

# DISCRETIZATION OF LAPLACIAN OPERATOR ON 19 POINTS STENCIL USING CYLINDRICAL MESH SYSTEM WITH THE HELP OF EXPLICIT FINITE DIFFERENCE SCHEME

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**Abstract:** In research and technology, discretization is essential for describing numerical evaluation of mathematical models. Computationally efficient, partial differential equations are used to provide promising numerical formulations with mathematical models. These equations must be solved for curved meshes with irregular boundaries and porous domains. Obtaining isotropic discrete solutions is very important for the numerical evaluation of partial differential equations. This guarantees stability, accuracy, and efficiency in numerical simulations. We have restricted the scope of this study to the Laplacian operator. This operator is fundamental to coarse grain models such as cell dynamic simulations. We have discretized the Laplacian on a cylindrical mesh structure with a mixed derivative on a 19-point stencil using an explicit finite-difference approach while maintaining model accuracy and computational simplicity. Graphical stability is described to explain the validity and numerical stability of this stencil based on a cylindrical mesh. The reduction of error describes the stability, consistency, and convergence of the scheme.

**Keywords:** Cell Dynamic Simulation Method, Finite Difference method, Laplacian operator, Discretization, 3-dimensional Molecule, Cylindrical mesh system, Stability, error analysis

## I. INTRODUCTION

The procedure of numerically approximating the continuous differential operator on a discrete grid, known as discretization of the Laplacian, makes it possible to compute approximate solutions. The finite difference technique and grid/mesh selection are crucial factors. Deconstructing the Laplacian into discrete forms has numerous significant uses in numerous fields. It makes it possible to model diffusion processes in domains such as image processing, fluid<sup>1</sup> transport, and heat transfer. It also makes it possible to simulate phenomena that are controlled by diffusion equations, such as those in biology, physics, and electromagnetic. Graph Laplacians are also applied to irregular structures in machine learning. All things considered, the discretized Laplacian is widely used in research, engineering, and data analysis whenever diffusion processes require numerical approximations. The Laplacian operator has several notable properties, one particularly important and used in engineering applications is its isotropy. Since isotropy is important

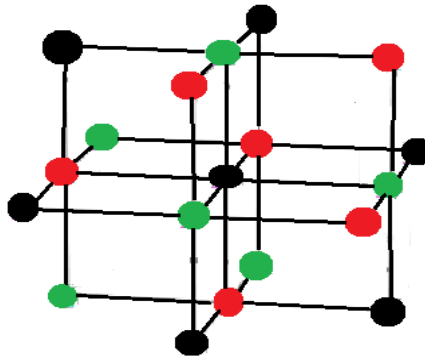
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to maintain the integrity of numerical modeling and simulated physical behavior, it has become a desirable property for the discretization of the Laplacian operator. These methods are often used to model a variety of block copolymers [1-4]. Several contemporary scholars have considered the use of the discrete isotropic Laplacian for various techniques. A study of two- and three-dimensional Laplacian proposals for a hybrid Boltzmann simulation approach has been proposed by Thampi *et al.* There are several excellent techniques for numerically estimating the discrete Laplacian operators and obtaining highly reliable isotropic results for the CDS model, but the best is the use of discretized stencils. For this purpose, 9- and 27-point numerical schemes are being prepared [5-6]. Through the use of finite difference schemes and a 5-point stencil, Inayat *et al.* derived the Laplacian operator on polar cylindrical and spherical mesh systems. Their submission included innovative results in both 2D and 3D domains [7-8]. Using mixed partial derivatives with forward and backward finite difference techniques (FDM), Rabnawaz *et al.* developed a 9-point discrete Laplacian operator using Taylor's approximation in polar mesh systems and also described the stability of the proposed scheme graphically [9-10]. Rabnawaz *et al.* studied 9-point stencils, which developed two unique schemes with different methods under the same Taylor series. Using the same basic finite-difference technique, they examined stability and compared their new findings [11-12]. Discretization of the Laplacian operator must retain certain structural properties for some fundamental applications. The need to preserve such properties of a continuous context motivates requirements such as symmetry and linear convergence accuracy, resulting in a wide range of discrete specifications. Establishing a consistent numerical method to discretize the Laplacian on meshes that faithfully represent the underlying continuous operator is the goal of this research. The objective is to create a logical discretization framework that replicates the qualities of the original Laplacian while maintaining important characteristics like precision, convergence, and symmetry [13-15]. Approximating the Laplacian in a rectangular coordinate and other systems has been done before, but the way it is now being done in a cylindrical coordinate system has not been done before [9-20]. This study aims to develop an accurate and consistent numerical approach based on the cylindrical mesh topology.

