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A BUFFERED FOURIER SPECTRAL METHOD FOR NON-PERIODIC PDE

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Abstract. Standard Fourier spectral method can be used to solve a lot of problems with periodic boundary conditions. However, for non-periodic boundary condition problems, standard Fourier spectral method is not efficient or even useless. This work has developed a new way to use Fourier spectral method for non-periodic boundary condition problems. First, the original function is normalized and then a smooth buffer polynomial is developed to extend the normalized function domain. The new function will be smooth and periodic with both function values and derivatives, which is easy to be treated by standard FFT for high resolution. This method has obtained high order accuracy and high resolution with a penalty of 25% over standard Fourier spectral method, as shown by our examples. The scheme demonstrates to be robust. The method will be further used for simulation of transitional and turbulent flow.

Key words. Fourier spectral method, FFT, non-periodic PDE, buffer zone, high resolution.

1. Introduction

Spectral methods are a class of techniques used in applied mathematics and scientific computing to numerically solve certain partial differential equations (PDEs). One of the spectral methods is Pseudo-Spectral Method which utilizes the efficient algorithm of fast Fourier transform (FFT) to solve differential and pseudo-differential equations in spatially periodic domains. It has emerged as a powerful computational technique for the simulation of complex smooth physical phenomena, and its exponential convergence rate depends on the smoothness and periodicity of the function in the domain of interest. As is known, Fourier spectral method is a high order method and can be used to resolve the small length scales, which is particularly important for simulation of turbulence and acoustic problems because of its high resolution. Since it's inception in early 1970's, spectral methods have been extensively used to solve a lot of problems including turbulence. However, classical pseudo-spectral method imposes restriction on boundary conditions which must be periodic. Such a restriction cannot be applied to practical flows that usually have non-periodic boundary conditions. To overcome this problem, people did a lot of work, for example, changing the basis functions to be Chebyshev polynomials or other polynomials. In that way, one can get Chebyshev spectral method and so on, refer to [20], but they have lower resolution than the original trigonometry polynomials. Also we can use windows to treat the boundary conditions, then the physical solution near the boundaries is obtained by a regularized dewindowing operation, and on the inner domain, the unmodified equations are solved, refer to [9]. There are other works which also deal with parts of the problems, like [7] through [14].

As is known, even the function value itself (not derivative) is periodic on the boundary, the classical Pseudo- spectral method may still not work. Therefore, modifying the function and making the some orders derivatives of the function to be periodic on the boundary is very important. The effort in this work is focused on solving the above problems, trying to use the classical Fourier spectral method to get

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the accurate derivatives of a function which is not periodic on boundary. Instead of using the classical Fourier spectral method directly for the problem, we first modify and extend the original function to get a new extended function (which is probably very different from the origin function), for which classical Fourier spectral method can be easily used. After getting the derivatives of the new function, we can easily recover the derivative of the original function.

The paper is organized as follows: Section 2 introduces the standard Fourier spectral method; Section 3 introduces our ideas and the new method; Section 4 gives some computational examples. The first part of Section 4 is for the derivative results. Here, we only focus on smooth functions, but we will continue to investigate for non-smooth functions. The other two parts of Section 4 give some preliminary results for the wave equation and Poisson equation.

2. Fourier Spectral Method

2.1. Fourier Interpolation. For a periodic sequence $\{x_n = 2\pi n/N, n = 0, 1, ...N\}$, the function $f(x)$ can be approximated by Fourier interpolation as:

$$I_N f = \sum_{k=-N/2}^{N/2} \frac{\tilde{f}_k}{\bar{c}_k} e^{ikx}, \tag{2.1}$$

here, $\bar{c}_k = \begin{cases} 1, & k = -N/2+1, ..., N/2-1; \\ 2, & k = \pm N/2. \end{cases}$ and $\tilde{f}_k = \frac{1}{N}\sum_{j=0}^{N-1} f_j e^{-ikx_j}$, $k = -N/2, ..., N/2$. The interpolation satisfies: $I_N f(x_n) = f(x_n), \quad n = 0, 1, ..., N-1$.

2.2. DFT. For a sequence $\{f(x_i)\}, \ \ i = 0, 1, ..., N-1$, the discrete Fourier transformation (DFT) is defined as:

$$\tilde{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f(x_j) e^{-2\pi ijk/N}, k = -N/2, ..., N/2-1. \tag{2.2}$$

The inverse transformation is:

$$f(x_j) = \sum_{k=-N/2}^{N/2-1} \tilde{f}_k e^{2\pi ijk/N}, j = 0, 1, ..., N-1. \tag{2.3}$$

2.3. Traditional Fourier spectral method for derivatives. Traditional Fourier spectral method for derivatives is based on the Fourier interpolation and use DFT/FFT to get coefficients of the DFT and then the original function derivatives. The original function is approximated by (2.1), and hence the derivative is:

$$f' = (I_N f)' = \sum_{k=-N/2}^{N/2} \frac{\tilde{f}_k}{\bar{c}_k} (ik) e^{ikx}$$

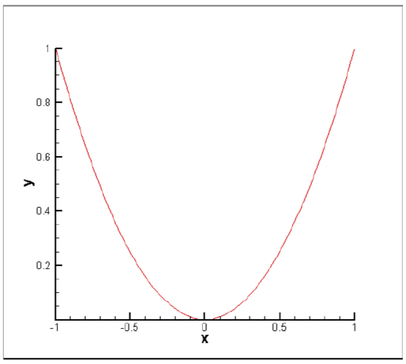
Therefore, if we want to get f' , we first use FFT to get the coefficients of DFT of f, and then multiply each of them with the corresponding number ik. After we perform the inverse DFT by FFT, the derivatives are available.

3. Buffered Fourier Spectral Method (BFSM)

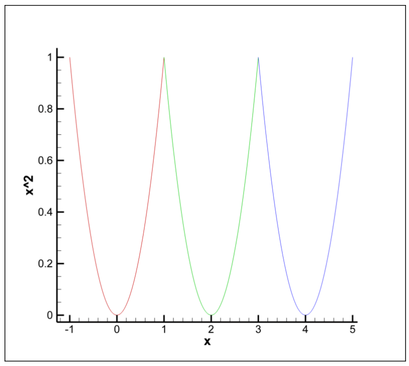
The boundary condition for using standard Fourier spectral method is periodic, which is too restrictive. Even for simple functions like $y = x^2, (-1 \le x \le 1)$, with periodic boundary condition but non-periodic derivatives, the result is still a disaster, referring to the following sections. However, most of practical engineering problems have non-periodic boundary conditions. Therefore, it is very important to modify the Fourier spectral method so that it can be used for problems with non-periodic boundary conditions. This is the major purpose of the current work. This modified Fourier spectral method, called as buffered Fourier spectral method or BFSM, can be described by two steps: 1. Normalization; 2. Smooth buffer extension.

3.1. Smooth buffer extension.

3.1.1. Problems with standard FFT. Let us take a simple example (Figure 1 (a)),$y = x^2, (-1 \leq x \leq 1)$, to explain how to develop a smooth buffer extension. This simple function can be artificially extended as a periodic function with T=2 as shown in Figure 1 (b) which we can use Fourier transform. However, it is not difficult to find that the derivative on the boundaries, i.e. x=-1 and 1, does not exist. If we use traditional FFT to calculate the derivatives, it will give a lot of oscillations (Gibbs Phenomenon) (Figure 1 (c)), but the exact derivative is $y' = 2x$ (Figure 1 (d)).



