

Project 5, FYS4150

Candidate 55

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1 About the problem

1.1 Notation

For finite differences I will use the the notation

$$u(t_n, x_i, y_j) = u_{i,j}^n$$

where $t_n = t_0 + n \cdot \Delta t$, $x_i = x_0 + i \cdot \Delta x$ and $y_j = y_0 + j \cdot \Delta y$. Thus it is important not to confuse u^n (u to the power of n) with $u_{i,j}^n$ (u evaluated at timestep n and position i,j).

2 The algorithm

We will solve the 1+1 dimensional diffusion equation by three different finite difference schemes in this project. Using the standard approximation of the second derivative in space, we use successively more elaborate approximations to the time derivative.

2.1 Forward Euler

Starting off with the Forward Euler (FE) approximation we get the following scheme

$$\begin{aligned} \frac{u_i^{n+1} - u_i^n}{\Delta t} &= \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \\ u_i^{n+1} &= \frac{\Delta t}{\Delta x^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n) + u_i^n \end{aligned} \quad (1)$$

So to solve the equation all we have to do is loop over the two variables and we are done.

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for n = 0,1, ... , N
  for i = 0,1, ... , N_x
    u_new[i] = dt dx2 *(u_prev[i+1]-2*u_prev[i] + u_prev[i-1]) + u_prev[i];
  u_prev = u_new;
end;

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2.2 Backward Euler

The Backward Euler (BE) approximation gives us a slightly more elaborate scheme seeing at it is an implicit one. The discretization gives

$$\begin{aligned}\frac{u_i^n - u_i^{n-1}}{\Delta t} &= \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \\ u_i^n - \frac{\Delta t}{\Delta x^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n) &= u_i^{n-1} \\ u_i^n \left(1 + 2\frac{\Delta t}{\Delta x^2}\right) - u_{i-1}^n \frac{\Delta t}{\Delta x^2} - u_{i+1}^n \frac{\Delta t}{\Delta x^2} &= u_i^{n-1}\end{aligned}$$

If we insert for a few steps we see that this takes the form of

$$\begin{pmatrix} \left(1 + 2\frac{\Delta t}{\Delta x^2}\right) & -\frac{\Delta t}{\Delta x^2} & 0 & \dots & 0 & 0 \\ -\frac{\Delta t}{\Delta x^2} & \left(1 + 2\frac{\Delta t}{\Delta x^2}\right) & -\frac{\Delta t}{\Delta x^2} & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & \dots \\ 0 & \dots & 0 & -\frac{\Delta t}{\Delta x^2} & \left(1 + 2\frac{\Delta t}{\Delta x^2}\right) & -\frac{\Delta t}{\Delta x^2} \\ 0 & \dots & 0 & -\frac{\Delta t}{\Delta x^2} & \left(1 + 2\frac{\Delta t}{\Delta x^2}\right) & -\frac{\Delta t}{\Delta x^2} \end{pmatrix} \mathbf{u}^n = \mathbf{u}^{n-1} \quad (2)$$

$$\mathbf{A} \mathbf{u}^n = \mathbf{u}^{n-1}$$

So for each timestep we need to multiply the inverse of \mathbf{A} with a vector \mathbf{u}^{n-1} containing the solution at the previous timestep. Looking a bit closer at equation (2) we realize two things. First of all, the matrix \mathbf{A} doesn't change at all throughout the computation so we can get away with invertig it once. Second, and perhaps more important, we already have a very efficient solver for this kind of problem from project 1.

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2.3 Crank Nicolson

Finally, we can use the Crank Nicolson approximation of the time derivative which is a special case of the so called theta -rule with $\theta = 0.5$.

