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TRUNCATION ERROR EQUIVALENT BOUNDARY CLOSURE SCHEMES FOR HIGH-ORDER SPATIAL DISCRETIZATION
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Abstract. *The time accurate simulations of initial value partial differential equations often require high-order spatial discretization schemes as well. The use of near boundary and boundary schemes with the same accuracy-order of the domain scheme, however, leads to numerical instability on uniform meshes. CFL numbers must, in turn, be reduced, which significantly increases CPU times. Two solutions are often employed to mitigate this issue:*
1) Mesh refinement at the boundaries and/or
2) Lower order near boundary and boundary schemes.

In the present paper, a preliminary study to better understand how the order of boundary and truncation error affects the numerical stability of the method giving a uniform mesh (case 2), limiting the maximum CFL that can be used in numerical simulations, is presented. Near boundary and boundary closure finite difference schemes are derived using the Taylor Series and are implement in methods to solve partial differential equations. Where the numerical stability will be analyzed using the Fourier/von Neumann criteria considering boundary schemes and will compare how the maximum value of CFL changed in comparison to when the closure are not considered .

Keywords: *Numerical Stability, Spatial Derivatives, Boundary, Order*

1. INTRODUCTION

Partial differential equations (PDE) are commonly used to model various natural phenomenon. The first step in a computational simulation using these equations utilizes the line method, which is known since the 60's (E. N. Sharmin and L. A. Chudov,1963). It consists of the transformation of PDEs into a system of ordinary equations (ODE). This only can be done with the discretization of the spatial derivatives, leaving the time derivatives in its continuous form. These spatial derivatives can be achieved by many methods, such as finite differences, finite volumes or finite elements, only to cite the most well-known methods. With this, the resulting system of ODEs can be resolved with one of various well established numerical solutions of the initial value problems, i.a. IVPs. The utilization of the line method for boundary value problems, i.e. BVPs, where the PDE is purely elliptical, requires the combined use of other techniques, known as the false transient method (W. E. Schiesser, 1991). In it, an artificial time derivative, in other words, that does not necessarily contain any physical meaning, is introduced in the elliptical PDE as to transform it in a parabolic or hyperbolic, changing the BVP into a IVP.

When a numerical solution of with low error is required, a spatial discretization of the PDE normally uses schemes with high precision order. Increasing the order of the spatial discretization signifies an increase in the rate at which the error decreases as the spacing between consecutives points in the spatial mesh decreases. For this reason, compact formulations became popular (S. K. Lele, 1992). As they can obtain high order while using fewer number of points than explicit formulations, turning the line method more numerically stable. More modern version where posteriorly developed to become more efficient the calculations of the second derivatives (K. Mahesh, 1998). However, the terms containing the second derivative are very important, explicit formulations of high order are still more efficient (K. F. S. Santiago and L. S. de B. Alves, 2017).

One of the difficulties in the use of high order schemes of both explicit and compact formulations for points inside the spatial domain is associated with the boundary conditions; (M. H. Carpenter, D. Gotlieb and S. Abarbanel, 1993),(C. D. Pruett, T. A. Zang, C. L. Chaang and M. H. Carpenter, 1995) and (S. S. Abarbanel, A. E. Chertock and A. Yefet, 2000). In the boundary, as well as for points sufficiently near it, the discretization utilized in the interior of the domain needs to be modified as to not utilize points outside de spatial domain. However, the resulting line method becomes numerically unstable if the modified discretization maintains the same order of precision as the spatial discretization used in the interior of the domain. For example, methods that use compact formulations of sixth order in the interior of the domain must reduce the order of this formation by three in the boundary as to maintain numerical stability. This way, the order of the global spatial method resulting from the line method is reduced to the fourth order. Increasing the order even further in the interior of the domain makes it necessary to decrease the order in the boundary even further, limiting the global order of the resulting method. This can be a serious problem, since the global order is one above the one of the boundary (B. Gustafsson, 1995).

Therefore, a better understanding of how the precision order and the truncation error of boundary closure schemes interact and limit a method's numerical stability could greatly existing methods and possibly aid in the development of new ones.

2. DISCRITAZTION OF BOUNDARY DERIVATIVES

The discretization of the 1st and 2nd derivatives is performed by the expansion of Taylor series around *n* number points and by solving the resulting linear system for the specified derivative with the desirable order. The nature of the approximations studied for boundary and near boundary points were centered, forward, partially forward, backward and partially backward discretization of 2nd, 3rd and 4th.