(a)



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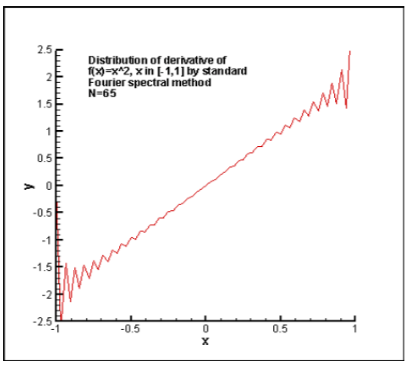
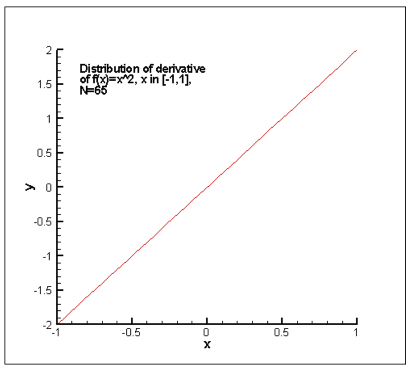


(c)



(d)

FIGURE 1. **sample figures** (a) graphic for $y = x^2, x \in [-1, 1]$; (b) Extended periodic function; (c) Traditional FFT results for y'; (d) Exact results for y'.

3.1.2. Extended smooth buffer functions. In order to solve the above Gibbs problem, we first split the original function with gaps (Figure 2 (a)). We then use a smooth polynomial to fill the gaps as a buffer zone (Figure 2 (b)). Note that the function is periodic and we can then use 8 points, 4 points from left end and 4 points from right end to construct the buffer polynomial. Assume and are the left and right ends of the domain of interest, we can have following 8 points to construct the buffer polynomial (Figure 2 (c)): $f(b-3\Delta x), f(b-2\Delta x), f(b-\Delta x), f(b)$ and $f(a), f(a+\Delta x), f(a+2\Delta x), f(a+3\Delta x)$ since $f(b+\delta) = f(a), f(b+\delta+\Delta x) = f(a+\Delta x), f(b+\delta+2\Delta x) = f(a+2\Delta x), f(b+\delta+3\Delta x) = f(a+3\Delta x)$, according to the periodic boundary condition. Here,δ is the length of the buffer zone. The buffer polynomial then can be written as

$$P(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 + a_6 x^6 + a_7 x^7,$$

where, $a_0 - a_7$ can be determined by the given 8 points. Apparently, the buffer polynomial is determined by left and right ending 8 points and the length of δ which determines the number of buffer points. Here we use $\delta = 25\% * (b-a)$. Actually, we obtain a new periodic function as shown in Figure 2 (d), which is periodic and is at least 7th order smooth. The extended function with buffer must be very easy for FFT to find interpolation and derivatives.

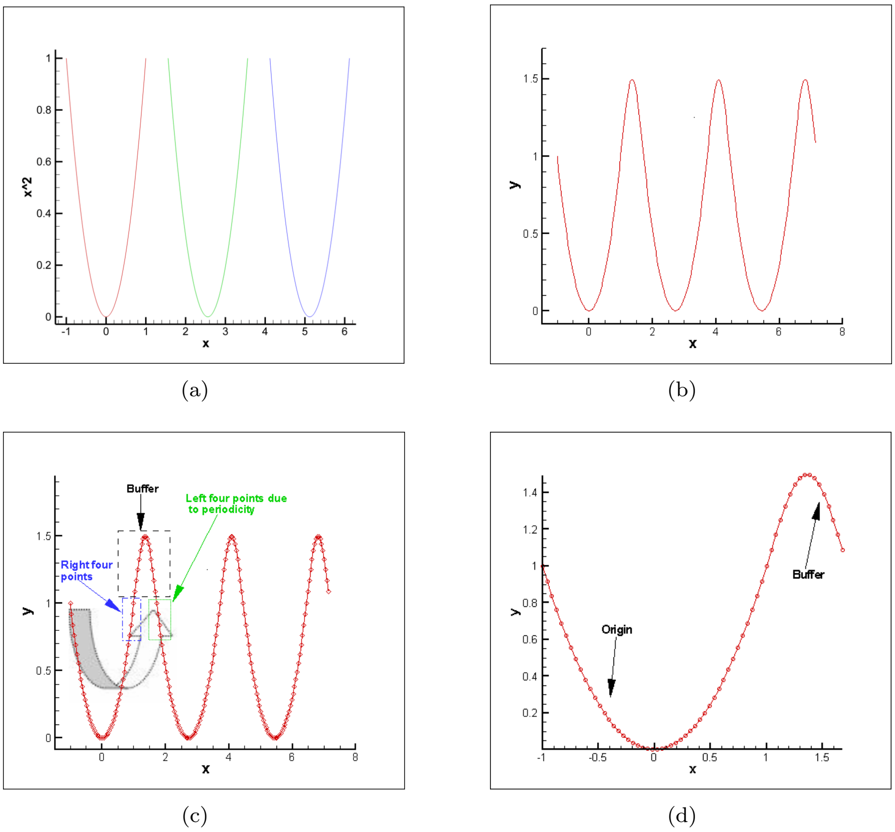


FIGURE 2. **sample figures** (a) Split periodic function; (b) Buffered periodic function; (c) Buffer polynomial can be constructed by 4 left end points and 4 right end points ; (d) New extended function with a buffer if a 7th order smooth polynomial .

The idea to construct an extended periodic function with high order polynomial as a buffer zone is the key of this BFSM method. Of course, the cost will be increased by 25% and the derivative obtained in buffer zone is non-physical and will be abandoned. However, the resolution will be much higher in comparison with regular finite difference for derivatives. Note here that the penalty of 25% is reasonable and meets the needs of most of the problems, and the using of 4 points at each end of the domain just keeps high order of accuracy, but these numbers can vary according to one's needs and the optimization could be case-related. However, the penalty of 25% is reasonable.

In the case if the function is not periodic in the function value, even we use the buffered domain to do FFT and get the derivative, serious oscillations (Gibbs phenomena) may still exist at most of these cases, and the results are not acceptable. Therefore, we still need to do some recoverable modification of the boundary conditions first, that is here called "normalization".

3.1.3. Normalization of the original function. In order to normalize the original function, we first shift the function up so that the values of two ends of the function are positive. Note that shifting up has no affect on the derivative of the original function since $(f + c)' = f'$. Second, we divide the function by a linear function $g(x)$, which links the two end points of the new function by a straight line, i.e. $F(x) = (f(x) + c)/g(x)$. Here, we use linear function because it is easy to be constructed and the derivatives of a linear function are simple. By this procedure, the new function will be periodic in the function values on the boundary. The last step is to add a buffer domain (see section 3.1.2) to make the two ends of the function periodic not only for function value but also for the first, second, or even higher order derivatives. After doing all of these, we can use standard Fourier spectral method to get the derivatives for the new extended function $F(x)$, which is periodic in function, first, second, and higher order derivatives. Then we can cut the added buffer part, and recover the derivative of the original function.

For FFT, we have to set up a point number to be 2^N and we use 1/4 points of the whole number as the buffer. For example, if we set the number of all points to be 64 (with the right end point, it should be 65), the physical domain $[a, b]$ occupies 48 points, and the number of buffer points is 16. One can change this if necessary. Note that the second step of normalization is also important since the large difference between two end point values will cause serious oscillations which are not acceptable, and it cannot be removed even more points are used to do the interpolation.

