

Project 5 - Partial Differential Equation

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Abstract

1 Introduction

2 Theory

2.1 Equation

In this project we are solving the partial differential equation:

$$\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{\partial u(x, t)}{\partial t}, t > 0, x \in [0, 1] \quad (1)$$

We have the initial condition:

$$u(x, 0) = 0 \quad (2)$$

And boundary conditions when $t > 0$:

$$u(0, t) = 0, u(L, t) = 1 \quad (3)$$

Here $L = 1$.

The steady state solution can be found easily by solving the laplace equation which is the harmonic solution. So we have to write our problem on a form that is easier to solve. We introduce:

$$w(x, t) = u(x, t) - v(x) \quad (4)$$

Where $v(x)$ is the steady state solution.

This gives us:

$$w(0, t) = 0 - 0 = 0 \quad (5)$$

$$w(L, t) = u(L, t) - v(L) = 1 - 1 = 0 \quad (6)$$

$$w(x, 0) = u(x, 0) - v(x) = 0 - x = -x \quad (7)$$

We can then solve the equation:

$$w_{xx} = w_t \quad (8)$$

This partial differential equation can be seen as the temperature gradient in a rod of length L . It is also dimensionless in our case since there are no constants multiplied to the equation and x goes from zero to one.

To solve this equation we are looking for a solution by separating the variables:

$$w(x, t) = X(x)T(t) \quad (9)$$

If we take the partial derivatives of this expression we get:

$$w_{xx} = X''(x)T(t), \text{ and } w_t = X(x)T'(t) \quad (10)$$

So if we set put this in the equation (8) we get:

$$\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} = \text{constant} = -\lambda \quad (11)$$

We see that this must be equal to a constant and that it therefore is an eigenvalue problem. We put a minus sign in front of the eigenvalue for convention.

This gives us the equations:

$$w(0, t) = X(0)T(t) = 0, w(1, t) = X(1)T(t) = 0 \quad (12)$$

If we let $T(t) = 0$ we get the trivial solution, which we are not interested in. The two-dimensional diffusion equation is given by eq(13).

$$\frac{\partial^2 u(x, y, t)}{\partial x^2} + \frac{\partial^2 u(x, y, t)}{\partial y^2} = \frac{\partial u(x, y, t)}{\partial t} \quad (13)$$

with $t \in [0, \infty)$ and $x, y \in [0, 1]$.

We choose to only look for the steady state solution with the boundary conditions:

$$u(0, 0, t) = X(0)Y(0)T(t) = 0$$

$$u(1, 0, t) = X(1)Y(0)T(t) = 0$$

$$u(0, 1, t) = X(0)Y(1)T(t) = 0$$

$$u(1, 1, t) = X(1)Y(1)T(t) = 0$$

The initial conditions are chosen for simplicity.

2.2 Algorithms

For solving PDE's we have two different kinds of algorithms: explicit and implicit. An example of an explicit algorithm is the Forward Euler. What defines an explicit algorithm is that it takes basis in the forward timestep when differentiating and is therefore straightforward to program. In the implicit scheme, however, we calculate the differential by using the previous timestep and it becomes a series of matrix equations which can be solved using for example Gaussian elimination or LU-decomposition. Examples of implicit schemes are backward Euler and Crank-Nicolson.

2.2.1 Forward Euler

In forward euler we are approximating the time derivative by:

$$u_t \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} = \frac{u(x_i, t_j + \Delta t) - u(x_i, t_j)}{\Delta t} \quad (14)$$

We are also using a centered difference in space with the approximation as you can see in equation (15).

$$u_{xx} \approx \frac{u(x_i + \Delta x, t_j) - 2u(x_i, t_j) + u(x_i - \Delta x, t_j))}{\Delta x^2}. \quad (15)$$

Setting these two equations equal to eachother gives:

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \quad (16)$$

$$\Rightarrow u_{i,j+1} = \alpha u_{i-1,j} + (1 - 2\alpha)u_{i,j} + \alpha u_{i+1,j} \quad (17)$$

And this is the form we choose for solving this. By looking at this equation we also see that stability requires (eq. (18))

$$\alpha = \frac{\Delta t}{\Delta x^2} < 0.5 \quad (18)$$

Else the second term vanishes, and our solution for the new time step is wrong.

We can implement this just by looping over the timesteps, followed by looping over the x values where $x \in [0, 1]$.

