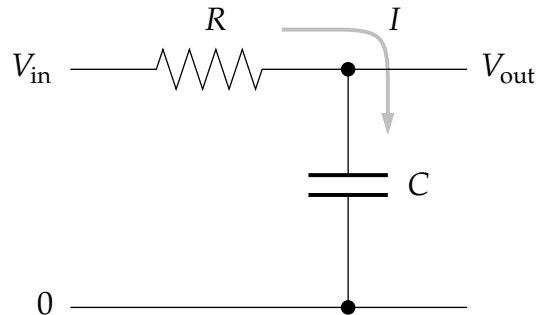


COMPUTATIONAL PHYSICS – PH 354

HOMEWORK DUE ON 18th April 2022

Exercise 1: A low-pass filter

Here is a simple electronic circuit with one resistor and one capacitor:



This circuit acts as a low-pass filter: you send a signal in on the left and it comes out filtered on the right.

Using Ohm's law and the capacitor law and assuming that the output load has very high impedance, so that a negligible amount of current flows through it, we can write down the equations governing this circuit as follows. Let I be the current that flows through R and into the capacitor, and let Q be the charge on the capacitor. Then:

$$IR = V_{\text{in}} - V_{\text{out}}, \quad Q = CV_{\text{out}}, \quad I = \frac{dQ}{dt}.$$

Substituting the second equation into the third, then substituting the result into the first equation, we find that $V_{\text{in}} - V_{\text{out}} = RC (dV_{\text{out}}/dt)$, or equivalently

$$\frac{dV_{\text{out}}}{dt} = \frac{1}{RC} (V_{\text{in}} - V_{\text{out}}).$$

- a) Write a program to solve this equation for $V_{\text{out}}(t)$ using the fourth-order Runge–Kutta method when in the input signal is a square-wave with frequency 1 and amplitude 1:

$$V_{\text{in}}(t) = \begin{cases} 1 & \text{if } [2t] \text{ is even,} \\ -1 & \text{if } [2t] \text{ is odd,} \end{cases} \quad (1)$$

where $\lfloor x \rfloor$ means x rounded down to the next lowest integer. Use the program to make plots of the output of the filter circuit from $t = 0$ to $t = 10$ when $RC = 0.01, 0.1$, and 1 , with initial condition $V_{\text{out}}(0) = 0$. You will have to make a decision about what value of h to use in your calculation. Small values give more accurate results, but the program will take longer to run. Try a variety of different values and choose one for your final calculations that seems sensible to you.

- b) Based on the graphs produced by your program, describe what you see and explain what the circuit is doing.

A program similar to the one you wrote is running inside most stereos and music players, to create the effect of the “bass” control. In the old days, the bass control on a stereo would have been connected to a real electronic low-pass filter in the amplifier circuitry, but these days there is just a computer processor that simulates the behavior of the filter in a manner similar to your program.

Exercise 2: The Lotka–Volterra equations

The Lotka–Volterra equations are a mathematical model of predator–prey interactions between biological species. Let two variables x and y be proportional to the size of the populations of two species, traditionally called “rabbits” (the prey) and “foxes” (the predators). You could think of x and y as being the population in thousands, say, so that $x = 2$ means there are 2000 rabbits. Strictly the only allowed values of x and y would then be multiples of 0.001, since you can only have whole numbers of rabbits or foxes. But 0.001 is a pretty close spacing of values, so it’s a decent approximation to treat x and y as continuous real numbers so long as neither gets very close to zero.

In the Lotka–Volterra model the rabbits reproduce at a rate proportional to their population, but are eaten by the foxes at a rate proportional to both their own population and the population of foxes:

$$\frac{dx}{dt} = \alpha x - \beta xy,$$

where α and β are constants. At the same time the foxes reproduce at a rate proportional the rate at which they eat rabbits—because they need food to grow and reproduce—but also die of old age at a rate proportional to their own population:

$$\frac{dy}{dt} = \gamma xy - \delta y,$$

where γ and δ are also constants.