Following is an example to introduce our method. The function we choose here is $f(x) = x^3, x \in [-1, 1]$, which has large difference between two end points.

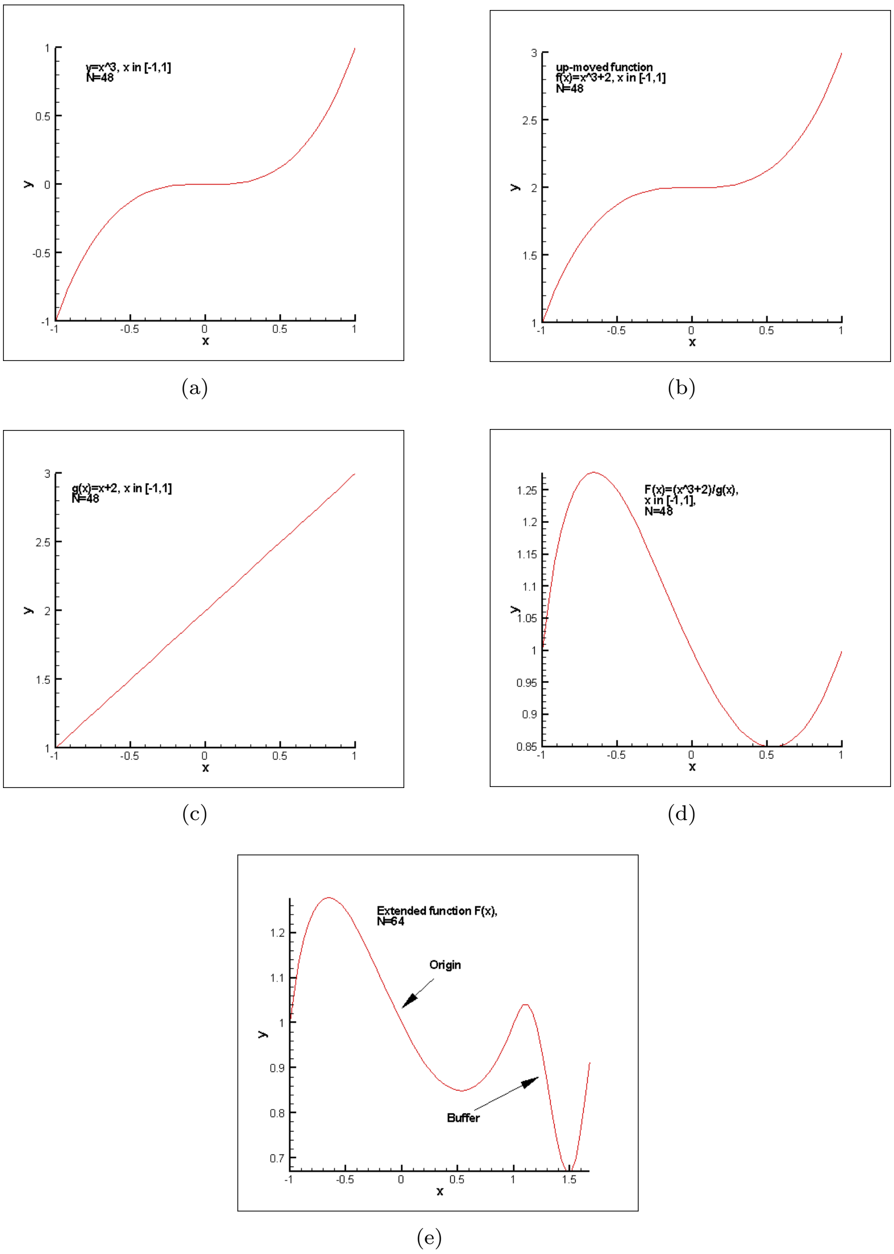


FIGURE 3. **Method steps** (a) Original function $f(x) = x^3$; (b) Up-moved function $f(x) + c$;(c) Linear function $g(x)$; (d) Normalized function $F(x) = (f(x) + c)/g(x)$; (e)Extended function with a polynomial buffer zone.

3.1.4. The chart of BFSM. The whole procedure can be described by the following chart:

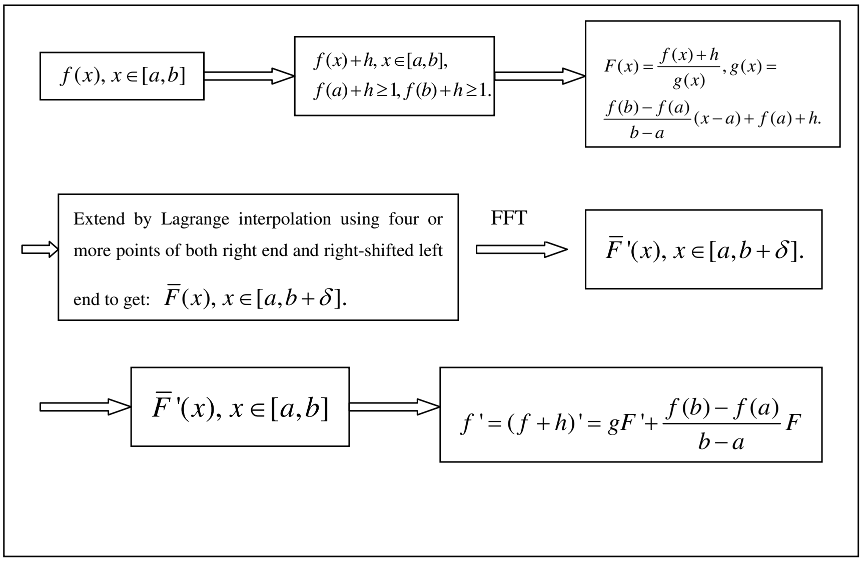


FIGURE 4. **the sketch of Buffered Fourier spectral method (BFSM)**

4. Computational Results by BFSM

4.1. Numerical Derivative.

4.1.1. Basic point of view on the new scheme development. Let us take an example. The 3-D time dependent Navier-Stokes equations in a general curvilinear coordinate can be written as:

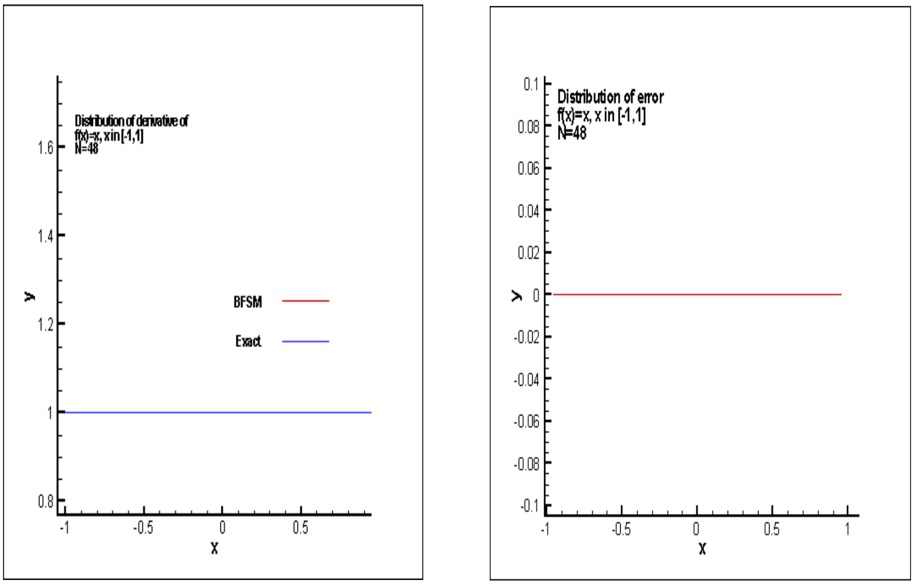
$$\frac{1}{J}\frac{\partial Q}{\partial t}+\frac{\partial\,(E-E_v)}{\partial\xi}+\frac{\partial\,(F-F_v)}{\partial\eta}+\frac{\partial\,(F-F_v)}{\partial\zeta}=0, \tag{4.1}$$

