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The conjugate gradient approach to solve two dimensions linear elliptic boundary value equations as a prototype of the reaction diffusion system

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ABSTRACT: This paper presents a numerical approach to solve the 2-dimensional reaction-diffusion problem, a crucial model in physics and chemistry, with applications ranging from pattern formation to material science. Focusing on addressing a stationary linear elliptic problem within a rectangular domain, boundary conditions are determined through a finite-difference formulation. The Conjugate-Gradient Method is employed for the numerical solution, facilitating efficient computation. Key findings are elucidated: Firstly, the grid size for the symmetric matrix A is intricately linked to a bijective function, enabling the transition of indices to grid points. Notably, the solution to this elliptic problem exhibits a concave-up profile. Secondly, various solvers such as the Conjugate Gradient, Gauss-Seidel, and Jacobi techniques are viable, with the Conjugate Gradient method chosen for its superior accuracy, especially when considering computational efficiency. Moreover, the relationship between grid size and solution accuracy is explored, revealing a proportional dependence. Refinement of the grid leads to increased iteration counts but reduced implementation time, owing to the linearity of the function ku. The convergence criterion ensures high accuracy in solutions, as demonstrated in the provided figures.

Keywords: 2D, elliptic boundary, reaction diffusion, system, gradient

1. INTRODUCTION

Reaction–diffusion systems (RDs) are mathematical representations of a variety of physical processes. The most common is the changing in the concentration of one or more chemicals over time and space: local chemical reactions, in which the chemicals are converted to one another; and diffusion, in which the chemicals disperse throughout the surface of the space. Reaction–diffusion systems are often utilized in chemistry [1]. However, the system may also be used to explain non-chemical dynamical processes. Ecology, physics (neutron diffusion theory), biology, and Geology, all provide examples [2-4]. Systems of reaction–diffusion are mathematically represented by semi-linear parabolic differential equations with partial coefficients [5].

A partial differential equation (PDE) is an equation that enforces relationships between a function's multiple partial derivatives [6]. The function is often seen as a "unknown" variable that needs resolution, analogous to how x is regarded as an unknown quantity in an algebraic problem that requires resolution. However, unambiguous formulae for partial differential equation solutions are sometimes hard to write down. As a result, a substantial amount of current mathematics and scientific research has been conducted on approaches for computer-aided numerical approximation of solutions to certain partial differential equations. The study of partial differential equations is a substantial component of pure mathematics, where the traditional focus is on identifying the general qualitative properties of solutions to

diverse partial differential equations [7]. The existence and smoothness of solutions to the Navier-Stokes equations, which were chosen as a Millennium Prize Problem in 2000, remain unresolved among several unaddressed concerns. In quantitatively oriented scientific subjects such as engineering and physics, partial differential equations are prevalent. These concepts, such as the Schrödinger equation and the Pauli equation, play a crucial role in the development of modern scientific understanding in several fields including sound, heat, diffusion, electrostatics, electrodynamics, thermodynamics, fluid dynamics, elasticity, general relativity, and quantum mechanics [8-13]. Additionally, these concepts arise from a range of mathematical concerns, including differential geometry and the calculus of variations. Notably, they are used to establish the Poincaré conjecture within the realm of geometric topology, among other significant applications [14]. The presence of many sources has contributed to the existence of a wide range of unique types of partial differential equations. Consequently, several strategies have been developed to address the particular difficulties that arise from these equations. As such, it is generally accepted that there is no "universal theory" of partial differential equations, with expert knowledge separated into multiple basically independent subfields [15]. The categories of partial differential equations include ordinary differential equations, which pertain to functions of a solitary variable. In 2020, the most actively studied extensions of the "PDE" paradigm are stochastic partial differential equations and nonlocal equations [16]. A variety of subjects, including as elliptic and parabolic partial differential equations, fluid mechanics, Boltzmann equations, and dispersive partial differential equations, fall within the category of classical themes. The aforementioned themes remain the focus of current academic inquiry [17].

