A survey of finite difference methods to solve partial differential equations and von Neumann analysis of their stability properties

René Ask, Kaspara Skovli Gåsvær & Maria Linea Horgen
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We reviewed several finite-difference methods to solve the one- and two-dimensional diffusion equation and their stability properties. We derived the upper-bounds on $r \equiv \Delta t/\Delta x^2$ using von Neumann stability analysis which we sought to confirm numerically. For the one-dimensional explicit scheme we found evidence of instability once r is chosen to be larger than the theoretically predicted upper-bound $r \leq 1/2$. We found no evidence of instability when using the implicit schemes for same values of r which is consistent with the prediction that they're unconditionally stable. In the two-dimensional case we only study an explicit scheme which we also found evidence of instability for when r was chosen to be larger than the predicted upper-bound $r \leq 1/4$. Comparatively, we found that the one-dimensional explicit scheme could not perform on par with the one-dimensional implicit schemes. We found no significant difference between the two implicit schemes in our qualitative analysis. We therefore recommend that future problems should be solved with the implicit schemes and suggest that a more thorough analysis of their errors is conducted in order to establish which method is to be preferred.

I. INTRODUCTION

Numerous problems in physics, biology and other branches of science can be modelled by partial differential equations. In the present article, the diffusion equation is of interest which can be used to model the diffusion of particles through a selectively permeable membrane, Brownian motion or even an action potential propagating through an axon in the brain. The vast majority of interesting and realistically modelled natural processes do, however, not allow themselves to be solved analytically, prompting a development of reliable numerical methods to unveil the thoughts of God.

We review three finite difference methods to solve the one-dimensional diffusion equation. One explicit method based on forward-Euler and two implicit methods, one which is based on the backward-Euler formula and one known as Crank-Nicolson which may be viewed as a combination of the two former methods. We present a derivation of the methods through Taylor expansions and provide an analysis of their stability properties through so-called von Neumann stability analysis. We perform tests to confirm that the derived stability criteria are sound. We move on to a two-dimensional explicit scheme similar to the one-dimensional one for which the same derivations and tests are performed. For codes and documentation, see our Github page here [1].

II. FORMALISM

A. The Diffusion Equation

The diffusion equation in its generic form is

$$\frac{\partial u(x,y,z,t)}{\partial t} = \nabla^2 u(x,y,z,t) \tag{1}$$

1. *The one-dimensional problem*

In the one-dimensional case we'll solve the diffusion equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2}, \qquad t > 0, \qquad x \in (0,1), \tag{2}$$

with the following constraints:

$$\begin{aligned} u(0,t) &= 0, \\ u(1,t) &= 1, \\ u(x,0) &= 0. \end{aligned} \tag{3}$$

To this end, it's convenient to define $v(x,t) = u(x,t) + f(x)$ which we require to be a solution of

$$\frac{\partial v(x,t)}{\partial t} = \frac{\partial^2 v(x,t)}{\partial x^2}, \qquad t > 0, \qquad x \in (0,1), \tag{4}$$

with the Dirichlet boundary condition $v(0,t) = v(1,t) = 0$. This leads to the initial condition

$$v(x,0) = \underbrace{u(x,0)}_{=0} + f(x) = f(x), \tag{5}$$

which prompts us to find an explicit expression for $f(x)$. Assume $u(x,t)$ is a solution of eq. (2) obeying eq. (3). By insertion of $v(x,t)$ into eq. (2), it follows that

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} = 0, \tag{6}$$

meaning $f(x) = Ax + B$ for some appropriate constants A and B. The boundary conditions of $v(x,t)$ imply

$$v(0,t) = \underbrace{u(0,t)}_{=0} + f(0) = 0, \tag{7}$$

which yields $B = 0$. Similarly

$$v(1,t) = \underbrace{u(1,t)}_{=1} + f(1) = 0, \tag{8}$$

so $A = -1$. Hence

$$v(x,0) = f(x) = -x. \tag{9}$$

Thus, to find $u(x,t)$ we'll instead find $v(x,t)$ as a means to an end and apply use the definition of $v(x,t)$ to obtain the desired function $u(x,t)$. The analytical solution of eq. (2) - which is derived in the appendix, see section VII A 1 - reads

$$u(x,t) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin(n\pi x) e^{-(n\pi)^2 t} + x. \tag{10}$$

2. *The two-dimensional problem*

Moving on to two spatial dimensions, we'll study a numerical scheme to solve the two-dimensional diffusion

$$\frac{\partial^2 v(x,y,t)}{\partial x^2} + \frac{\partial^2 v(x,y,t)}{\partial y^2} = \frac{\partial v(x,y,t)}{\partial t}, \tag{11}$$

We'll require that v obeys the following constraints:

$$\begin{aligned} v(0,y,t) &= v(1,y,t) = 0, \\ v(x,0,t) &= v(x,1,t) = 0, \\ v(x,y,0) &= f(x,y). \end{aligned} \tag{12}$$

The analytical solution to this problem will naturally end up as a Fourier series, so for simplicity we'll assume that the initial condition is the first term in a general Fourier series such that

$$f(x,y) = \sin(\pi x)\sin(\pi y). \tag{13}$$

The solution for any time t is then given as

$$v(x,y,t) = f(x,y) e^{-2\pi^2 t}, \tag{14}$$

which we derive in the appendix, see section VII A 2.

B. Discretization

In the one-dimensional case, we'll operate with the following notational conventions: $v(x_j, t_m) \equiv v_j^m$ where $x_j = j\Delta x$ and $t_m = m\Delta t$. We assume that we have $n+1$ coordinate gridpoints such that $\Delta x = 1/(n+1)$ and M distinct timesteps such that $\Delta t = T/M$, where T represents the total time of simulation. The initial- and boundary conditions in this discretized format is then

$$v_0^m = v_{n+1}^m = 0, \qquad v_j^0 = f(x_j) \equiv f_j. \tag{15}$$

In the two-dimensional case, we'll use $v(x_l, y_j, t_m) \equiv v_{lj}^m$, where $x_l = l\Delta x$, $y_j = j\Delta y$ and $t_m = m\Delta t$. We assume that there are $n+1$ grid points in the x- and y-direction and that there is a total of M timesteps. We shall use the same spacing in both directions in space such that $h \equiv \Delta x = \Delta y = 1/(n+1)$. The spacing in time is given by $\Delta t = T/M$ for some total time T. The constraints to which the solution of the two-dimensional diffusion equation must obey can be written as

$$v_{0,j}^m = v_{n+1,j}^m = v_{l,0}^m = v_{l,n+1}^m = 0, \qquad v_{l,j}^0 = f(x_l, y_j) \equiv f_{lj}. \tag{16}$$

C. Explicit Scheme

An explicit scheme is a prescription from which the state of a system at a time t_{m+1} can be computed explicitly from a complete description of the system at a time t_m. To obtain such a scheme for the diffusion equation we Taylor expand forwards in time about the point (x,t):

$$v(x, t+\Delta t) = v(x,t) + \frac{\partial v(x,t)}{\partial t}\Delta t + \mathcal{O}(\Delta t^2), \tag{17}$$

which naturally leads to

$$\frac{\partial v(x,t)}{\partial t} = \frac{v(x,t+\Delta t) - v(x,t)}{\Delta t} + \mathcal{O}(\Delta t). \tag{18}$$