For 1-D conservation law, it will be:

$$\frac{\partial Q}{\partial t}+\frac{\partial E}{\partial\xi}=0. \tag{4.2}$$

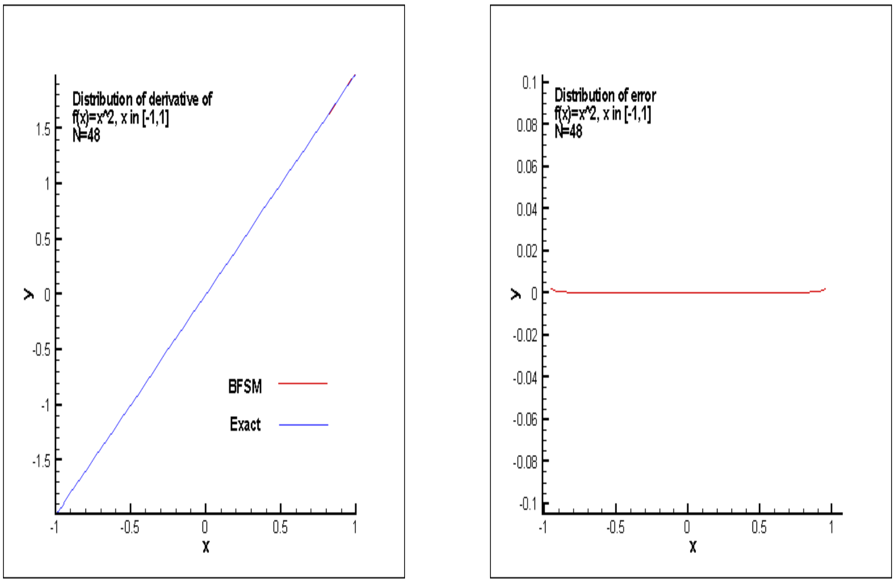
The critical issue for high order CFD is to find an accurate approximation of derivatives for a given discrete data set. The computer does not know any physical process but accepts a discrete data set as the input. The output is derivatives which are also a discrete data set. Therefore, it is critical to develop a high order scheme to achieve accurate derivative for a discrete data set.

4.1.2. Derivative using BFSM. The numerical derivatives approximated by BFSM are very accurate (see Figures 5-10). Following are several non-periodic functions we tested. One can see that the main error only appears on the boundary points, which are caused by the Lagrange interpolation of the function at the buffer points. However, they are located outside the domain $[a, b]$. And we can see these errors do not propagate into the domain $[a, b]$.



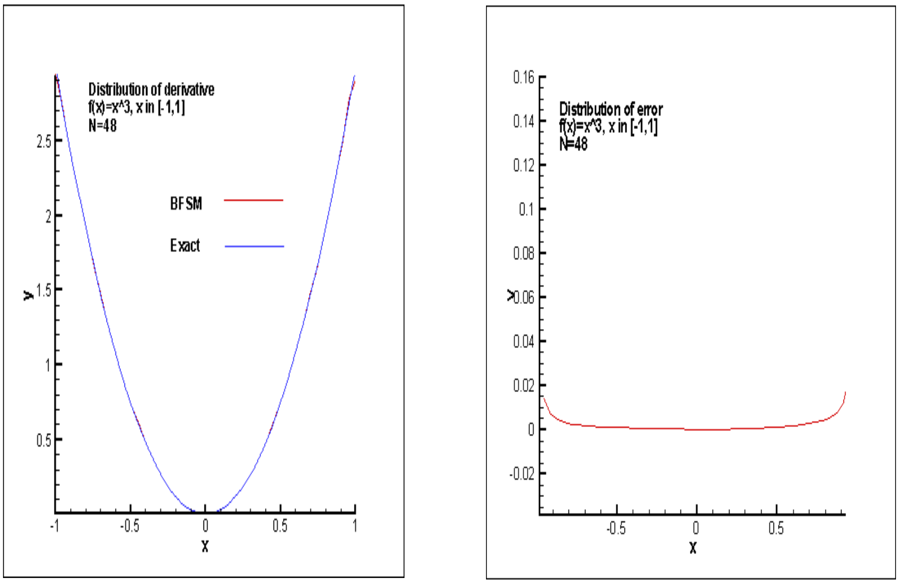
(a) (b)

FIGURE 5. $f(x) = x, x \in [-1, 1]$ (a) distribution of derivative of the function; (b) error by using BFSM;



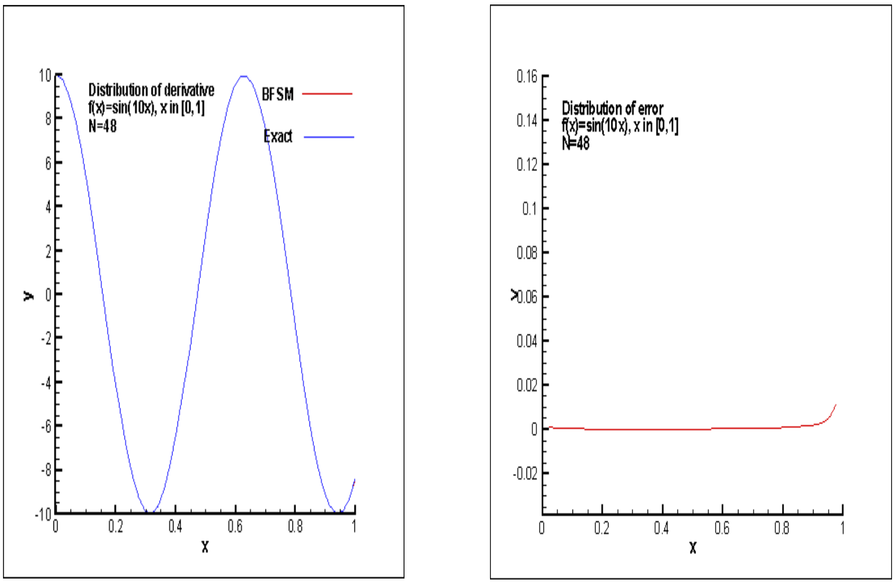
(a) (b)

FIGURE 6. $f(x) = x^2, x \in [-1, 1]$ (a) distribution of derivative of the function; (b) error by using BFSM;



