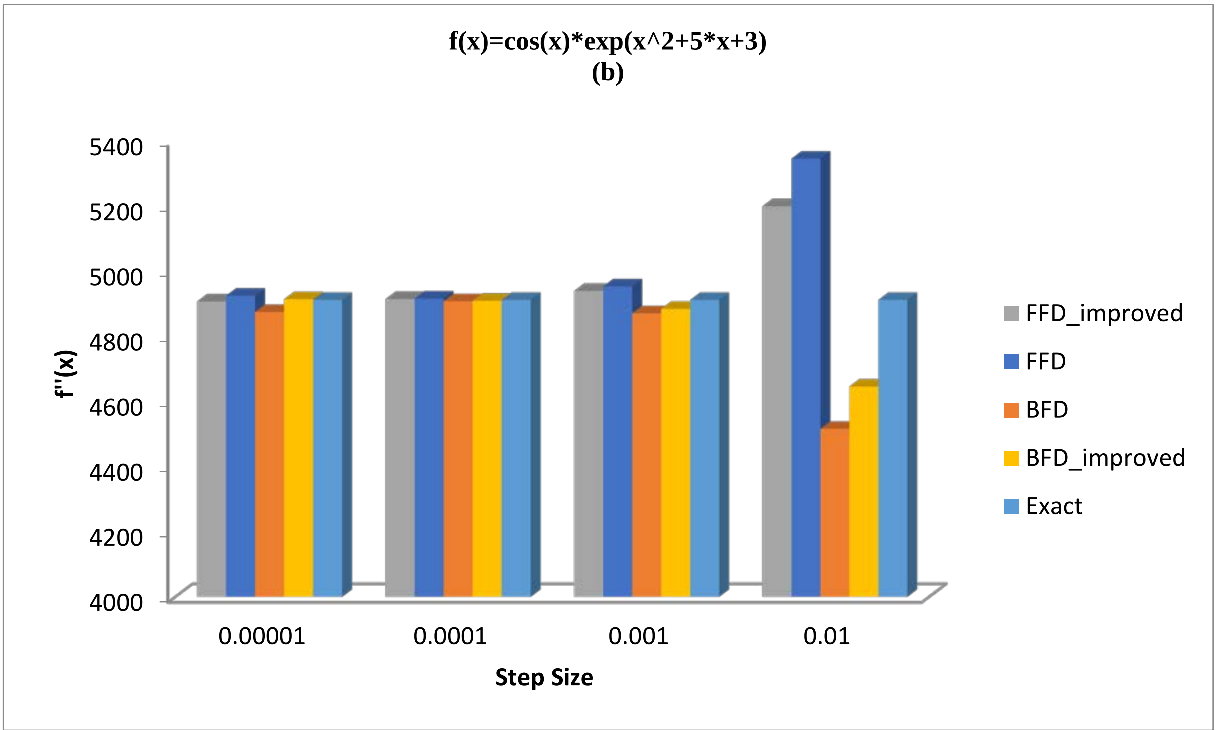




**Figure 5.** Numerical results for **(a)** second order derivative of f(x)= $\cos(x)e^{(x^2+5x+3)}$ (**b**) third order derivative of f(x)= $\cos(x)e^{(x^2+5x+3)}$

It is evident from Figures 1-5 that decreasing the step size increases the accuracy for both second and third order differentiations. When, step size is 0.00001, an almost exact solution is achieved.

*3.1 Performance Analyses of New Algorithm*

The performance analyses are conducted using both error and elapsed time computations. The results of the error computations for the example functions are presented in Figures 6-10.

