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NUMERICAL APPROXIMATION OF A NONLINEAR PARABOLIC PARTIAL DIFFERENTIAL EQUATION

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ABSTRACT

We consider the Allen-Cahn model of phase transitions. We approximate the problem using finite difference method in space coupled with several explicit and implicit methods in time and compare the solutions. We present some numerical experimental results of such approximations.

Key words: Numerical approximations, Allen-Cahn model, finite difference, Euler's method.

I. INTRODUCTION

A lot of practical life problems from mechanical, biological, chemical, physical and many other systems have been modeled by reaction diffusion systems and advection reaction diffusion systems. There are various such models that contains local [8, 10, 11, 16, 15] or nonlocal diffusion [14, 2, 4, 7, 6, 12, 13], and a lot of them contain both [5]. The key feature lies in the nonlinear reaction term and it balance between diffusion, advected diffusion and reaction terms. These type of models are typically complicated, interesting to scientists, challenging to understand substantially and analyze them.

Parabolic differential equations (PDE's) are commonly used in the fields of Engineering and Science for simulating physical processes. In a variety of cases, approximations are used to convert PDE 's to ordinary differential equations (ODE 's) or even to algebraic equations. However, because of the ever increasing requirement for more accurate modeling of physical process, engineers and scientists are more and more required to solve the actual PDE 's that govern the physical problem under investigated. The solutions of PDE 's describe possible physical reactions that have to be fixed through boundary conditions. These equations involve two or more independent variables that determine the behavior of the dependent variable as described by a differential equation, usually of second or higher order.
Consider the second-order nonlinear parabolic partial differential equation

$$u_t(x,t) = \varepsilon u_{xx}(x,t) + f(u(x,t)) . \qquad (1)$$

The equation (1) is known as the Allen-Cahn model of Phase transitions. For detail discussion please see [7, 17] and references therein. Here the initial function $u(x,0)$ and we consider boundary conditions

(a) the Dirichlet boundary condition $u(-1,t) = 0 = u(1,t)$ or
(b) the Neumann boundary condition $u_x(-1,t) = 0 = u_x(1,t)$,

ε is a nonnegative parameter and $f(u) = u - u^3$ which is a bistable nonlinearity associated with the ODE

$$u_t = f(u),$$

which has two stable equilibria at ± 1 and 0 is its unstable equilibrium. If $u(x,0) > 0$ solutions goes to 1 and if $u(x,0) < 0$ solution goes to -1.

There are different type of nonlinearity have been using for this type of models. $f(u) = k^2 u - u^3$ with k is a controlling parameter represents duffing equation and $f(u) = (u-\gamma)(1-u^2)$ with $-1 < \gamma < 1$ gives general Allen-cahn equation. In general, we present this nonlinearity as $f(u) = (u-\gamma)(k^2 - u^2)$; where $k \in \Re$. In some articles scientists also use $f(u) = u(u-1)(u-a)$ with $0 < a < 1$.

In [1], the author discussed numerical computations of a PDE. He developed a stable parallel algorithm to solve the problem. He discritized the problem by finite difference scheme in space and consider exponential operator to get exact solution in time. Then he developed a parallel algorithm to speed up the computation. In [7], Duncan et. al. consider non-local parabolic problem and discuss stability and coarsening of solutions. They also present one numerical example using piecewise constant basis functions in space. Several sequential numerical methods (implicit as well as explicit) have been for the solution of this problem proposed in the literatures [18, 19, 20].

In [8] author analysed accuracy of Crank-Nicolson and Richtmyer-Morton methods for local diffusion and advection operators for non-periodic problems whereas [10] discussed finite differences for linear variable coefficient local diffusion operator. In [11] and [16] authors well presented spectral methods for parabolic problem, in particular, [11] restricted themselves with the stability issues of Fourier spectral method. In [15] author discussed various issues of finite difference approximation of partial differential equations (PDE) in infinite domain. Author discussed welposedness, stability, accuracy and convergence of various finite difference approximations of time dependent PDE.

Here we consider numerical approximations of such model using several schemes in space and time. Then we compare the results. The article is organized in the following way. We start with discretising the problem using a finite difference scheme, then we find a bound on the spectral radius of semidiscerete matrix in Section II. In Section III we present several time discretisations whereas Section IV contains numerical experimental results. We finish our study in Section V with the conclussion.