## II. COMPUTATIONAL MOLECULE CONTAINING 19-POINT STENCIL

In Figure 1, A molecule is presented in the square grid, as well as computational molecule is shown in Figure 2.



*Figure 1: Computational molecule containing 19-point stencil in the square grid system*

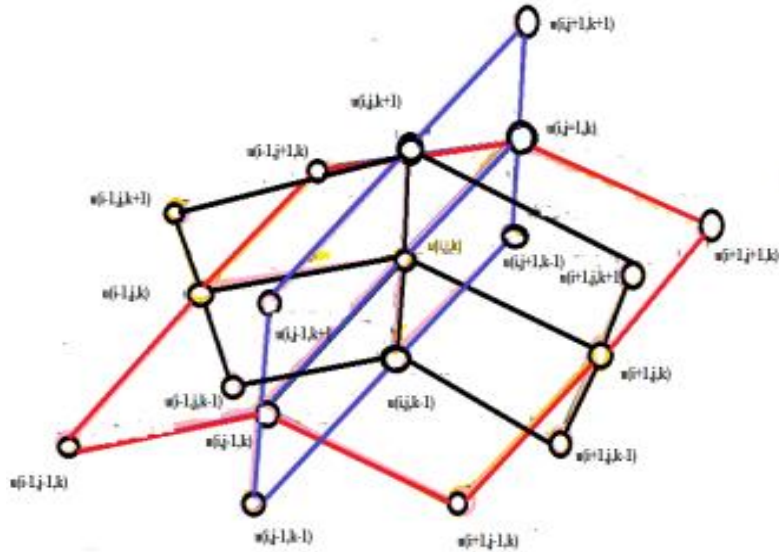


Figure 2: Computational molecule containing 19-point stencil in a cylindrical mesh system

### III. METHODOLOGY

As shown in Figure 1 and Figure 2, this study formulates the discretization of the Laplacian operator on a 19-point stencil in a cylindrical mesh system. Using a contemporary finite difference technique and Taylor series expansion, the discrete Laplacian operator was constructed. This method is preferred in order to achieve new isotropic outcomes for the discrete Laplacian operator. The discrete Laplacian operator finds extensive use in sophisticated materials modeling and computations (including soft and active materials) and cell dynamic simulation, as well as more general applications in science and engineering. The goal of this work is to use the same 19-point stencil discretization within a cylindrical mesh system using finite difference methods to produce innovative outcomes in each of these use cases. This is an example of three-dimensional research that uses the cylindrical coordinate system  $(r, \theta, z)$ . The following equations serve as the foundation for the discrete Laplacian operator formulation. For simulating a wide range of practical issues involving partial differential equations, cylindrical meshes work well. The suggested discretization method's higher-order accuracy suggests that it could be useful in a variety of application domains to accurately capture the characteristics of the underlying continuous Laplacian operator.

$$r_i = r_a + i(\Delta r)$$

$$\theta_j = j(\Delta \theta)$$

$$\theta_k = k(\Delta \varphi)$$

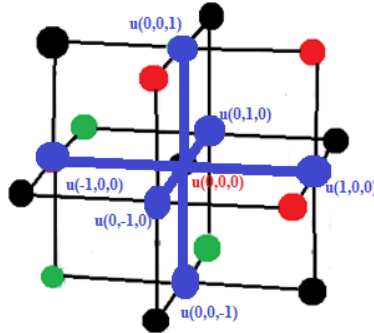
The above discretization values will be integrated into the governing equations to produce innovative numerical approximation results with isotropic behavior. The discretization of first and second-order derivatives using 3-point stencils and explicit methods is made possible by the finite difference approximations presented below. The higher-order 19-point Laplacian discretization that is suggested is based on these fundamental approximations. An effective method for implicit solutions is to compute derivatives as weighted averages of nodal values using the approximations below. The method begins with typical finite difference techniques and proceeds to a novel higher-order Laplacian discretization designed for cylindrical meshes. These basic approximations are critical for the overall accuracy and rotational symmetry qualities of the proposed discretization approach, with an emphasis on isotropic outcomes.