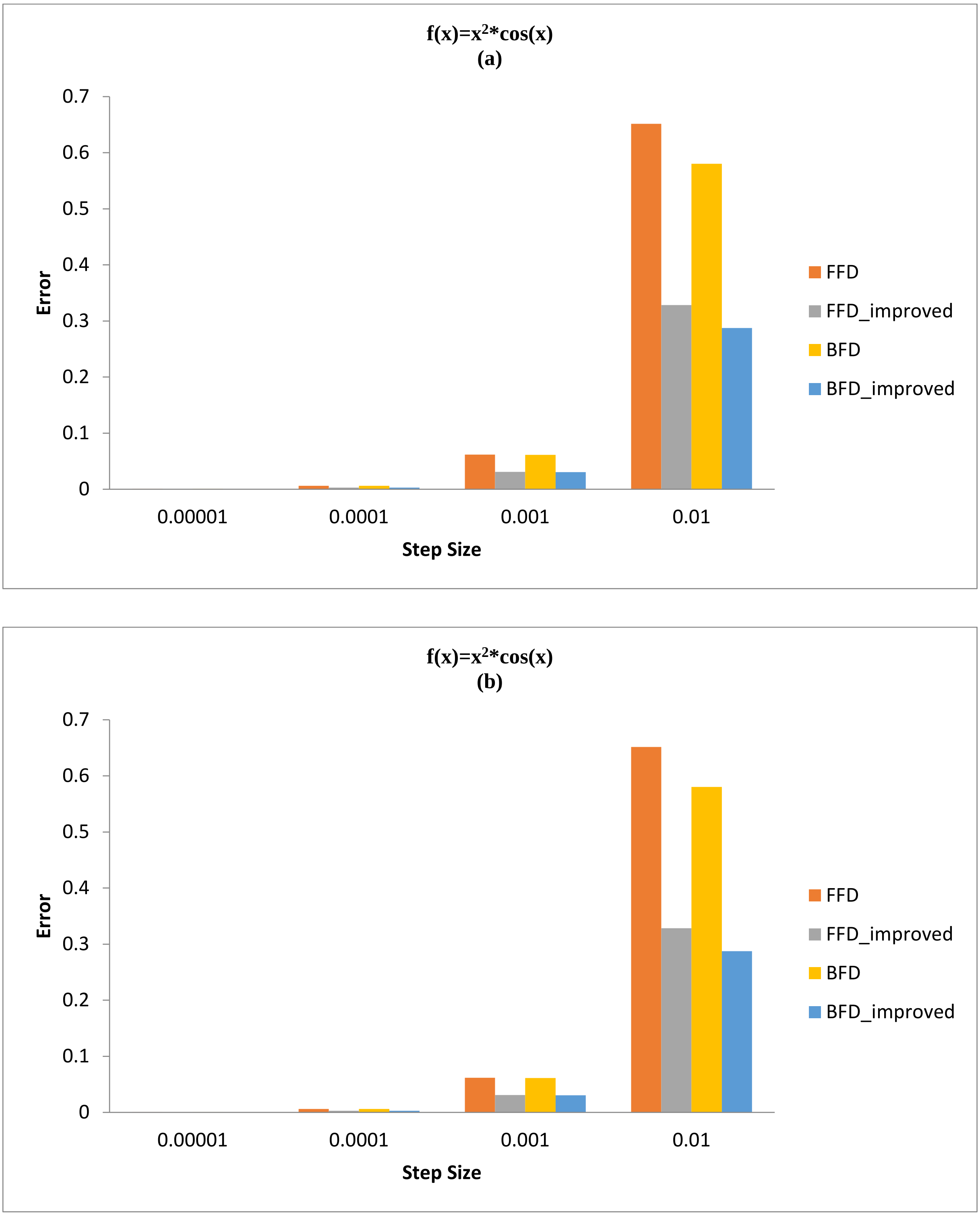



**Figure 6.** Numerical results for **(a)** second order derivative of f(x)= $x^2$cos(x) **(b)** third order derivative of f(x)= $x^2$cos(x)