Boundary value difficulties occur in several disciplines of physics, as they occur in every physical differential equation [18]. The use of boundary value issues is often employed in order to tackle difficulties associated with the wave equation, such as the identification of normal modes. The Sturm-Liouville problems represent a substantial category of boundary value problems. The analysis of these circumstances involves the use of the eigenfunctions of a differential operator. In order for a boundary value problem to be applicable, it is essential that it be well-posed. This suggests that, given the input of the issue, there is a singular solution that is infinitely dependent on the input. A significant amount of theoretical research in the field of partial differential equations focuses on determining the degree to which boundary value problems arise in both scientific and practical scenarios. The Dirichlet problem, which included the determination of harmonic functions (solutions to Laplace's equation), was one of the first boundary value difficulties investigated. The Dirichlet principle was found to offer the solution to this problem [19].

To handle boundary value problems numerically, one might refer to the finite-difference methods (FDM). These methods consist of a set of numerical techniques that aim to solve differential equations by approximating derivatives using finite differences [20]. Discreteization is used to estimate the solution value at specified locations, including both the geographical domain and, if appropriate, the time period. The process entails partitioning the domain into a limited number of iterations and resolving algebraic equations that include finite disparities and values derived from adjacent spots. Finite difference methods are used to transform nonlinear ordinary differential equations (ODE) or partial differential equations (PDE) into a system of linear equations that may be solved using matrix algebra techniques. Contemporary numerical analysis has seen the widespread use of Finite Difference Method (FDM) due to its efficient execution of linear algebra computations, as well as its relatively simple implementation [21]. Along with finite element techniques, FDM are one of the most frequently used ways for numerical solution of PDEs nowadays. At present, several methods are used to solve nonlinear equations [22-40].

This work aims to find the numerical solution of an RD system in 2D by using the conjugate-gradient method when considering linear elliptic equations. However, the organizations of the present work in the following manner: section 3, a brief introduction to the Reaction-Diffusion system with two variables of unknowns has been investigated. In section 4, we explore how to discretize RD in two dimensions. In Section 5, the Conjugate-Gradient algorithm is shown as a numerical solver for the RD system. Section 6 deals with a specific type of RD system, namely the linear elliptic equation, which is solved using conjugate-gradient algorithms. Finally, section 7 concludes the paper.

2. Methodology

2.1 Reaction-Diffusion Problems

It is most normal for reaction-diffusion equations (RD) to appear in frameworks containing numerous collaboration components (e.g., chemical responses). These equations are commonly used to depict pattern-formation phenomena across a variety of natural, chemical, and physical frameworks.

A one-dimensional reaction-diffusion equation comprises a response and a diffusion component, and so has the following typical structure:

$$u_t = D\Delta u + g(u) \tag{1}$$

where $u_t = \frac{\partial u}{\partial t}$ and $u = u(\alpha, t)$ is a state variable that depicts substance or population density, etc., at a position $\alpha \in \Omega \subset R^n$ at time t (Ω is an unrestricted set). Δ signifies the Laplace operator.

The first term on the right facets denotes "diffusion," with D denoting the diffusion coefficient. For additional requirements, D is also represented as a diagonal diffusion matrix. The second term, $g(u)$, is a simple feature that refers to procedures that really "alter" the current u, i.e., something occurs to it (birth, death, chemical reaction, … etc.), rather than just spread in space. Additionally, it is feasible that the response term is dependent not only on u, but also on its principal subsidiary, i.e., and explicitly on α. The 1-dimensional model of RD is of the shape [41].