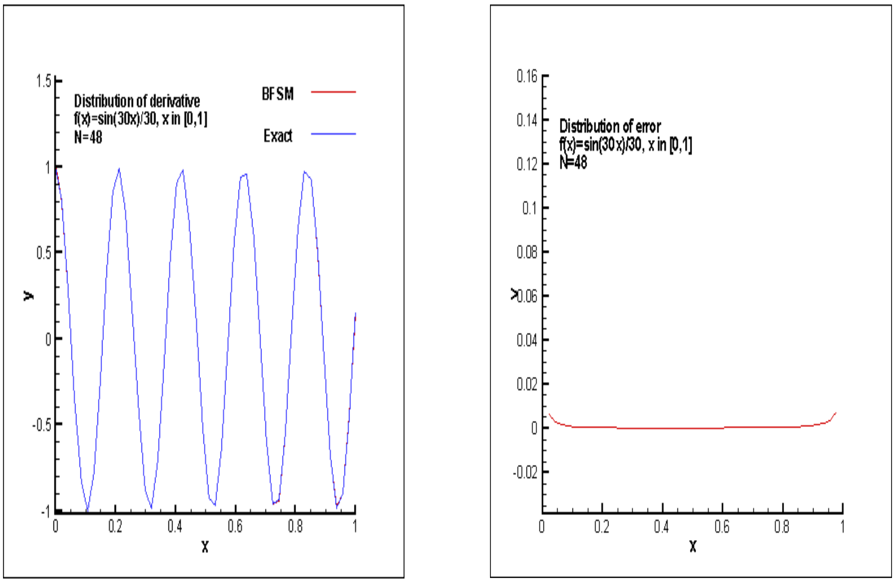
(a) (b)

FIGURE 7. $f(x) = x^3, x \in [-1, 1]$ (a) distribution of derivative of the function; (b) error by using BFSM;



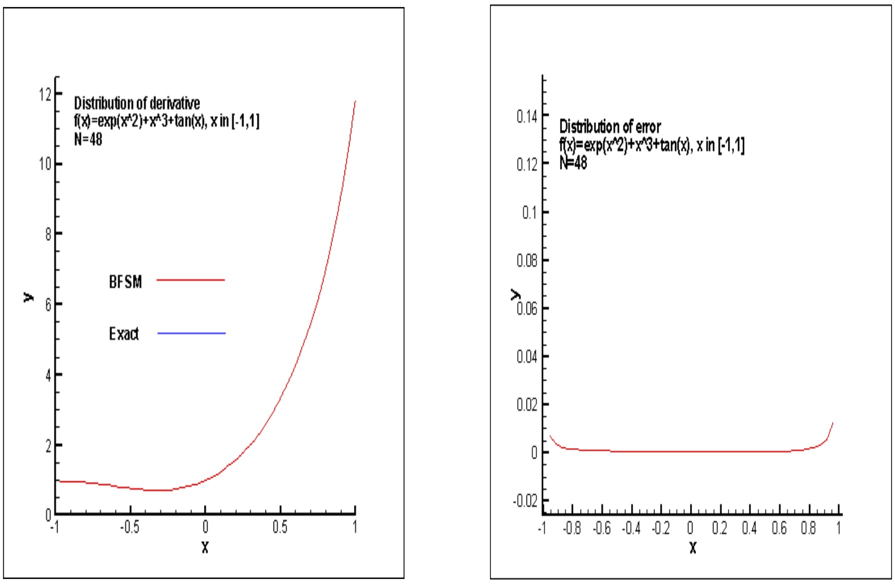
(a) (b)

FIGURE 8. $f(x) = sin(10x), x \in [0, 1]$ (a) distribution of derivative of the function; (b) error by using BFSM;



(a) (b)

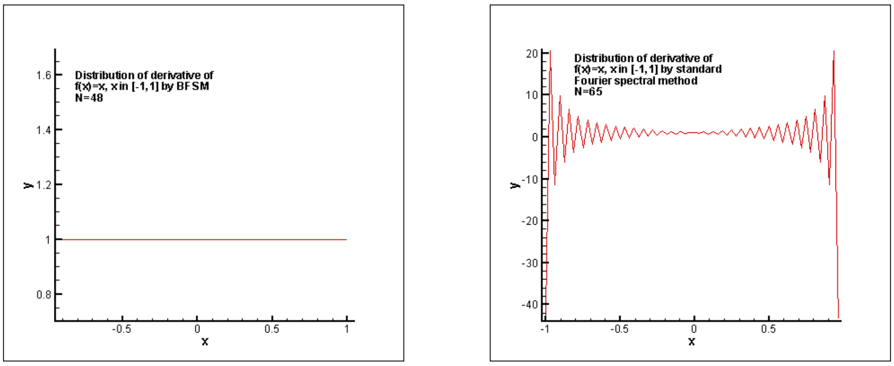
FIGURE 9. $f(x) = \frac{1}{30}sin(30x), x \in [0, 1]$ (a) distribution of derivative of the function; (b) error by using BFSM;



(a) (b)

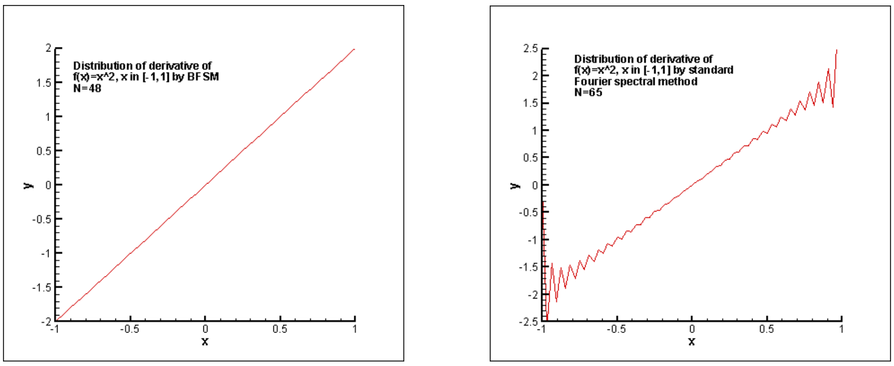
FIGURE 10. $f(x) = e^{x^2} + x^3 + tan(x), x \in [-1, 1]$ (a) distribution of derivative of the function; (b) error by using BFSM;

4.1.3. Comparison between our BFSM and the standard spectral method. Following figures give us a picture that our new method can obtain accurate derivatives for those functions which are non-periodic (see Figures 11 and 13-14). For standard Fourier spectral method, the approximation of derivatives contains a lot of oscillations, even for the function which is periodic on the boundary, such as $f(x) = x^2, x \in [-1, 1]$ (see Figure 11). For the functions which are non-periodic on the boundary, the standard Fourier spectral approximation of the derivatives are very oscillatory and cannot be accepted (see Figure 14). Note that our comparisons use different grids here for two different methods because for our new scheme we discard 25% of 64 points, but we do not need cut 25% for the standard method. Since the grids used for standard Fourier spectral method is finer, the comparison is acceptable.



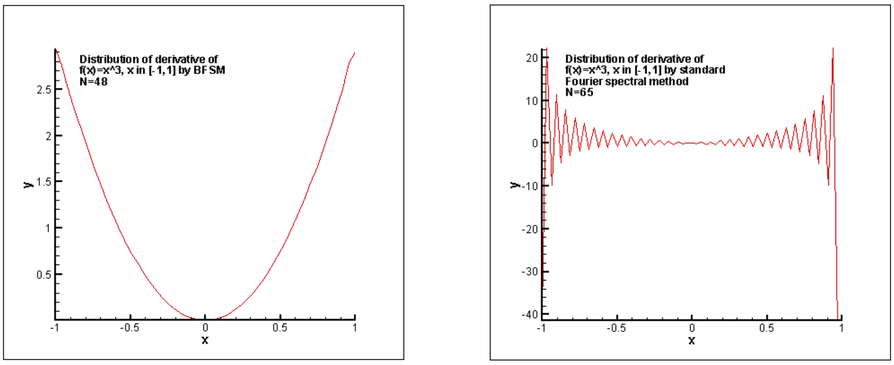
(a) (b)

FIGURE 11. **comparison between new method and standard spectral method for derivative of $f(x) = x, x \in [-1, 1]$:** $f'(x) = 0$. (a) BFSM; (b) standard spectral method.