Similarly, we'll Taylor expand about (x,t) forwards and backwards in coordinate space. Expanding forwards yields:

$$v(x+\Delta x, t) = v(x,t) + \frac{\partial v(x,t)}{\partial x}\Delta x + \frac{\partial^2 v(x,t)}{\partial x^2}\frac{\Delta x^2}{2!} + \frac{\partial^3 v(x,t)}{\partial x^3}\frac{\Delta x^3}{3!} + \mathcal{O}(\Delta x^4). \tag{19}$$

Similarly, expanding backwards gives:

$$v(x-\Delta x, t) = v(x,t) - \frac{\partial v(x,t)}{\partial x}\Delta x + \frac{\partial^2 v(x,t)}{\partial x^2}\frac{\Delta x^2}{2!} - \frac{\partial^3 v(x,t)}{\partial x^3}\frac{\Delta x^3}{3!} + \mathcal{O}(\Delta x^4). \tag{20}$$

Adding these two equations gives us

$$v(x+\Delta x, t) + v(x-\Delta x, t) = 2v(x,t) + \frac{\partial^2 v(x,t)}{\partial x^2}\frac{\Delta x^2}{2!} + \mathcal{O}(\Delta x^4). \tag{21}$$

Solving this with respect to the second derivative leads to

$$\frac{\partial^2 v(x,t)}{\partial x^2} = \frac{v(x+\Delta x,t) - 2v(x,t) + v(x-\Delta x,t)}{\Delta x^2} + \mathcal{O}(\Delta x^2). \tag{22}$$

Inserting the expression for the time derivative from eq. (18) and our newly derived second derivative of x into the diffusion equation (2) gives us

$$\frac{v(x,t+\Delta t) - v(x,t)}{\Delta t} = \frac{v(x+\Delta x,t) - 2v(x,t) + v(x-\Delta x,t)}{\Delta x^2} + \mathcal{O}(\Delta x^2, \Delta t), \tag{23}$$

which clearly carries a truncation error $\mathcal{O}(\Delta x^2, \Delta t)$. In the more compact notation defined earlier, we can derive the explicit formula

$$v_j^{m+1} = r\left(v_{j+1}^m - 2v_j^m + v_{j-1}^m\right) + v_j^m, \tag{24}$$

with $r \equiv \Delta t/\Delta x^2$.

D. Implicit Scheme

In an implicit scheme, the state of a system at two adjacent times t_m and t_{m+1} depend on each other, which leads to a set of linear equations which can be solved using techniques from linear algebra. In our specific case, we'll apply the backward-Euler formula (in time) which leads to a tridiagonal matrix equation which can be solved with the Thomas algorithm which is thoroughly explored here [2]. In the following we derive the matrix equation starting from Taylor expansions of $v(x,t)$. Expanding forwards and backwards in coordinate space at a time $t+\Delta t$ gives us two equations:

$$\begin{aligned} v(x \pm \Delta x, t+\Delta t) = v(x, t+\Delta t) \pm \frac{\partial v(x,t+\Delta t)}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 v(x,t+\Delta t)}{\partial x^2}\Delta x^2 \\ \pm \frac{1}{3!}\frac{\partial^3 v(x,t+\Delta t)}{\partial x^3}\Delta x^3 + \mathcal{O}(\Delta x^4). \end{aligned} \tag{25}$$

Adding these equations together yields

$$v(x+\Delta x, t+\Delta t) + v(x-\Delta x, t+\Delta t) = 2v(x,t+\Delta t) + \frac{\partial^2 v(x,t+\Delta t)}{\partial x^2}\Delta x^2 + \mathcal{O}(\Delta x^4), \tag{26}$$

which we can solve for the second derivative:

$$\frac{\partial^2 v(x,t+\Delta t)}{\partial x^2} = \frac{v(x+\Delta x,t+\Delta t) - 2v(x,t+\Delta t) + v(x-\Delta x,t+\Delta t)}{\Delta x^2} + \mathcal{O}(\Delta x^2). \tag{27}$$

Now, using the same Taylor expansion in time as with the explicit method and inserting it into the diffusion equation we get

$$\frac{v(x,t+\Delta t) - v(x,t)}{\Delta t} = \frac{v(x+\Delta x,t+\Delta t) - 2v(x,t+\Delta t) + v(x-\Delta x,t+\Delta t)}{\Delta x^2} + \mathcal{O}(\Delta x^2, \Delta t). \tag{28}$$

Clearly the truncation error of this scheme goes as $\mathcal{O}(\Delta x^2, \Delta t)$ just like it did with the explicit method. Compactifying our notation a bit, the implicit scheme can be written neatly as

$$\frac{v_j^{m+1} - v_j^m}{\Delta t} = \frac{v_{j+1}^{m+1} - 2v_j^{m+1} + v_{j-1}^{m+1}}{\Delta x^2}. \tag{29}$$

This equation can be rearranged into

$$v_j^{m+1} + r\left(-v_{j-1}^{m+1} + 2v_j^{m+1} - v_{j+1}^{m+1}\right) = v_j^m, \tag{30}$$

with $r \equiv \Delta t/\Delta x^2$, which is equivalent to the matrix equation

$$\begin{bmatrix} 1+2r & -r & 0 & \cdots & 0 \\ -r & 1+2r & -r & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & -r \\ 0 & \cdots & 0 & -r & 1+2r \end{bmatrix} \begin{bmatrix} v_1^{m+1} \\ v_2^{m+1} \\ \vdots \\ \vdots \\ v_n^{m+1} \end{bmatrix} = \begin{bmatrix} v_1^m \\ v_2^m \\ \vdots \\ \vdots \\ v_n^m \end{bmatrix}. \tag{31}$$

We can rewrite this in the more compact notation

$$(I + rA)\boldsymbol{v}_{m+1} = \boldsymbol{v}_m, \tag{32}$$

where I is the identity matrix and A is the tridiagonal matrix

$$A \equiv \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{bmatrix}. \tag{33}$$

E. Crank-Nicolson in one dimension

In this section we derive the Crank-Nicolson scheme. We'll do this by Taylor expansions about the point (x, t') where $t' = t + \Delta t/2$ using a step size of $\Delta t/2$. Expanding forwards in time and forwards and backwards in space gives us the following:

$$\begin{aligned}v(x \pm \Delta x, t + \Delta t) = v(x, t') \pm \frac{\partial v(x,t')}{\partial x}\Delta x + \frac{\partial v(x,t')}{\partial t}\frac{\Delta t}{2} + \frac{1}{2}\frac{\partial^2 v(x,t')}{\partial x^2}\Delta x^2 \\ \pm \frac{\partial^2 v(x,t')}{\partial x \partial t}\frac{\Delta x \Delta t}{2} \pm \frac{\partial^3 v(x,t')}{\partial x^3}\frac{\Delta x^3}{3!} + \mathcal{O}(\Delta x^4, \Delta t^2).\end{aligned} \tag{34}$$

Similarly, expanding backwards in time and forwards and backwards in space gives us:

$$\begin{aligned}v(x \pm \Delta x, t - \Delta t) = v(x, t') \pm \frac{\partial v(x,t')}{\partial x}\Delta x - \frac{\partial v(x,t')}{\partial t}\frac{\Delta t}{2} + \frac{1}{2}\frac{\partial^2 v(x,t')}{\partial x^2}\Delta x^2 \\ \mp \frac{\partial^2 v(x,t')}{\partial x \partial t}\frac{\Delta x \Delta t}{2} \pm \frac{\partial^3 v(x,t')}{\partial x^3}\frac{\Delta x^3}{3!} + \mathcal{O}(\Delta x^4, \Delta t^2).\end{aligned} \tag{35}$$