$$u_r = \frac{u_{1,0,0} - u_{-1,0,0}}{2(\Delta r)} \quad (1)$$

$$u_{rr} = \frac{u_{1,0,0} - 2u_{0,0,0} + u_{-1,0,0}}{(\Delta r)^2} \quad (2)$$

$$u_{\theta\theta} = \frac{u_{0,1,0} - 2u_{0,0,0} + u_{0,-1,0}}{(\Delta\theta)^2} \quad (3)$$

$$u_{zz} = \frac{u_{0,0,1} - 2u_{0,0,0} + u_{0,0,-1}}{(\Delta z)^2} \quad (4)$$



**Figure 3:** In this graph blue vertices and lines are involved in derivation, which can be seen in equation no (1), (2), (3), and (4).

In Figure 3, a three-dimensional view of stencils is provided for which the equations (1), (2), (3) and (4) are derived.

#### IV. METHODOLOGY ADOPTED IN DISCRETIZATION OF LAPLACIAN OPERATOR ON CYLINDRICAL MESH SYSTEM

The summation form of the Laplacian operator is

$$\nabla^2 u = \sum_{k=1}^n \frac{\partial^2 u}{\partial x_k^2} \quad (5)$$

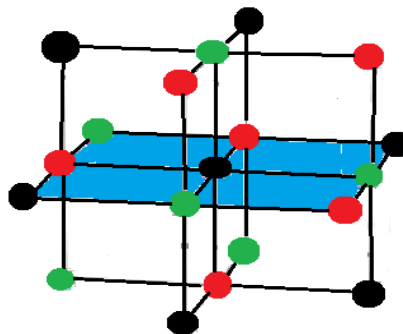
The Laplacian operator in 3D in the Cartesian coordinate system can be written mathematically as

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \quad (6)$$

The Laplacian operator in cylindrical form can be written as

$$\nabla^2 u = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\partial^2 u}{\partial z^2} \quad (7)$$

Now we have provided the derivation of first-order approximation concerning  $r$ ,  $\frac{\partial u}{\partial r}$ . We have also presented the derivation of second-order approximations  $\frac{\partial^2 u}{\partial r^2}$ ,  $\frac{\partial^2 u}{\partial \theta^2}$  and  $\frac{\partial^2 u}{\partial z^2}$  by Taylor expansion. In the following figures 4-11, stencils are shown in square grid form for clear understanding, however computations are being carried out by considering a cylindrical system.



**Figure 4:** Approximation of 2<sup>nd</sup> order partial derivatives by variation in  $r$  and  $\theta$ , but  $z$  is fixed

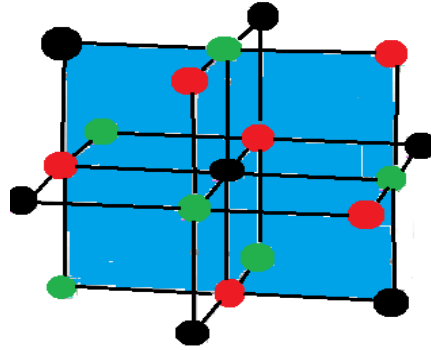


Figure 5: Approximation of 2<sup>nd</sup> order partial derivatives by variation in  $r$  and  $z$ , but  $\theta$  is fixed

$$\frac{\partial^2 u}{\partial r^2} = \frac{1}{6(\Delta r)^2} [u_{1,1,0} + u_{1,-1,0} + u_{-1,1,0} + u_{-1,-1,0} + u_{1,0,1} + u_{1,0,-1} + u_{-1,0,1} + u_{-1,0,-1} + 2u_{(1,0,0)} + 2u_{(-1,0,0)} - 2u_{(0,1,0)} - 2u_{(0,-1,0)} - 2u_{(0,0,1)} - 2u_{(0,0,-1)} - 4u_{(0,0,0)}] \quad (8)$$