- a) Write a program to solve these equations using the fourth-order Runge–Kutta method for the case $\alpha = 1$, $\beta = \gamma = 0.5$, and $\delta = 2$, starting from the initial condition $x = y = 2$. Have the program make a graph showing both x and y as a function of time on the same axes from $t = 0$ to $t = 30$.
- b) Describe in words what is going on in the system, in terms of rabbits and foxes.

Exercise 3: The Lorenz equations

One of the most celebrated sets of differential equations in physics is the Lorenz equations:

$$\frac{dx}{dt} = \sigma(y - x), \quad \frac{dy}{dt} = rx - y - xz, \quad \frac{dz}{dt} = xy - bz,$$

where σ , r , and b are constants. (The names σ , r , and b are odd, but traditional—they are always used in these equations for historical reasons.)

These equations were first studied by Edward Lorenz in 1963, who derived them from a simplified model of weather patterns. The reason for their fame is that they were one of the first incontrovertible examples of *deterministic chaos*, the occurrence of apparently random motion even though there is no randomness built into the equations.

- a) Write a program to solve the Lorenz equations for the case $\sigma = 10$, $r = 28$, and $b = \frac{8}{3}$ in the range from $t = 0$ to $t = 50$ with initial conditions $(x, y, z) = (0, 1, 0)$. Have your program make a plot of y as a function of time. Note the unpredictable nature of the motion.
- b) Modify your program to produce a plot of z against x . You should see a picture of the famous “strange attractor” of the Lorenz equations, a lopsided butterfly-shaped plot that never repeats itself.

Exercise 4: Harmonic and anharmonic oscillators

The simple harmonic oscillator arises in many physical problems, in mechanics, electricity and magnetism, and condensed matter physics, among other areas. Consider the standard oscillator equation

$$\frac{d^2x}{dt^2} = -\omega^2x.$$

- a) Write a program to solve the equations for the case $\omega = 1$ in the range from $t = 0$ to $t = 50$. A second-order equation requires two initial conditions, one on x and one on its derivative. For this problem use $x = 1$ and $dx/dt = 0$ as initial conditions. Have your program make a graph showing the value of x as a function of time.
- b) Now increase the amplitude of the oscillations by making the initial value of x bigger—say $x = 2$ —and confirm that the period of the oscillations stays roughly the same.
- c) Modify your program to solve for the motion of the anharmonic oscillator described by the equation

$$\frac{d^2x}{dt^2} = -\omega^2 x^3.$$

Again take $\omega = 1$ and initial conditions $x = 1$ and $dx/dt = 0$ and make a plot of the motion of the oscillator. Again increase the amplitude. You should observe that the oscillator oscillates faster at higher amplitudes. (You can try lower amplitudes too if you like, which should be slower.)

- d) Modify your program so that instead of plotting x against t , it plots dx/dt against x , i.e., the “velocity” of the oscillator against its “position.” Such a plot is called a *phase space* plot.
- e) The *van der Pol oscillator*, which appears in electronic circuits and in laser physics, is described by the equation

$$\frac{d^2x}{dt^2} - \mu(1 - x^2)\frac{dx}{dt} + \omega^2 x = 0.$$

Modify your program to solve this equation from $t = 0$ to $t = 20$ and hence make a phase space plot for the van der Pol oscillator with $\omega = 1$, $\mu = 1$, and initial conditions $x = 1$ and $dx/dt = 0$. Try it also for $\mu = 2$ and $\mu = 4$ (still with $\omega = 1$). Make sure you use a small enough value of the time interval h to get a smooth, accurate phase space plot.

Exercise 5: Trajectory with air resistance

Many elementary mechanics problems deal with the physics of objects moving or flying through the air, but they almost always ignore friction and air resistance to make the equations solvable. If we’re using a computer, however, we don’t need solvable equations.