$$u_t = D\Delta^2 u + g(u, \alpha, \nabla u) \tag{2}$$

with $u(\alpha, t) \in R^m, \alpha \in [0, M] = \Omega$ together with initial condition

$$u(\alpha, 0) = g(\alpha),\ \alpha \in \Omega \tag{3}$$

and the boundary condition that follows

$$u(0,t) = u(L,t) = 0,\ \forall t > 0 \tag{4}$$

Condition in Eq. 4 is also known as Dirichlet boundary condition Eqs. 3 and 4. The analytical solution of Eq. 2 with the conditions Eqs. 3 and 4 is widely discussed in many sources, for example, Eqs. 1 and 5. In real-life scenarios, RD can apply to higher-dimensional problems, where some modifications are required to the model to be convenient for the problem size. Thus, for 2-dimensional model, the RD can be represented as:

$$u_t = D\left(u_{\alpha\alpha} + u_{\beta\beta}\right) + g(u) \tag{5}$$

Noticing that $u_{\alpha\alpha} = \frac{\partial^2 u}{\partial \alpha^2}$ and $u_{\beta\beta} = \frac{\partial^2 u}{\partial \beta^2}$ plus u is defined here as $u = u(\alpha, \beta, t) = (u, v)^T,\ x \in [a, b],$ and $\beta \in [c, d]$, and $g(u) = (g_1(u, v), g_2(u, v))^T$ is defined here as the local reaction kinetics. The diffusion coefficient D is presented as the following diagonal matrix,

$$D = \begin{bmatrix} d_u & 0 \\ 0 & d_v \end{bmatrix} \tag{6}$$

Moreover, the initial condition in Eq. 3 is specified and $u_0 = (u_0, v_0)^T$ is steady state solution of Eq. 5 which means $g_1(u_0, v_0) = g_2(u_0, v_0) = 0$. make up for the boundary condition in Eq. 4 on both the x- and y-axes [42-45]. The RD system in Eq. 5 contains a family of partial differential problems IVP discussed in many references, including [41-48]. In support of the above, it should be noted that the analytics of this system has been reviewed and investigated by many references in order to determine whether the system has a solution, see [44-47]. In studying these kinds of equations, RD has a more prevalent numerical approach that will be more conducive to our purposes in this paper.

2.2 Discretization of RD in 2-Dimensions

The discretization in PDE presented in a grid with two variables like α and β with two indices j and k respectively. Assume that $u_{j,k} = u(j\Delta\alpha, k\Delta\beta)$ and $\alpha_j = j\Delta\alpha, \beta_k = k\Delta\beta$, where $0 < \Delta\alpha, \Delta\beta$, Fig. 2.

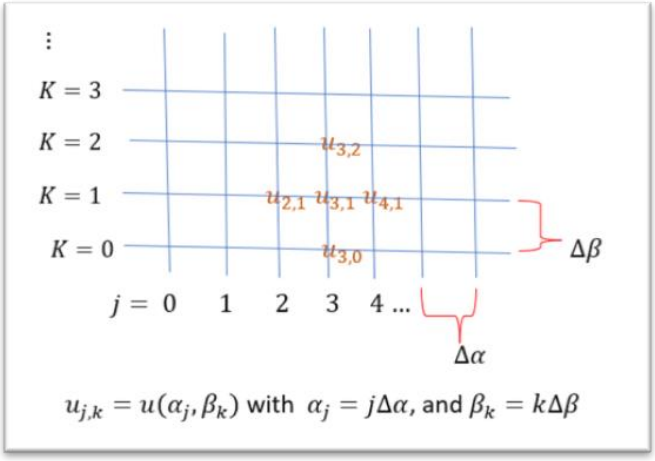

FIGURE 1. - Discretization of PDE variables in 2D

When dealing with boundary value problems that contain a 2nd order ODE, by solving the second order ODE with the two boundary conditions, we get a system of N-2 linear equations for the interior points (points in orange hue in Fig. 1). A matrix manipulation method was utilized in order to solving linear equations type N-2 for the inner locations. If the initial value equation involves a 1st order ODE, then the value of u_0 must be known.

A finite difference scheme is then used for $(du/d\alpha)$ to determine $u_j, j = 1,2, \ldots$ successively. We will talk about how the type of boundary-value problems is related to PDEs Partial Differential Equations in two dimensions, for more details, see [46].

