MSE 493/593 Homework #3/Lab3
Fall 2011 October 10, 2011
Thornton

MSE 493/593
Computational Approaches in Materials Science and Engineering
Homework #3
Due October 17, 2011

The purpose of this lab and assignment is to learn about the finite difference method and apply it to solve the diffusion equation, an important equation in materials science and engineering. This assignment is ungraded, but must submit to show you have done the work (I will record pass or not pass). The solution will be available on October 12, 2011.

Euler's method is a first order explicit time stepping scheme. It approximates the change rate from the current value, f^n, where *f*(*x*) is the right hand side of the differential equation. The resulting discretized evolution equation is given by

$$y^{n+1} = y^n + f^n \Delta t \ .$$

All notations are consistent with the lecture notes, with *n* denoting the step in time.
We will apply this time stepping scheme to solve the dimensionless diffusion equation, i.e.,

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2},$$

which has an analytic solution,

$$C_{analytic}(x,t) = \sqrt{\frac{t_0}{t}} \exp\left(\frac{-(x-x_0)^2}{4t}\right).$$

We take x_0 to be the center of computational domain. For spatial difference, use the centered differencing scheme,

$$\left.\frac{\partial^2 C}{\partial x^2}\right|^n = \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2}.$$

1. [10 points] Write a simulation program in a language of your choice. Use computational **domain of size of 20** with **201 mesh points** (i.e., $\boldsymbol{\Delta x}$ **= 0.1**). Set the initial condition for *C* to $\boldsymbol{C(x, t_0) = C_{analytic}(x,t_0)}$, with $\boldsymbol{t_0}$ **= 0.1**. Use **periodic boundary conditions**. The simulation should **start with** $\boldsymbol{t_0}$ and **end with** $\boldsymbol{t_f}$ **= 1**. with time step size of $\boldsymbol{\Delta t}$ **=4E-3**. As mentioned earlier, x_0 to be the center of computational domain, i.e,. $\boldsymbol{x_0}$ **= 10**. (Hint: you may find Matlab command "circshift" useful.)

2. [10 points] Verify analytically that this scheme is first-order in time and second-order in space. Here, nth-order means the error is of the order $(\Delta x)^n$. (This is the standard definition when discussing the errors in derivatives.)

3. [10 points] Derive (analytically) the amplification factor, *g*, and the condition for Δt such that $|g| \leq 1$.

4. [10 points, 5 points each] Perform simulation starting $t = t_0$ with two different setups.

(a) With Δt =4E-3, plot the solution at $t = 1$. Overplot with $C_{analytic}(x, t=1)$. Obtain the maximum difference (in magnitude) between the numerical solution and the analytical solution.

(b) With Δt =6E-3, plot the solutions at four different times, after 100, 105, 110, and 115 iterations. Comment on the result based on your finding in #3.

5. [20 points; 5 points each for (a) and (b), 10 points for (c)] Perform a simulation with varying Δx. I suggest using 10 cases, starting with N_x = number of grid points = 201 with 100 incremental steps (i.e., the second case has 301 points, the third case has 401 points, etc. (Keep the size of domain to be 20.) Use $\Delta t = 0.4\ (\Delta x)^2$ for each run. (a) Comment on why I chose this expression for Δt. (b) Obtain the maximum difference between the numerical solution and the analytical solution for each case at t=1, and plot them against Δx. (Hint: you should get an approximately quadratic curve.) (c) Explain the dependence of the maximum error on Δx based on your answer in #2. (Hint: consider the truncation errors at each time step (both in time and space); the stability condition ensures that it does not grow in time.)