Exercises for Advanced Topics in High Performance Scientific Computing

WS 15/16, Nr.: 0000003213, 02.10.011, Rechnerraum

Exercise Sheet 1 (until October 21, 2015)

Exercise 1*

Write a library in C or C++ for calculating the numerical solution of initial value ordinary differential equations, i.e. ordinary differential equations of the form

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(t, y), \quad y(T_0) = Y_0$$

for a specified function $f(t, y)$, with the initial value Y_0 given at the initial time T_0. We want to calculate a numerical solution in the time interval $T_0 < t < T_1$ where T_1 is the final time. To solve this equation numerically, we require the user to specify an integration step size, which we denote by h.

Develop the library functions for the solution of the initial value ordinary differential equations using two methods: the forward Euler method; and a Runge-Kutta method. Using a step size h, we define the points $t_i, i = 0, 1, 2, ..., N$ by

$$t_i = T_0 + ih,$$

where h is chosen so that $t_N = T_1$. The numerical solution at these points is denoted by $y_i, i = 0, 1, 2, ..., N$. These values of y_i are determined by the numerical technique chosen.

For the forward Euler method, we set $y_0 = Y_0$. For $i = 1, 2, ..., N$, y_i is given by

$$y_i = y_{i-1} + hf(t_{i-1}, y_{i-1}) \ .$$

For the fourth order Runge-Kutta method, we set $y_0 = Y_0$. For $i = 1, 2, ..., N$, we calculate y_i using the following formulae:

$$k_1 = hf(t_{i-1}, y_{i-1}), \tag{1}$$

$$k_2 = hf\left(t_{i-1} + \frac{1}{2}h, y_{i-1} + \frac{1}{2}k_1\right), \tag{2}$$

$$k_3 = hf\left(t_{i-1} + \frac{1}{2}h, y_{i-1} + \frac{1}{2}k_2\right), \tag{3}$$

$$k_4 = hf(t_{i-1} + h, y_{i-1} + k_3), \tag{4}$$

$$y_i = y_{i-1} + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{5}$$

Compare the performance of the C/C++ implementations of the ordinary differential equation solvers with corresponding implementations in Matlab for a sufficiently large number of time steps to get accurate timings.

* Place all source files of the exercises in a folder named `Exercise1` in your home directory on the `mephisto.uni-graz.at` cluster.