Consider, for instance, a spherical cannonball shot from a cannon standing on level ground. The air resistance on a moving sphere is a force in the opposite direction to the motion with magnitude

$$F = \frac{1}{2}\pi R^2 \rho C v^2,$$

where R is the sphere's radius, ρ is the density of air, v is the velocity, and C is the so-called *coefficient of drag* (a property of the shape of the moving object, in this case a sphere).

- a) Starting from Newton's second law, $F = ma$, show that the equations of motion for the position (x, y) of the cannonball are

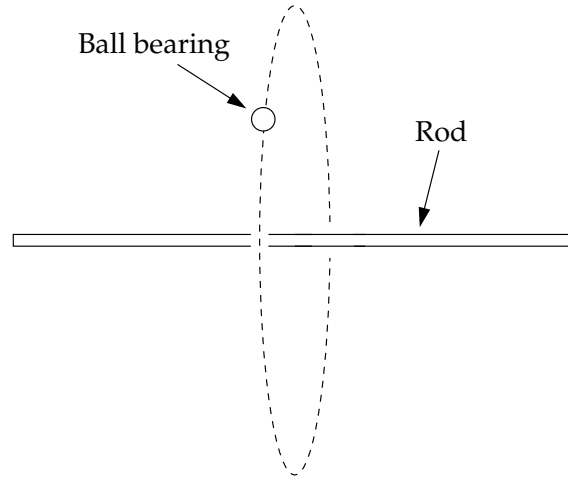
$$\ddot{x} = -\frac{\pi R^2 \rho C}{2m} \dot{x} \sqrt{\dot{x}^2 + \dot{y}^2}, \quad \ddot{y} = -g - \frac{\pi R^2 \rho C}{2m} \dot{y} \sqrt{\dot{x}^2 + \dot{y}^2},$$

where m is the mass of the cannonball, g is the acceleration due to gravity, and \dot{x} and \ddot{x} are the first and second derivatives of x with respect to time.

- b) Change these two second-order equations into four first-order equations using the methods you have learned, then write a program that solves the equations for a cannonball of mass 1 kg and radius 8 cm, shot at 30° to the horizontal with initial velocity 100 ms^{-1} . The density of air is $\rho = 1.22 \text{ kg m}^{-3}$ and the coefficient of drag for a sphere is $C = 0.47$. Make a plot of the trajectory of the cannonball (i.e., a graph of y as a function of x).
- c) When one ignores air resistance, the distance traveled by a projectile does not depend on the mass of the projectile. In real life, however, mass certainly does make a difference. Use your program to estimate the total distance traveled (over horizontal ground) by the cannonball above, and then experiment with the program to determine whether the cannonball travels further if it is heavier or lighter. You could, for instance, plot a series of trajectories for cannonballs of different masses, or you could make a graph of distance traveled as a function of mass. Describe briefly what you discover.

Exercise 6: Space garbage

A heavy steel rod and a spherical ball-bearing, discarded by a passing spaceship, are floating in zero gravity and the ball bearing is orbiting around the rod under the effect of its gravitational pull:



For simplicity we'll assume that the rod is of negligible cross-section and heavy enough that it doesn't move significantly, and that the ball bearing is orbiting around the rod's mid-point in a plane perpendicular to the rod.

- a) Treating the rod as a line of mass M and length L and the ball bearing as a point mass m , show that the attractive force F felt by the ball bearing in the direction toward the center of the rod is given by

$$F = \frac{GMm}{L} \sqrt{x^2 + y^2} \int_{-L/2}^{L/2} \frac{dz}{(x^2 + y^2 + z^2)^{3/2}},$$

where G is Newton's gravitational constant and x and y are the coordinates of the ball bearing in the plane perpendicular to the rod. The integral can be done in closed form and gives

$$F = \frac{GMm}{\sqrt{(x^2 + y^2)(x^2 + y^2 + L^2/4)}}.$$

Hence show that the equations of motion for the position x, y of the ball bearing in the xy -plane are

$$\frac{d^2x}{dt^2} = -GM \frac{x}{r^2 \sqrt{r^2 + L^2/4}}, \quad \frac{d^2y}{dt^2} = -GM \frac{y}{r^2 \sqrt{r^2 + L^2/4}},$$

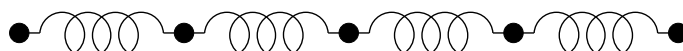
where $r = \sqrt{x^2 + y^2}$.

