Exercise 5. Diffusion and Parabolic Equations. Example Solution.

1. Write a computer code to solve the diffusive equation

$$\frac{\partial \psi}{\partial t} = D\frac{\partial^2 \psi}{\partial x^2} + s(x)$$

For constant, uniform diffusivity D and constant specified source $s(x)$. Use a uniform x-mesh with N_x nodes. Consider boundary conditions to be $\psi = \psi_1$ at $x = 0$ and $\frac{\partial \psi}{\partial x} = 0$ at $x = 1$ (the domain boundaries).

Construct a matrix $\mathbf{D} = D_{ij}$ such that $\mathbf{D}.\psi = \nabla^2\psi$. Use it to implement the FTCS scheme

$$\psi^{(n+1)} = (\mathbf{I} + \Delta t\mathbf{D})\psi^{(n)} + \Delta t\, s,$$

paying special attention to the boundary conditions.

Solve the time-dependent problem, for $t = 0 \to 1$, when $D = 1$, $s = 1$, $N_x = 50$, $\psi_1 = 0$, with initial condition $\psi = 0$ at $t = 0$ storing your results in a matrix $\psi(x,t) = \psi_{j_x,j_t}$, and plotting that matrix at the end of the solution, for examination.

Experiment with various Δt to establish the dependence of the accuracy and stability of your solution on Δt. In particular,

(i) find experimentally the value of Δt above which the scheme becomes unstable.

(ii) estimate experimentally the value of Δt at which $\psi(t = 1)$ is accurate to 1%.

Solution

I wrote my code so that N was a parameter, and it could run multiple cases of dt for that parameter. I chose my mesh so that the first point was at $x = 0$, but the final point was beyond $x = 1$ by an amount such that $x_{N-1/2} = 1$. This allows me to define the $d\psi/dx = 0$ boundary condition by just two terms in the difference matrix, `D`. Let me illustrate with $N = 6$.

```
x =
   0.00000
   0.22222
   0.44444
   0.66667
   0.88889
   1.11111

D =
  -2   0   0   0   0   0
   1  -2   1   0   0   0
```

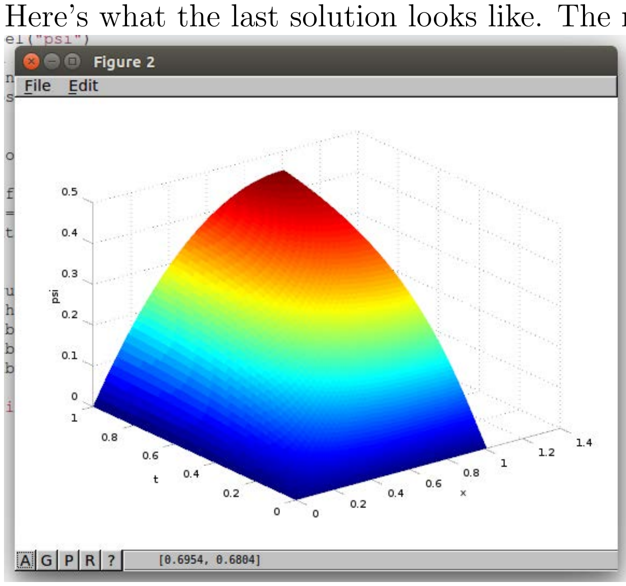
0	1	-2	1	0	0
0	0	1	-2	1	0
0	0	0	1	-2	1
0	0	0	0	2	-2

Then setting $s = 0$ at the first and last positions: 1, and N, implements the boundary conditions.

When the solution is completed, I find the maximum value of psi: maxpsi. That's going to be my measure of accuracy. There are other choices; it's not terribly important what you choose. Since I know theoretically what the stability criterion is, I start by running ten cases up to the theoretical stability limit of `dt=0.0002126`. (Now using $N = 50$: the specified value.)

nsteps	dt	maxpsi
47045	0.0000213	0.453754
23522	0.0000425	0.453756
15681	0.0000638	0.453759
11761	0.0000850	0.453762
9409	0.0001063	0.453765
7840	0.0001276	0.453768
6720	0.0001488	0.453771
5880	0.0001701	0.453774
5227	0.0001913	0.453776
4704	0.0002126	0.453779

Here's what the last solution looks like. The maxpsi is the value at $x = 1$, $t = 1$.

