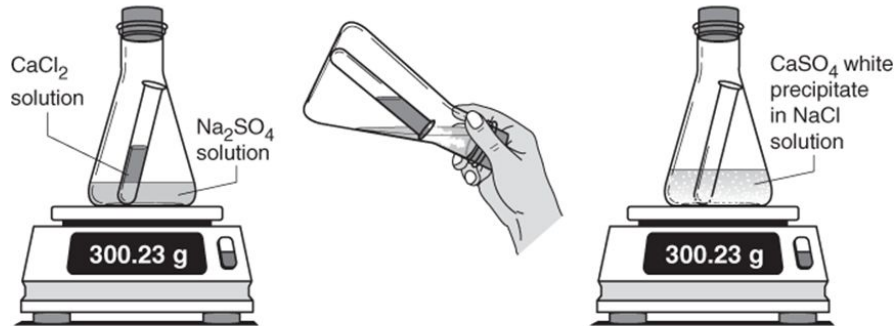


Conservation

MATH1090: Directed Study in Differential Equations

http://people.sc.fsu.edu/~jburkardt/classes/math1090_2020/conservation/conservation.pdf

Conservation of mass



mass (g) of reactants = mass (g) of products

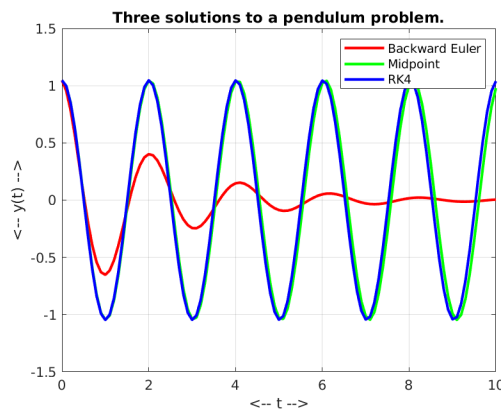
Physical laws often require the conservation of some quantity.

Conservation

If a physical law requires that mass be conserved, or that we stay on the surface of the earth, can an ODE solver produce solutions that satisfy this requirement?

1 The meaning of conservation

In your study of the pendulum equation last week, you produced approximate solutions using several different methods. Especially when the number of steps used was low, there seemed to be something obviously wrong with the solution produced by the backward Euler method.



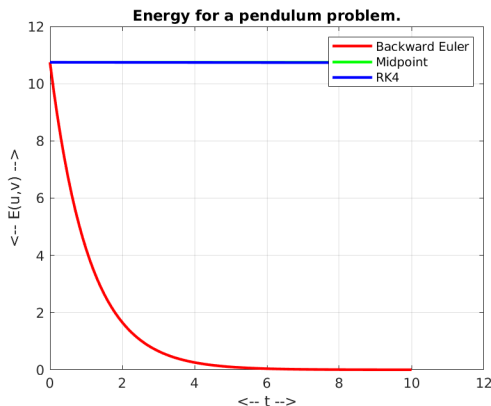
The backward Euler solution dwindles down to zero.

We know that a real pendulum will also (slowly) stop swinging, but that doesn't excuse the behavior of the backward Euler solution. Our mathematical equation does not include a friction term. Moreover, if we increase the number of steps taken, the backward Euler method does a better and better job of approximation, and the model solution begins to swing back and forth approximately the same distance on each beat.

So this makes us ask, why did the midpoint and RK4 method do so well?

The RK4 method is a high order method, so we can expect that it is able to do a good job of modeling the (frictionless) pendulum. But why is the midpoint method doing so well, when it is only of second order? The explanation lies in the fact that any exact solution to the pendulum problem will satisfy a conservation law: the conservation of energy. For our model, this means that, for at any time t , then energy $E(t)$ cannot change, and so the quantities $u(t)$ and $v(t) = u'(t)$ must satisfy:

$$E(t) = \frac{g}{l}u(t)^2 + v(t)^2 = \frac{g}{l}u(0)^2 + v(0)^2 = \text{constant}$$



The energy of the backward Euler method decays exponentially.

From the plot, it looks like the backward Euler method does a terrible job of conserving energy, while both midpoint and RK4 are perfect. In fact, the RK4 method is not perfect at conserving energy; it just does a very good job of approximating the true solution, and the true solution conserves energy. By contrast, the midpoint method does a “pretty good” job of approximating the solution (as an order 2 solver) but does a perfect job of energy conservation.