2.2.2 Backward Euler

This is an implicit scheme where we approximating the time derivative by:

$$u_t \approx \frac{u(x, t) - u(x, t - \Delta t)}{\Delta t} = \frac{u(x_i, t_j) - u(x_i, t_j - \Delta t)}{\Delta t} \quad (19)$$

By setting $u_t = u_{xx}$ we get the equation:

$$u_{i,j-1} = \alpha u_{i-1,j} + (1 - 2\alpha)u_{i,j} - \alpha u_{j+1,i} \quad (20)$$

We then introduce the matrix:

$$\begin{bmatrix} 1 + 2\alpha & -\alpha & 0 & 0 & \dots & 0 \\ -\alpha & 1 + 2\alpha & -\alpha & 0 & \dots & 0 \\ 0 & -\alpha & 1 + 2\alpha & -\alpha & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & & \vdots \\ 0 & 0 & 0 & \dots & & 1 + 2\alpha \end{bmatrix}$$

We see that we can formulate this as a matrix multiplication problem:

$$\hat{A}V_j = V_{j-i} \quad (21)$$

which means we can rewrite our differential equation problem to:

$$V_j = \hat{A}^{-1}V_{j_1} = \hat{A}^{-1}(\hat{A}^{-1}V_{j_2}) = \dots = \hat{A}^{-j}V_0 \quad (22)$$

To solve this matrix equation we utilize the Gaussian elimination for tridiagonal matrixes which we solved in project 1.

2.2.3 Crank Nicolson

In Cranc-Nicolson we use a time centered scheme where

$$u(x_i, t_{j+1/2}) \approx \quad (23)$$

This gives the equation :

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \frac{1}{2} \left(\frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{(\Delta x)^2} + \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} \right) \quad (24)$$

We can write this as:

$$-\alpha u_{i+1,j+1} + (1+2\alpha)u_{i,j+1} - \alpha u_{i-1,j+1} = \alpha u_{i+1,j} + (1-2\alpha)u_{i,j} + \alpha u_{i-1,j} \quad (25)$$

Giving the matrix equation:

$$\hat{A}V_{j+1} = \hat{B}V_j \quad (26)$$

or

$$\hat{A}V_{j+1} = b_j \quad (27)$$

where we find V_{j+1} by using a forward euler and solving the matrix equation as in backward euler by using Gaussian elimination.

2.3 Jacobi

For an explicit solution to the 2-dimensional problem, $U_{x,t}$ and $U_{y,t}$ are given by eq(17). Combining these results in the explicit Jakobi-algorithm (28).

$$u(i, j, t+dt) = u(i, j, t) + \alpha * (u(i+1, j, t) + u(i-1, j, t) - 4 * (i, j, t) + u(i, j+1, t) + u(i, j-1, t)) \quad (28)$$

3 Execution

3.0.1 Forward Euler

For the forward Euler algorithm we start by solving $U(x,0)$, hereby referenced as U_0 , and define α as given by eq(17) with $dx=0.1$ and $dt=dx*dx*0.25$, as dictated by the restrictions for the stability for the explicit scheme (eq(18)). We then call the forward step method (see below) for a given number of timesteps, each run increasing the total time T by dt .

```
vec forward_step(double n, double alpha, vec u, vec unew) {
    for (int i=1; i<n; i++) {
        unew(i) = alpha*u(i-1) + (1-2*alpha) * u(i) + alpha*u(i+1);
    }
    return unew;
}
```

3.0.2 Backward Euler

In the implicit Backward Euler scheme we use Gaussian elimination to advance in space and time, implemented in code below. Here, as eq (20) shows, b -value is defined as $1+2\alpha$, and $a=c=-\alpha$, v being the solution given at a previous timestep, with the same initial condition as for the forward Euler scheme. We run the Gaussian elimination for each timestep dt until $T(i) = \text{final } T$.