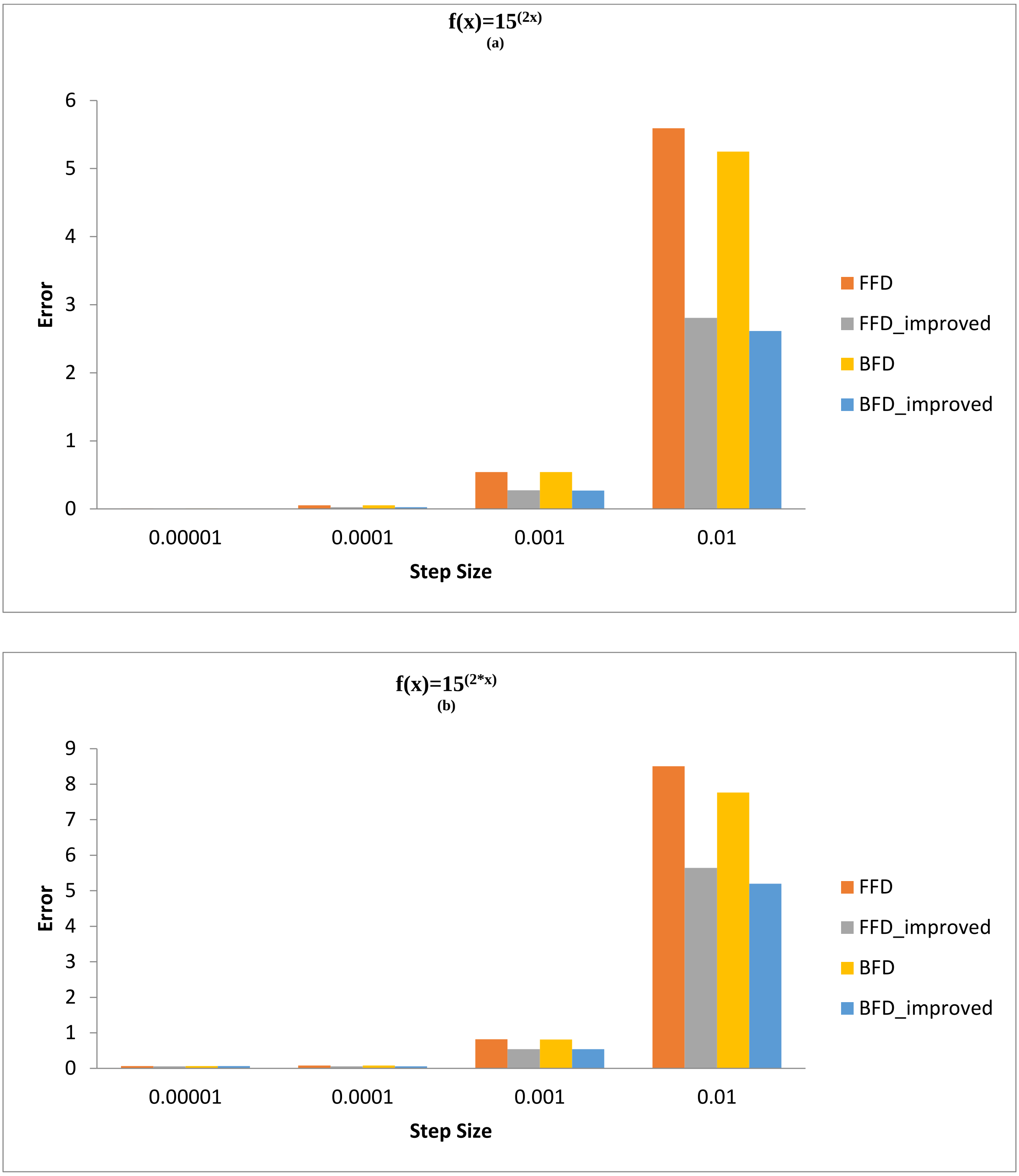



**Figure 7.** Numerical results for **(a)** second order derivative of f(x)=$15^{2x}$ **(b)** third order derivative of f(x)=$15^{2x}$