The first derivative term in Eq. 5 is expressed as Laplace equation with boundary conditions which given as follows

$$\frac{\partial^2 u}{\partial \alpha^2} + \frac{\partial^2 u}{\partial \beta^2} = 0 \tag{7}$$

with assumed rectangular boundary conditions

$$u(\alpha,1) = 2, u(\alpha,0) = 1, u(0,\beta) = 1, u(1,\beta) = 2 \tag{8}$$

where: $u(\alpha,\beta)$ is presumed so that $\alpha, \beta \in [0,1]$

The four boundary conditions in Eq. 8 will represent a square domain for Eq. 7 as shown in Fig. 2.

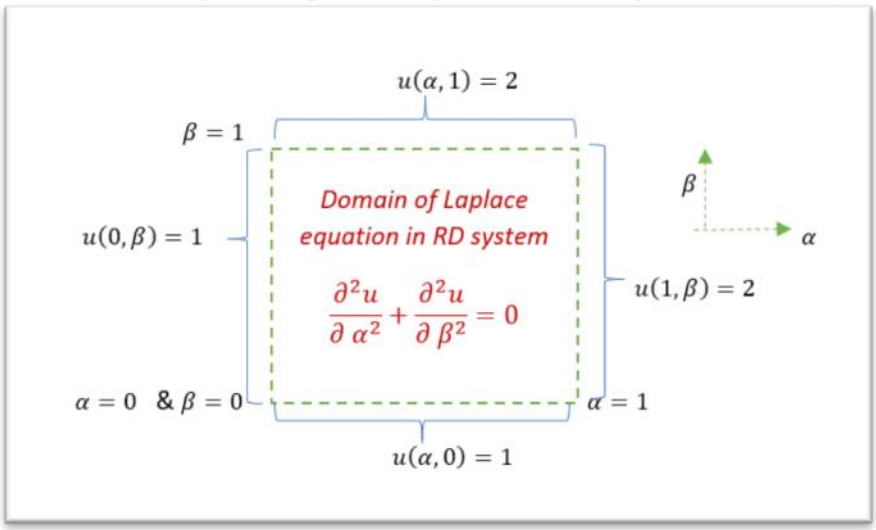

FIGURE 2. - Domain of PDE in 2D

The points on the 4 walls (boundary conditions in Eq. 8) are known, while the interior points in the square are not. The task is to determine the unknown points, which need an approximation scheme for this problem. For a grid of (j,k), we consider the order-two central-difference scheme to approximate the second partial derivative in the RD system (or Laplace), which leads to having the following two equations, see [49].

$$\frac{\partial^2 u}{(\partial \alpha)^2} = \frac{u(\alpha-\Delta\alpha,\beta)-2u(\alpha,\beta)+u(\alpha+\Delta\alpha,\beta)}{(\Delta\alpha)^2} \tag{9}$$

where all terms with β in Eq. 9 have the same index k.

$$\frac{\partial^2 u}{(\partial \beta)^2} = \frac{u(\alpha,\beta-\Delta\beta)-2u(\alpha,\beta)+u(\alpha,\beta+\Delta\beta)}{(\Delta\beta)^2} \tag{10}$$

where all terms with α in Eq. 10 have the same index j.

Applying Eqns. 9 and 10 to the original Laplace Eq. 7, we get the finite central-difference equation for a grid point (j,k),

$$u_{j-1,k} - 2u_{j,k} + u_{j+1,k} \Big/ (\Delta\alpha)^2 + u_{j,k-1} - 2u_{j,k} + u_{j,k+1} \Big/ (\Delta\beta)^2 = 0 \tag{11}$$

when $\Delta\alpha = \Delta\beta$ The outcome is

$$u_{j-1,k} + u_{j+1,k} + u_{j,k-1} + u_{j,k+1} - 4u_{j,k} = 0, \text{ at grid point } (j,k) \tag{12}$$

The partial derivatives $\left(\frac{\partial^2 u}{\partial \alpha^2}, \frac{\partial^2 u}{\partial \beta^2}\right)$ are calculated by Eq. 12 at grid point (j,k) with discretized values of u for (j,k) and its four neighbors-at tops, bottom, left, and right, for more details see [49].

Scilab is an open-source alternative to MATLAB [13]. It places less emphasis on syntactic compatibility with MATLAB; however, it is sufficiently comparable for some authors to assert that it is simple to transfer skills between them [14].