$$\begin{aligned}\frac{u_i^n - u_i^{n-1}}{\Delta t} &= \frac{1}{2\Delta x^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n) + \frac{1}{2\Delta x^2} (u_{i+1}^{n-1} - 2u_i^{n-1} + u_{i-1}^{n-1}) \\ u_i^n - \frac{\Delta t}{2\Delta x^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n) &= u_i^{n-1} + \frac{\Delta t}{2\Delta x^2} (u_{i+1}^{n-1} - 2u_i^{n-1} + u_{i-1}^{n-1}) \\ u_i^n (2 + 2C) - Cu_{i+1}^n - Cu_{i-1}^n &= u_i^{n-1} (2 - 2C) + Cu_{i+1}^{n-1} + Cu_{i-1}^{n-1}\end{aligned}$$

where $C = \frac{\Delta t}{\Delta x^2}$. This can also be expressed as a linear algebra problem

$$(2\mathbf{I} + C\mathbf{B})\mathbf{u}^n = (2\mathbf{I} - C\mathbf{B})\mathbf{u}^{n-1} \quad (3)$$

Again we observe that we will need to invert a matrix, but this time we will also need to do a matrix-vector multiplication.

$$\begin{aligned}(2\mathbf{I} + C\mathbf{B})\mathbf{u}^n &= (2\mathbf{I} - C\mathbf{B})\mathbf{u}^{n-1} = \tilde{\mathbf{u}}^{n-1} \\ \mathbf{u}^n &= (2\mathbf{I} + C\mathbf{B})^{-1} \tilde{\mathbf{u}}^{n-1}\end{aligned}$$

This is the same problem as we had in the BE case, only with a modified right-hand side

2.4 2+1 dimensional diffusion equation

For simplicity we will only use explicit schemes for the 2+1 dimensional case. That is we will discretize using the FE and a centered difference approximation. These are both very straightforward to discretize and implement

$$\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} = \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} + \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2}$$

This leads us to the same scheme as in 1 only with one more dimension.

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

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n-1}}{2\Delta t} = \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} + \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2}$$

3 Analytic solution

As a comparison we can find the analytic solution to this problem as follows.

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}, \quad u(x, 0) = u(d, t) = 0 \quad (4)$$

$$x \in [0, d], \quad D = d = u(0, t) = 1 \quad (5)$$

We see right away that the boundary $x = 0$ could give us some problems, so we start off with a small trick

$$u(x, t) = v(x, t) = u(x, t) - u_s(x)$$

where the $u_s = 1 - x$ term is the steady-state solution to equation 4. This trick leaves us with new boundary conditions on $u(x, t)$

$$v(0, t) = u(0, t) - u_s(0, t) = 1, \quad u_s(0, t) = 1 \implies u(0, t) = 0$$

which makes the whole procedure much simpler. We now assume that $u(x, t)$ can be separated into factors

$$u(x, t) = F(x)G(t) \implies \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \rightarrow F(x) \frac{\partial G}{\partial t} = G(t) \frac{\partial^2 F}{\partial x^2}$$

$$\frac{1}{G(t)} \frac{\partial G}{\partial t} = -k^2 = \frac{1}{F(x)} \frac{\partial^2 F}{\partial x^2}$$

We start with the simplest of the equations which is the time dependence

$$\frac{1}{G(t)} \frac{\partial G}{\partial t} = -k^2$$

$$G(t) = Ce^{-k^2 t}$$

and leave it like this for now. The x-dependent equation is somewhat more complicated

$$\frac{1}{F(x)} \frac{\partial^2 F}{\partial x^2} = -k^2$$

$$F(x) = A \sin(kx) + B \cos(kx)$$

$$F(0) = A \sin(0) + B \cos(0) = 0 \implies B = 0$$

$$F(d) = A \sin(kd) = 0 \implies k = \frac{m\pi}{d} = \pi m, \quad A = A_m$$

we now combine all the equations to determine $v(x, t)$

$$v(x, t) = 1 - x + \sum_{m=1}^{\infty} B_m e^{-(m\pi)^2 t} \sin(m\pi x)$$

$$v(x, 0) = 1 - x + \sum_{m=1}^{\infty} B_m \sin(m\pi x)$$

$$\implies \int_0^1 \sin(m\pi x) \sin(n\pi x) dx = \delta_{mn} = \int_0^1 (x - 1) \sin(m\pi x) dx = -\frac{2}{m\pi} = B_m$$

This gives us the full analytical solution

$$v(x, t) = 1 - x - \frac{2}{\pi} \sum_{m=1}^{\infty} \frac{1}{m} e^{-(m\pi)^2 t} \sin(m\pi x) \quad (6)$$

which satisfies all initial and boundary conditions.