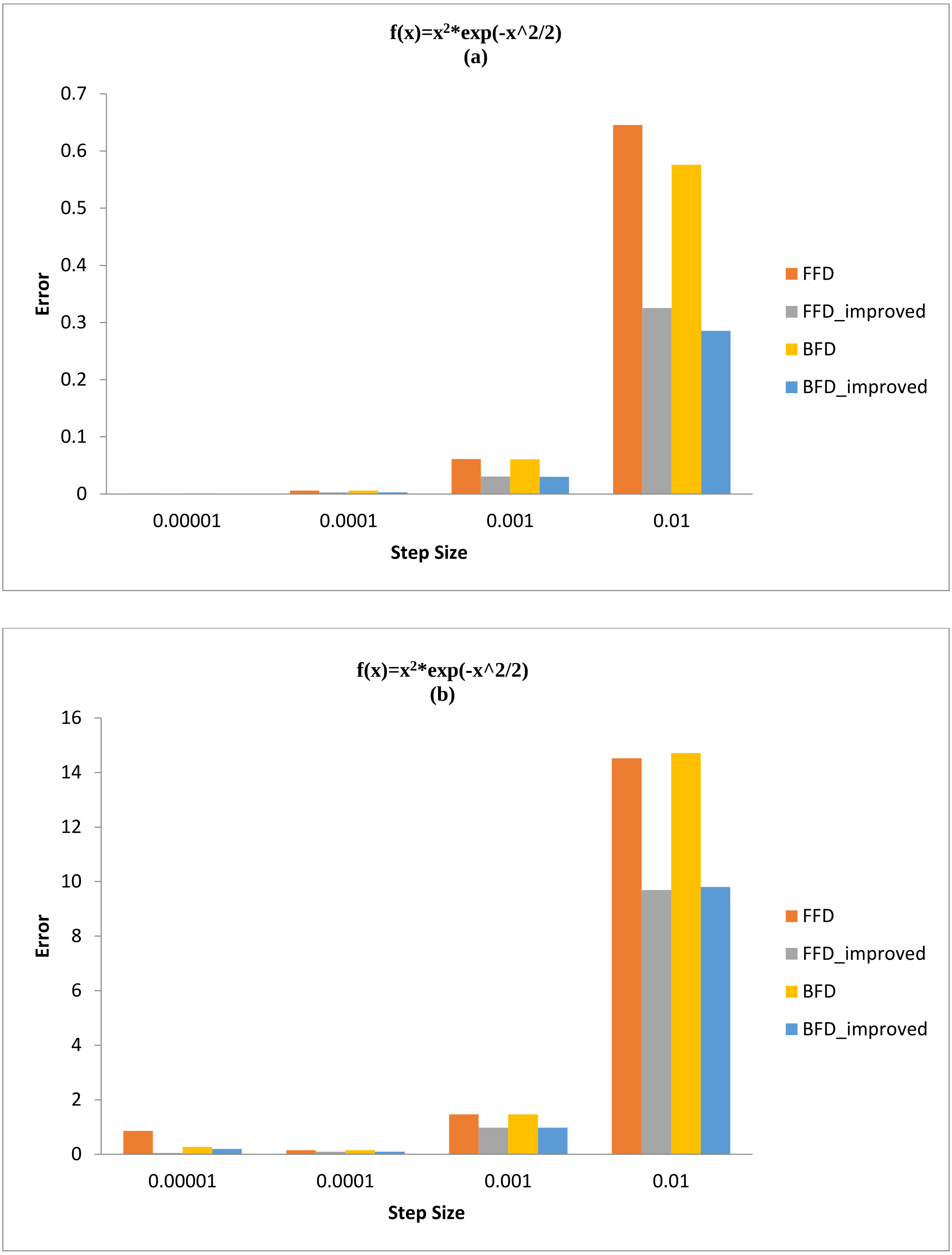
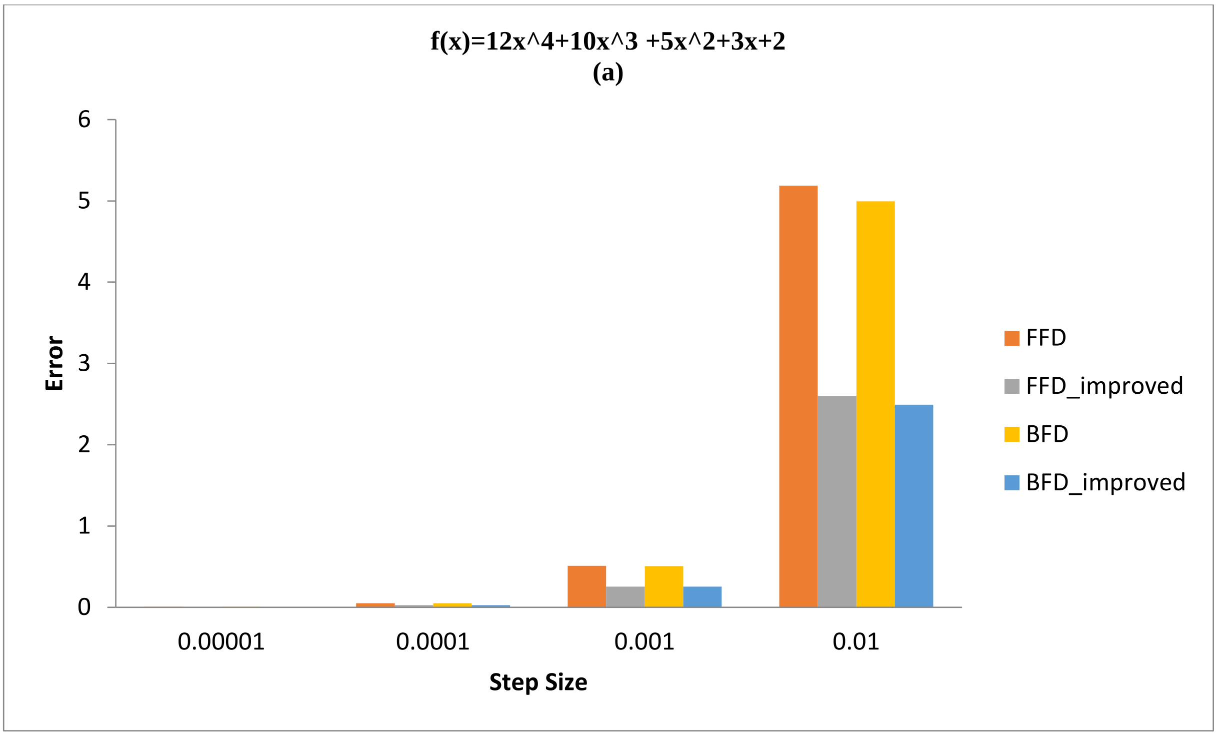



**Figure 8.** Numerical results for **(a)** second order derivative of f(x)= $x^2e^{-\frac{x^2}{2}}$ **(b)** third order derivative of f(x)= $x^2e^{-\frac{x^2}{2}}$ x