An ODE solver which is able to perfectly conserve a quantity, or satisfy some constraint, is called **symplectic**. The midpoint method is symplectic for any conservation quantity that is no more than quadratic polynomial expression in terms of the solution variables. The energy $E(t)$ is such an expression.

2 SIR: A hidden conservation

A model of disease is known as Susceptible/Infected/Recovered or **SIR**. A population of $N = 1000$ people is divided into three groups. Initially, there might be just one member of the I group and no one in R . Then, over time, the populations change by

$$\begin{aligned} \frac{dS}{dt} &= -\alpha SI + \gamma R \\ \frac{dI}{dt} &= +\alpha SI - \beta * I \\ \frac{dR}{dt} &= +\beta I - \gamma R \end{aligned}$$

Now define $N(t) = S(t) + I(t) + R(t)$. It should be obvious that we want $\frac{dN}{dt} = 0$. In fact, if we add our three ODE's, we get that hidden equation exactly. In other words, our ODE system, if solved exactly, should conserve the quantity N . In this case, even if we didn't know that, we would be very surprised and unhappy if at time $t = 500$, for instance, our total population of 1000 was now suddenly 993!

In other cases, a physical system may include a constraint or conservation quantity, and a good ODE model will incorporate that condition...and a good ODE solve should be accurate enough to approximately conserve that quantity. On the other hand, for certain kinds of conservation quantities, some ODE solvers can guarantee conservation. In particular, we expect the midpoint method to be able to conserve a quantity $H(t)$ as long as it is expressed as a polynomial of quadratic degree or less in the variables.

3 Cycling on a sphere

The “sphere” differential equation system describes the change in the position (x, y, z) of a particle along a closed loop on the surface of the unit sphere:

$$i1 = 1.6, i2 = 1, i3 = \frac{2}{3}$$

$$\frac{\partial x}{\partial t} = \left(\frac{1}{i3} - \frac{1}{i2}\right)zy$$

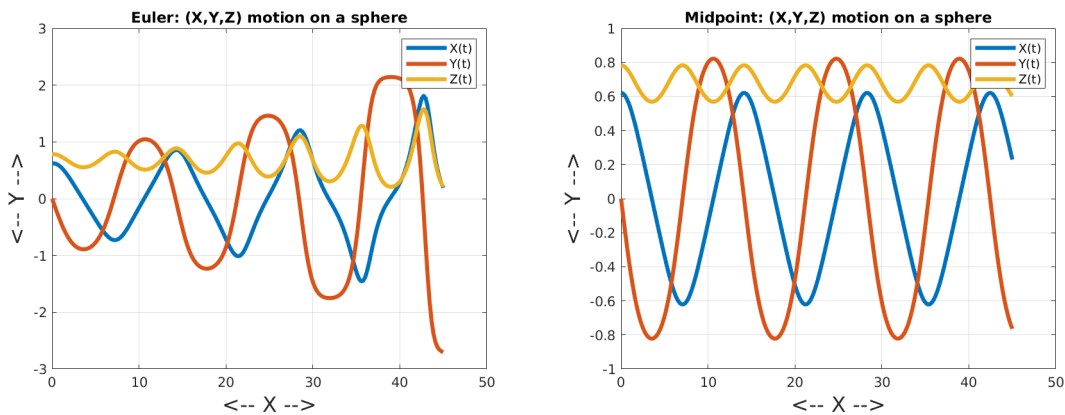
$$\frac{\partial y}{\partial t} = \left(\frac{1}{i1} - \frac{1}{i3}\right)xz$$

$$\frac{\partial z}{\partial t} = \left(\frac{1}{i2} - \frac{1}{i1}\right)yx$$

This means that the true solution must satisfy

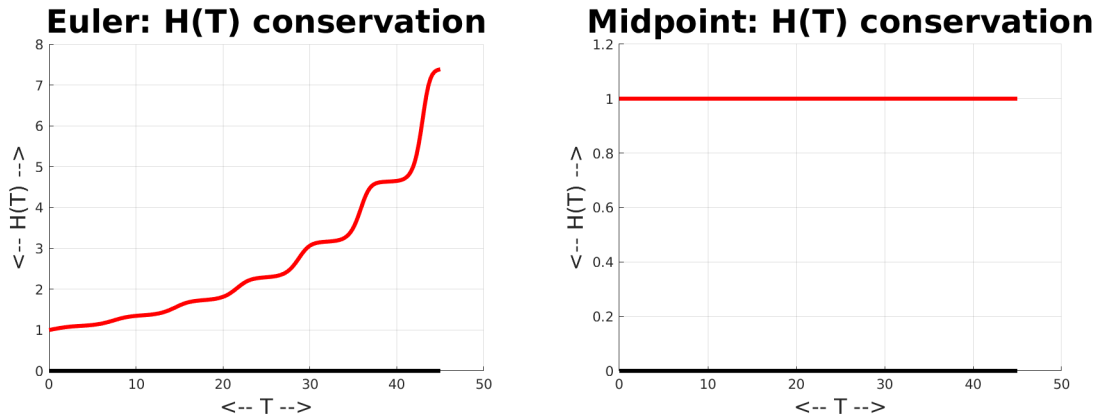
$$h(t) = x(t)^2 + y(t)^2 + z(t)^2 = 1 \text{ for all time } t$$