II. THE PROBLEM AND ITS DISCRETISATIONS

We consider $2N+1$ points over the interval $[-1, 1]$ and $h=\frac{1}{N}$. We define $x_i = -1+ih$, $0 \le i \le 2N+1 = N_h$. We approximate u_{xx} in space by

$$u_{xx}(x_i,t) = \frac{u_i - 2u_{i+1} + u_{i-1}}{h^2} \qquad (2)$$

for all $1 \le i \le N_h$. Then (1) can be approximated by

$$u_t(t) = Au + f(u). \qquad (3)$$

Now when the boundary condition (a) is used

$$A = \begin{pmatrix} -2 & 1 & 0 & 0 & \cdots \\ 1 & -2 & 1 & 0 & \vdots \\ 0 & 1 & -2 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & -2 \end{pmatrix}.$$

And using the boundary condition (b) we have $u_1(t) - u_{-1}(t) = 0$ gives $u_1(t) = u_{-1}(t)$ and $u_{N_h+1}(t) - u_{N_h-1}(t) = 0$ gives $u_{N_h+1}(t) = u_{N_h-1}(t)$. So

$$A = \begin{pmatrix} -2 & 2 & 0 & 0 & \cdots \\ 1 & -2 & 1 & 0 & \vdots \\ 0 & 1 & -2 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 2 & -2 \end{pmatrix}$$

The matrix obtained from (2) has some specialty. In most cases A is a toeplitz matrix.

Definition 1: Toeplitz matrix: A Toeplitz matrix is a matrix which is constant along each of its diagonals.

Now consider the matrix the A of the form

$$A = \begin{pmatrix} b & a & 0 & 0 & \cdots \\ a & b & a & 0 & \vdots \\ 0 & a & b & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & a \\ 0 & \cdots & 0 & a & b \end{pmatrix}. \qquad (3a)$$

of order N_h which depends on space discretisation. The eigenvalues and eigenvectors [21] of A are of the form

$$\lambda_i = b + 2a\sqrt{\frac{c}{a}}\cos\left(\frac{i\pi}{N_h+1}\right)$$

and

$$x_i = \begin{bmatrix} \left(\frac{c}{a}\right)^{\frac{1}{2}} \sin\left(\frac{1.i\pi}{N_h+1}\right) \\ \left(\frac{c}{a}\right)^{\frac{2}{2}} \sin\left(\frac{2.i\pi}{N_h+1}\right) \\ \left(\frac{c}{a}\right)^{\frac{3}{2}} \sin\left(\frac{3.i\pi}{N_h+1}\right) \\ \vdots \\ \left(\frac{c}{a}\right)^{\frac{N_h}{2}} \sin\left(\frac{N_h.i\pi}{N_h+1}\right) \end{bmatrix}$$

for each $i = 1, 2, \cdots, N_h$.

Lemma 1:
The spectral radius of the toeplitz tridiagonal matrix of type $(3a)$ is bounded and

$$\frac{a\pi^2}{(N+1)^2} \le |\lambda_i| \le 4|a|$$

where the matrix A is defined by $(3a)$.

Proof:
From the definition of the eigenvalue of A we have

$$\lambda_i = b + 2a\sqrt{\frac{c}{a}}\cos\left(\frac{i\pi}{N_h+1}\right)$$

For all $i = 1, 2, \cdots, N_h$.

Now in the matrix A of type $(3a)$ $2|a| = |b|$ and $|a| = |c|$. Then we have

$$\lambda_i = 2|a|\left|1 + \cos\left(\frac{i\pi}{N_h+1}\right)\right|$$

$$= 2|a|2\sin^2\left(\frac{i\pi}{2(N_h+1)}\right)$$

So, we can write

$$2|a|2\sin^2\left(\frac{i\pi}{2(N+1)}\right) \le 4|a|,$$

for all $i = 1, 2, \cdots, N_h$. Thus the proof follows from inspection.

In Figure 1 we plot spectral radius and stiffness ratio of the matrix A considering both boundary conditions. We notice that in both cases the spectral radius and stiffness ratio are computationally same and the spectral radius is of $O(N_h{}^2)$ which reflects the Lemma 1.