Scilab Image Processing toolkit or SIP, aims to perform imaging tasks like filtering, blurring, edge detection, thresholding, histogram manipulation, segmentation, mathematical morphology, color image processing, etc. These processes are important for problem-solving in a variety of real-world applications, from automobile motion planning to autonomous medical picture diagnosis [15].

SIP offers the following advantageous features: First: Input/Output of image files in a variety of formats, such as BMP, JPEG, GIF, PNG, TIFF, XPM, and PCX. Second: a multitude of features with an adaptable interface and error handling. Third: Function documentation with examples [16-27].

2.3 Conjugate Gradient Method for Solving RD

Hestenes and Stefiel pioneered the Conjugate Gradient technique in 1952. They published a paper entitled "Conjugate Gradient Method for Solving Linear Equations" [50, 51], which presented this method for solving linear algebraic equations.

$$Ax = b \tag{13}$$

In the above system, $A = a_{j,k}$ is real-positive and symmetric definite matrix of size $m \times m$, the vector of unknowns is $x = (x_1, x_2, \dots, x_m)^T \in \mathbb{R}^m$, and the right-hand side $b = (b_1, b_2, \dots, b_m)^T \in \mathbb{R}^m$ is already given. In the case of dense matrices, conjugate gradient requires $2n^2 + O(n^2)$ arithmetic operations, while, standard

$$n^2/_3 + O(n^2)$$

Gaussian elimination method requires only operations as $\to \infty$, see [52]. When dealing with sparse systems that are too large to handle directly or through other direct procedures, the conjugate gradient is often used as an iterative strategy. Large sparse systems are often a side effect of solving partial differential equations or optimization problems computationally [53].

Two non-zero vectors γ_1 and γ_2 are conjugates (in terms of the symmetric positive-definite matrix A) if and only if they are.

$$\gamma_1{}^T A\, \gamma_2 = 0 \tag{14}$$

Eq. 14 defines an inner product on the left-hand side.

$$\gamma_1{}^T A\, \gamma_2 = \langle \gamma_1, \gamma_2 \rangle_A := \langle A\gamma_1, \gamma_2 \rangle = \langle \gamma_1, A^T \gamma_2 \rangle = \langle \gamma_1, A\, \gamma_2 \rangle \tag{15}$$

In other words, if γ_1 and γ_2 are orthogonal on each other with regard to the inner product in Eq. 15, then they are conjugate. To be conjugate is indeed a symmetric relationship, which means that if γ_1 and γ_2 are conjugate, then γ_2 is conjugate to γ_1. Assume that the set

$$\Gamma = \{\gamma_1, \gamma_2, \dots, \gamma_m\} \tag{16}$$

To contain all mutual conjugate vectors of rank m concerning matrix A. Hence, for all $j \neq k$ if $\gamma_j{}^T A\, \gamma_k = 0$, then Γ is a base for $\mathbb{R}^m$, and the solution x^* of Eq. 13 is expressed as

$$x^* = \sum_{j=0}^{m} c_j\, \gamma_j \Rightarrow Ax^* = \sum_{j=0}^{m} c_j A\, \gamma_j = \gamma_m{}^T A x^* = \sum_{j=0}^{m} c_j\, \gamma_m{}^T A\, \gamma_j \Rightarrow \gamma_m{}^T b = \sum_{j=0}^{m} c_j \langle \gamma_m, \gamma_j \rangle_A$$

$$= c_m \langle \gamma_m, \gamma_m \rangle_A \Rightarrow c_m = \frac{\langle \gamma_m, b \rangle}{\langle \gamma_m, \gamma_m \rangle_A}$$

Thus, for solving $Ax = b$, conjugate gradient determines the series of n conjugate directions and then computes the parameters cm [54].