Forward Substitution

```
double m;
for (int k=2; k<=n; k++) {
    m = a/b(k-1);
    b(k) = b_value - m*c;
    v(k) -= m*v(k-1);
}
```

Backward Substitution

```
u(n)= v(n)/b(n);
for (int k= n-1; k>0; k--) {
    u(k) = (1.0/b(k))*(v(k) - c*u(k+1));
}

u(0) = 0;
u(n) = 0;
```

3.0.3 Crank-Nicolson

Crank-Nicolson, being a combination of the explicit and implicit schemes, first runs forward step and then uses this updated solution v in the gaussian elimination for each timestep $T(i)$.

```
void crank_Nicolson(int n, int t_steps, double alpha, double dx, double dt) {
    char* method = "crank_nicolson";
    initializePrint(method, n, dx, dt, t_steps);
    double a_value, c_value, b_value;
    vec b(n+1);
    a_value = c_value = -alpha;
    b_value = 1 + 2*alpha;

    vec u(n+1);
    vec v(n+1);

    //making the vectors
    for (int k=1; k<n; k++){
        b(k) = b_value;
        u(k) = func(dx,k);
    }

    b(0) = b(n) = b_value;
    u(0) = 0.0;
```

```

u(n) = 1.0;

//GaussElim(a_value,b, b_value,c_value,u,n,v);
for (int t=1;t<=t_steps;t++) {
    v = forward_step(n,alpha,u,v);
    v(0) = 0.0;
    v(n) = 1.0;
    u = GaussElim(a_value,b, b_value,c_value,n,u,v);
    if (t%10==0 || t==1) {
        double time = t*dt;
        printtofile(time,v,n);
    }
}
}

```

3.1 Jacobi

Implementing the jacobi-algorithm is quite straight forward using eq.(28). $U(x,y,0)=A_{old}$ = solution for $t=0$ found by separation of variables.

```

void jakobi_solver (double dx, double dt) {
    double n = 1.0/dx;
    double t_steps = 1000;
    mat A_old = zeros<mat>(n+1,n+1);
    for (int i=1;i<n;i++) {
        for (int j=1;j<n;j++) {
            A_old(i,j) = func(dx,i,j);
        }
    }

    double alpha = dt/(dx*dx);
    mat A_new = zeros<mat>(n+1,n+1);
    for (int t=1;t<=t_steps;t++) {
        for (int i=1;i<n;i++) {
            for (int j=1;j<n;j++) {
                A_new(i,j) = A_old(i,j) + alpha*(A_old(i+1,j)
                    + A_old(i-1,j) - 4*A_old(i,j) + A_old(i,j+1) + A_old(i,j-1));
            }
        }
        A_old = A_new;
    }
}

```

4 Results

4.1 Closed form solutions

4.1.1 Solution to the 1D heat equation

To solve the equation (1) we need to look for seperable solutions on the form:

$$w(x, t) = X(x)T(t) \quad (29)$$

If we set this in in the equation (1) we get:

$$\frac{\partial}{\partial t}(X(x)T(t)) = \frac{\partial^2}{\partial x^2}(X(x)T(t)) \quad (30)$$

To simplify the notation we write:

$$T'(t)X(x) = T(t)X''(x) \quad (31)$$

Which we can write:

$$\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} \quad (32)$$

We see that each side depends on a different variable R.H.S depends on x and L.H.S depends on t , so therefore this mus be equal to a constant. This is because if we change one and keep the other fixed the value must be the same. This constant we set to $-\lambda$ by convention so the equations to solve becomes:

$$X''(x) + \lambda X(x) = 0 \quad (33)$$

$$T'(t) + \lambda T(t) = 0 \quad (34)$$

With the boundary conditions:

$$w(0, t) = X(0)T(t) = 0 \quad (35)$$

$$w(1, t) = X(1)T(t) = 0 \quad (36)$$

From these boundary conditions we see that $X(0) = X(1) = 0$ because if $T(t) = 0$ we would only get the trivial solutions which we are not interested in.

So we solve the $X(x)$ equation first.

This is an equation which we have solved nmany times before. First we have the case $\lambda < 0$ which gives the solution:

$$X(x) = Ae^{\sqrt{k}x} + Be^{-\sqrt{k}x}, \lambda = -k \quad (37)$$

if we set in the boundary conditions we get that $X(0) = A + B$ and then $X(1) = Ae^{\sqrt{k}} + Be^{-\sqrt{k}} = A(e^{2\sqrt{k}} - 1)$ and since k must be positive this gives that $A = B = 0$ which is the trivial solution which we are not interested in.

When $\lambda = 0$ this gives $A = B = 0$ which are also trivial solutions.