- b) Convert these two second-order equations into four first-order ones. Then, working in units where $G = 1$, write a program to solve them for $M = 10$, $L = 2$, and initial conditions $(x, y) = (1, 0)$ with velocity of $+1$ in the y direction. Calculate the orbit from $t = 0$ to $t = 10$ and make a plot of it,

meaning a plot of y against x . You should find that the ball bearing does not orbit in a circle or ellipse as a planet does, but has a precessing orbit, which arises because the attractive force is not a simple $1/r^2$ force as it is for a planet orbiting the Sun.

Exercise 7: Vibration in a one-dimensional system

Previously we had studied the motion of a system of N identical masses (in zero gravity) joined by identical linear springs like this:



As we showed, the horizontal displacements ξ_i of masses $i = 1 \dots N$ satisfy equations of motion

$$\begin{aligned} m \frac{d^2 \xi_1}{dt^2} &= k(\xi_2 - \xi_1) + F_1, \\ m \frac{d^2 \xi_i}{dt^2} &= k(\xi_{i+1} - \xi_i) + k(\xi_{i-1} - \xi_i) + F_i, \\ m \frac{d^2 \xi_N}{dt^2} &= k(\xi_{N-1} - \xi_N) + F_N. \end{aligned}$$

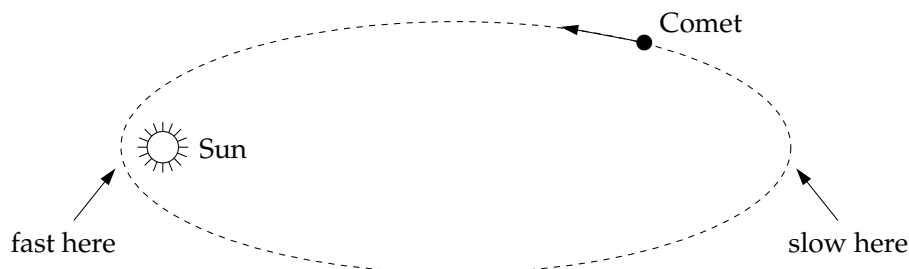
where m is the mass, k is the spring constant, and F_i is the external force on mass i . In Example 6.2 we showed how these equations could be solved by guessing a form for the solution and using a matrix method. Here we'll solve them more directly.

- a) Write a program to solve for the motion of the masses using the fourth-order Runge–Kutta method for the case we studied previously where $m = 1$ and $k = 6$, and the driving forces are all zero except for $F_1 = \cos \omega t$ with $\omega = 2$. Plot your solutions for the displacements ξ_i of all the masses as a function of time from $t = 0$ to $t = 20$ on the same plot. Write your program to work with general N , but test it out for small values— $N = 5$ is a reasonable choice.

You will need first of all to convert the N second-order equations of motion into $2N$ first-order equations. Then combine all of the dependent variables in those equations into a single large vector \mathbf{r} to which you can apply the Runge–Kutta method in the standard fashion.

Exercise 8: Cometary orbits

Many comets travel in highly elongated orbits around the Sun. For much of their lives they are far out in the solar system, moving very slowly, but on rare occasions their orbit brings them close to the Sun for a fly-by and for a brief period of time they move very fast indeed:



This is a classic example of a system for which an adaptive step size method is useful, because for the large periods of time when the comet is moving slowly we can use long time-steps, so that the program runs quickly, but short time-steps are crucial in the brief but fast-moving period close to the Sun.