To discuss the algorithm of Conjugate-Gradient, suppose r_p is the result of Eq. 13, at step p, and we call it a residual function, as follows

$$r_p = b - Ax_p \tag{17}$$

Then for any two residuals r_j and r_k are orthogonal if $r_j{}^T r_k = 0$, $\forall\, j \neq k$; also recall the orthogonal vectors γ_j and γ_k i.e. $\gamma_j{}^T A\, \gamma_k = 0$. However, each of r_j and γ_j forms a distinct orthogonal base concerning the standard inner product. Thus, a solution x_k can be thought of as a projection of x, thus a solution to Eq. 13 can be written, but at first, an input vector $x_0 = 0$ should be considered [52]. As a result, an iterative algorithm can be expressed as follows

Algorithm 1: Conjugate Gradient Method for Solving RD System

Step 1: set an initial residual $r_0 = b - Ax_0$

Step 2: if r_0 is small enough, then x_0 is the solution

Step 3: set $\gamma_0 = r_0$

Step 4: set $j = 0$

Step 5: loop $j = 0: m$

Step 6: $c_j = \frac{r_j^T r_j}{\gamma_j^T A \gamma_j}$

Step 7: $x_{j+1} = x_j + c_j \gamma_j$

Step 8: $r_{j+1} = r_j - c_j A \gamma_j$

Step 9: if r_{j+1} small enough, then exit the loop

Step 10: $d_j = \frac{r_{j+1}^T r_{j+1}}{r_j^T r_j}$

Step 11: $\gamma_{j+1} = r_{j+1} + d_j \gamma_j$

Step 12: $j = j + 1$

Step 13: end loop

Step 14: then x_{j+1} is the resulted solution

For more clarity see Fig. 4,

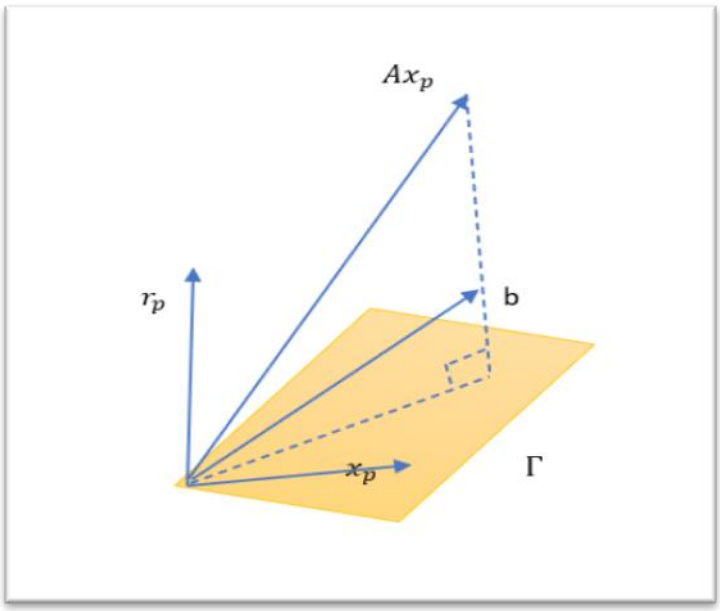

FIGURE 3. - The solution x_p in the base Γ so that $r_p = b - Ax_p \perp \Gamma$

3. Results and Discussion

3.1 Numerical Treatment of Linear Elliptic Reaction-Diffusion System

The 2-D linear elliptic equation is a common RD system type, an expression of the boundary value problem. Based on Eq. 5, this type can be expressed in the following form

$$u_t = D\left(u_{\alpha\alpha} + u_{\beta\beta}\right) \text{ with } D\left(u_{\alpha\alpha} + u_{\beta\beta}\right) = \kappa\, u \tag{18}$$

This equation is shown in the domain Ω, where $(\alpha, \beta) \in [0, M] \times [0, N] = \Omega$. To start finding the solution, one needs to consider a boundary condition $\Omega|_{\partial\Omega}$, see [41]. We will find the numerical solution of problem Eq. 18 by using the conjugate gradient method. A source code in Fortran 90 is built-up for this problem and the solution obtained based on two algorithms: Algorithm 1 mentioned before and the following Algorithm 2,