The last possibility is the harmonic equation which is:

$$X(x) = A\cos(\sqrt{\lambda}x) + B\sin(\sqrt{\lambda}x) \quad (38)$$

And with our boundary conditions it gives $X(0) = A = 0$ and $X(1) = B \sin(\sqrt{\lambda}) = 0$. This means that $\sin \lambda = 0$ This gives us the eigenvalue $\lambda = (n\pi)^2$ for any positive integer. This gives the solution:

$$X(x) = b_n \sin(n\pi x) \quad (39)$$

The solution for $T(t)$ is then given by:

$$T'(t) = -n^2 * \pi^2 T(t) \quad (40)$$

Which is well known as

$$T(t) = c_n e^{-(n\pi)^2 t} \quad (41)$$

So the the solution becomes:

$$w(x, t) = \sum_{n=1}^{\infty} B_n * \sin(n * \pi x) e^{-(n^2 \pi^2 t)} \quad (42)$$

With the initial condition

$$w(x, 0) = \sum_{n=1}^{\infty} B_n * \sin(n * \pi x) \quad (43)$$

multiply with $\sin(m\pi x)$ on both sides and use the orthogonality of $\sin(m\pi x)$ and $\sin(n\pi x)$

And this gives:

$$\sum_{n=1}^{\infty} b_n \int_0^1 \sin(n\pi x) \sin(m\pi x) dx = \frac{1}{2} b_n = - \int_0^1 \sin(m\pi x) x dx \quad (44)$$

This gives the integral

$$b_n = -2 \int_0^1 x \sin(m\pi x) \quad (45)$$

solving this by using partial integration and simplifying gives:

$$b_n = (-1)^m \left(-\frac{1}{m\pi} \right), m = 1, 2, \dots \quad (46)$$

So setting this into the whole solution from equation (4) we get:

$$u(x, t) = v(x) + w(x, t) = x + \sum_{n=1}^{\infty} (-1)^n \left(\frac{2}{n\pi} \right) \sin(n\pi * x) e^{-(n\pi)^2 t} \quad (47)$$

4.2 3D- Heat equation

4.2.1 Analytical Solution

The equation (13), as the 2D equation, is solved by assuming separation of solutions:

$$u(x, y, t) = X(x)Y(y)T(t) \quad (48)$$

With the boundary conditions $u(0, y, t) = u(1, y, t) = 0$ and $u(x, 0, t) = u(x, 1, t) = 0$ Using this, the equation takes the form:

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} = \frac{T'(t)}{T(t)} \quad (49)$$

By the same logic as in the 2D-case this becomes:

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} = -\lambda \quad (50)$$

If we first keep y constant and varies x we get the equation:

$$X''(x) + (\lambda + \frac{Y''(y)}{Y(y)})X(x) = 0 \rightarrow X''(x) + (\lambda + \mu)X(x) = 0 \quad (51)$$

As in the 2D-case when we get the equations:

$$Y''(y) + (\lambda + \mu)Y(y) = 0 \quad (52)$$

in both dimensions, giving

$$X(x) = b_n \sin(n\pi x) \quad (53)$$

$$Y(y) = c_m \sin(m\pi y) \quad (54)$$

And the time equation then becomes:

$$T(t) = d_{n,m} e^{-(m^2\pi^2 + n^2\pi^2)t} \quad (55)$$

So the equation becomes with $m = n = 1$ and $b_n c_n d_{n,m} = 1$

$$u(x, y, t) = \sin(\pi x) \sin(\pi y) e^{-2\pi^2 t} \quad (56)$$

4.2.2 Error Analysis

To calculate the error we use taylor expansion which are defined:

$$u_n = \frac{f^{(n)}(b)}{n!} \quad (57)$$

So to calculate the error in the forward difference for $u'(t)$ we make a Taylor expansion around t_n :

$$u(t_{n+1}) = u(t_n) + u'(t_n)\Delta t + \frac{1}{2}u''(t_n)\Delta t^2 + \mathcal{O}(\Delta t^3) \quad (58)$$

This gives the error:

$$R = \frac{1}{2}u''(t_n)\Delta t + \mathcal{O}\Delta t^2 \quad (59)$$

This means that the forward euler has an error in time in the first order. For backwards euler we taylor expand $u(t_{n-1})$ and get:

$$R = \frac{1}{2}u''(t_n)\Delta t + \mathcal{O}\Delta t^2 \quad (60)$$

So the same as in the Forward Euler scheme

In Crank-Nicolson we use a time centered scheme so we have to taylor expand $u_{n+1/2}$ and $u_{n-1/2}$ and combine these.