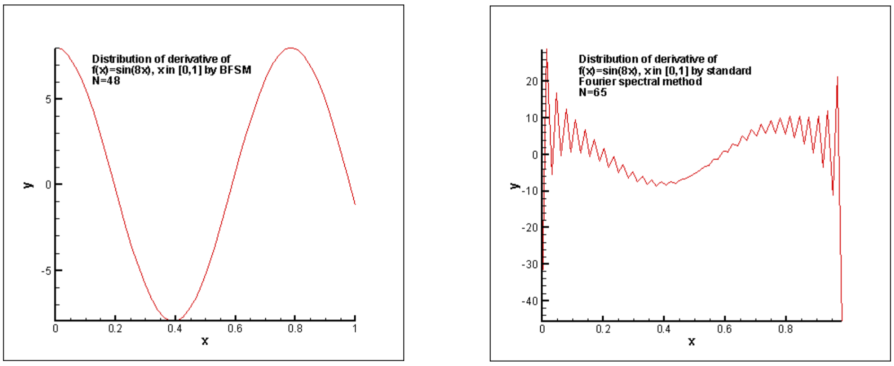
(a) (b)

FIGURE 12. **comparison between new method and standard spectral method for derivative of $f(x) = x^2, x \in [-1, 1]$:** $f'(x) = 2x$. (a) BFSM; (b) standard spectral method.



(a) (b)

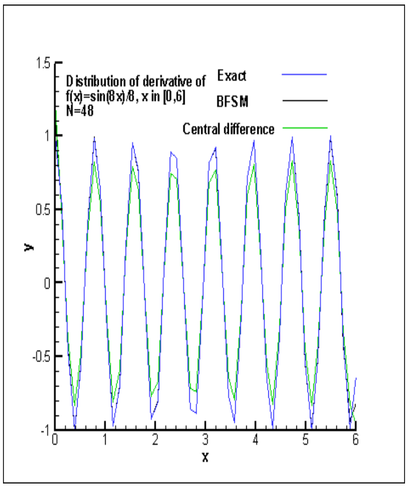
FIGURE 13. **comparison between new method and standard spectral method for derivative of** $f(x) = x^3, x \in [-1, 1]$: $f'(x) = 3x^2$. (a) BFSM; (b) standard spectral method.



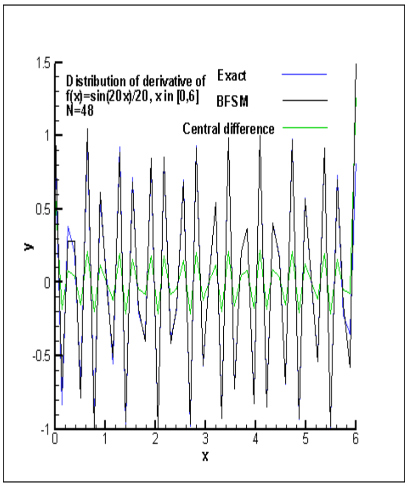
(a) (b)

FIGURE 14. **comparison between new method and standard spectral method for derivative of** $f(x) = sin(8x), x \in [0, 1]$: $f'(x) = 8 * cos(8x)$. (a) BFSM; (b) standard spectral method.

4.1.4. Comparison between BFSM and the 2nd order central difference method. In the following figures, we compare our new method with the central finite difference scheme. We try to approximate the derivative of $f(x) = sin(8x)/8, x \in [0, 6]$ and $f(x) = sin(20x)/20, x \in [0, 6]$. These are high frequency waves and we want to compare the capability for high resolution between BFSM and the central finite difference method. From Figure 15 (a), we see that the central difference does not work well and has visible large errors even for $f(x) = sin(8x)/8, x \in [0, 6]$, but Buffered Fourier Spectral Method works very well except for the boundary points due to the artificial interpolation polynomial. For the higher frequency function $f(x) = sin(20x)/20, x \in [0, 6]$, the central difference loses accuracy and the results are completely unacceptable, but our new method works very well. From these two graphs, we see that although we use only 48 points in [0, 6], our results are nearly the same as the exact solution (the blue one and the black one overlap each other), which means our new method has high order accuracy and high resolution. But the results approximated by central difference are not acceptable and even worse for higher frequencies (Figure 15 (b)). This clearly shows BFSM has much higher resolution than standard central finite difference schemes.



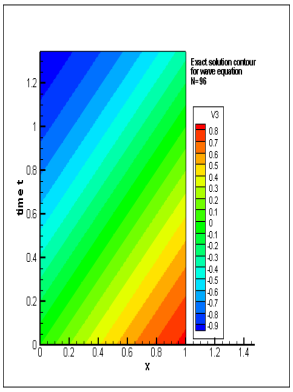
(a)



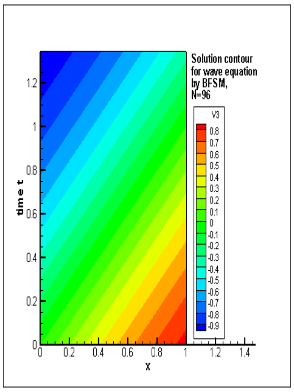
(b)

FIGURE 15. **comparison between BFSM and central difference method** (a) comparison of derivative of $f(x) = sin(8x)/8, x \in [0,6], N = 48$; (b) comparison of derivative of $f(x) = sin(20x)/20, x \in [0,6], N = 48$.

4.2. The BFSM method for wave equation. For a wave equation $u_t + cu_x = 0, u(0,x) = f(x)$, we solved the equation under different initial boundary conditions and different grids. The exact solution is $u(t,x) = f(x - ct)$. In addition, we made comparisons between our new method and second order central difference scheme. For time marching, both methods use the 4th order Runge-Kutta method and both central and BFSM methods are conditionally stable. We use a Courant number 0.5 for all following calculations. One should note that all boundary conditions are not periodic here. Figures 16, 17, 18, 19 give us a picture that our method is of fourth order, which is determined by the interpolation on the boundary. And these figures also show us that the Buffered Fourier Spectral Method can obtain high resolution. By the comparisons in Figure 17 and Figure 18, one can easily see that the 2nd-order central difference results are just simply not acceptable after some time steps, but our new method still works very well. For the initial boundary condition $f(x) = sin(20x), x \in [0,6]$, our new method still can resolve the high frequency waves and obtain nearly same results as the exact solution. On the other hand, the second order central difference scheme can work for the initial boundary condition of $f(x) = sin(x), x \in [0,1]$ with large errors, but completely failed for the initial boundary conditions of $f(x) = sin(8x), x \in [0,6]$ and $f(x) = sin(20x), x \in [0,6]$. We also tested up-winding schemes (1st order) for the boundary condition $f(x) = sin(8x), x \in [0,6]$, the results of which are not acceptable .