Before we add these four equations, it's useful to compactify our notation. Let $v(x, t') \equiv v_j^{m+1/2}$, $v(x \pm \Delta x, t) \equiv v_{j\pm1}^m$ and $v(x \pm \Delta x, t + \Delta t) \equiv v_{j\pm1}^{m+1}$. Now, adding the equations gives:

$$v_{j+1}^{m+1} + v_{j-1}^{m+1} + v_{j+1}^m + v_{j-1}^m = 4v_j^{m+1/2} + 2\frac{\partial^2 u(x,t')}{\partial x^2}\Delta x^2 + \mathcal{O}(\Delta x^4, \Delta t^2). \tag{36}$$

The only problem now is the term containing $v_j^{m+1/2}$. To get around this we Taylor expand forwards and backwards in time about (x, t')

$$v(x, t' \pm \Delta t/2) = v(x, t') \pm \frac{\partial v(x,' t)}{\partial t}\Delta t + \mathcal{O}(\Delta t^2). \tag{37}$$

Adding the two equation gives

$$v(x, t) + v(x, t + \Delta t) = 2v(x, t') + \mathcal{O}(\Delta t^2), \tag{38}$$

which we can solve for $v_j^{m+1/2}$. We essentially then replace the term with the average of its adjacent values in time:

$$v_j^{m+1/2} = \frac{1}{2}\left(v_j^m + v_j^{m+1}\right) + \mathcal{O}(\Delta t^2), \tag{39}$$

which by insertion in to eq. (36) gives us

$$v_{j+1}^{m+1} + v_{j-1}^{m+1} + v_{j+1}^m + v_{j-1}^m = 2v_j^m + 2v_j^{m+1} + 2\frac{\partial^2 u(x,t')}{\partial x^2}\Delta x^2 + \mathcal{O}(\Delta x^4, \Delta t^2), \tag{40}$$

which may be solved with respect to the second derivative:

$$\frac{\partial^2 v(x,t')}{\partial x^2} = \frac{1}{2}\left[\frac{v_{j+1}^m - 2v_j^m + v_{j-1}^m}{\Delta x^2} + \frac{v_{j+1}^{m+1} - 2v_j^{m+1} + v_{j-1}^{m+1}}{\Delta x^2}\right] + \mathcal{O}(\Delta x^2, \Delta t^2). \tag{41}$$

Now, we move onto the time derivative of $v(x, t')$. The idea is to perform a symmetric time difference scheme about t':

$$v(x, t' \pm \Delta t/2) = v(x, t') \pm \frac{\partial v(x,t')}{\partial t}\frac{\Delta t}{2} + \frac{1}{2!}\frac{\partial^2 v(x,t')}{\partial t^2}\frac{\Delta t^2}{4} + \mathcal{O}(\Delta t^3). \tag{42}$$

Subtracting the two equations gives us:

$$v(x, t + \Delta t) - v(x, t) = \frac{\partial v(x,t')}{\partial t}\Delta t + \mathcal{O}(\Delta t^3), \tag{43}$$

which leads to the following expression for the time derivative:

$$\frac{\partial v(x,t')}{\partial t} = \frac{v(x,t+\Delta t) - v(x,t)}{\Delta t} + \mathcal{O}(\Delta t^2). \tag{44}$$

Evidently, the method can be summarized as

$$\frac{v_j^{m+1} - v_j^m}{\Delta t} = \frac{1}{2}\left[\frac{v_{j+1}^m - 2v_j^m + v_{j-1}^m}{\Delta x^2} + \frac{v_{j+1}^{m+1} - 2v_j^{m+1} + v_{j-1}^{m+1}}{\Delta x^2}\right] + \mathcal{O}(\Delta x^2, \Delta t^2). \tag{45}$$

Clearly, the method carries a truncation error of $\mathcal{O}(\Delta x^2, \Delta t^2)$. The last equation can be rewritten into

$$v_j^{m+1} + \rho\left(2v_j^{m+1} - v_{j+1}^{m+1} - v_{j-1}^{m+1}\right) = v_j^m + \rho\left(-2v_j^m + v_{j+1}^m + v_{j-1}^m\right), \tag{46}$$

where $\rho = \Delta t / 2\Delta x^2$. This can be recast into a matrix equation which we shall derive below:

$$\begin{bmatrix} v_1^{m+1} + \rho\left(2v_1^{m+1} - v_2^{m+1} - v_0^{m+1}\right) \\ v_2^{m+1} + \rho\left(2v_2^{m+1} - v_3^{m+1} - v_1^{m+1}\right) \\ \vdots \\ v_n^{m+1} + \rho\left(2v_n^{m+1} - v_{n+1}^{m+1} - v_{n-1}^{m+1}\right) \end{bmatrix} = \begin{bmatrix} v_1^m + \rho\left(-2v_1^m + v_2^m + v_0^m\right) \\ v_2^m + \rho\left(-2v_2^m + v_3^m + v_1^m\right) \\ \vdots \\ v_n^m + \rho\left(-2v_n^m + v_{n+1}^m + v_{n-1}^m\right) \end{bmatrix}. \tag{47}$$

which may be factorized in the following way.

$$\begin{bmatrix} 1+2\rho & -\rho & 0 & \cdots & 0 \\ -\rho & 1+2\rho & -\rho & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & -\rho \\ 0 & \cdots & 0 & -\rho & 1+2\rho \end{bmatrix} \begin{bmatrix} v_1^{m+1} \\ v_2^{m+1} \\ \vdots \\ \vdots \\ v_n^{m+1} \end{bmatrix} = \begin{bmatrix} 1-2\rho & \rho & 0 & \cdots & 0 \\ \rho & 1-2\rho & \rho & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \rho \\ 0 & \cdots & 0 & \rho & 1-2\rho \end{bmatrix} \begin{bmatrix} v_1^m \\ v_2^m \\ \vdots \\ \vdots \\ v_n^m \end{bmatrix} \tag{48}$$

Clearly, by defining vectors the $\boldsymbol{v}_m = \left(v_1^m, v_2^m, ..., v_n^m\right)^T$ and $\boldsymbol{v}_{m+1} = \left(v_1^{m+1}, v_2^{m+1}, ..., v_n^{m+1}\right)^T$, the equation can be rewritten as

$$(I + \rho A)\boldsymbol{v}_{m+1} = (I - \rho A)\boldsymbol{v}_m \equiv \boldsymbol{q}_m, \tag{49}$$

where I is the identity matrix and A is the tridiagonal Toeplitz matrix defined in eq. (33). The i-th vector matrix product-element is given by

$$q_i^m = \rho v_{i-1}^m + (1-2\rho)v_i^m + \rho v_{i+1}^m. \tag{50}$$

At this point, we can apply the Thomas algorithm to compute the time evolution of $v(x,t)$. We'll get back to this algorithm in section III.

