

Homework Set 3

ASTR 5900, Computational Physics & Astrophysics

Due 2024 February 29, 11:59pm

Carry out the following work and write up an informal report showing the output (e.g., plots/graphs) and answers to questions. Put all together into a single pdf file and upload to Canvas. Also turn in the (documented) code you have written to perform the main numerical tasks (code for making plots isn't necessary). Code can either be included in the pdf document, or you can send me a link to a github repository, where I can see the code.

1. Write your own code(s) to carry out a numerical integration using both the Euler Method and a Runge-Kutta Method (either 2nd order or 4th order).

- (a) Use your code to solve the equation

$$\frac{dy}{dx} = y^2 + 1$$

and compare your answer with the exact solution $y = \tan(x)$. Also compare (and show and comment on) your results for both the Euler and Runge-Kutta methods, using the same number of steps for each.

- (b) At what value of x does your numerical solution start to break down, and how does that relate to the derivative of $y(x)$? Use a plot and/or table of numbers to show this breakdown.
- (c) Show that a decrease in step size increases your accuracy. Do you notice a difference in *how much* the accuracy improves for the Euler method, versus the Runge-Kutta?

In real problems, we usually perform a numerical integration on a function for which there is no known analytic solution. If you have no way to know the true/exact solution, you can still check your numerical result by running several cases with different step sizes. This is called a *convergence study*. If your solution is working, you should see the final solution asymptotically approaching some value, as the step-size decreases. If your solution is indeed converging, you can then use the differences in your last few cases (with the smallest step sizes) to estimate the uncertainty/precision of your final answer.

- (d) Pretend like you don't know the exact solution to the equation above. Do a convergence study, calculating the fractional difference between your highest-resolution (smallest step-size) case and a few other lower-resolution cases (make a range of step sizes over at least a factor of 10-100). Plot the fractional difference as a function of step size on a log-log scale. Show the Euler and Runge-Kutta methods on the same plot. The *slope* in this log-log plot is often referred to as the *order* of convergence. Comment on what you see.
- (e) Now consider the exact/known solution. Does your smallest fractional difference, between your two highest-resolution cases, well-represent the actual difference between your best solution and the exact solution (i.e., is this a good measure of the uncertainty in your result?)?

2. Consider the surface of a star with a temperature of 10,000 K, where the speeds of atoms are described by a Maxwell-Boltzmann velocity distribution. Namely, the fraction $f(v)$ of particles with a speed between v and $v + dv$ is given by

$$f(v)dv = \left[\frac{m}{2\pi kT} \right]^{\frac{3}{2}} 4\pi v^2 \exp\left(-\frac{mv^2}{2kT}\right) dv$$

- (a) Plot this probability density distribution of velocities for hydrogen atoms. This step is just for fun and for you to be able to double-check for bugs (e.g., check that the peak is where you expect, the numbers on the axes make sense, etc.).
- (b) Using your own numerical integrator, calculate what fraction of the hydrogen atoms are moving fast enough for the kinetic energy to be enough to excite the atom from the ground state ($n=1$) into the first excited state ($n=2$). This requires an integration from the minimum speed to a speed of "infinity." Determine how precise is your solution (i.e., what is your error bar?), considering both the convergence as you decrease your stepsize and also the convergence as you end your integration at larger velocities (approaching "infinity").

Optional Exercises (or possible ideas for presentations later in the semester):

(A) To make a numerical integration more accurate, we have seen that one can add more (smaller) steps and/or use a higher-order numerical method. Either of these solutions will require more work (more computations) for your code. Another way to improve accuracy (which sometimes can actually save work) is to be more clever about your step size. Can you think of a way to have a *variable* step size (i.e., one that varies *during the integration*) that automatically takes bigger (smaller) steps when the integral is changing slowly (quickly)? Think carefully about what criteria you might use to define "quickly" or "slowly." Pick a problem to solve (e.g., from one above or another of your choosing), implement a variable-step integrator, and show a case where you have achieved a more accurate solution with a variable step than with the same number of steps using a fixed-step version.

(B) Use a 2nd- or 4th-order Runge-Kutta to evaluate Bessel functions, which are normally given by the differential equations

$$z^2 \frac{d^2 w}{dz^2} + z \frac{dw}{dz} + (z^2 - \nu^2)w = 0$$

but which can be broken down into two linear differential equations

$$\begin{aligned} \frac{dw}{dz} &= V \\ \frac{dV}{dz} &= -\frac{1}{z}V + \left(\frac{\nu^2}{z^2} - 1\right)w \end{aligned}$$

where w is the Bessel function of order ν and V is its first derivative. This example is mathematically analogous to the situation in evaluating the position and velocity of a particle (with specified acceleration/force). The initial conditions should be evaluated at $z_0 = 0^+$, meaning at some small increment away from zero. The solution for the first kind ($\nu = 0$) of Bessel function $J(z)$ is given by

$$J_0(z_0) = 1. \quad J'_0(z_0) = 0$$

and for $\nu > 0$

$$J_\nu(z_0) = \frac{1}{\nu!} \left(\frac{z_0}{2}\right)^\nu. \quad J'_\nu(z_0) = \frac{1}{2^\nu} \frac{z_0^{\nu-1}}{(\nu-1)!}.$$