The differential equation obeyed by a comet is straightforward to derive. The force between the Sun, with mass M at the origin, and a comet of mass m with position vector \mathbf{r} is GMm/r^2 in direction $-\mathbf{r}/r$ (i.e., the direction towards the Sun), and hence Newton's second law tells us that

$$m \frac{d^2 \mathbf{r}}{dt^2} = - \left(\frac{GMm}{r^2} \right) \frac{\mathbf{r}}{r}.$$

Canceling the m and taking the x component we have

$$\frac{d^2 x}{dt^2} = -GM \frac{x}{r^3},$$

and similarly for the other two coordinates. We can, however, throw out one of the coordinates because the comet stays in a single plane as it orbits. If we orient our axes so that this plane is perpendicular to the z -axis, we can forget about the z coordinate and we are left with just two second-order equations to solve:

$$\frac{d^2 x}{dt^2} = -GM \frac{x}{r^3}, \quad \frac{d^2 y}{dt^2} = -GM \frac{y}{r^3},$$

where $r = \sqrt{x^2 + y^2}$.

- a) Turn these two second-order equations into four first-order equations, using the methods you have learned.
- b) Write a program to solve your equations using the fourth-order Runge–Kutta method with a *fixed* step size. You will need to look up the mass of the Sun and Newton’s gravitational constant G . As an initial condition, take a comet at coordinates $x = 4$ billion kilometers and $y = 0$ (which is somewhere out around the orbit of Neptune) with initial velocity $v_x = 0$ and $v_y = 500 \text{ m s}^{-1}$. Make a graph showing the trajectory of the comet (i.e., a plot of y against x).

Choose a fixed step size h that allows you to accurately calculate at least two full orbits of the comet. Since orbits are periodic, a good indicator of an accurate calculation is that successive orbits of the comet lie on top of one another on your plot. If they do not then you need a smaller value of h . Give a short description of your findings. What value of h did you use? What did you observe in your simulation? How long did the calculation take?

- c) Make a copy of your program and modify the copy to do the calculation using an adaptive step size. Set a target accuracy of $\delta = 1$ kilometer per year in the position of the comet and again plot the trajectory. What do you see? How do the speed, accuracy, and step size of the calculation compare with those in part (b)?
- d) Modify your program to place dots on your graph showing the position of the comet at each Runge–Kutta step around a single orbit. You should see the steps getting closer together when the comet is close to the Sun and further apart when it is far out in the solar system.

Exercise 9: Write a program to solve the differential equation

$$\frac{d^2x}{dt^2} - \left(\frac{dx}{dt}\right)^2 + x + 5 = 0$$

using the leapfrog method. Solve from $t = 0$ to $t = 50$ in steps of $h = 0.001$ with initial condition $x = 1$ and $dx/dt = 0$. Make a plot of your solution showing x as a function of t .

Exercise 10: Orbit of the Earth

Use the Verlet method to calculate the orbit of the Earth around the Sun. The equations of motion for the position $\mathbf{r} = (x, y)$ of the planet in its orbital plane are the same as those for any orbiting body and are derived in Exercise 8.10 on page 361. In vector form, they are

$$\frac{d^2\mathbf{r}}{dt^2} = -GM\frac{\mathbf{r}}{r^3},$$

where $G = 6.6738 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$ is Newton's gravitational constant and $M = 1.9891 \times 10^{30} \text{ kg}$ is the mass of the Sun.

The orbit of the Earth is not perfectly circular, the planet being sometimes closer to and sometimes further from the Sun. When it is at its closest point, or *perihelion*, it is moving precisely tangentially (i.e., perpendicular to the line between itself and the Sun) and it has distance $1.4710 \times 10^{11} \text{ m}$ from the Sun and linear velocity $3.0287 \times 10^4 \text{ m s}^{-1}$.