F. Explicit scheme in the 2-dimensional case

The diffusion equation in 2-dimensions is

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}. \tag{51}$$

As a reminder: we'll denote $v(x_l, y_j, t_m) \equiv v_{lj}^m$. Assuming that $\Delta x = \Delta y \equiv h$, we can discretize the equation as

$$\frac{v_{lj}^{m+1} - v_{lj}^m}{\Delta t} = \frac{v_{l+1,j}^m - 2v_{lj}^m + v_{l-1,j}^m}{h^2} + \frac{v_{l,j+1}^m - 2v_{lj}^m + v_{l,j-1}^m}{h^2}, \tag{52}$$

which we may rearrange as

$$v_{lj}^{m+1} = v_{lj}^m(1-4r) + r\left[v_{l+1,j}^m + v_{l-1,j}^m + v_{l,j+1}^m + v_{l,j-1}^m\right], \tag{53}$$

with boundary- and initial conditions

$$v_{0,j}^m = v_{n+1,j}^m = v_{l,0}^m = v_{l,n+1}^m = 0, \qquad v_{l,j}^0 = f(x_l, y_j) \equiv f_{lj}. \tag{54}$$

This method clearly carries the same truncation error in space and time as the explicit scheme in one-dimension, that is, the error is of the order $\mathcal{O}(h^2, \Delta t)$.

G. Stability analysis

In this section we will follow the treatment presented here [4]. To assess the stability of the methods, we'll apply von Neumann analysis which is to require that the time-dependent part of the discrete solution is bounded by the maximum value of the time-dependent part of the solution for the continuous case. The discrete solution of eq. (2) can be written as

$$v_j^m = (a_k)^m e^{ik\pi x_j}, \tag{55}$$

where $x_j \equiv j\Delta x$ and $k = 0, \pm1, \pm2, ...$; Mathematically, then, the criterion to impose is

$$|(a_k)^m| \leq \max_{t\in[0,\infty)} \left| e^{-k^2 t} \right| = 1. \tag{56}$$

1. *Explicit scheme*

Inserting the discrete solution into eq. (24) for the explicit scheme produces the following equation

$$\frac{(a_k)^{m+1} - (a_k)^m}{\Delta t} e^{ik\pi j\Delta x} = \frac{e^{ik\pi(j-1)\Delta x} - 2e^{ik\pi j\Delta x} + e^{ik\pi(j+1)\Delta x}}{\Delta x^2}(a_k)^m, \tag{57}$$

which can be rewritten into

$$\frac{a_k - 1}{\Delta t} = \frac{e^{ik\pi\Delta x} - 2 + e^{-ik\pi\Delta x}}{\Delta x^2} = 2\left[\frac{\cos(k\pi\Delta x) - 1}{\Delta x^2}\right]. \tag{58}$$

Using the trigonometric identity

$$\sin\left(\frac{x}{2}\right) = \pm\sqrt{\frac{1-\cos x}{2}},$$

we obtain the relation

$$a_k = 1 - 4r\sin^2\left(\frac{k\pi\Delta x}{2}\right). \tag{59}$$

From eq. (56), the following criterion for r arises

$$\left|1 - 4r\sin^2\left(\frac{k\pi\Delta x}{2}\right)\right| = \left|4r\sin^2\left(\frac{k\pi\Delta x}{2}\right) - 1\right| \leq |4r - 1| \leq 1, \tag{60}$$

from which it follows that the upper-bound on r to attain a stable simulation is

$$r \leq \frac{1}{2}. \tag{61}$$

What this is means is that r must be chosen accordin to eq. (61) to obtain a stable numerical simulation. When an upper-bound on r exists for a finite difference scheme, we refer to the scheme as *conditionally* stable, a classification which the explicit scheme is subordinated.

2. *Implicit scheme*

Inserting eq. (55) into eq. (29) yields

$$\frac{(a_k)^{m+1} - (a_k)^m}{\Delta t} e^{ik\pi j\Delta x} = \frac{e^{ik\pi(j-1)\Delta x} - 2e^{ik\pi j\Delta x} + e^{ik\pi(j+1)\Delta x}}{\Delta x^2}(a_k)^{m+1}, \tag{62}$$

which may be rearranged as

$$a_k - 1 = 2ra_k \left[\cos\left(k\pi\Delta x\right) - 1\right] = -4ra_k \sin^2\left(\frac{k\pi\Delta x}{2}\right). \tag{63}$$

Thus

$$a_k = \frac{1}{1 + 4r\sin^2\left(\frac{k\pi\Delta x}{2}\right)} \leq 1 \tag{64}$$

for all choices of r. Clearly, *any* choice of r is acceptable to obtain as stable solution. By convention, such a method is classified as *unconditionally* stable since any choice of r provides a stable simulation.

3. The Crank-Nicolson Scheme

We'll show here that Crank-Nicolson scheme is unconditonally stable in the same way the implicit scheme from last section was. We use the same ansatz as before and inserting it into eq. (45) yields:

$$\frac{(a_k)^{m+1} - (a_k)^m}{\Delta t} e^{ik\pi j\Delta x} = \frac{1}{2}\left[(a_k + 1)\frac{e^{ik\pi(j-1)\Delta x} - 2e^{ik\pi j\Delta x} + e^{ik\pi(j+1)\Delta x}}{\Delta x^2}(a_k)^m\right], \tag{65}$$

which can be rearranged as

$$a_k - 1 = -4\rho(a_k + 1)\sin^2\left(\frac{k\pi\Delta x}{2}\right). \tag{66}$$

with $\rho \equiv \Delta t/2\Delta x^2$. Solving this equation for a_k yields

$$a_k = \frac{1 - 4\rho\sin^2\left(\frac{k\pi\Delta x}{2}\right)}{1 + 4\rho\sin^2\left(\frac{k\pi\Delta x}{2}\right)} \leq 1, \tag{67}$$

for all choices of ρ. Thus, in the von Neumann sense, the algorithm is unconditionally stable.

4. 2-dimensional explicit scheme

The discrete solution in the 2-dimensional case is almost identical to the one in one dimension, except we have to take the second spatial variable into account.

$$v_{l,j}^m = (a_k)^m e^{ik\pi(x_l + y_j)} = (a_k)^m e^{ik\pi\Delta x(l+j)}. \tag{68}$$

As in the previous cases, we insert the discrete solution into the 2-dimensional diffusion equation. With some rewriting we obtain the following relation

$$\frac{a_k - 1}{\Delta t} = \frac{2e^{ik\pi\Delta x} - 4 + 2e^{-ik\pi\Delta x}}{\Delta x^2} = -8r\sin^2\left(\frac{k\pi x}{2}\right). \tag{69}$$

From eq. (56), it easily follows that

$$r \leq \frac{1}{4}. \tag{70}$$

In other words, the explicit scheme is two dimensions is properly classified as conditionally stable because there exists an upper-bound on r for which the method provides a stable simulation.

III. ALGORITHMS

The implementation of the explicit scheme is summarized below.

Algorithm 1 Explicit scheme

for $j = 1, 2, ..., n$ **do** ▷ Impose the initial condition $v(x, 0) = f(x)$
  $v_j^0 = f_j$
for $m = 0, 1, ..., M$ **do**
  for $j = 1, 2, ..., n$ **do**
    $v_j^{m+1} = (1 - 2r)v_j^m + r(v_{j+1}^m + v_{j-1}^m)$ ▷ Compute solution forward in time step at grid point j.