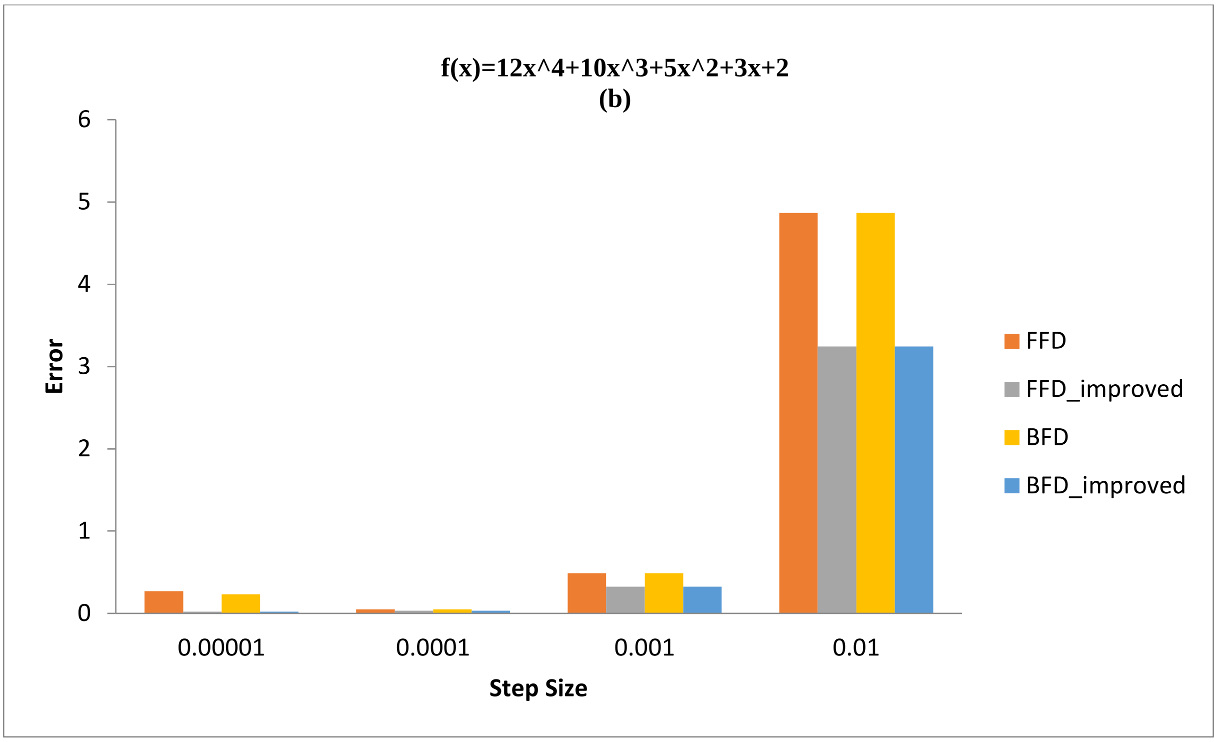
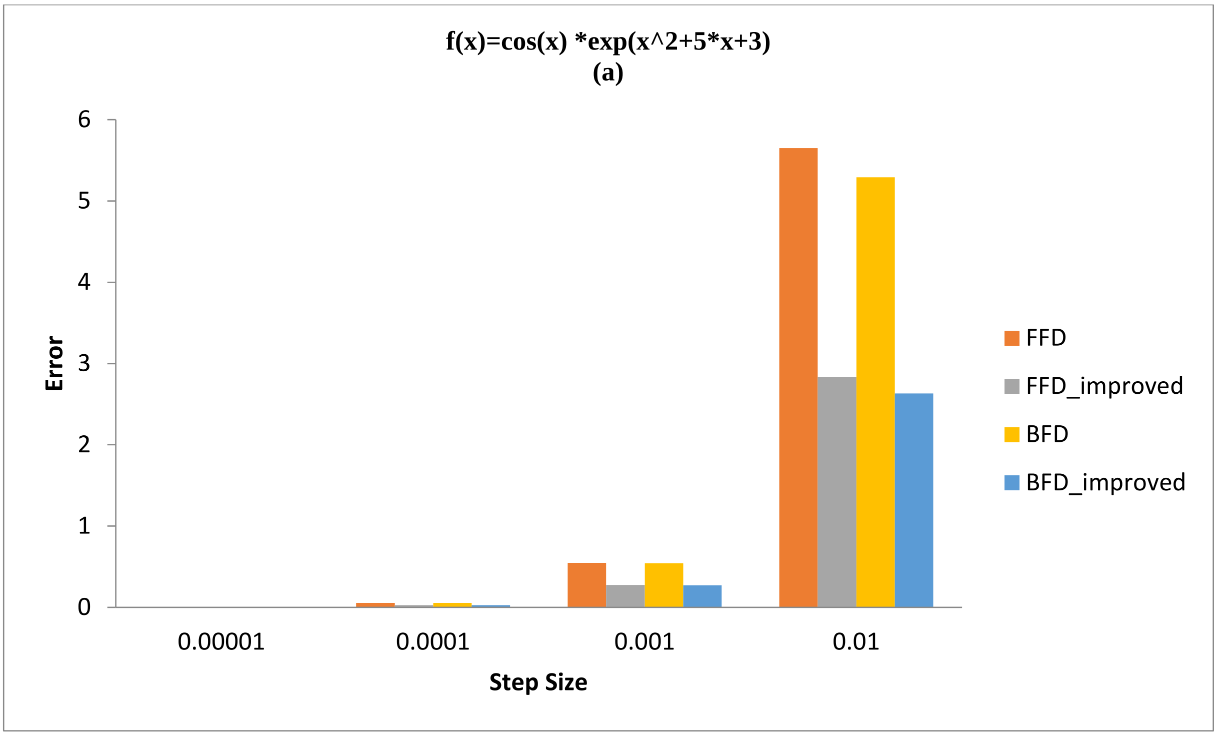




