1. In this exercise, you are asked to find “one-sided” finite difference formulas for derivatives. These are useful for approximating derivatives of functions at or near the boundary of their domain. (a) Construct a second order, one-sided finite difference formula that approximates the derivative $f'(x)$ using the values of $f(x)$ at the points $x, x+h$ and $x+2h$. (b) Find a finite difference formula for $f''(x)$ that involves the same values of $f$. What is the order of your formula? (c) Test your formulas by computing approximations to the first and second derivatives of $f(x) = e^{x^2}$ at $x = 1$ using step sizes $h = .1, .01$ and .001. What is the error in your numerical approximations? Are the errors compatible with the theoretical orders of the finite difference formulae? Discuss why or why not. (d) Answer part (c) at the point $x = 0$.

Solution:

(a) $f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} + O(h^2)$.

(b) $f''(x) = \frac{f(x) - 2f(x+h) + f(x+2h)}{h^2} + O(h)$, which is of order 1.

(c) The errors in computing $f'(1) = 5.43656$ are, respectively, $-.245$, $-.00186$, $-.000182$, which is compatible with a second order approximation because each decrease in step size by $\frac{1}{10} = 10^{-1}$ decreases the error by approximately $(\frac{1}{10})^2 = 10^{-2}$. The errors in computing $f''(1) = 16.3097$ are, respectively, $6.89114$, $.555923$, $.0544864$, which is comparable with a first order approximation.

(d) The errors in computing $f'(0) = 0$ are, respectively, $-3.0505 \times 10^{-3}$, $-3.0005 \times 10^{-6}$, $-3.0000 \times 10^{-9}$, which indicates that we have a third order approximation. The errors in computing $f''(0) = 2$ are, respectively, $.0710$, $.000700$, $.0000070$, which indicates a second order approximation. The reason for the observed increase in order is that the leading term in the Taylor error formulas is proportional to $h^3 f'''(x)$ which, at $x = 0$, is zero, and hence the errors have one more order in $h$. 
2. (a) Design an explicit numerical method for solving the initial-boundary value problem

\[ u_t = \gamma u_{xx} + s(x), \quad u(t, 0) = u(t, 1) = 0, \quad u(0, x) = f(x), \quad 0 \leq x \leq 1, \]

for the heat equation with a source term \( s(x) \).  

(b) Test your scheme on the particular problem for \( \gamma = \frac{1}{6} \), 

\[ s(x) = x(1-x)(10-22x), \quad f(x) = \begin{cases} 
2 \left| x - \frac{1}{6} \right| - \frac{1}{3}, & 0 \leq x \leq \frac{1}{3}, \\
0, & \frac{1}{3} \leq x \leq \frac{2}{3}, \\
\frac{1}{2} - 3 \left| x - \frac{5}{6} \right|, & \frac{2}{3} \leq x \leq 1, 
\end{cases} \]

using space step sizes \( h = .1 \) and .05, and a suitably chosen time step \( k \).  

(c) What is the long term behavior of your solution? Can you find a formula for its eventual profile?  

(d) Design an implicit scheme for the same problem. Does the behavior of your numerical solution change? What are the advantages of the implicit scheme?

Solution:

(a) Setting \( u^{(i)} = (u_{i,1}, \ldots, u_{i,n-1})^T \approx (u(t_i, x_1), \ldots, u(t_i, x_{n-1}))^T \) to be the approximation to the solution at the interior nodes at time \( t_i \), we have

\[ u^{(i+1)} = A u^{(i)} + b^{(i)} + k s, \quad u^{(0)} = f, \]

where \( A \) is the tridiagonal matrix and \( b^{(i)} \) is the vector in (11.20), while \( s = (s(x_1), \ldots, s(x_{n-1}))^T \) is the sample vector of the forcing function \( s(x) \) at the interior nodes, while \( f = (f(x_1), \ldots, f(x_{n-1}))^T \) is the sample vector of the initial data.
(b) For $h = .1$, we choose $k = .025$ to satisfy the stability criterion (11.25) with 
$\mu = .4167$. The numerical solution at times $t = 0, .05, .1, .15, .2$ and, much later, at 
$1.5$ is graphed below:

(The poor approximation of the initial data is due to the relatively small number 
of sample points, but does not seriously affect the subsequent numerical solution.

For $h = .05$, we choose $k = .005$, with $\mu = .3333$. The numerical solution at times $t = 0, .05, .1, .15, .2$ and $1.5$ is

which is slightly more accurate.
(c) The solution tends, at an exponential rate, to an equilibrium temperature $u^*(x)$ which is the solution to the equilibrium boundary value problem $u_{xx}^* + s(x) = 0, \quad u^*(0) = u^*(1) = 0$. For the particular forcing function in part (b), $u^*(x) = -\frac{33}{5} x^5 + 16 x^4 - 10 x^3 + \frac{3}{5} x$, which is very close to the final figure in the two sets of graphs.

\[ \hat{A} u^{(i+1)} = u^{(i)} + b^{(i+1)} + k s, \quad u^{(0)} = f, \]

where $\hat{A}, b^{(i+1)}$ are as in (11.28) and $s$ is the same sample vector as in part (a). The numerical solution with $h = .05$, $k = .025$, is plotted below:

The Implicit Method is unconditionally stable, and hence we do not have to worry about the size of $k = \Delta t$. Also, we can use longer time steps to approximate the solution with less work.