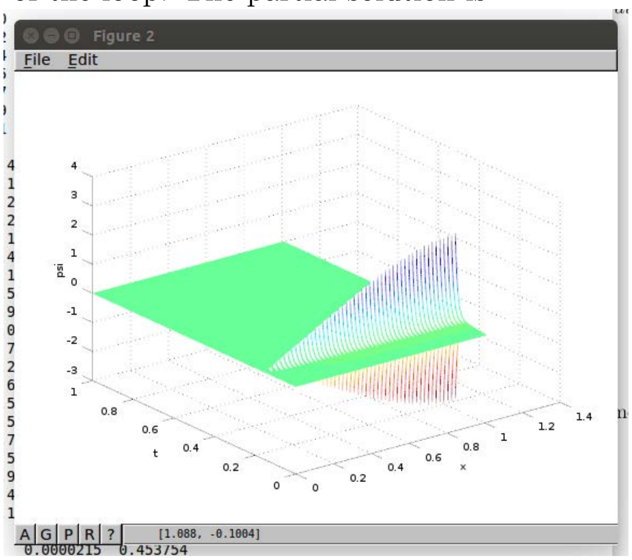


Now I increase the range of the dt to 1.01 times bigger. Here's what I get instead:

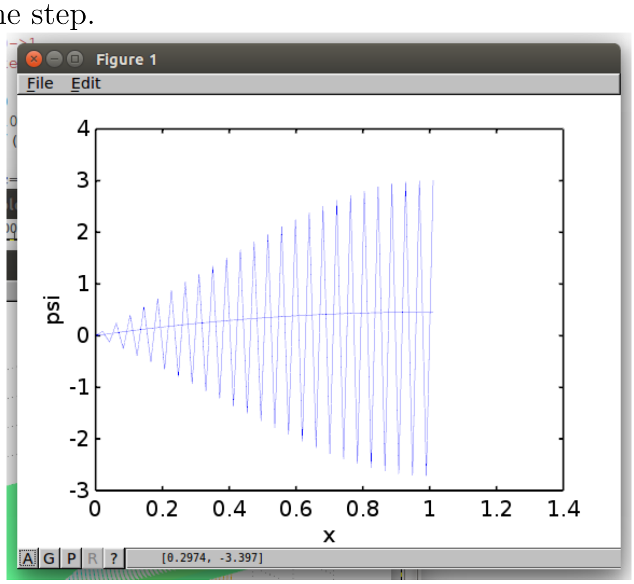
nsteps	dt	maxpsi
46579	0.0000215	0.453754
23289	0.0000429	0.453756
15526	0.0000644	0.453759

11644	0.0000859	0.453762
9315	0.0001074	0.453765
7763	0.0001288	0.453768
6654	0.0001503	0.453771
5822	0.0001718	0.453774
5175	0.0001932	0.453777
4657	0.0002147	0.000000

The last case is unstable and the maxpsi is unset because when I detect it is unstable I jump out of the loop. The partial solution is



And here's a comparision of the unstable solution with the prior stable ones at the last time step.



(i) The cases dt = 0.0002126 and 0.0002147 bracket the experimental stability limits, in excellent agreement with theory.

(ii) This part of the question is (accidentally, sorry) a trick. There is no stable dt for which the time accuracy is worse than 1%. Look at my first list of maxpsi. With tiny dt, it gives

0.453754 and twice as large dt changes only the last significant figure. The least accurate stable case is then with dt=0.0002126. It gets 0.453779. That's different from the tiny dt case by only $0.453779 - 0.453754 = 0.000025$ which is a fractional error of only 5.5×10^{-5}, which is far less than 1%. The answer is that effectively any stable dt (≤ 0.0002126) gives a time-step accuracy much better than 1%.

I haven't actually shown that the solution is accurate to this level. It is converged in time-step to this level, but there is presumably also uncertainty arising from finite spatial differences. I can play around with different values of N to discover the degree of spatial convergence. Here are some examples:

```
N     nsteps      dt     maxpsi
10     1430    0.0006993  0.440490
20     6777    0.0001476  0.449460
30    16084    0.0000622  0.451934
40    29351    0.0000341  0.453087
50    47045    0.0000213  0.453754
60    67767    0.0000148  0.454187
70    92915    0.0000108  0.454492
```

where I've shown only the tiny `dt=0.1*dtmax` cases which have the most accurate time-stepping. What we see is that the spatial convergence at $N = 50$ is to approximately 1 part in 454, i.e. roughly 0.2%. That is the rough level of the error.

Please notice, I don't need to know an "exact" solution to make these estimates. I estimate on the basis of seeing the trends in my solutions as I vary the time and space steps. That's the way one usually has to work in practice.

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2. Develop a modified version of your code to implement the θ-implicit scheme:

$$(\mathbf{I} - \Delta t \theta \mathbf{D})\psi^{(n+1)} = (\mathbf{I} + \Delta t(1-\theta)\mathbf{D})\psi^{(n)} + \Delta t\, s,$$

in the form

$$\psi^{(n+1)} = \mathbf{B}^{-1}\mathbf{C}\psi^{(n)} + \mathbf{B}^{-1}\Delta t\ s$$

Experiment with Δt and different θ values, for the same time-dependent problem and find experimentally the value of θ for which instability disappears for all Δt.

Also choose a Δt value for which the FTCS ($\theta = 0$) scheme is stable; then find experimentally the approximate optimum value of θ (at that fixed Δt) which produces the most accurate results.

Solution

Not done in its entirety. But clearly the Δt optimum value isn't going to be very meaningful because we already know we are not dominated by time error but space error. The second part would have made more sense if it had asked for the θ that allows the biggest steps for some specified time accuracy.

22.15 Essential Numerical Methods
Fall 2014