Algorithm 2: Linear Solver

Step 1: $u = 1; m = 64; n = m \times m$

Step 2: for $i = 1, m$
Step 3: for $j = 1, m$
Step 4: $D = \frac{u_{i+1,j}+u_{i,j+1}+u_{i-1,j}+u_{i,j-1}-4u_{i,j}}{h^2} = \kappa u_{i,j}$
Step 5: end
Step 6: end
Step 7: for k= 1, m
Step 8: set $P(i,j) = (j-1)\,n + i$
Step 9: set $(u_{i+1,j} = u_{p+1};\ u_{i-1,j} = u_{p-1};\ u_{i,j+1} = u_{p+n};\ u_{i,j-1} = u_{p-n};\ u_{i,j} = u_p)$
Step 10: $u_{p+1} + u_{p-1} + u_{p+n+}u_{p-n} - 4u_p = h^2 \kappa\, u_p$
Step 11: end

We notify that $\kappa = 1, D = 0.01$, containing $\Omega = [0,1] \times [0,1]$ as rectangular domain and boundary condition $\Omega|_{\partial\Omega} = 1$. We continue to find the solution for problem $P1$ (problem of linear elliptic solver) by using Algorithm 1 to get the final result. After implementing Algorithm 2 above, we ran some tests to show the accuracy and the efficiency of the method we solved, and it is in Table 1.

Table 1. - Test problem for Linear Solver algorithm 2

Test	Iter	Grid-Size (m)	Time (sec)
1	65	32	0.180
2	122	64	0.800
3	236	128	0.442
4	473	265	0.297

A sample of the results of Test 2 in Table 1 is shown in Table 2, where the number of iterations is in the first column, the solution X is in the second column, the residual is in the third column, the maximum value of the solution X is in the fourth column, and the minimum value of X is in the fifth column. Note the grid size ($m = 64$).

Table 2. - Sample of solutions for problem $P1$: Algorithm 2 and Algorithm 1 in Gfortran, with $m = 64$

Nit	X	Resd	Max-Val	Min-Val
1	0.1998793E-02	0.1931965E-02	0.9740633E+00	0.0000000E+00
2	0.1428013E-02	0.1351284E-02	0.9444863E+00	0.0000000E+00
3	0.1267772E-02	0.8697530E-02	0.1096118E+01	0.0000000E+00
4	0.9547615E-03	0.7609555E-03	0.9715253E+00	0.0000000E+00
5	0.8540408E-03	0.6897023E-03	0.9492763E+00	0.0000000E+00
6	0.6951369E-03	0.5835200E-03	0.9624640E+00	0.0000000E+00
7	0.6222733E-03	0.5559316E-03	0.1005777E+01	0.0000000E+00
8	0.5274140E-03	0.4720334E-03	0.9542296E+00	0.0000000E+00

To visualize the solution, a variety of grid sizes (m) were applied, and Gnuplot was used to plot the results; for the resulting data, we ran the command to generate the final plots, which are represented in Figs. 4, 5, 6, and 7.