$$u(t_{n+1/2}) = u(t_n) + \frac{1}{2}u'(t_n)\Delta t + \frac{1}{4}u''(t_n)\Delta t^2 + \frac{1}{12}u'''(t_n)\Delta t^3 + \frac{1}{48}u^{(4)}(t_n)\Delta t^4 + \frac{1}{240}u^{(5)}(t_n)\Delta t^5 + \mathcal{O}(\Delta t^6) \quad (61)$$

and

$$u(t_{n-1/2}) = u(t_n) - \frac{1}{2}u'(t_n)\Delta t + \frac{1}{4}u''(t_n)\Delta t^2 - \frac{1}{12}u'''(t_n)\Delta t^3 + \frac{1}{48}u^{(4)}(t_n)\Delta t^4 - \frac{1}{240}u^{(5)}(t_n)\Delta t^5 + \mathcal{O}(\Delta t^6) \quad (62)$$

If we subtract the last from the first we get the error:

$$R = \frac{1}{24}u'''(t_{n+1/2})\Delta t^2 + \mathcal{O}(\Delta t^4) \quad (63)$$

But to get the full error we have to take in consideration the standard arithmetic mean wich is:

$$\frac{1}{2}(u(t_{n+1/2}) + u(t_{n-1/2})) \quad (64)$$

This has the error term:

$$R = \frac{1}{8}u''(t_{n+1/2})\Delta + \frac{1}{384}u''''(t_n)\Delta t^4 + \mathcal{O}(\Delta t^6) \quad (65)$$

If we add these two we get the total error in time as:

$$R = (\frac{1}{24}u'''(t_{n+1/2}) + \frac{1}{8}u''(t_n))\Delta t^2 + \mathcal{O}\Delta t^4 \quad (66)$$

So the error in the Crank-Nicolson scheme is Δt^2

And the error in spatial differential for all three is equal to by usin taylor expansion:

$$R_x = \frac{1}{12}u''''(x_n)\Delta x^2 + \mathcal{O}(\Delta x^4) \quad (67)$$

So the error in x is of the second order.

In figure (1) and (2) we see the numerical calculations against the analytical for two times $t_1 = 0.025$ and $t_2 = 0.65$. And in table (??) we see the realtive error at the different time points. Where the relative error is calculated with the max value and $\epsilon = |1 - u_{num}/u_{analytical}|$.

4.3 2D PDE

Explicit numeric solutions for different values of dx and dt are figured in plots ((3), (5), (5), (6), (7), (8), (9), (10), (11), (12), (13), (14)).

5 Discussion

5.1 2D

We see in figure (1) that all the solutions are very correct which is not strange considering it has only calculated approximately 10 timesteps. But in figure (2)

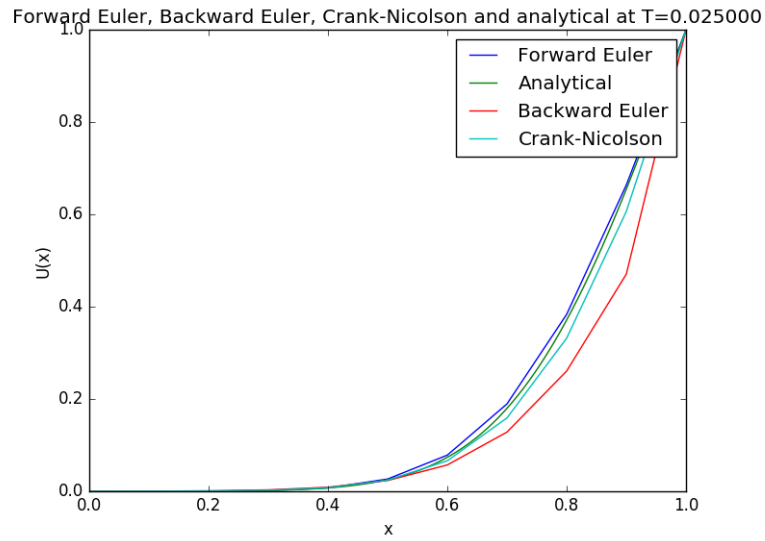


Figure 1: The three schemes with the analytical solution for when $T = 0.025$ and $dt = 0.0025$