To implement the implicit scheme, we used the Thomas algorithm for a tridiagonal matrix on the generic form

$$T \equiv \begin{bmatrix} b_1 & c_1 & 0 & \cdots & \cdots & \cdots \\ a_1 & b_2 & c_2 & 0 & \cdots & \cdots \\ 0 & a_2 & b_3 & 0 & \cdots & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{n-2} & b_{n-1} & c_{n-1} \\ 0 & 0 & \cdots & 0 & a_{n-1} & b_n \end{bmatrix}. \tag{71}$$

The algorithm that follows solves the general equation $T\boldsymbol{v}_{m+1} = \boldsymbol{v}_m$ which combines the implicit one-dimensional scheme with the Thomas algorithm.

Algorithm 2 Implicit scheme

for $m = 0, 1, ..., M$ **do**
  for $j = 1, 2, ..., n$ **do** ▷ Forward substitution
    $b_j = b_j - a_{j-1}c_{j-1}/b_{j-1}$
    $v_j^m = v_j^m - a_{j-1}v_{j-1}^m/b_{j-1}$
  for $j = n, n-1, ..., 1$ **do** ▷ Backward substitution
    if $j = n$ **then**
      $v_j^{m+1} = v_j^m/b_j$
    else
      $v_j^{m+1} = (v_j^m - c_j v_{j+1}^{m+1})/b_j$

The algorithm for solving the PDE using the Crank-Nicolson method combined with the Thomas algorithm can be summarized in the following way.

Algorithm 3 Crank-Nicolson

for $m = 0, 1, ..., M$ **do**
  for $j = 1, 2, ..., n$ **do** ▷ Forward substitution
    $q_i = \rho v_{i-1}^m + (1 - 2\rho)v_i^m + \rho v_{i+1}^m$
    $b_j = b_j - a_{j-1}c_{j-1}/b_{j-1}$
    $q_j = q_j - a_{j-1}q_{j-1}/b_{j-1}$
  for $j = n, n-1, ..., 1$ **do** ▷ Backward substitution
    if $j = n$ **then**
      $v_j^{m+1} = q_j/b_j$
    else
      $v_j^{m+1} = (q_j - c_j v_{j+1}^{m+1})/b_j$

The foundation to solve the two-dimensional equation was laid in eq. (53). The algorithm is an explicit scheme and is summarized below.

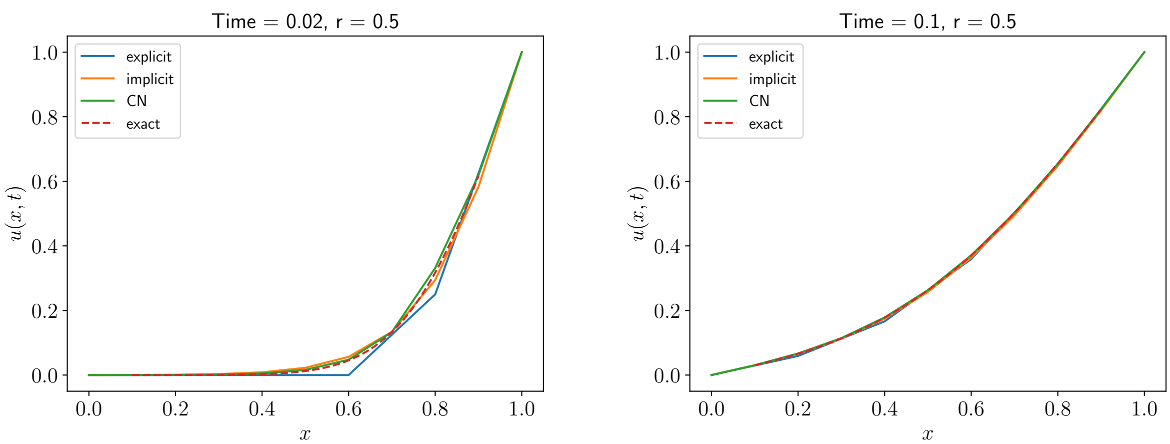
Algorithm 4 2D explicit scheme

for $l = 1, 2, ..., n$ **do**
  for $j = 1, 2, ..., n$ **do**
    $v_{lj}^0 = f_{ij}$ ▷ Initial condition
for $m = 1, 2, ..., M$ **do** ▷ Compute the time evolution
  for $l = 1, 2, ..., n$ **do**
    for $j = 1, 2, ..., n$ **do**
      $v_{lj}^{m+1} = v_{lj}^m(1 - 4r) + r\left[v_{l+1,j}^m + v_{l-1,j}^m + v_{l,j+1}^m + v_{l,j-1}^m\right]$

IV. RESULTS

A. The 1-dimensional implementations

FIG. 1 and 2 displays a comparison between the three finite difference methods that solves the one-dimensional diffusion equation and the analytical solution in eq. (88).



(a) (b)

FIG. 1. In figure **(a)** we show the numerical solution for all three one-dimensional algorithms versus the exact solution (red dashed line) truncated after 1001 terms at a time $t = 0.02$. In figure **(b)** we show the numerical solution for all three methods versus the exact solution (red dashed line) at a time $t = 0.1$. In both figures the blue line shows the explicit scheme, the orange shows the implicit scheme, the green shows the Crank-Nicolson scheme. The parameters were set to $r = 0.5$, $\Delta x = 0.1$ and $\Delta t = r(\Delta x)^2$.

By working with a multivariable function, $u(x, t)$, we can visualize the time evolution of our system and compare it with the expected evolution from the analytical expression. FIG. 3 displays this time evolution for $t \in (0, 1)$ and $x \in (0, 1)$ and the comparison with the analytical solution in eq. (88) for the Crank-Nicolson scheme. The results where computed with $r = 0.25$, $\Delta x = 0.01$ and $\Delta t = r(\Delta x)^2$. Qualitatively, the numerical solution appears to be in agreement with the analytical solution.

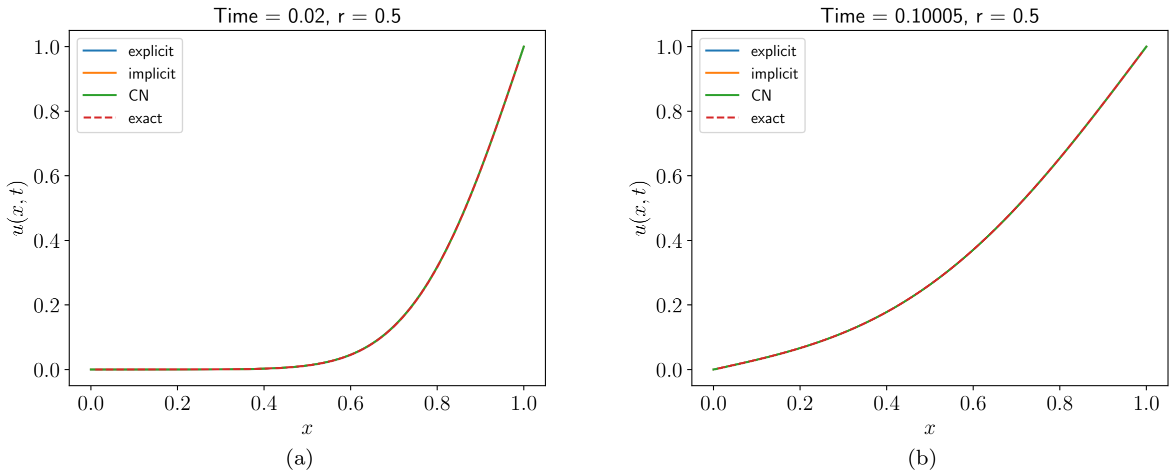


FIG. 2. In figure **(a)** we show the numerical solution for all three one-dimensional algorithms versus the exact solution (red dashed line) truncated after 1001 terms at a time $t = 0.02$. In figure **(b)** we show the numerical solution for all three methods versus the exact solution (red dashed line) at a time $t = 0.10005$. In both figures the blue line shows the explicit scheme, the orange shows the implicit scheme, the green shows the Crank-Nicolson scheme.