4 Results

5 Stability and precision

To get a feeling of how good the numerical schemes are we will analyze their errors and stability criterions individually.

5.1 Forward Euler

Let us first look at the truncation error of this scheme. If we do a Taylor expansion of $u(x + \Delta x, t)$, $u(x - \Delta x, t)$ and $u(x, t + \Delta t)$, assuming $\Delta x, \Delta t \rightarrow 0$ we get the following

$$\begin{aligned} u(x + \Delta x, t) &= u(x, t) + \frac{\partial u(x, t)}{\partial x} \Delta x + \frac{\partial^2 u(x, t)}{2\partial x^2} \Delta x^2 + \mathcal{O}(\Delta x^3) \\ u(x - \Delta x, t) &= u(x, t) - \frac{\partial u(x, t)}{\partial x} \Delta x + \frac{\partial^2 u(x, t)}{2\partial x^2} \Delta x^2 + \mathcal{O}(\Delta x^3) \\ u(x, t + \Delta t) &= u(x, t) + \frac{\partial u(x, t)}{\partial t} \Delta t + \mathcal{O}(\Delta t^2) \end{aligned}$$

These are the local errors, meaning that our complete scheme gives the error of

$$\begin{aligned} \frac{u^{n+1} - u^n}{\Delta t} &\approx \frac{\partial u(x, t)}{\partial t} + \mathcal{O}(\Delta t) \\ \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} &\approx \frac{\partial^2 u(x, t)}{\partial x^2} + \mathcal{O}(\Delta x^2) \end{aligned}$$

Let us also look at the stability of the scheme, but by in slightly different way than what has been done in the rest of the course. Let us assume that the solution of the diffusion equation takes the form

$$u(x, t) = A^n e^{ikq\Delta x} \quad (7)$$

Where A^n is a damping factor which is time dependent. If we insert this expression 7 into the scheme 1 we get

$$\begin{aligned} A^n e^{ikq\Delta x} (A - 1) &= C A^n e^{ikq\Delta x} (e^{i(q+1)k\Delta x} - 2e^{iqk\Delta x} + e^{i(q-1)k\Delta x}) \\ A - 1 &= C (e^{ik\Delta x} - 2 + e^{-ik\Delta x}) \\ A &= 1 - 4C (\cos(k\Delta x) - 1) = 1 - 4C \sin^2(k\Delta x/2) \end{aligned}$$

Note that x_i has been replaced by x_q . This means that the final solution is on the form

$$u_q^n = (1 - 4C \sin^2(k\Delta x/2))^n e^{ikq\Delta x}$$

It is obvious that we need $-1 \leq A \leq 1$ to avoid divergence. $A \leq 1 \implies C \geq 0$ is not of too much interest, however if we insert for

$$\begin{aligned} -1 \leq A &\implies 1 - 4C \sin^2(k\Delta x/2) \geq -1 \\ C &\leq \frac{1}{2 \sin^2(k\Delta x/2)} \end{aligned}$$

and $\max(\sin^2(k\Delta x/2)) = 1$ we are left with

$$C = \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2} \quad (8)$$

5.2 Backward Euler

The truncation error of the BE scheme is very similar to the FE case. In fact it is obvious that the spacial part is identical, so we only need to redo the time dependence.

$$u(x, t - \Delta t) = u(x, t) - \frac{\partial u(x, t)}{\partial t} \Delta t + \mathcal{O}(\Delta t^2)$$

And so the complete scheme gives an error of

$$\begin{aligned} \frac{u^n - u^{n-1}}{\Delta t} &\approx \frac{\partial u(x, t)}{\partial t} + \mathcal{O}(\Delta t) \\ \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} &\approx \frac{\partial^2 u(x, t)}{\partial x^2} + \mathcal{O}(\Delta x^2) \end{aligned}$$