- a) Write a program to calculate the orbit of the Earth using the Verlet method with a time-step of $h = 1$ hour. Make a plot of the orbit, showing several complete revolutions about the Sun. The orbit should be very slightly, but visibly, non-circular.
- b) The gravitational potential energy of the Earth is $-GMm/r$, where $m = 5.9722 \times 10^{24} \text{ kg}$ is the mass of the planet, and its kinetic energy is $\frac{1}{2}mv^2$ as usual. Modify your program to calculate both of these quantities at each step, along with their sum (which is the total energy), and make a plot showing all three as a function of time on the same axes. You should find that the potential and kinetic energies vary visibly during the course of an orbit, but the total energy remains constant.
- c) Now plot the total energy alone without the others and you should be able to see a slight variation over the course of an orbit. Because you're using the Verlet method, however, which conserves energy in the long term, the energy should always return to its starting value at the end of each complete orbit.

Exercise 11: Quantum oscillators

Consider the one-dimensional, time-independent Schrödinger equation in a

harmonic (i.e., quadratic) potential $V(x) = V_0 x^2 / a^2$, where V_0 and a are constants.

- a) Write down the Schrödinger equation for this problem and convert it from a second-order equation to two first-order ones. Find the energies of the ground state and the first two excited states for these equations when m is the electron mass, $V_0 = 50 \text{ eV}$, and $a = 10^{-11} \text{ m}$. Note that in theory the wavefunction goes all the way out to $x = \pm\infty$, but you can get good answers by using a large but finite interval. Try using $x = -10a$ to $+10a$, with the wavefunction $\psi = 0$ at both boundaries. (In effect, you are putting the harmonic oscillator in a box with impenetrable walls.) The wavefunction is real everywhere, so you don't need to use complex variables, and you can use evenly spaced points for the solution—there is no need to use an adaptive method for this problem.

The quantum harmonic oscillator is known to have energy states that are equally spaced. Check that this is true, to the precision of your calculation, for your answers. (Hint: The ground state has energy in the range 100 to 200 eV.)

- b) Now modify your program to calculate the same three energies for the anharmonic oscillator with $V(x) = V_0 x^4 / a^4$, with the same parameter values.
- c) Modify your program further to calculate the properly normalized wavefunctions of the anharmonic oscillator for the three states and make a plot of them, all on the same axes, as a function of x over a modest range near the origin—say $x = -5a$ to $x = 5a$.

To normalize the wavefunctions you will have to evaluate the integral $\int_{-\infty}^{\infty} |\psi(x)|^2 dx$ and then rescale ψ appropriately to ensure that the area under the square of each of the wavefunctions is 1. Either the trapezoidal rule or Simpson's rule will give you a reasonable value for the integral. Note, however, that you may find a few very large values at the end of the array holding the wavefunction. Where do these large values come from? Are they real, or spurious?

One simple way to deal with the large values is to make use of the fact that the system is symmetric about its midpoint and calculate the integral of the wavefunction over only the left-hand half of the system, then double

the result. This neatly misses out the large values.

Exercise 12: The three-body problem

Three stars, in otherwise empty space, are initially at rest, with the following masses and positions, in arbitrary units:

	Mass	x	y
Star 1	150	3	1
Star 2	200	−1	−2
Star 3	250	−1	1

(All the z coordinates are zero, so the three stars lie in the xy plane.)

- a) Show that the equation of motion governing the position \mathbf{r}_1 of the first star is

$$\frac{d^2\mathbf{r}_1}{dt^2} = Gm_2 \frac{\mathbf{r}_2 - \mathbf{r}_1}{|\mathbf{r}_2 - \mathbf{r}_1|^3} + Gm_3 \frac{\mathbf{r}_3 - \mathbf{r}_1}{|\mathbf{r}_3 - \mathbf{r}_1|^3}$$

and derive two similar equations for the positions \mathbf{r}_2 and \mathbf{r}_3 of the other two stars. Then convert the three second-order equations into six equivalent first-order equations, using the techniques you have learned.

- b) Working in units where $G = 1$, write a program to solve your equations and hence calculate the motion of the stars from $t = 0$ to $t = 2$. Make a plot showing the trails of all three stars (i.e., a graph of y against x for each star).