**Figure 9.** Numerical results for **(a)** second order derivative of f(x)= $12x^4 + 10x^3 + 5x^2 + 3x + 2$ **(b)** third order derivative of f(x)= $12x^4 + 10x^3 + 5x^2 + 3x + 2$



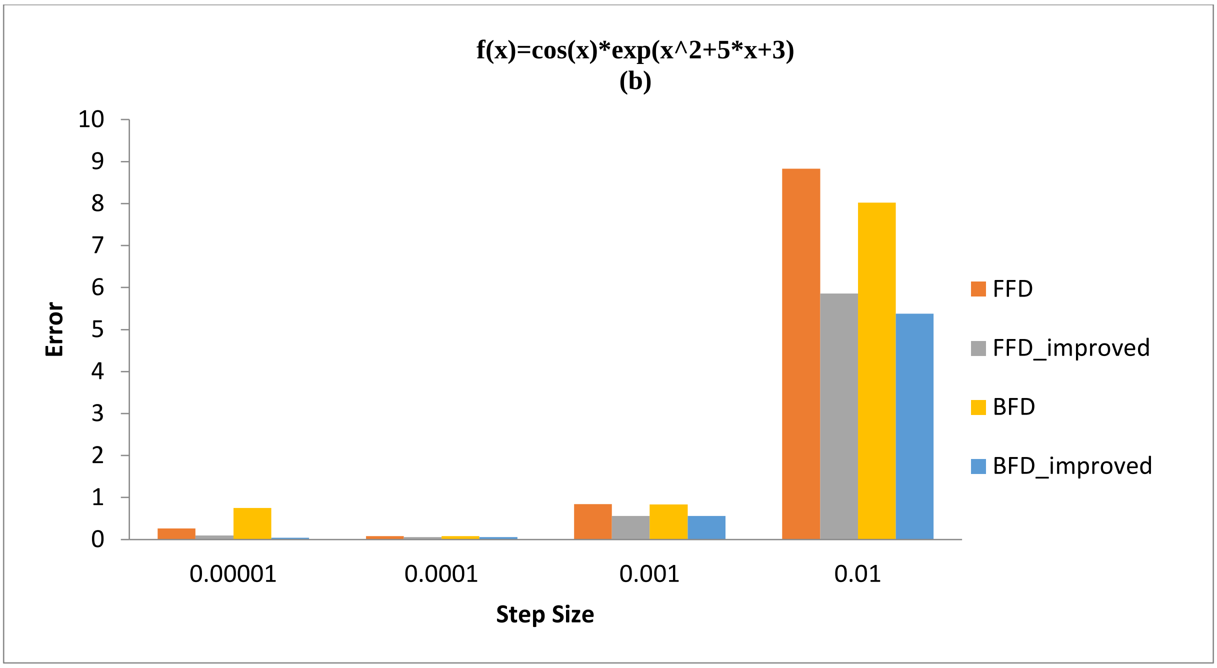




**Figure 10.** Numerical results for **(a)** second order derivative of f(x)= cos $(x)e^{(x^2+5x+3)}$ **(b)** third order derivative of f(x)= cos $(x)e^{(x^2+5x+3)}$

It is proved that error approaches zero for both second and third order computations in Figures 6-10. Exact results can be obtained by improved methods when step size gets the value: 0.00001.

Elapsed time of the new algorithm is displayed in Figures 11-15 for each function.