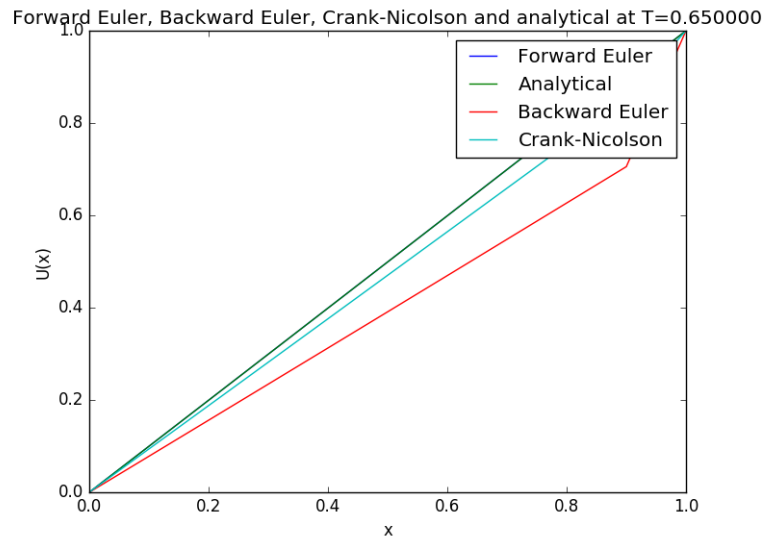


Figure 2: The three schemes with the analytical solution for when $T = 0.025$ and $dt = 0.65$