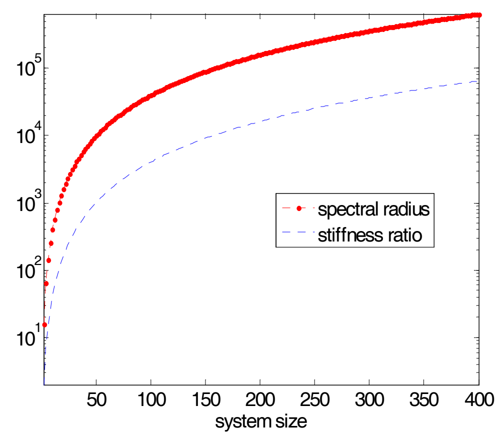

Figure 1: Spectral radius and stiffness ratio of the stiffness matrix A with both boundary conditions. We notice that both the spectral radius and stiffness ratio grows as system size grows and it is of $O(N_h{}^2)$.

III. THE TIME DISCRETISATION

Now for time discretisation we use the following schemes.
Applying explicit Euler formula to (3)

$$\frac{u^{n+1} - u^n}{\nabla t} = Au^n + f(u^n)$$

And so

$$u^{n+1} = u^n + \nabla t\left(Au^n + f(u^n)\right) \tag{4}$$

which can be solved easily using one iteration per time steps.

Applying implicit Euler formula to (3)

$$\frac{u^{n+1}-u^n}{\nabla t} = Au^{n+1} + f(u^{n+1}),$$

which can be written as

$$u^{n+1} = u^n + \nabla t\, Au^{n+1} + \nabla t\, f(u^{n+1}). \qquad (5)$$

Here is a problem of getting solutions in each time steps since (5) is a nonlinear system of equations. We start solving the problem using Newton's method for nolinear system. Actually solving the problem in such a way gives better stability and accuracy than the explicit solver (4) but has a difficulty of solving nonlinear system of equations per time steps.

To avoid the difficulty we linearise the problem by replacing u^{n+1} by u^n in f. That linearization can give an alternative of solving the nonlinear system. Thus (5) can be written as

$$u^{n+1} = u^n + \nabla t\, Au^{n+1} + \nabla t\, f(u^n),$$

and thus

$$u^{n+1}(I-\nabla t\, A) = u^n + \nabla t\, f(u^n). \qquad (6)$$

We experienced another problem while solving the linear system (6). That is to invert the matrix $(I-\nabla t\, A)$.

To avoid computing $(I-\nabla t\, A)^{-1}$, we approximate the inverse by

$$(I-\nabla t\, A)^{-1} \approx I + \nabla t A + O(\nabla t^2)$$

when $\nabla t \to 0$ which is $O(\nabla t^2)$ accurate. We observe that numerical scheme (6) with such an approximation of inverse of $(I-\nabla t\, A)^{-1}$ is stable.

IV. RESULTS

Here we present numerical experimental results for the schemes discussed above. In most cases we consider $N = 32$, $u_0 = \sin(2\pi x^2)$, and vary ∇t and ε.

We start with Explicit Euler's method with two different choices of ∇t. We notice from Figure 2 that solution converges to steady state and is bounded when ∇t is small (which is relative to N), whereas for larger choice of ∇t solution diverges (see Figure 3).

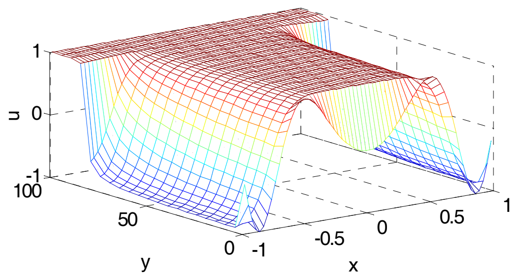

Figure 2: Explicit Euler solver with $N = 32$, $\nabla t = 0.01$, $u_0 = \sin(2\pi x^2)$ and $\varepsilon = 0.001$. We notice that solutions converge to single steady sate 1.