In Figure 4 and Figure 5 the approximations of the 2<sup>nd</sup> partial derivative by considering variations  $r$ ,  $\theta$ , and  $r, z$  axis are formulated which is given above in equation 8. The above equation (8) is the approximation of the 2<sup>nd</sup> order derivative w.r.t  $r$  on a 9-point sub-stencil.

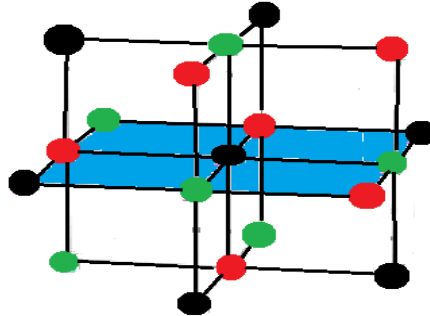


Figure 6: Approximation of 2<sup>nd</sup> order partial derivatives by variation in  $r$  and  $\theta$ , but  $z$  is fixed

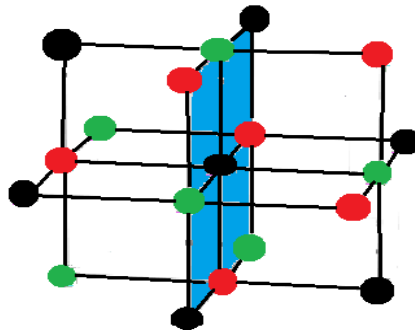


Figure 7: Approximation of 2<sup>nd</sup> order partial derivatives by variation in  $\theta$  and  $z$ , but  $r$  is fixed

$$\frac{\partial^2 u}{\partial \theta^2} = \frac{1}{6(\Delta \theta)^2} [u_{1,1,0} + u_{1,-1,0} + u_{-1,1,0} + u_{-1,-1,0} + u_{0,1,1} + u_{0,1,-1} + u_{0,-1,1} + u_{0,-1,-1} + 2u_{(0,1,0)} + 2u_{(0,-1,0)} - 2u_{(1,0,0)} - 2u_{(-1,0,0)} - 2u_{(0,0,1)} - 2u_{(0,0,-1)} - 4u_{(0,0,0)}] \quad (9)$$

The graphs are shown in Figure 6 and Figure 7 by combining variations in both  $(r, \theta)$  and  $(\theta, z)$ , new formulations for the approximations of the 2<sup>nd</sup> order derivative w.r.t  $\theta$  are shown in equation (9). The numerical approximations given in equation (9) are obtained on a 9-point sub-stencil in a cylindrical mesh system.

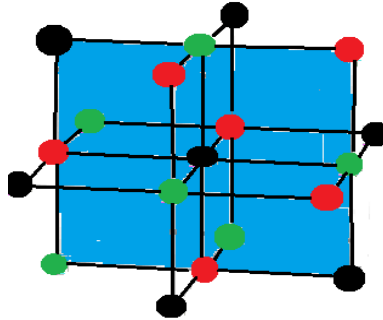


Figure 8: Approximation of 2<sup>nd</sup> order partial derivatives by variation in  $r$  and  $z$ , but  $\theta$  is fixed