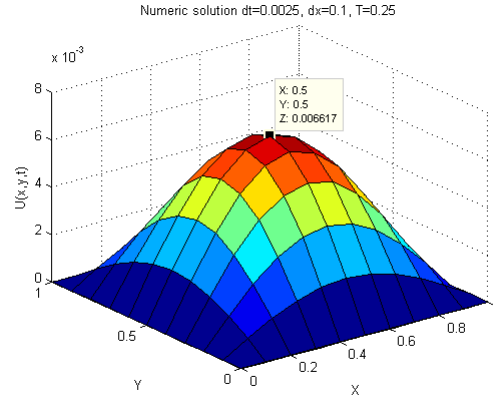


Figure 3: Explicit solution for $dx=0.1$, $\alpha = 0.25$, $T=0.25$

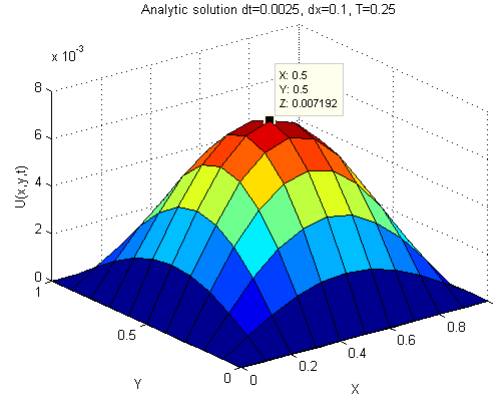


Figure 4: Analytical solution for $dx=0.1$, $\alpha = 0.25$, $T=0.25$

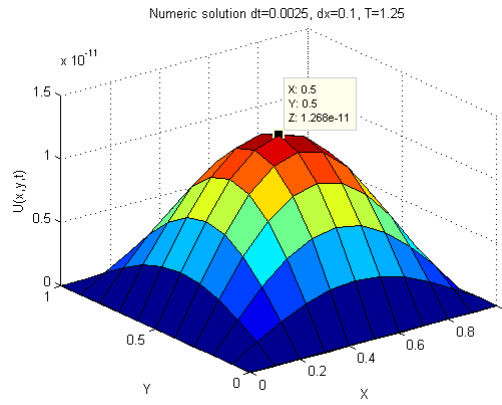


Figure 5: Explicit solution for $dx=0.1$, $\alpha = 0.25$, $T=1.25$

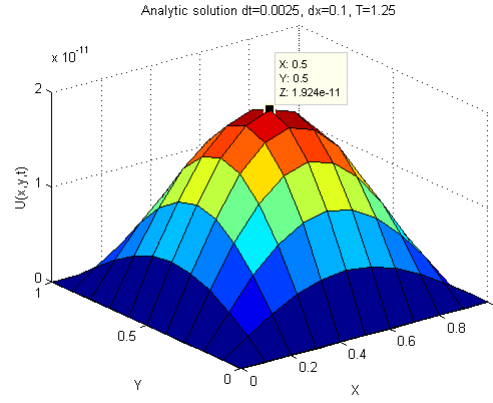


Figure 6: Analytical solution for $dx=0.1$, $\alpha = 0.25$, $T=1.25$

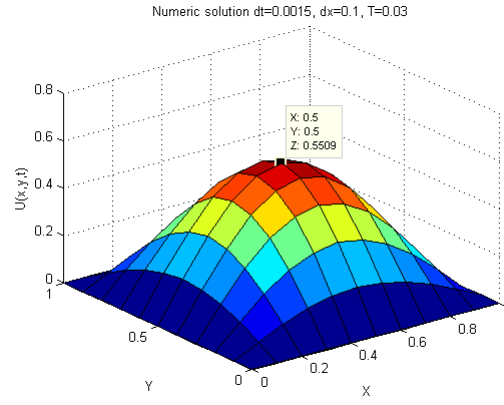


Figure 7: Explicit solution for $dx=0.1$, $\alpha = 0.15$, $T=0.03$

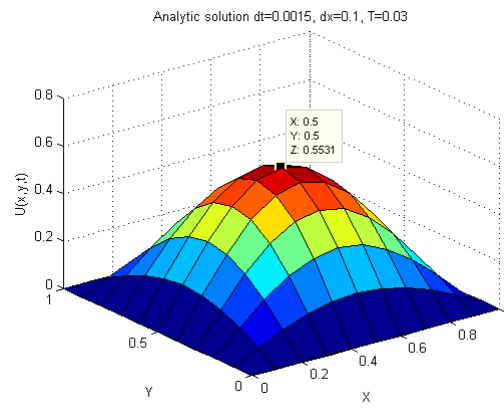


Figure 8: Analytical solution for $dx=0.1$, $\alpha = 0.15$, $T=0.03$

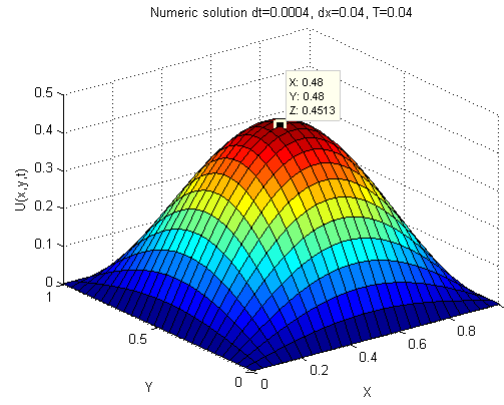


Figure 9: Explicit solution for $dx=0.04$, $\alpha = 0.25$, $T=0.04$

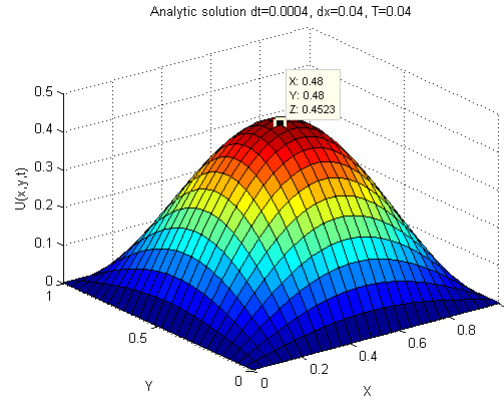


Figure 10: Analytic solution for $dx=0.04$, $\alpha = 0.25$, $T=0.04$

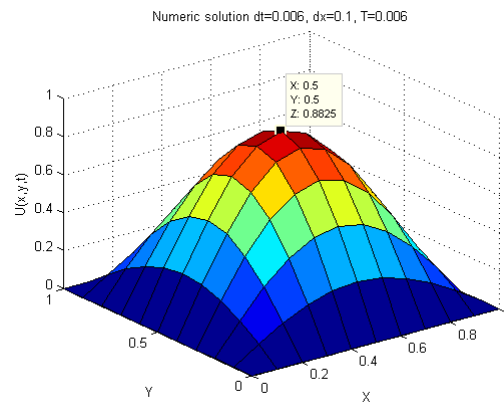


Figure 11: Explicit solution for $dx=0.1$, $\alpha = 0.6$, $T=0.006$

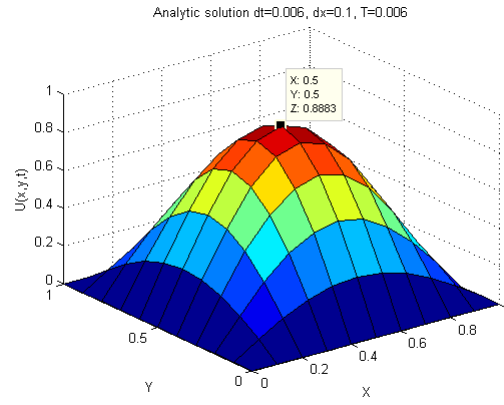


Figure 12: Analytical solution for $dx=0.1$, $\alpha = 0.6$, $T=0.006$

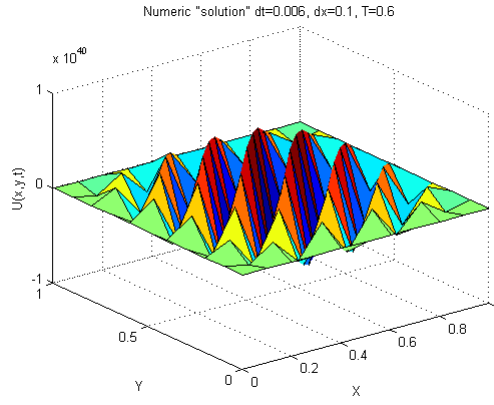


Figure 13: Explicit solution for $dx=0.1$, $\alpha = 0.6$, $T=0.6$

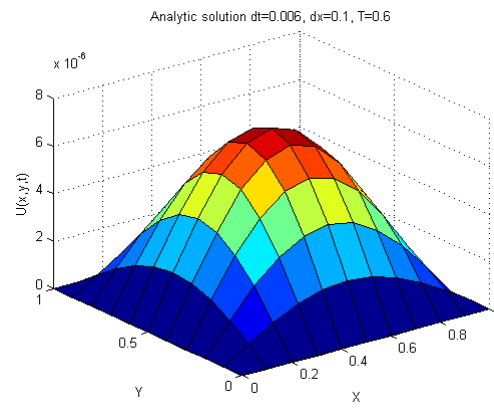


Figure 14: Analytical solution for $dx=0.1$, $\alpha = 0.25$, $T=0.6$

we see that the one that most closely resembles the analytical solution is Forward Euler, followed by Crank Nicolson and lastly Backward Euler. For these plots we have used as stated before the timestep: $\Delta t = 0.0025$. So the truncation error in Forward and Backward Euler is both $\epsilon = 0.0025$ and in Crank Nicolson it is $\epsilon = 6.25 * 10^{-6}$. Since the truncation error is the error committed by one step of the method, and it assumes the earlier step is the exact solution it will be an