To validate the discretization the nature of precision order and error behavior were studied the periodic function giving by Eq. (1) and Eq. (2) for 4th order inner domain approximations.

$$F(x) = \cos(x + 1.5\pi)\ ;\ \frac{dF}{dx}(x) = -\sin(x + 1.5\pi)\ ;\ \ x \in [0,2\pi] \tag{1}$$

$$F(x) = \cos(x + \pi)\ ;\ \frac{d^2F}{dx^2}(x) = -\cos(x + \pi)\ ;\ \ x \in [0,2\pi] \tag{2}$$

It also observed how the absolute error varies as the scheme's order increases for a giving mesh was analyzed. The results for boundary schemes with a 4th order inner domain are presented, where Fig. 1 through Fig. 4 are for the 1st derivative and Fig. 5 through Fig. 8 the 2nd derivative

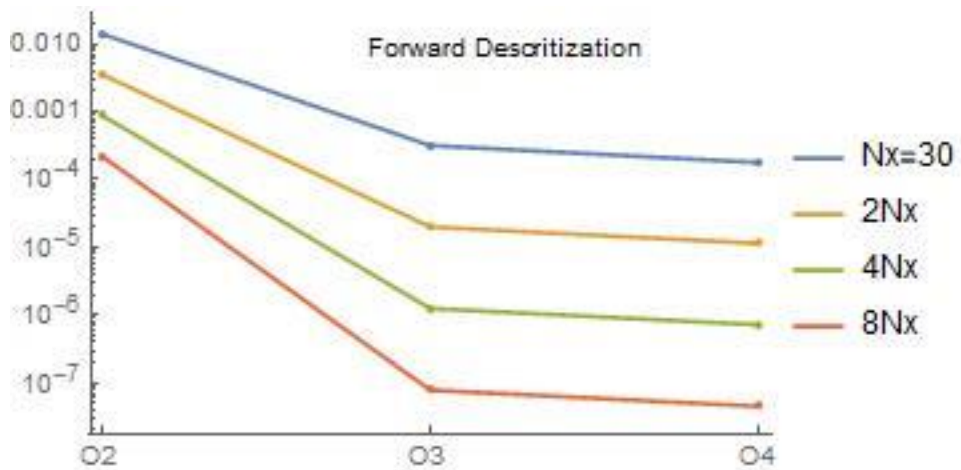

Figure 1. Absolute error by order of forward discretization of the 1st derivative used in the boundary of 4th order inner domain approximation evaluated in a mesh of *Nx* points.

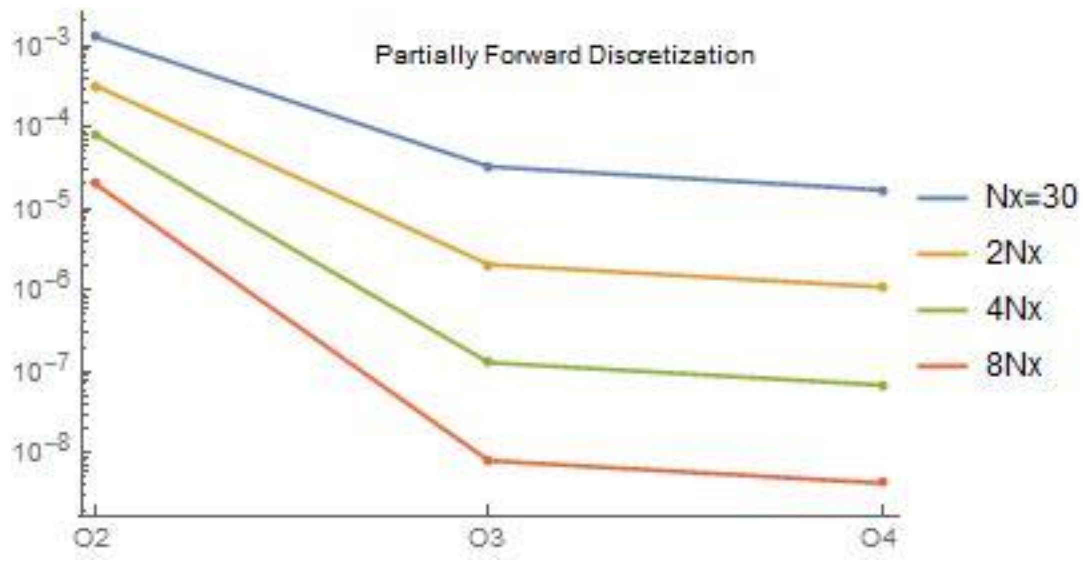

Figure 2. Absolute error by order of partially forward discretization of the 1st derivative used in the boundary of 4th order inner domain approximation evaluated in a mesh of *Nx* points.