At time $t = 0$, we start the system at $(x, y, z) = (\cos(0.9), 0.0, \sin(0.9))$, and take 200 steps to time $t = 45$. Compare the solutions from the Euler and midpoint methods:



The Euler and midpoint solutions to the sphere problem.

Another way to consider the quality of the solutions is to plot the conserved quantity $h(t)$. Here, we see that something is clearly wrong with the Euler solution, which is flying off the surface of the sphere:



The Euler and midpoint conserved quantity plots.

4 A Kepler Equation

We can use Kepler's equations of planetary motion to define a simple two-body problem:

$$\begin{aligned} \frac{\partial q_1}{\partial t} &= p_1 \\ \frac{\partial p_1}{\partial t} &= \frac{-q_1}{(q_1^2 + q_2^2)^{3/2}} \\ \frac{\partial q_2}{\partial t} &= p_2 \\ \frac{\partial p_2}{\partial t} &= \frac{-q_2}{(q_1^2 + q_2^2)^{3/2}} \end{aligned}$$

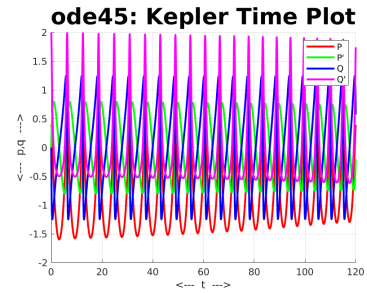
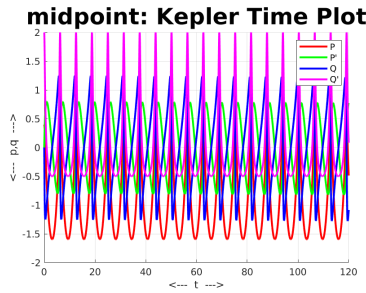
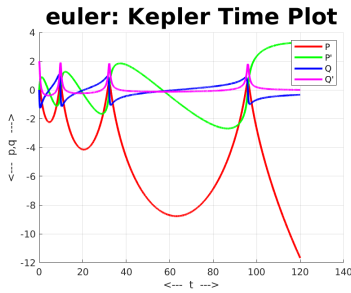
Exact solutions of this equation must conserve the quantity:

$$h = \frac{p_1^2 + p_2^2}{2} - \frac{1}{\sqrt{q_1^2 + q_2^2}}$$

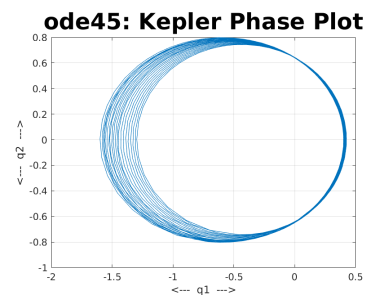
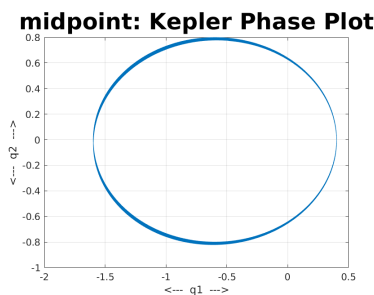
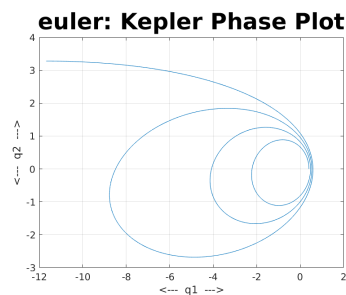
For our test problem, we integrate over $0 \leq t \leq 120$, using an initial condition of