To do this calculation properly you will need to use an adaptive step size method—the stars move very rapidly when they are close together and very slowly when they are far apart. An adaptive method is the only way to get the accuracy you need in the fast-moving parts of the motion without wasting hours uselessly calculating the slow parts with a tiny step size. Construct your program so that it introduces an error of no more than 10^{-3} in the position of any star per unit time.

Exercise 13: Lane-Emden equations

The equations of stellar structure can be simplified enormously if we assume a polytropic equation of state relating pressure and density ($p = K\rho^{(1+1/n)}$),

where $n = 1/(\gamma - 1)$ is related to the polytropic index. The equations for mass conservation and hydrostatic equilibrium are:

$$\frac{dM(r)}{dr} = 4\pi r^2 \rho,$$

$$\frac{dp}{dr} = -\frac{GM(r)}{r^2} \rho$$

We can define new variables θ, ξ such that, $\rho = \lambda \theta^n$, $p = K \lambda^\gamma \theta^{n+1}$, and $r = \xi \sqrt{\frac{(1+n)K}{4\pi G} \lambda^{(1/n-1)}}$. The scaled mass is defined as $M = m 4\pi \lambda \left[\frac{(1+n)K}{4\pi G} \lambda^{(1/n-1)} \right]^{3/2}$. Thus, the normalized first order Lane-Emden equations are:

$$\frac{dm}{d\xi} = \xi^2 \theta^n, \quad (2)$$

$$\frac{d\theta}{d\xi} = -\frac{m}{\xi^2}. \quad (3)$$

subject to boundary conditions $m = 0$ at $\xi = 0$ (mass enclosed vanishes at the origin), and $\theta = 0$ at $\xi = \xi_*$ (density vanishes at the stellar surface). Solve the Lane-Emden equations for index $n = 3$. The difficulty with solving this equation is that ξ_* is not known a priori.

(a) First, try solving the system using ‘shooting by hand.’ Integrate Eqs. 2 & 3 as an initial value problem using θ at $\xi = 0$ between 1 and 10. In each case plot the solution from $\xi = 0$ to ξ_* (ξ_* will be different for each initial guess; a bigger star for a larger core temperature) on the same graph. Estimate roughly the value of θ at $\xi = 0$ that gives $\xi_* = 2$. Because of coordinate singularity at $\xi = 0$, you will need to start your integrations from $r = \epsilon$ where $\epsilon \ll 1$. Taylor series expansion for m, θ , using Eqs. 2 & 3, gives $m \approx m(0) + (dm/d\xi)_0 \epsilon + \dots = \epsilon^3 \theta_0^3$ and similarly $\theta \approx \theta_0$, where $\theta_0 = \theta(0)$.

(b) Now implement an automated shooting method using Newton-Raphson iteration that finds the value of θ at $\xi = 0$ which gives $\xi_* = 2$. How does your value differ from the intuitive approach in (a)?

Exercise 14: Stiff ODEs

Consider the following set of ODEs

$$\begin{aligned} \frac{du}{dt} &= 998u + 1998v, \\ \frac{dv}{dt} &= -999u - 1999v \end{aligned}$$

with boundary conditions $u(0) = 1$ and $v(0) = 0$. What step-size should be chosen to integrate this equation using an explicit method such as forward Euler? These equations can be integrated analytically. Solve this equation using the forward Euler scheme and an implicit backward Euler scheme using a step-size $\Delta t = \Delta t_{\text{stab}}/2$ and $10\Delta t_{\text{stab}}$. Of course the explicit solution blows up because of numerical instability for the latter choice. How does the implicit method compare with the analytic solution? Higher order implicit methods, which we haven't covered in this course, are useful for stiff ODEs. These equations are stiff because the growth rate of the two independent solutions of these homogeneous ODEs differ by orders of magnitude. Such equations can arise in chemical kinetics where some rate coefficients are much larger compared to others.