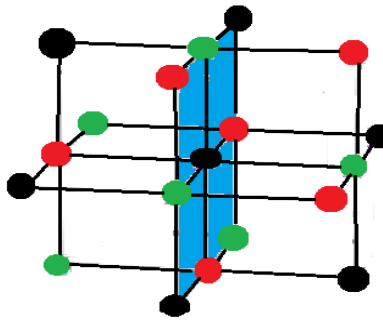


Figure 9: Approximation of 2<sup>nd</sup> order partial derivatives by variation in  $\theta$  and  $z$ , but  $r$  is fixed

$$\frac{\partial^2 u}{\partial z^2} = \frac{1}{6(\Delta z)^2} [u_{1,0,1} + u_{1,0,-1} + u_{-1,0,1} + u_{-1,0,-1} + u_{0,1,1} + u_{0,1,-1} + u_{0,-1,1} + u_{0,-1,-1} + 2u_{(0,0,1)} + 2u_{(0,0,-1)} - 2u_{(1,0,0)} - 2u_{(-1,0,0)} - 2u_{(0,1,0)} - 2u_{(0,-1,0)} - 4u_{(0,0,0)}] \quad (10)$$

Both graphs are shown in Figure 8 and Figure 9 by combining variations in both  $(r, z)$  and  $(\theta, z)$  new formulations for the approximations of 2<sup>nd</sup> order derivative w.r.t  $z$  are shown in equation (9). The numerical approximations given in equation (9) are obtained on a 9-point sub-stencil in a cylindrical mesh system.

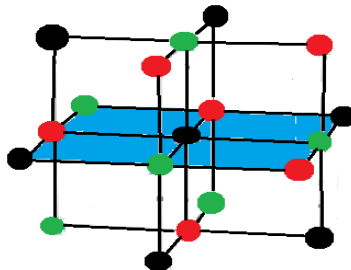


Figure 10: Approximation of 2<sup>nd</sup> order partial derivatives by variation in  $r$  and  $\theta$ , but  $z$  is fixed

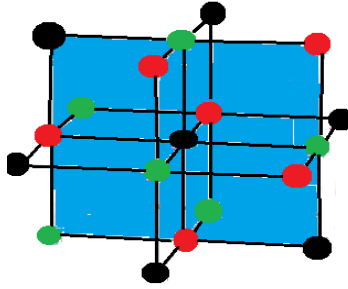


Figure 11: Approximation of 2<sup>nd</sup> order partial derivatives by variation in  $r$  and  $z$ , but  $\theta$  is fixed

$$\frac{\partial u}{\partial r} = \frac{1}{12(\Delta r)} [u_{1,1,0} + u_{1,-1,0} - u_{-1,1,0} - u_{-1,-1,0} + u_{1,0,1} + u_{1,0,-1} - u_{-1,0,1} - u_{-1,0,-1} + 2u_{1,0,0} - 2u_{-1,0,0}] \quad (11)$$

The graphs are shown in Figure 10 and Figure 11 by combining variations in both  $(r, \theta)$  and  $(r, z)$  new formulations for the approximations of 1st order derivative with respect to  $r$  are shown in equation (9). The numerical approximations given in equation (9) are obtained on a 9-point sub-stencil in a cylindrical mesh system. After substitution of obtained 1<sup>st</sup> order and 2<sup>nd</sup> order derivatives, equation 7 becomes.

$$\nabla^2 u = w[a_1 + a_2 + a_3 + a_4] \quad (12)$$

where

$$w = \frac{6r^2(\Delta r)^2(\Delta\theta)^2(\Delta z)^2}{4(r^2(\Delta\theta)^2(\Delta z)^2 + (\Delta r)^2(\Delta z)^2 + r^2(\Delta\theta)^2(\Delta r)^2)}$$

$$a_1 = \frac{1}{6(\Delta r)^2} \{u_{1,1,0} + u_{1,-1,0} + u_{-1,1,0} + u_{-1,-1,0} + u_{1,0,1} + u_{1,0,-1} + u_{-1,0,1} + u_{-1,0,-1} + 2u_{(1,0,0)} + 2u_{(-1,0,0)} - 2u_{(0,1,0)} - 2u_{(0,-1,0)} - 2u_{(0,0,1)} - 2u_{(0,0,-1)}\}$$

$$a_2 = \frac{1}{12r(\Delta r)} \{u_{1,1,0} + u_{1,-1,0} - u_{-1,1,0} - u_{-1,-1,0} + u_{1,0,1} + u_{1,0,-1} - u_{-1,0,1} - u_{-1,0,-1} + 2u_{1,0,0} - 2u_{-1,0,0}\}$$