$$y = \begin{bmatrix} 1 - e \\ 0 \\ 0 \\ \sqrt{\frac{1+e}{1-e}} \end{bmatrix}$$

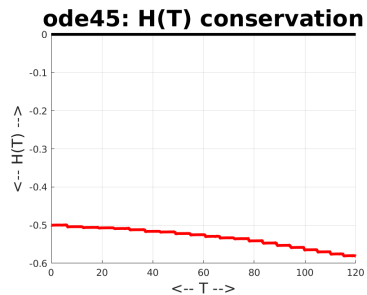
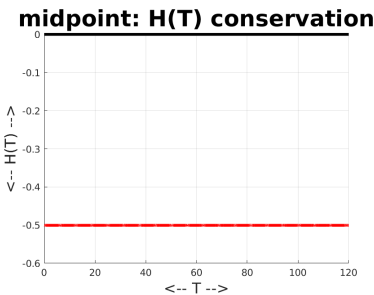
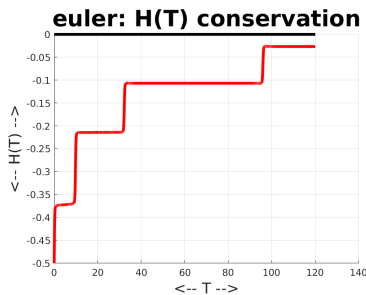
where the eccentricity $e = 0.6$. As ODE solvers we use `euler()`, `midpoint_fixed()`, and MATLAB's `ode45()`. While `ode45()` chooses its own stepsize adaptively, we used 10,000 steps for the two fixed step methods.



The time plots.



The phase plots for (q_1, p_1) .



The conservation plots.

The time plot by itself tells us that even 10,000 steps was not enough to get a reliable answer from `euler()`. Surprisingly, the solution from `ode45()` also has problems. The time plot curves gradually diminish in size, the phase plot curve clearly does not repeat, and the conservation curve is not constant. By contrast, `midpoint_fixed()` returns a solution that maintains its size, gives a cyclic phase plot, and conserves energy, as far as we can tell from looking at a plot.

Theoretically, we can only prove that the midpoint method conserves quantities that are defined in terms of polynomials that are at most quadratics. The conserved quantity for the Kepler problem includes a term that does not satisfy this requirement, and so we should expect that the midpoint method will not exactly conserve it. However, as we can see, it nonetheless does so well that it's hard to detect any significant loss.

5 Conservation for the predator-prey problem

Recall the predator prey example: at any time t , we have populations of $u(t)$ prey and $v(t)$ predators, which might be rabbits and foxes. The equation that models the changes in population is:

$$\begin{aligned}\frac{du}{dt} &= \alpha u - \beta uv \\ \frac{dv}{dt} &= -\gamma v + \delta uv\end{aligned}$$

where $\alpha, \beta, \gamma, \delta$ are positive parameters which control the relationship between the predators and prey.

For our experiments, we used $\alpha = 2, \beta = 1, \gamma = 1, \delta = 1$, an initial time $t_0 = 0$, and initial conditions

$$\begin{aligned}u(t_0) &= 4.0 \\ v(t_0) &= 2.0\end{aligned}$$

and we wanted to compute the solution out to time $t = 250$.

We already saw that the Euler method needed to take about 1,000,000 steps to get an answer whose values showed regular oscillation, and whose phase plane made what looked like a closed curve. Methods that were more accurate were able to use much fewer steps to get a reasonable solution.

We showed that the predator-prey system has a conserved quantity:

$$H(u, v) = \delta(u) - \gamma \ln(u) + \beta v - \alpha \ln(v)$$

or, for our choice of parameters:

$$H(u, v) = u - \ln(u) + v - 2 \ln(v)$$

For a given ODE solver, we are interested in how well the various methods do in conserving this quantity over time. This will be your task for next week.

6 Report

Try to create time, phase, and conservation plots for the predator prey problem, as it is solved by several ODE solvers.

The web page supplies the codes `euler()`, `midpoint_fixed()`, `predator_deriv()` and `predator_conserved()`, which you will need.

You will also need to write codes to solve the predator prey problem with various ODE solvers. Look at the codes `kepler_euler()`, `kepler_midpoint()`, and `kepler_ode45()`. Create corresponding programs for the predator-prey problem.

We know that `euler()` needs a lot of steps to get a reasonable result. Perhaps you can use fewer steps for the midpoint method. Let `ode45()` choose its own stepsize.

Bring your plots to our next meeting, at 1:00pm, Thursday, 05 March, room Thackeray 624.