

CHE 581

Extra Credit Problem (+5 points)

Due: Friday, 27 Feb 2019

You have already coded up the problem 22.1. I would like you to revisit that problem, and do a proper “convergence” analysis. Basically, this just means examining how the time step size influences the solution. We know that as we cut the time step, the solution should improve. The question we want to answer now is, what time step size would be required for a particular error limit?

For this problem, you happen to have the analytical solution. So, you can compute two types of error as you decrease the mesh size: (1) The true percent relative error (tpre) and the present relative error (pre). Note: The percent relative error can only be computed after you have a first numerical solution. At each time in the domain, t_i , the pre is given by

$$\varepsilon_a(t_i) = \frac{(\text{approximation at } t_i \text{ using } \Delta t_2) - (\text{approximation at } t_i \text{ using } \Delta t_1)}{(\text{approximation at } t_i \text{ using } \Delta t_2)} \times 100$$

I would like you to compute the tpre and the pre for the following partitions of time. Each of these computations results in a decrease in Δt (and, hence, a more accurate solution). The pre will have to be computed for the results between two simulations with decreasing time step (i.e., you can compare the results of grid 2 with those of grid 1).

Grid	n (intervals)	n(points)	Δt
1	40	41	2/40
2	80	81	2/80
3	160	161	2/160
4	320	321	2/320
5	640	641	2/640

Note that, in principle, we can compute our error metrics at each time point for which we have a solution. To make things easier, and concrete, compute the following averages for the error

$$\varepsilon_{ave} = \frac{1}{41} \sum_{i=1}^{l=41} \varepsilon_a(t_i)$$

where the t_i are taken at the 41 points defined for grid 1. Thus, for example, you will use only every other point in grid 2 to compare with all points in grid 1, and every 4th point in grid 3 to compare with every other point in grid 2 (this way, each comparison has exactly 41 comparison points).

Please plot both (1) your predictions of the function for the 5 different grids, and (2) the tpre and pre as a function of Δt (this plot will have only 5 time points on it, and you can compute the pre for only 4 of those).