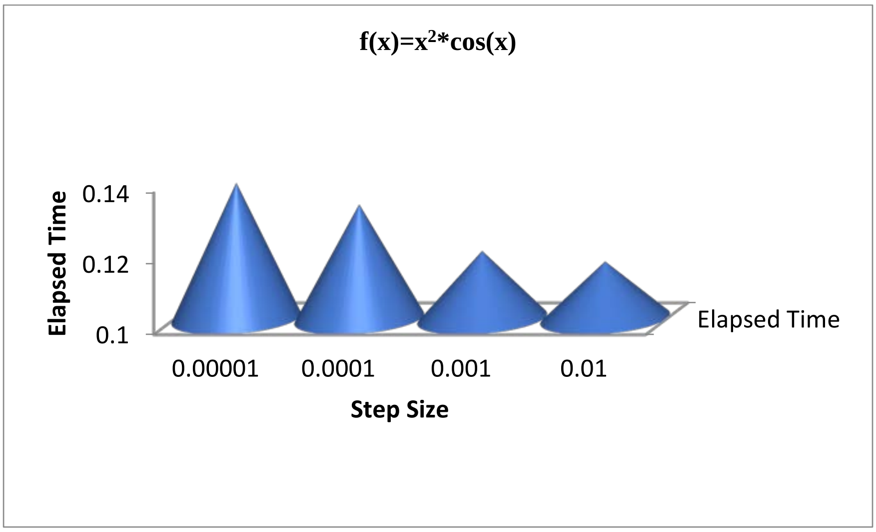



**Figure 11.** For f(x)= $x^2\cos(x)$

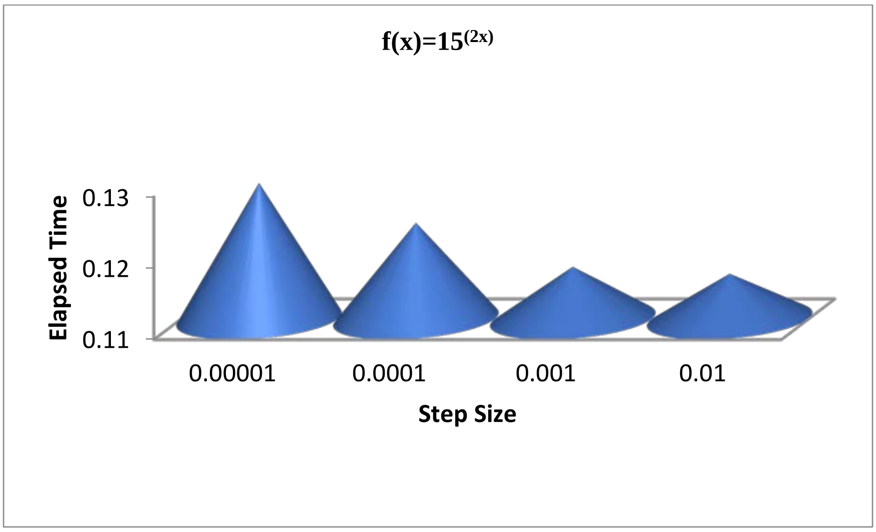



**Figure 12.** For f(x)= $15^{(2x)}$

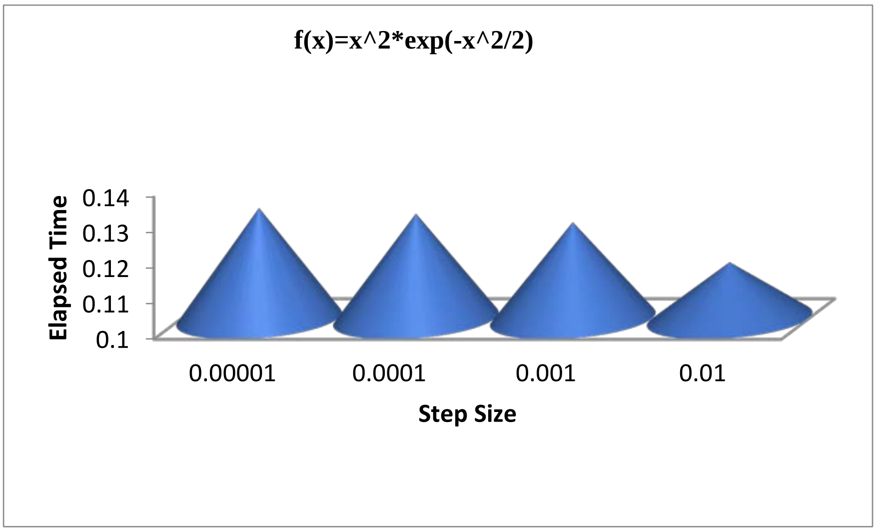



**Figure 13.** For f(x)= $x^2 e^{\left(\frac{-x^2}{2}\right)}$

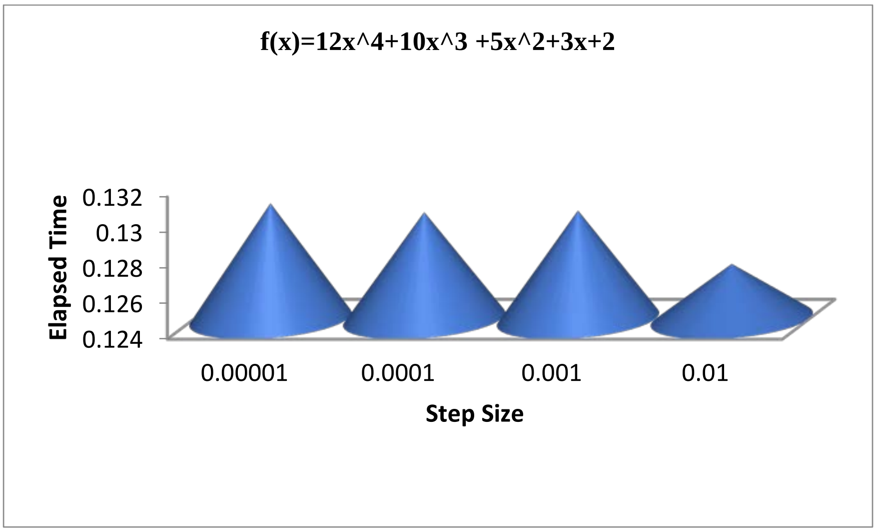



**Figure 14.** For f(x)= $12x^4 + 10x^3 + 5x^2 + 3x + 2$

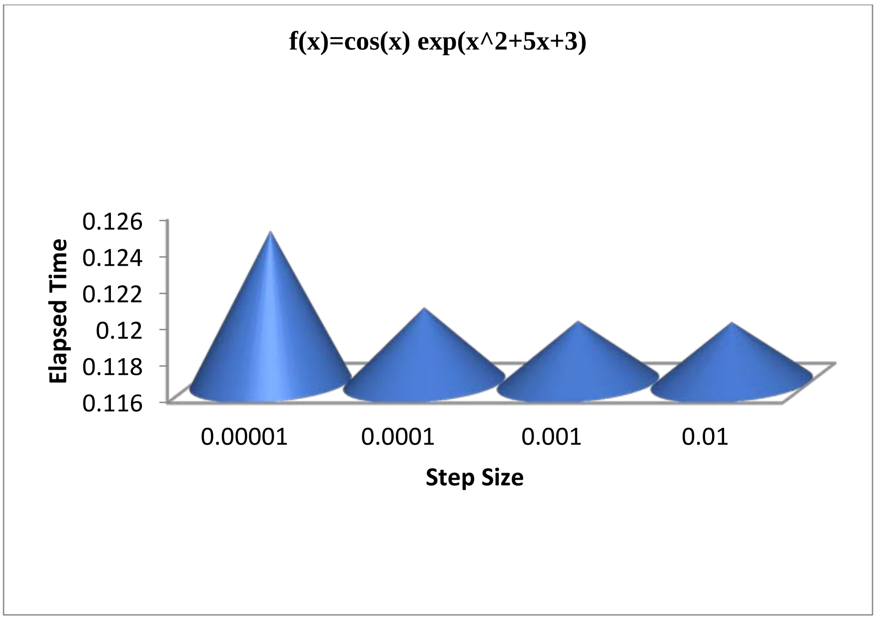



**Figure 15.** For f(x)= $\cos(x)e^{(x^2+5x+3)}$

Smallest step size leads to a little increase in computation duration for each function. This situation is demonstrated in Figures 11-15.

## IV. CONCLUSIONS

This paper presents alternative methods with use of CFD, BFD, FFD for second and third order derivative calculations. Exact solutions are obtained. So, there is no need to use extra terms for higher accuracy in second and third order differentiations. It is the first time in the literature that finite difference techniques are employed in new forms for numerical differentiation of second and third order.

It is also shown that new methods composing of CFD, BFD and FFD can be conveniently employed with any step size. BFD_improved and FFD_improved can be used confidently instead of BFD and FFD.

For comparison purposes, various numerical examples have been selected and presented in Table 1. Within this context, a general algorithm has been designed, enabling simultaneous computations for both second and third order numerical differentiations, along with error and elapsed time calculations. This is another novel aspect of the paper.

The findings presented in Figures 1-5 demonstrate that the improved methods achieve highly accurate derivative approximations with small step sizes for both second and third order differentiations, particularly when the step size is 0.00001.

This observation is further validated in Figures 6-10, which show the error computations for both second and third order differentiations.

Although the smallest step size leads to an increase in elapsed computation time for each example, as illustrated in Figures 11-15, employing the smallest step size remains the most convenient and accurate approach for calculations.

The highest accuracy is achieved with a step size of 0.00001. The proposed methods in this paper can be effectively used by instructors and students in calculus courses for a wide range of functions. Additionally, these methods have potential applications in solving both Ordinary Differential Equations (ODEs) and Partial Differential Equations (PDEs).

Consequently, these methods are valuable for both academic and practical applications in calculus, enhancing the accuracy and efficiency of numerical differentiation.

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