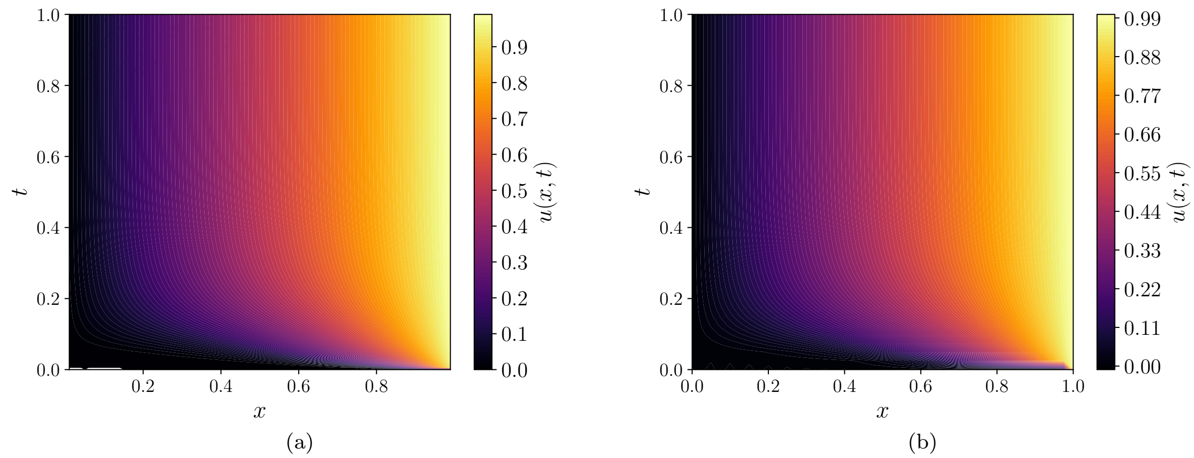


FIG. 3. Figure **(a)** shows the time evolution of $u(x,t)$ for $t \in (0,1)$ and $x \in (0,1)$. The result was computed using the Crank-Nicolson scheme with $r = 0.25$, $\Delta x = 0.01$ and $\Delta t = r(\Delta x)^2$. Figure **(b)** shows the time evolution of the analytical solution truncated after 1001 terms.

B. Results of the two-dimensional explicit method

In FIG. 4 the numerical- and analytical solution for the two-dimensional explicit scheme are graphically displayed. The results were computed for a total time of $t \approx 0.5$, $r = 0.25$ and a stepsize $h = 0.01$.

C. Stability analysis

1. In one dimension

FIG. 5 shows the numerical solutions for the one dimensional schemes for two different values of r (and ρ for the Crank-Nicolson scheme). The choice for $r, \rho \in \{0.5, 0.505\}$ were made based on the von Neumann stability analysis in section II G.

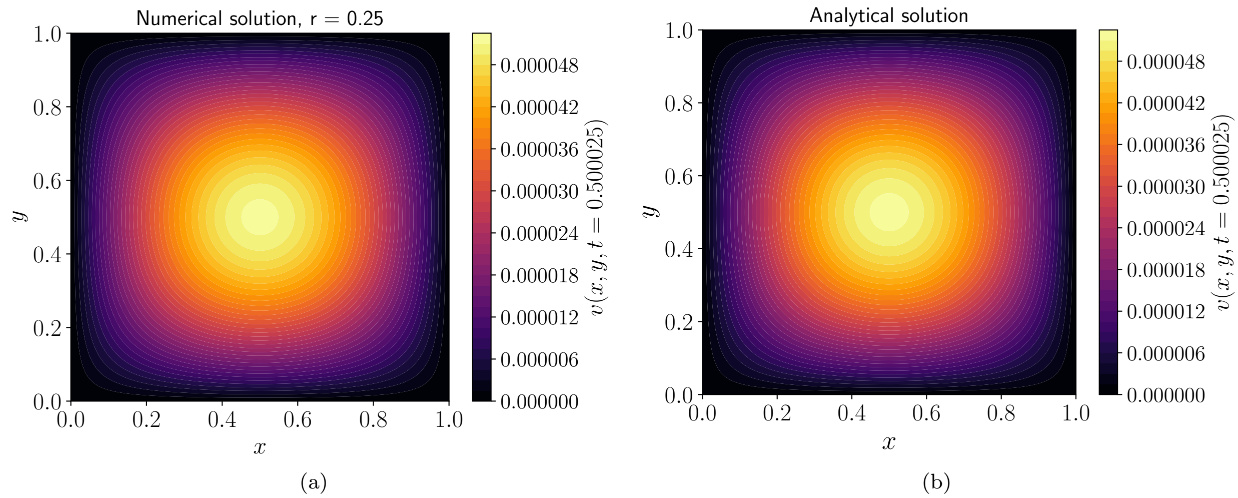


FIG. 4. Figure **(a)** shows the computed solution $v(x, y, t)$ at $t \approx 0.5$ using $r = 0.25$ using $h = 0.01$ and $\Delta t = rh^2$. Figure **(b)** shows the analytical solution truncated after 10^4 terms for the same time t.