(a)



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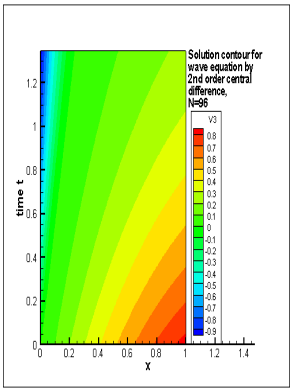
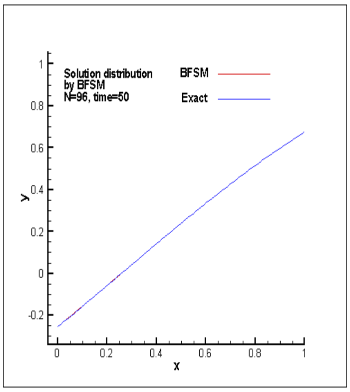


(c)



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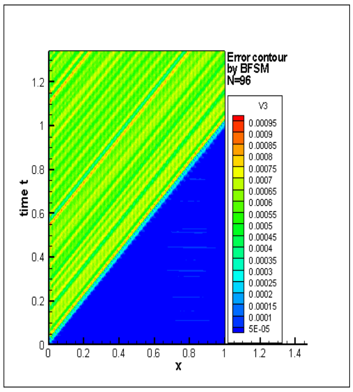
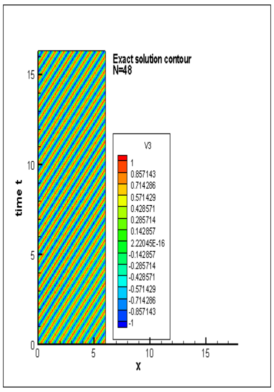
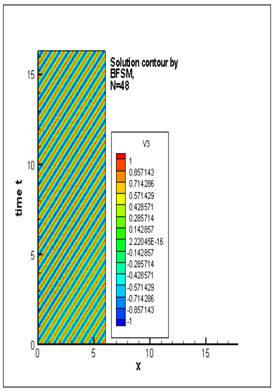


(e)

FIGURE 16. **comparison between new method and central difference method, N=96, for initial condition:** $f(x) = sin(x), x \in [0, 1]$. (a) Exact solution; (b) BFSM; (c) Central difference; (d) solution distribution u at t=50 by BFSM;(e) error contour by BFSM.



(a)



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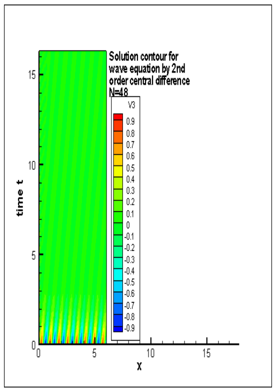
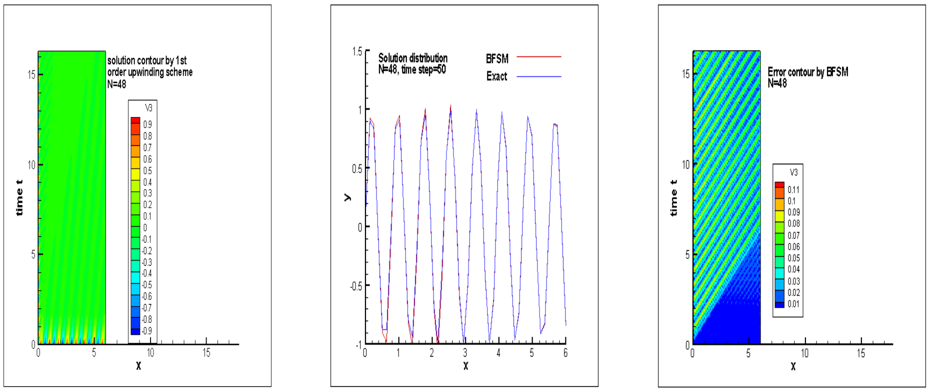
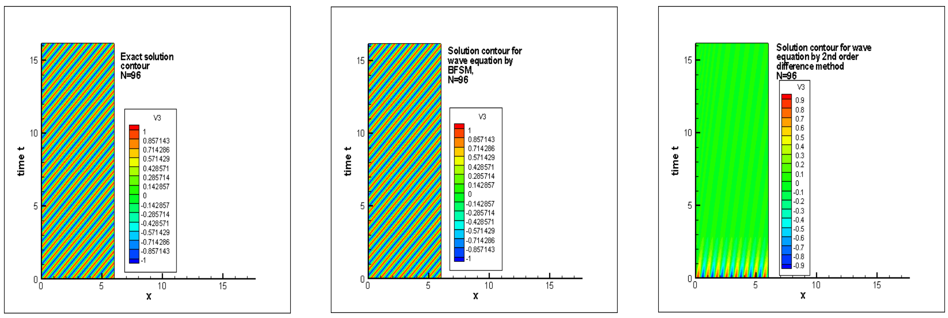


(c)

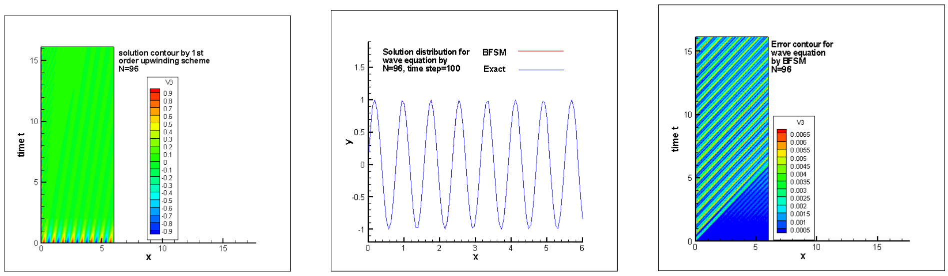


(d) (e) (f)

FIGURE 17. **comparison between new method and central difference method, N=96 for initial condition:** $f(x) = sin(8x), x \in [0, 6]$**.** (a) Exact solution; (b) BFSM; (c) Central difference; (d) solution distribution u at t=50 by BFSM;(e) error contour by BFSM; (f) error contour by BFSM.

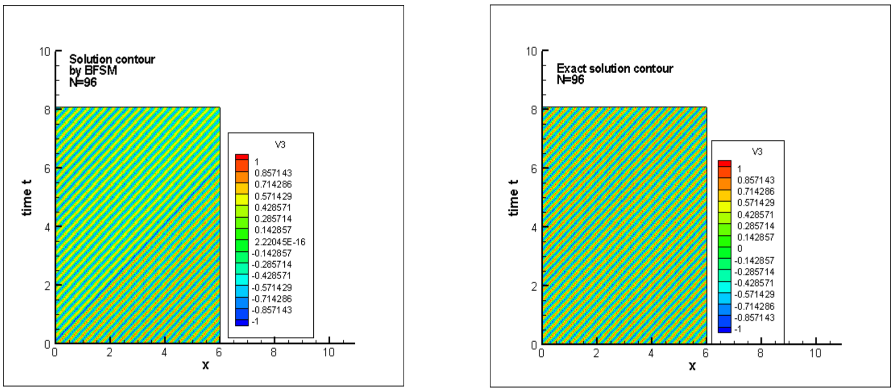


(a) (b) (c)



(d) (e) (f)

FIGURE 18. **comparison between new method and central difference method, N=96 for initial condition:** $f(x) = sin(8x), x \in [0, 6]$**.** (a) Exact solution; (b) BFSM; (c) Central difference; (d) solution distribution u at t=100 by BFSM;(e) error contour by BFSM; (f) error contour by BFSM.



(a) (b)

FIGURE 19. **solution contour by BFSM, N=96 for initial condition:** $f(x) = sin(20x), x \in [0, 6]$**.** (a) BFSM; (b) Exact solution.