We can investigate the stability of the BE scheme in the same way as we did for the FE scheme. Assume again that we have a general solution on the form 7. Insert it in 2 as follows

$$\begin{aligned} A^n e^{ikq\Delta x} (1 - A^{-1}) &= C A^n \left(e^{ik(q+1)\Delta x} - 2e^{ikq\Delta x} + e^{ik(q-1)\Delta x} \right) \\ A^{-1} &= 1 - 4C \sin^2(k\Delta x/2) \\ A &= \frac{1}{1 - 4C \sin^2(k\Delta x/2)} \end{aligned}$$

giving us the general term

$$u_q^n = \left(\frac{1}{1 - 4C \sin^2(k\Delta x/2)} \right)^n e^{ikq\Delta x}$$

but now we have that $0 \leq A \leq 1$.

$$\begin{aligned} \frac{1}{1 - 4C \sin^2(k\Delta x/2)} &\leq 1 \\ 1 \leq 1 - 4C \sin^2(k\Delta x/2) &\implies C \geq 0 \end{aligned}$$

The other limitation ($A \geq 0$) gives us nothing and thus the scheme is stable for all values of Δt and Δx .

5.3 Crank Nicolson

The truncation error of the CN scheme is slightly more intricate to calculate because we need to Taylor expand around $t' = t + \Delta t/2$

$$\begin{aligned} u(x + \Delta x, t + \Delta t) &= u(x, t') + \frac{\partial u(x, t')}{\partial x} \Delta x + \frac{\partial u(x, t')}{\partial x} \Delta t/2 + \frac{\partial^2 u(x, t')}{2\partial x^2} \Delta x^2 + \frac{\partial^2 u(x, t')}{2\partial t^2} \Delta t^2/4 \\ &\quad + \frac{\partial^2 u(x, t')}{\partial x \partial t} \Delta x \Delta t/2 + \mathcal{O}(\Delta x^3) \\ u(x - \Delta x, t + \Delta t) &= u(x, t') - \frac{\partial u(x, t')}{\partial x} \Delta x + \frac{\partial u(x, t')}{\partial x} \Delta t/2 + \frac{\partial^2 u(x, t')}{2\partial x^2} \Delta x^2 + \frac{\partial^2 u(x, t')}{2\partial t^2} \Delta t^2/4 \\ &\quad - \frac{\partial^2 u(x, t')}{\partial x \partial t} \Delta x \Delta t/2 + \mathcal{O}(\Delta x^3) \\ u(x + \Delta x, t) &= u(x, t') + \frac{\partial u(x, t')}{\partial x} \Delta x - \frac{\partial u(x, t')}{\partial x} \Delta t/2 + \frac{\partial^2 u(x, t')}{2\partial x^2} \Delta x^2 + \frac{\partial^2 u(x, t')}{2\partial t^2} \Delta t^2/4 \\ &\quad - \frac{\partial^2 u(x, t')}{\partial x \partial t} \Delta x \Delta t/2 + \mathcal{O}(\Delta x^3) \\ u(x - \Delta x, t) &= u(x, t') - \frac{\partial u(x, t')}{\partial x} \Delta x - \frac{\partial u(x, t')}{\partial x} \Delta t/2 + \frac{\partial^2 u(x, t')}{2\partial x^2} \Delta x^2 + \frac{\partial^2 u(x, t')}{2\partial t^2} \Delta t^2/4 \\ &\quad + \frac{\partial^2 u(x, t')}{\partial x \partial t} \Delta x \Delta t/2 + \mathcal{O}(\Delta x^3) \\ u(x, t + \Delta t) &= u(x, t') + \frac{\partial u(x, t')}{\partial t} \Delta t/2 + \frac{\partial^2 u(x, t')}{2\partial t^2} \Delta t^2/4 + \mathcal{O}(\Delta t^3) \\ u(x, t) &= u(x, t') - \frac{\partial u(x, t')}{\partial t} \Delta t/2 + \frac{\partial^2 u(x, t')}{2\partial t^2} \Delta t^2/4 + \mathcal{O}(\Delta t^3) \end{aligned}$$

Which means that the error of the whole scheme scales like

$$\begin{aligned} \frac{\partial u(x, t')}{\partial t} &\approx \frac{\partial u(x, t')}{\partial t} + \mathcal{O}(\Delta t^2) \\ \frac{\partial^2 u(x, t')}{\partial x^2} &\approx \frac{\partial^2 u(x, t')}{\partial x^2} + \mathcal{O}(\Delta x^2) \end{aligned}$$

6 Final comments