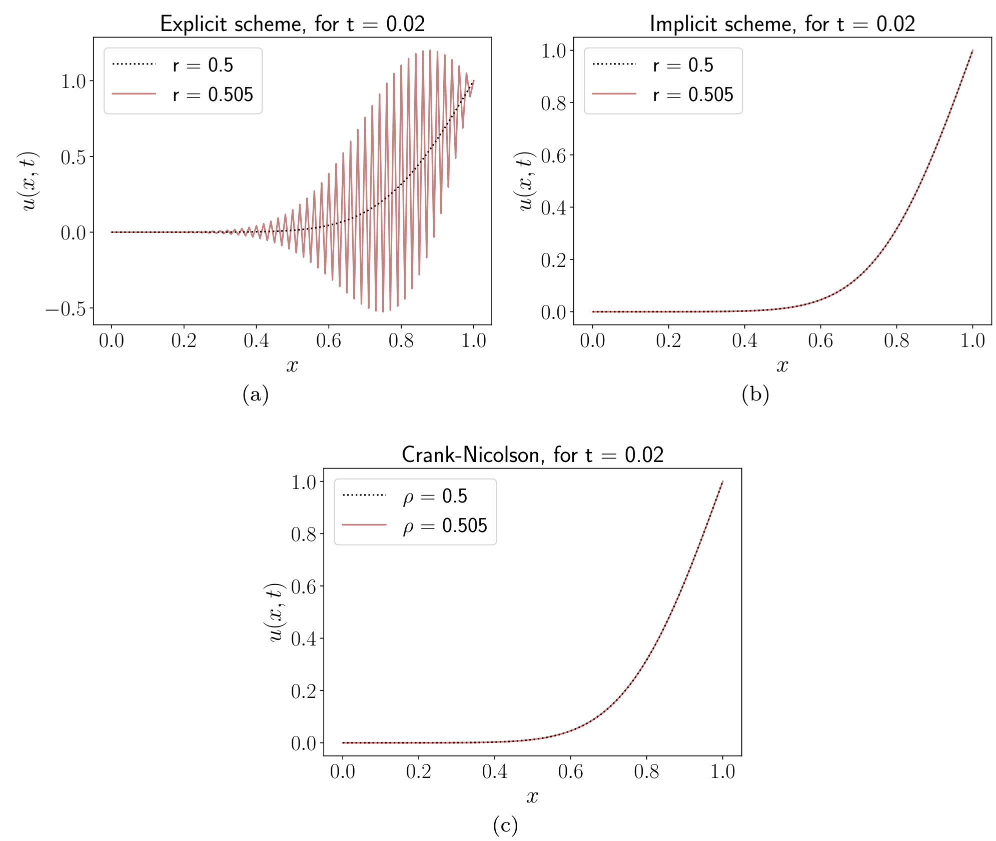


FIG. 5. The figures display the numerical solutions for two different values of $r \equiv \Delta t/\Delta x$, where $r = 0.5$ which corresponds to the stability criterion imposed for the explicit scheme. Here $\Delta x = 0.01$ were chosen. For the Crank-Nicolson scheme we used $\rho = 0.5$ and $\Delta t = 2\rho(\Delta x)^2$. From the plots, it is evident that the explicit scheme is conditionally stable.

As expected, the explicit scheme appears to be conditionally stable.

2. In two dimensions

FIG. 6 displays the numerical solution for $r = 0.251$ which is larger than the predicted upper-bound of stable choices of r. Even the non-astute reader may observe that this simulation led to unstable results, precisely as predicted by the analysis performed earlier.

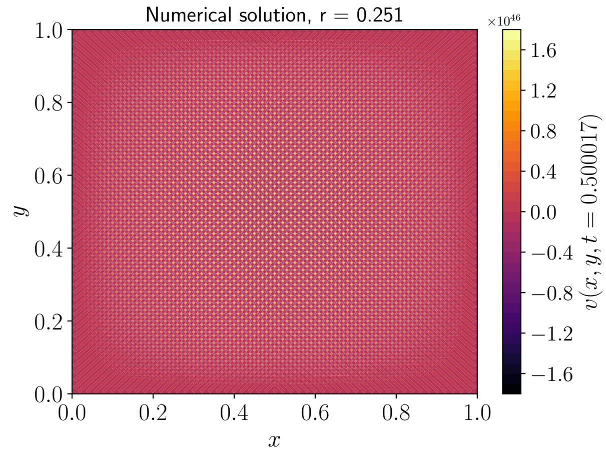


FIG. 6. The figure shows the numerical solution in units of 10^{46} using $r = 0.251$ with $h = 0.01$ at a time $t \approx 0.5$. Here the solution is clearly diverging from the analytical solution in shown in FIG. 4(b).

V. DISCUSSION

A. A comparison of the one-dimensional methods

By studying FIG. 1(a), we see that the methods which most closely reproduces the analytical solution is the implicit scheme and the Crank-Nicolson method when $\Delta x = 0.1$. The explicit scheme misses the mark significantly. Clearly the Crank-Nicolson scheme is expected to be better than the explicit scheme due to the higher order truncation error. It is not obvious, however, why the implicit scheme produces so much better results than the explicit method since they both carry the same order in time and space with respect to their truncation error. Inspecting FIG. 1(b), we see that the methods are closer to an equal footing once the simulation approaches the steady state solution which is likely due to the fact that the time-derivative of the true solution is of a much lesser magnitude than it is initially. Ostensibly, the explicit method manages to catch up with the other methods towards the end.

B. The two-dimensional explicit scheme

Inspecting FIG. 4(a), we see that it reproduces the qualitative features of the analytical solution shown in FIG. 4(b). Although the functions values $v(x, y, t)$ appear to be on par with one another, we didn't do any extensive analysis of the error in this case and propose this as a further topic of study.

C. Confirmation of stability properties

The one-dimensional explicit scheme was predicted to fail for $r > 0.5$. In FIG. 5(a) we observe that the computed solution for $r > 0.5$ oscillates about the solution computed with $r = 0.5$, which can be seen as a confirmation of the stability criterion derived for the method earlier. The other methods which are shown in FIG. 5(b) and 5(c) present no such instability for the same choices of r (technically ρ in the case of Crank-Nicolson) which is consistent with the fact that they mathematically are unconditionally stable.

Onto the stability properties of the two-dimensional scheme. From FIG. 4(a) and 6, the predicted stability properties does indeed seem to be confirmed. For the case with $r = 0.25$ the solution is stable while for $r = 0.2505$, the solution is dramatically different and running the computations for a few more iterations would likely lead to overflow even though the steady state of the system is $v(x,y,\infty) = 0$. We do, however, acknowledge that to truly confirm this stability criterion one ought to test for several other values of r close to the predicted one and suggest that this is a possible further problem to scrutinize.

VI. CONCLUSION

In this article we've reviewed several finite difference schemes to solve diffusion equation both with one and two spatial dimensions. For these methods, we studied the numerical solutions and found general agreement with the analytically derived solutions. We derived stability properties using von Neumann analysis and tested the methods numerically in search for agreement with the predicted values of r. For both explicit schemes, we found evidence of instability by slightly increasing r beyond the predicted upper-bound to attain stability. We found no evidence of instability in the implicit schemes studied in this article which is consistent with the prediction that they are unconditionally stable. In the one-dimensional case, we found that the implicit scheme and Crank-Nicolson scheme performed much better than the explicit scheme for large step spatial step sizes Δx, but no significant difference between the two others. We therefore recommend either of the two methods to solve the one-dimensional diffusion equation. In two dimensions, we simply developed an explicit scheme which reproduced the qualitative features of the analytical solution. We did not engage in an extensive study of the accuracy of this method and suggest that this can be a future research topic. We also suggest investigating more advanced implicit methods in the two-dimensional case may bear fruits unexplored in this article.

VII. APPENDIX

A. Analytical solutions of the diffusion equation

1. *In the one-dimensional case*

Solving the partial differential equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2}, \tag{72}$$

with the boundary- and initial conditions

$$\begin{aligned} u(0,t) &= 0, \\ u(1,t) &= 1, \\ u(x,0) &= 0, \end{aligned} \tag{73}$$

is done in the following manner: As explained in section II A 1, we introduce the function

$$v(x,t) = u(x,t) + f(x), \tag{74}$$

where $f(x) = -x$. The boundary conditions then changes to $v(0,t) = v(1,t) = 0$, while the initial condition reads

$$v(x,0) = f(x) = -x. \tag{75}$$

First step in obtaining the analytical solution to the diffusion equation in one dimension is to make an educated guess about the solution. We simply guess that the solution is separable with respect to x and t, and make the ansatz

$$v_n(x,t) = X_n(x)T_n(t). \tag{76}$$

Inserting this into eq. (72) yields

$$X_n T_n' = X_n'' T_n. \tag{77}$$

Next we divide both sides in eq. (77) with $X_n T_n$ to obtain the following relation,

$$\frac{T_n'}{T_n} = \frac{X_n''}{X_n} = -k_n^2, \tag{78}$$

where k_n^2 is a constant. The left- and right side of the expression above is only dependent of their respective variables, hence, both expressions must be equal to a shared constant. Eq. (78) can now be recast into two ordinary differential equations:

$$T_n' = -k_n^2 T_n, \tag{79}$$
$$X_n'' = -k_n^2 X_n. \tag{80}$$

Looking at eq. (79), and requiring on physical grounds that the solution $u(x,t) \to 0$ when $t \to \infty$, it is evident that the time-dependent part of the solutions reside in the subspace,

$$T_n \propto e^{-k_n^2 t}. \tag{81}$$

Eq. (80) is easily recognised as a harmonic oscillator, which has the general solution

$$X_n = A_n \cos(k_n x) + B_n \sin(k_n x), \tag{82}$$

for some constants A_n and B_n. The boundary conditions gives $A_n = 0$, and the constant k_n^2.