4.3. The modified method for Poisson equation. We now use our new method for Poisson equation with non-periodic boundary conditions. The problem is defined as follows:

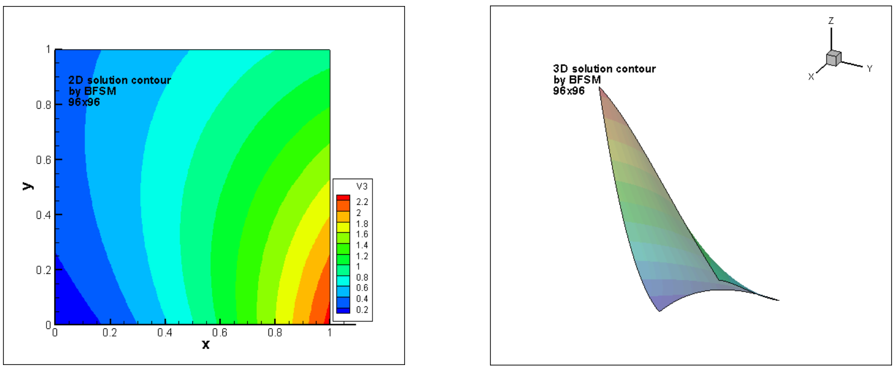
$$\begin{cases} \Delta u = 0, \quad (x, y) \in [0, 1] \times [0, 1]; \\ u(x, 0) = e^x \sin(x); \ u(0, y) = e^{-y} \sin(y); \\ u(1, y) = e^{1-y} \sin(1 + y); \ u(x, 1) = e^{x-1} \sin(x + 1). \end{cases}$$

The exact solution is $u(x, y) = e^{x-y} sin(x + y), (x, y) \in [0, 1] \times [0, 1]$. We solve the equation by using following equation for iteration:

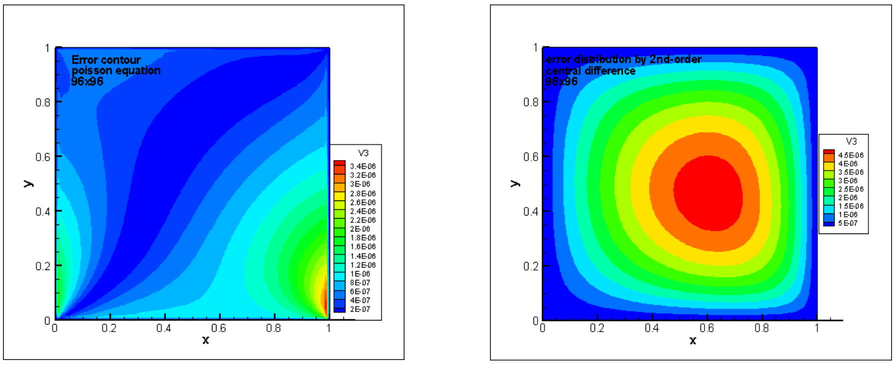
$$u_{t+1} = u_t + \Delta t(u_{xx} + u_{yy}).$$

The convergence tolerance is set to be $|u_{t+1} - u_t| \leq 10^{-12}$, and we use 6 points at each end of the boundary to do the interpolation.

Following figures are our results.

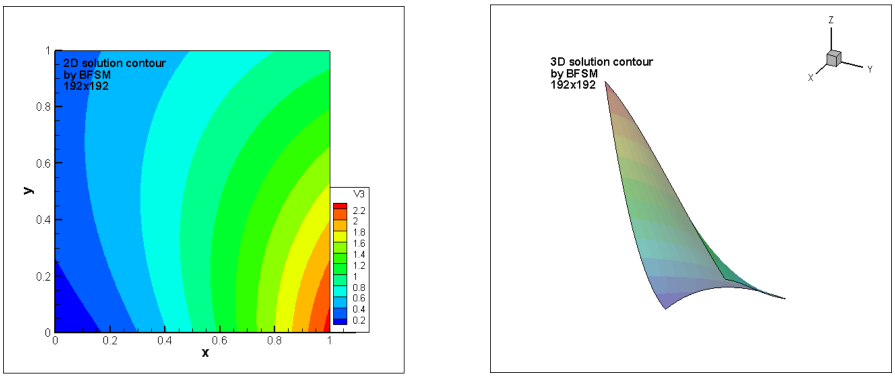


(a) (b)

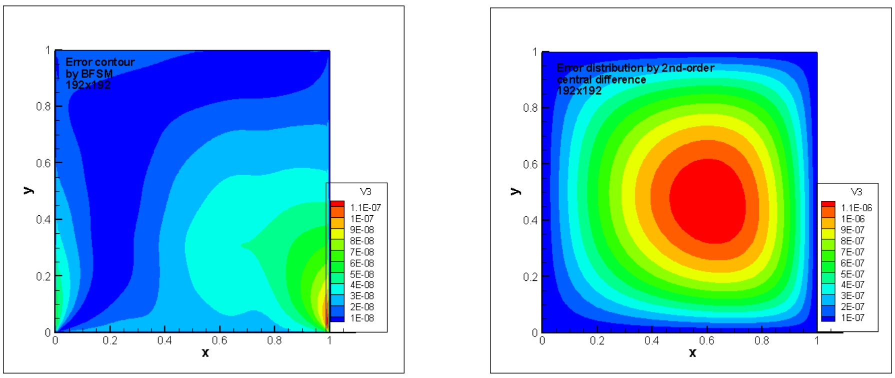


(c) (d)

FIGURE 20. **solution and error contour, grids:** 96×96**.** (a) 2D solution contour; (b) 3D solution contour; (c) error contour;(d) error contour by 2nd order central difference.



(a) (b)



(c) (d)

FIGURE 21. **solution and error contour, grids:** 192×192**.** (a) 2D solution contour; (b) 3D solution contour; (c) error contour by BFSM; (d) error contour by 2nd order central difference.

Maximum error comparison		
Grids	BFSM	2nd-order central difference
96×96	$3.5847E-6$	$4.8255E-6$
192×192	$1.1874E-7$	$1.1971E-6$

From the above table, we can see the order of accuracy for BFSM is 5, which is partially determined by the boundary treatment. However, the 2nd order central difference has only 2nd order of accuracy. From those Figures, we can get a picture that for BFSM, the largest error primarily appears on the boundary, and is related to the function value difference between two end points, while the error for central difference occupies most of the middle area. From the error figures, we can see that near the bottom of the left and right sides, the errors are larger than other area. This is because the difference of function (or solution) values between those two end points in the x direction is large. However, near both tops and bottom sides, the errors are not large since the differences between these two end points in y direction are smaller. In the interior area, the BFSM solution is very accurate, almost same as the exact solution. In general, we say that the large errors happen only near the boundary which is caused by the manually extending the function and doing the polynomial interpolation. However, this is acceptable because of the non-periodicity of the function.

5. Conclusion

1. Using smooth buffer and normalization, the non-periodic smooth function can be extended to a periodic function which is smooth in functions and derivatives, and therefore the standard Fourier spectral method can be use to such a new buffered function.

2. The Buffered Fourier Spectral Method (BFSM) can get very accurate numerical derivatives for non-periodic functions. Large errors only happen near the boundary because of the non-periodicity of the function or solution and polynomial interpolation.

3. The Buffered Fourier Spectral Method keeps high resolution and high order accuracy for smooth PDEs, and the order of accuracy is determined by the interpolation on the boundary. Non-smooth PDEs are still open for further research.

4. With some penalty over the standard FSM method, BFSM still keeps high order of accuracy and high resolution for non-periodic PDEs.

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