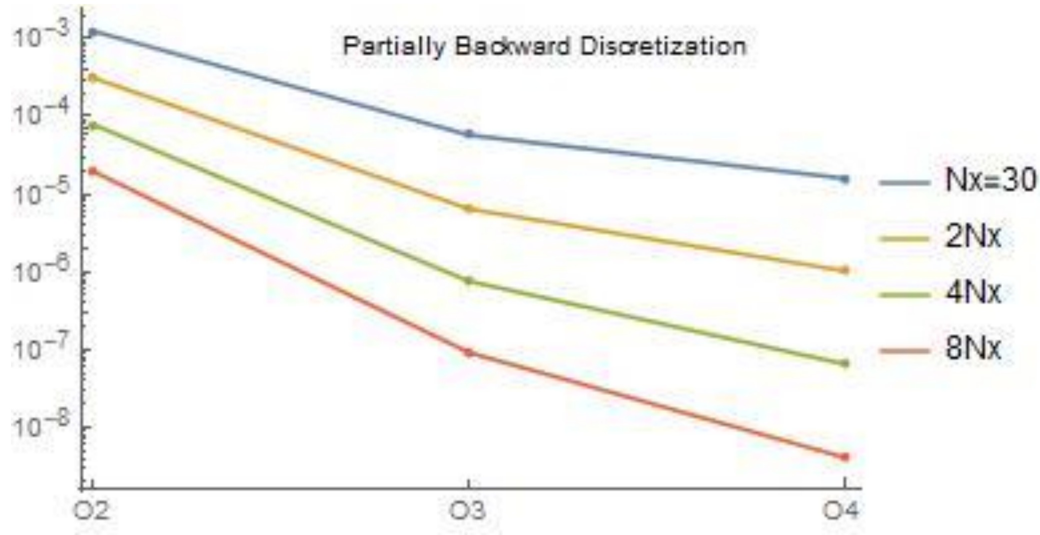

Figure 3. Absolute error by order of partially backward discretization of the 1st derivative used in the boundary of 4th order inner domain approximation evaluated in a mesh of *Nx* points.

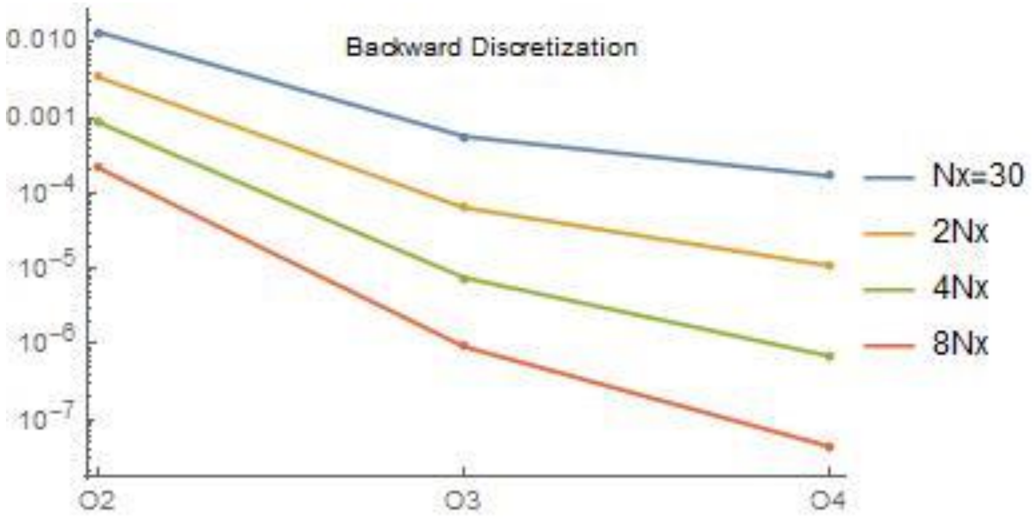

Figure 4. Absolute error by order of backward discretization of the 1st derivative used in the boundary of 4th order inner domain approximation evaluated in a mesh of *Nx* points.

3. MODEL AND STABILITY

The model was based on the partial differential equation represented in equation Eq. (4).

$$\frac{\partial y}{\partial t} + U \cdot \frac{\partial y}{\partial x} = V \cdot \frac{\partial^2 y}{\partial x^2} \tag{4}$$

For the time derivative, the Euler discretization was adopted, and a 4th centered scheme was implemented in the interior of the spatial domain.