accumulated error. But in our plot (figure (2)) we see that the Forward Euler method is incredible correct. This is because the initial values are tailored for the forward Euler method. But if we had chosen other timesteps then the forward Euler method would have failed miserably, while the two other methods will be stable for all chosen timesteps and position steps.

Number of FLOPS in the forward Euler scheme is $\propto n$ for every timestep, and in backward Euler which uses gaussian elimination on a tridiagonal matrix also have number of FLOPS $\propto n$. Crank-Nicolson scheme is a combination of these two so number of FLOPS will be $\propto 2n$. These round off errors are for every timestep, so the errors will accumulate with time but as we see all the round off errors are proportional with n for every timestep so the error coming from the round off will be approximately the same for the three methods.

5.2 3D

We see from the 3D-plots that the explicit method gives results very close to the analytical solution for closely defined α 's. Because of the stability limitations care must be taken when choosing optimal resolution in the plots. A reduction in dx in order to increase accuracy means a dx^2 increase in the number of timesteps needed to analyse the time evolution of the solution up to a point T , meaning we are using a lot more computer power.

Figure (13) shows the results of not obeying the stability requirements of the explicit scheme after only 100 timesteps.

6 Conclusion

7 Codes

8 Sources

The sources we have used is: Computational Physics, Lecture notes Fall 2015 (Morten Hjort-Jensen)

Knut Mørken: Numerical Algorithms and Digital Representation, Compendium 2012 (Knut Mørken)

http://hplgit.github.io/num-methods-for-PDEs/doc/pub/trunc/sphinx/./_main_trunc001.html#example-the-backward-difference-for

(Hans Petter Langtangen)