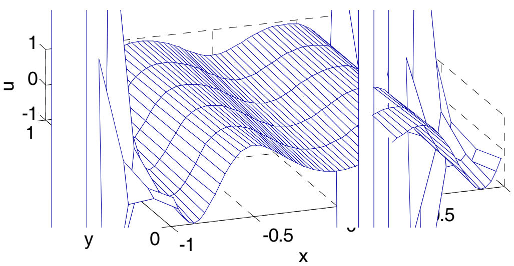

Figure 3: Explicit Euler solver with $N = 32$, $\nabla t = 0.1$, $u_0 = \sin(2\pi x^2)$ and $\varepsilon = 0.001$. Here we experience that after very little iteration, solutions become unstable (the vertical lines of the figure are jumps of the solutions).

Then we consider an implicit solver with full discrete nonlinear scheme (5), linear approximate scheme (6) and approximate inverse of the co-efficient matrix in (6). We observe that schemes (5) and (6) gives same steady state with any suitable choice of ∇t (see Figure 4 and Figure 5) with two different choices of ε. We also experiment solutions for the scheme (6) with approximate inverse of $(I-\nabla t\, A)^{-1}$ and notice that approximate inverse computation version scheme also stable and converges (see Figure 6), but it converges to a state different from ones shown in Figure 5 with same choices of initial function and ε.

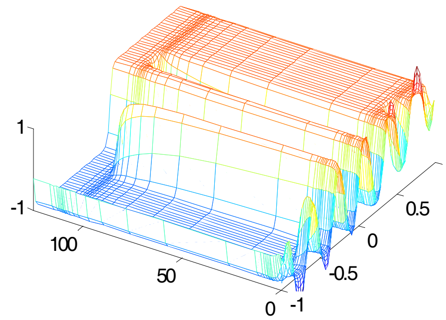

Figure 4: This plot with $u_0 = x + \sin(6\pi x)$, $\varepsilon = 0.0005$. implicit euler's method for all t=[0, 125]. N=64.

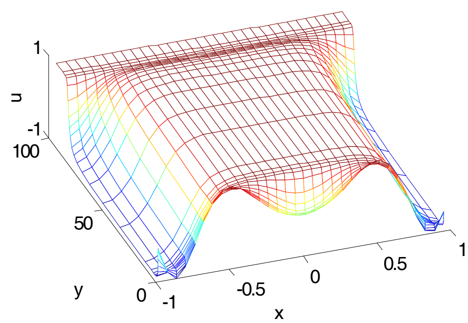

Figure 5: Implicit Euler solver with $N = 32$, $\nabla t = 0.1$, $u_0 = \sin(2\pi x^2)$ and $\varepsilon = 0.001$. Here we notice that solutions go to the steady state single steady state $1$and the solutions are stable. We also notice that the scheme (*6*) also converges to that same state as the scheme (5) does.

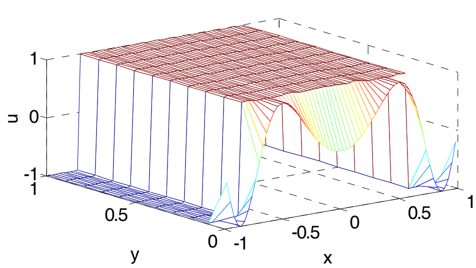

Figure 6: Linearised implicit Euler solver with $N = 32$, $\nabla t = 0.1$, $u_0 = \sin(2\pi x^2)$ and $\varepsilon = 0.001$ with approximate inverse of $(I - \nabla t\, A)^{-1}$. Here we notice that solutions are stable and converge to a two jump steady state with ± 1.

V. CONCLUSSION

In this paper couple of schemes have been presented for the parabolic equation subject to suitable boundary conditions. The second-order spatial derivative was discretized to result in an approximating system of ODEs. We find bounds for the spectral radius of such a discretisation. We notice that the system of ordinary differential equation obtained from the space discretisation gives a stiff system (see Figure 1). We consider several explicit and implicit solvers in time. Then we move to approximate the full non-linear algebraic equation to a linear problem. We also approximate the inverse of the Jacobian matrix for the algebraic system. We also notice that stability of solution depends on time steps for the explicit approximation in time (Figure 2 and Figure 3). We notice that an implicit solver and its approximate versions converge fast to the steady state. The two approximate version (linearization and approximate inverse of a matrix for implicit Euler) works fine, stable and converges to the final state ± 1 (See Figure 4, Figure 5 and Figure 6).

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