The numerical parameters that govern the analyses and delimitate the region of stability of the method are *CFL* and Vnn defined through Eq. (5) and Eq. (6).

$$CFL = \frac{U \cdot dt}{dx} \tag{5}$$

$$Vnn = \frac{V \cdot dt}{dx^2} \tag{6}$$

To analyze the impact of the different precision order truncation error on limiting the maximum value of *CFL* possible while maintaining stability the value of Vnn was fixed.

3.1 Single Equation Analysis

For a numerical method to be stable, Fourier criteria states that the method amplification factor, *G*, should be accordance with Eq. (7) (J. C. Tannehill, D. A. Anderson and R. H. Pletcher, 1997).

$$|G| \leq 1 \tag{7}$$

When analyzing the amplification factor of the inner domain in function of *CFL* and Vnn for 4th order schemes it was found that *G* is given by Eq. (8). As a result, the transition between a stable and unstable method happens for a *CFL* between *0.73096* and *0.73014* when Vnn was fixed at 1/3.

$$G = 1 + \frac{CFL}{12} e^{-2i\beta}\left(-1 + 8e^{i\beta} - 8e^{3i\beta} - e^{4i\beta}\right) - \frac{Vnn}{12} e^{-2i\beta}\left(-1 + 16e^{i\beta} - 30e^{2i\beta} + 16e^{3i\beta} - e^{4i\beta}\right) \tag{8}$$

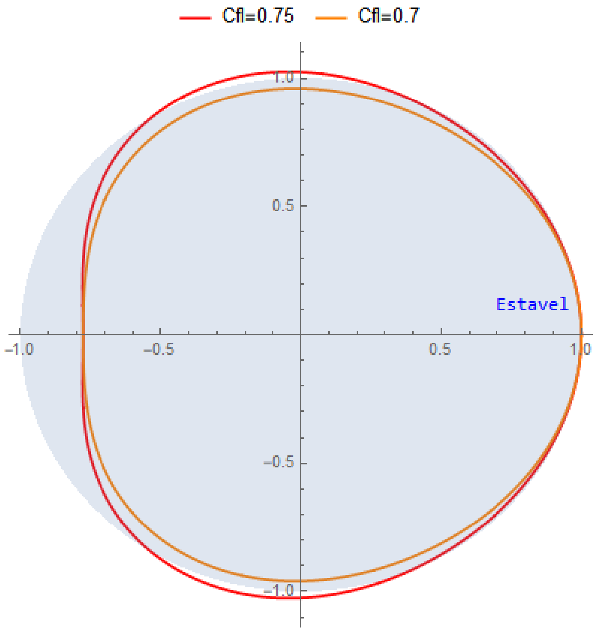

Figure 5. The absolute value of Amplification factor of 4th order method for different *CFL*s and delimitated in blue is the region of stability

3.2 Analysis for Systems of Equations

This analysis is similar to the single equation, but instead of an amplification factor, G, we have amplification matrix [X].

$$\boldsymbol{T}^{n+1} = [X]\boldsymbol{T}^{n} \tag{9}$$

Where the stability of the finite-difference calculation is governed by the eigenvalue structure of [X] (J. C. Tannehill, D. A. Anderson and R. H. Pletcher, 1997).

$$|\lambda_{max}| \leq 1 \tag{10}$$

Before refining the results of this analysis, a study of numerical precision and mesh convergence were carried out. The criteria of numerical precision were as followed, the percentage error of λ_{max}, between the refence precision of 250 significant digits and y significant digits, should be equal or less than 10^{-5}%. For all conditions of closure schemes a precision of 37 was adopted. For mesh convergence, the percentage difference of λ_{max} between to two sequential mesh size (N_x) should be equal or less than 10^{-5}%. For all conditions of closure schemes a mesh of 50 points was adopted.

$$N_x \; \epsilon \; [10, 50, 100, 250, 500, 750, 1000, 1250, 1500] \tag{11}$$

3.2.1 Analysis Periodic Boundary

When analyzing eigenvalue of the system with periodic boundary conditions in function of *CFL* and Vnn for 4th order schemes it was found the transition between a stable and unstable method happens for a *CFL* between *0.72892* and *0.72824* when Vnn was fixed at 1/3.

