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MTH 552 Winter 2017

Homework #5

Due Wednesday, March 1, 2017

1. See attached work.
2. a. The attached code has been modified as directed. The results of the evaluation with each of the different solvers can be found below. The code was modified for each of the solvers to use an absolute tolerance of 1x10-7 in order for the ODE45 solvers to be able to produce qualitatively correct plots, and for the stiff solvers (ode23s and ode15s) to produce results that did not have mass fractions (which each of the values c1 – c5 are assumed to represent) with negative values. Any negative values for the mass fractions would not show up in the plot due to the use of the semilogy plotting. Even with this very small absolute tolerance, a significant amount of “noise” showed up in the c3 plot using the ODE45 solvers. The noise could be made negligible by decreasing the tolerance further, but the tolerance of 1x10-7 was considered sufficient for the purposes of this exercise.

The number of time steps required and the number of evaluations of *f* can be found on each plot below. As can be seen, the stiff solvers (ode23s and ode15s) outperformed ODE45 by a substantial margin. This is because the Oregonator equation is known to be a stiff equation that has even been used as a test equation in studies of stiff systems of equations1. ode23s and ode15s use implicit methods to improve their stability and are consequentially much better for solving stiff systems than explicit methods2. ode45 and ode45v4 performed poorly, requiring a very large number of steps because they are explicit methods. The performance of the implicit solvers was similar, however ode15s appeared to have the best performance for the given and assumed criteria. The solvers all took many steps as soon as the integration started, and took very few steps in the latter half of the integration. The two implicit methods appear to have taken many steps in three distinct areas, as seen by the large slopes of the lower right subplot of each figure.

ode45 and ode45v4 behaved slightly differently due to slightly different tolerance parameters being used. ode45v4 used a single tolerance value of 1x10-7, while ode45 had 2 different tolerances that were calculated differently (AbsTol and RelTol). Had these numbers been the same in both cases, the methods would perform identically.

b. The Oregonator represents a model of a chemical reaction and is named as such because it was developed by Richard Field and Richard M. Noyes at the University of Oregon. Its name is a combination of the great state of Oregon and an oscillator3, though the cool sounding name would seem to be a likely motivation.

1. G. Söderlind, L. Jay, and M. Calvo, Stiffness 1952-2012: Sixty years in search of a definition, BIT Numerical Mathematics 55 (2014) 531–558.
2. <https://www.mathworks.com/videos/solving-odes-in-matlab-7-stiffness-ode23s-ode15s-117651.html>
3. <https://en.wikipedia.org/wiki/Oregonator>