$$a_3 = \frac{1}{6r^2(\Delta\theta)^2} \{u_{1,1,0} + u_{1,-1,0} + u_{-1,1,0} + u_{-1,-1,0} + u_{0,1,1} + u_{0,1,-1} + u_{0,-1,1} + u_{0,-1,-1} + 2u_{(0,1,0)} + 2u_{(0,-1,0)} - 2u_{(1,0,0)} - 2u_{(-1,0,0)} - 2u_{(0,0,1)} - 2u_{(0,0,-1)}\}$$

$$a_4 = \frac{1}{6(\Delta z)^2} \{u_{1,0,1} + u_{1,0,-1} + u_{-1,0,1} + u_{-1,0,-1} + u_{0,1,1} + u_{0,1,-1} + u_{0,-1,1} + u_{0,-1,-1} + 2u_{(0,0,1)} + 2u_{(0,0,-1)} - 2u_{(1,0,0)} - 2u_{(-1,0,0)} - 2u_{(0,1,0)} - 2u_{(0,-1,0)}\}$$

Equation (12) is the new numerical formulation for the isotropic discretization of Laplacian operator on a 19-point stencil by employing a cylindrical mesh system. These new numerical formulations along with allied formulations equation (8) to equation (11) are also beneficial in solving or discretization of partial differential equations involving 1<sup>st</sup> and 2<sup>nd</sup> order derivatives.

Numerical example 1:

$$f(r, \theta, \phi) = u_{i,j,k} = r + 2k - \cos\theta$$

$$r_i = r_a + i(\Delta r)$$

$$\theta_j = j(\Delta\theta)$$

$$\phi_k = k(\Delta\phi)$$

$$i = j = k = 0, 1, 2, 3 \dots \dots l, M, N$$

For the above problem, we set the parameters.

$$\Delta r = 0.1 \text{ units}, \quad \Delta\theta = \frac{\pi}{180} \text{ radians}, \quad \Delta\phi = \frac{\pi}{180} \text{ radians}$$

### V. STABILITY OF THE PROPOSED SCHEME

The function  $f(r, \theta, \phi)$  is examined through FORTRAN codes and evaluated results are shown in Table 1. A comparison of analytical and approximated results is provided in the form of an error evaluation.

**Table 1 Numerical Results Of Laplacian Operator On 19-Point Stencils In Cylindrical Mesh System**

R	$\theta$	z	Analytical value	Approximate value	Error	Error
1.1	0.017	0.1	0.300152305	0.300453653	-0.000301349	-3.01E-04
1.1	0.017	0.2	0.500152305	0.500453653	-0.000301349	-3.01E-04
1.1	0.017	0.3	0.700152305	0.700453653	-0.000301349	-3.01E-04
1.1	0.017	0.4	0.900152305	0.900453653	-0.000301349	-3.01E-04
1.1	0.017	0.5	1.100152305	1.100453653	-0.000301349	-3.01E-04
1.2	0.035	0.1	0.400609173	0.40092123	-0.000312057	-3.12E-04
1.2	0.035	0.2	0.600609173	0.60092123	-0.000312057	-3.12E-04
1.2	0.035	0.3	0.800609173	0.80092123	-0.000312057	-3.12E-04
1.2	0.035	0.4	1.000609173	1.00092123	-0.000312057	-3.12E-04
1.2	0.035	0.5	1.200609173	1.20092123	-0.000312057	-3.12E-04
1.3	0.052	0.1	0.501370465	0.501692614	-0.000322149	-3.22E-04
1.3	0.052	0.2	0.701370465	0.701692614	-0.000322149	-3.22E-04
1.3	0.052	0.3	0.901370465	0.901692614	-0.000322149	-3.22E-04
1.3	0.052	0.4	1.101370465	1.101692614	-0.000322149	-3.22E-04
1.3	0.052	0.5	1.301370465	1.301692614	-0.000322149	-3.22E-04

#### A. Error analysis

**Table 2 Error analysis by depreciating the value of  $\Delta r$  in the approximated Laplacian operator on 19-point stencil**