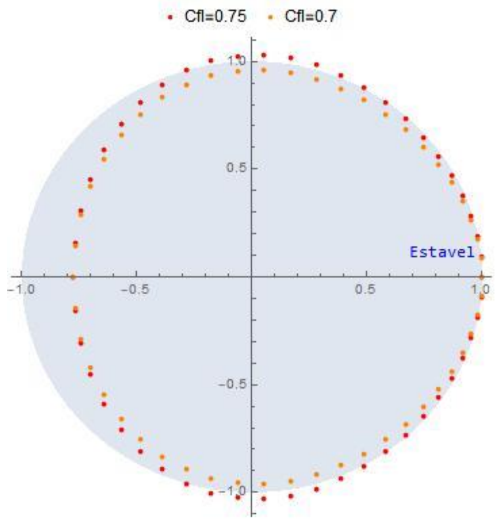

Figure 6. The eigenvalues of the Amplification Matrix of 4th order with periodic boundary for different *CFL*s and delimitated in blue is the region of stability

3.2.2 Analysis 2^{nd} order Boundary

When analyzing eigenvalue of the system with 2^{nd} order closing schemes in function of *CFL* and Vnn for 4th order schemes it was found the transition between a stable and unstable method happens for a *CFL* between 0.*94690* and *0.94660* when Vnn was fixed at 1/3.

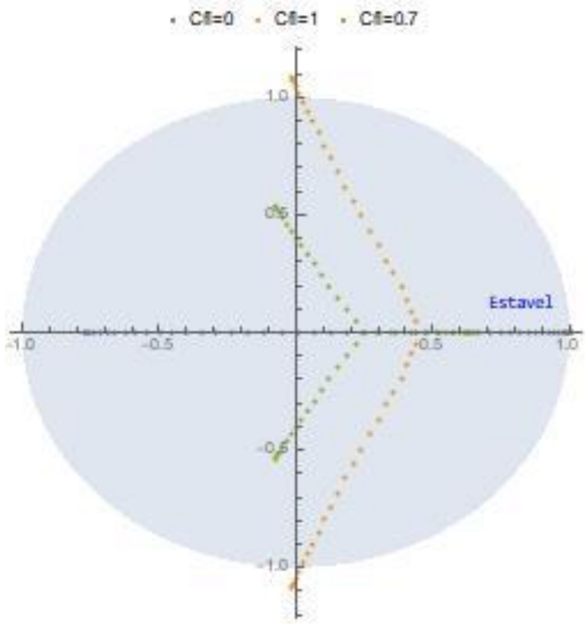

Figure 7. The eigenvalues of the Amplification Matrix of 4^{th} order 2^{nd} order boundary for different *CFL*s and delimitated in blue is the region of stability

3.2.3 Analysis 3th order Boundary

When analyzing eigenvalue of the system with 3^{rd} order closing schemes function of *CFL* and Vnn for 4th order schemes it was found the transition between a stable and unstable method happens for a *CFL* between *0.94675* and *0.94650* when Vnn was fixed at 1/3.

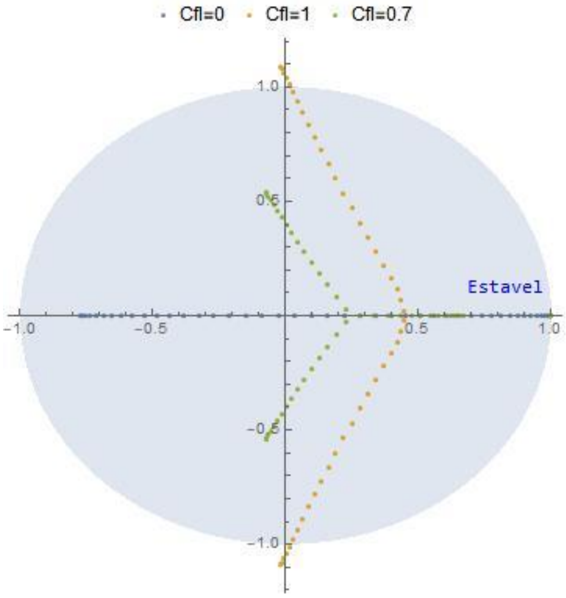

Figure 7. The eigenvalues of the Amplification Matrix of 4th order 3rd order boundary for different *CFL*s and delimitated in blue is the region of stability

4. FINAL REMARKS

As can be seen from the study, although global order is expected to be reduced, begin closer to the closure than the interior of the domain, when lower order schemes are applied at the boundary a great increase the region of stability is observed. The gain in numerical stability with further reduction in order is of reduced magnitude.

Therefore, its expected that if new closure schemes, with the same order as the interior of the domain, are developed that the methods derived from them will not be as numerically stable as the current methods applied. Where the transition between stability and instability will most likely be between the periodic closure's range and the third order's.

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