$$X_k(1) = B_n \sin(k_n \cdot 1) = 0 \qquad \Rightarrow \qquad k_n = n\pi \quad \text{for} \quad n = 1, 2, ... \tag{83}$$

From eq. (82) and (83) it follows that the solution is of the form

$$v_n(x,t) = e^{-k_n^2 t} B_n \sin(k_n x), \tag{84}$$
$$v(x,t) = \sum_{n=1}^{\infty} B_n \sin(n\pi x) e^{-(n\pi)^2 t}. \tag{85}$$

In the last step we applied the principle of superposition. It states that any linear combination of particular solutions creates a new solution. To decide the Fourier constants $\{B_n\}_{n=1}^{\infty}$, we make us of the initial condition

$$\sum_{n=1}^{\infty} B_n \sin(n\pi x) = -x. \tag{86}$$

From [3] the Fourier constants is determined by the integral

$$\begin{aligned} B_n &= 2\int_0^1 f(x) \sin(n\pi x) dx, \\ &= -2\int_0^1 x \sin(n\pi x) dx = \frac{2}{n\pi}(-1)^n. \end{aligned} \tag{87}$$

Hence, the solution of the one dimensional diffusion equation is given by

$$u(x,t) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin(n\pi x) e^{-(n\pi)^2 t} + x. \tag{88}$$

2. In the two-dimensional case

In this section we derive an analytical solution to the two-dimensional diffusion equation

$$\frac{\partial v}{\partial t} = \nabla^2 v, \tag{89}$$

where we impose the constraints

$$\begin{aligned} v(0,y,t) &= v(1,y,t) = 0, \\ v(x,0,t) &= v(x,1,t) = 0, \\ v(x,y,0) &= f(x,y) \end{aligned} \tag{90}$$

where the initial condition is defined as

$$f(x,y) = \sin(\pi x)\sin(\pi y), \tag{91}$$

with $\alpha > 0$. Again we make the ansatz

$$v_{mn}(x,y,t) = Z_{nm}(x,y)T_{nm}(t). \tag{92}$$

Plugging this into eq.(89) gives us

$$T_{nm}\frac{\partial^2 Z_{nm}}{\partial x^2} + T_{nm}\frac{\partial^2 Z_{nm}}{\partial y^2} = Z_{nm}\frac{\partial T_{nm}}{\partial t}. \tag{93}$$

Next we divide both sides by $Z_{nm}T_{nm}$,

$$\frac{1}{Z_{nm}}\frac{\partial^2 Z_{nm}}{\partial x^2} + \frac{1}{Z_{nm}}\frac{\partial^2 Z_{nm}}{\partial y^2} = \frac{1}{T_{nm}}\frac{\partial T_{nm}}{\partial t} = -k_{nm}^2, \tag{94}$$

where $k_{mn} > 0$ is a real parameter. This must be the case since the LHS of the equation is only dependent on position coordinates and the RHS is only dependent upon the time t. Fixing, say, t and varying x and y freely or vice versa must imply that both sides are constant for all (x,y,t) in order for the equation to hold. The time-dependent part of the function is the same as in the one-dimensional case:

$$T_{nm} \propto \exp\left(-k_{nm}^2 t\right) \tag{95}$$

We are now left with the equation

$$\frac{\partial^2 Z_{nm}}{\partial x^2} + \frac{\partial^2 Z_{nm}}{\partial y^2} = -k_{nm}^2 Z_{nm}, \tag{96}$$

for which we again assume a separation of variables

$$Z_{nm}(x,y) = X_n(x)Y_m(y). \tag{97}$$

Inserting this into eq.(96) gives us

$$\frac{\partial^2 X_n}{\partial x^2}Y_m + \frac{\partial^2 Y_m}{\partial y^2}X_n = -k_{nm}^2 X_n Y_m, \tag{98}$$

and dividing both sides with X_nY_m results in

$$\frac{1}{X_n}\frac{\partial^2 X_n}{\partial x^2} + \frac{1}{Y_m}\frac{\partial^2 Y_m}{\partial y^2} = -k_{nm}^2. \tag{99}$$

Same as for the time dependent part of the solution, each of these spatial parts must be equal to a constant, which is to say

$$\frac{1}{X_n}\frac{\partial^2 X_n}{\partial x^2} = -k_n^2, \quad \frac{1}{Y_m}\frac{\partial^2 Y_m}{\partial y^2} = -k_m^2, \quad k_{nm}^2 = k_n^2 + k_m^2. \tag{100}$$

As in the one dimensional case, these equations can be recognised as a harmonic oscillator which have the solutions

$$X_n = A_n\cos(k_n x) + B_n\sin(k_n x), \qquad Y_m = C_m\cos(k_m y) + D_m\sin(k_m y), \tag{101}$$

where, from the boundary conditions, we get that

$$X_n = C_n\sin(n\pi x), \qquad k_n = n\pi, \tag{102}$$

$$Y_m = C_m\sin(m\pi y), \qquad k_m = m\pi. \tag{103}$$

Again we invoke the principle of superposition,

$$v(x,y,t) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} C_{nm}\sin{(n\pi x)}\sin{(m\pi y)}e^{-t[(n\pi)^2+(m\pi)^2]}. \tag{104}$$

The Fourier coefficients, $\{C_{nm}\}_{n,m=1}^{\infty}$, are then determined by

$$C_{nm} = 4\int_0^1\int_0^1 f(x,y)\sin{(n\pi x)}\sin{(m\pi y)}dxdy, \tag{105}$$

from [3]. Solving eq. (105) is trivial since we've chosen the initial condition $f(x,y)$ to coincide with the term $n=m=1$ such that

$$C_{nm} = \begin{cases} 1, & n=m=1 \\ 0, & \text{otherwise} \end{cases} \tag{106}$$

It thus follows that the solution is

$$v(x,y,t) = f(x,y)e^{-2\pi^2 t} = \sin(\pi x)\sin(\pi y)e^{-2\pi^2 t}. \tag{107}$$

[1] Link to our Github repository with code documentation. `https://github.com/reneaas/ComputationalPhysics/tree/master/projects/project5`.

[2] Kaspara Skovli Gåsvær, Maria Linea Horgen, Anders Bråte. An analysis of numerical methods for solving second order linear differential equations. `https://github.com/reneaas/ComputationalPhysics/blob/master/projects/project1/report/PROSJEKT1.pdf`.

[3] Karl Rottmann. *Matematisk formelsamling*, page 175. Universitetsforlaget, 2019.

[4] Aslak Tveito, Ragner Winther. *Introduction to Partial Differential equations: A Computational Approach*, chapter 4.2-4.3. Springer, 2005.