$\Delta r$	Result	Error
0.1	-0.000301349	-3.01E-04
0.01	-0.000112463	-1.12E-04
0.001	-5.15899E-05	-5.16E-05
0.0001	-5.07689E-05	-5.08E-05
0.00001	-5.07606E-05	-5.08E-05
0.000001	-5.07606E-05	-5.08E-05

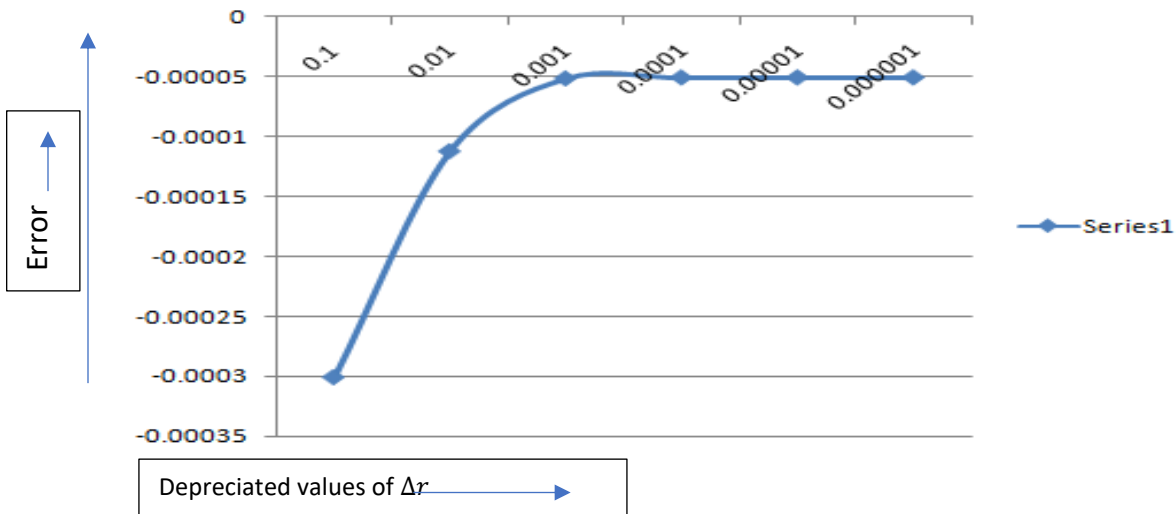


Figure 12: Graphically representation error analysis

To assess the suggested discretization plan for the Laplacian operator, an error analysis was done in Table 2 and Figure 12. It was found that the error in the solution converged to a value of  $-5.08E - 05$  when the grid spacing ( $\Delta r$ ) approached zero. The scheme consistently maintains a consistent degree of accuracy, as evidenced by its stable convergence with  $\Delta r$ . The Laplacian approximation method's stability and dependability are further validated by the modest, negative error value.

## VI. STABILITY ANALYSIS

To investigate the suggested discretization of the Laplacian operator, a stability analysis is done. The response of the scheme can be seen by gradually increasing the grid spacing  $\Delta r$ . The solution error stays within its bounds and falls off to a small negative value in a predictable manner. This behavior reveals the unconditional stability of the approach across a large variety of grid sizes.

## VII. CONCLUSION

An essential first step in numerically solving diffusion problems is discretizing the Laplacian. Since computers are unable to evaluate the continuous Laplacian directly, an approximation using discrete grids is necessary. The accuracy, stability, and convergence of solutions are strongly impacted by the discretization scheme selection. Wide-ranging simulations in research and engineering are made possible by the development of reliable and effective discretizations of the Laplacian. This paper presents a novel 19-point stencil to approximate Laplacian in cylindrical mesh. In this study, the discretization process is illustrated step-by-step in a very simple way and all steps of their computational approximation are described. The validity of the scheme is described numerically from the table and the stability of the scheme is described by determining the convergence. Fortran codes are used to keep the entire process numerically transparent and for visual appreciation the stability and error evaluation of the scheme is presented graphically using Maple.

The results show that this scheme is stable and can be used in real life to solve problems that require solving equilibrium problems by numerical simulations

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