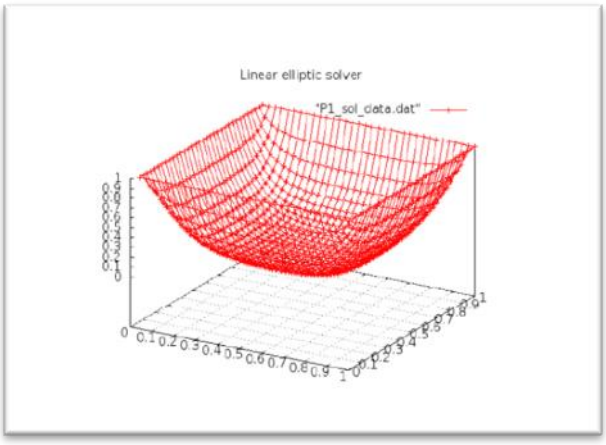

FIGURE 4. - The solution to $P1$ with a grid size of $m = 32$

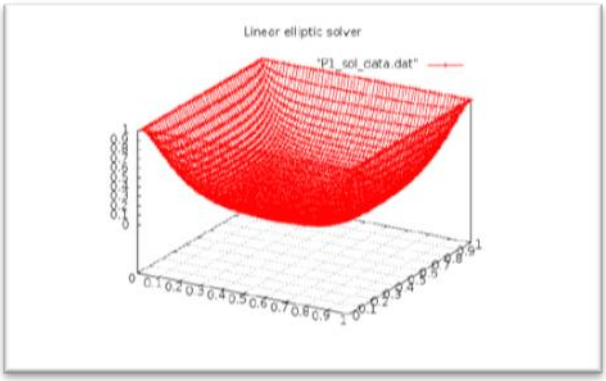

FIGURE 5. - The solution to $P1$ with a grid size of $m = 64$

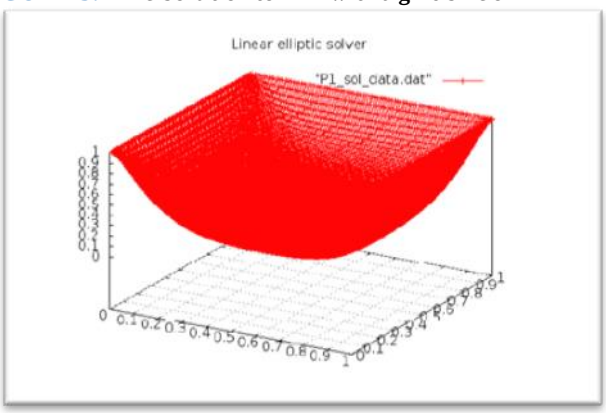

FIGURE 6. - The solution to $P1$ with a grid size of $m = 128$

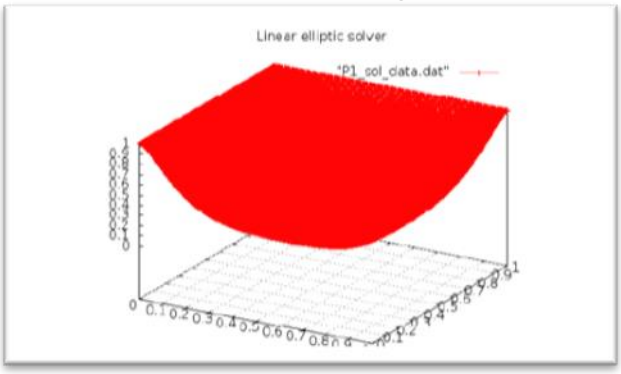

FIGURE 7. - The solution to $P1$ with a grid size of $m = 256$

4. Conclusions

A numerical solution for the problem of 2-dimensional Reaction-Diffusion, which has many applications in physics and chemistry have been provided in this work. The work addresses a stationary linear elliptic problem in a rectangular domain, with boundary conditions determined by the Finite-Difference formula. However, two FORTRAN codes were developed to implement the numerical solution, linear solver and Conjugate-Gradient method. The findings are summarized in the following:

1. The grid size for the symmetric matrix A depends on the bijective function $P: \{1, \dots, n\} \times \{1, \dots, n\} \to \{1, \dots, n^2\}$ to switch the index of the entries u_{ij} to grid point u_p; the solution for this problem is concave-up since it is an elliptic problem.
2. Many solvers can be implemented for symmetric matrices like the conjugate gradient, Gauss-Seidel technique, and Jacobi techniques. Each of them gives the right solution, but we choose conjugate gradient because it provides high accuracy. And also, the efficiency of the used computer affects the answer.
3. The size of the grid in the problem affects proportionally with the solution; since as long as we refine the problem's grid size, the iteration count is raised, while the implementing time is decreased, which is probably because of the linearity of the function κu.
4. The convergent test for this problem is $\|u_i - u_{i+1}\| \leq Tol$, where $Tol = 10^{-12}$, this convergent assures good accuracy for the solution, check Figs. 4, 5, 6, and 7.
5. In future work, we will tackle a semi-linear elliptic boundary-value problem using the same method as in this study.

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CONFLICTS OF INTEREST

The authors declare no conflict of interest

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