The University of Sydney
Applied Mathematics Honours

Computational Projects in Applied Mathematics 2009

Project 4: Symplectic Integrators

Hamiltonian systems evolve in a phase space which has very specific properties. When integrating Hamilton's equations numerically, it is very desirable to use numerical methods which conserve this structure, otherwise erroneous and unrealistic features can be introduced into the solutions. This project gives examples of the types of disasters that can occur, and shows how a special class of methods, known as symplectic integrators, can be used to make a much better job of solving Hamiltonian systems numerically. A symplectic integrator approximates the system by a mapping or sequence of mappings over a timestep τ. The mapping is designed to conserve certain quantities known as *Poincaré invariants*, which can be shown to be conserved quantities of the original continuous-time differential system. Details and background on this will be given in the lectures.

1. First, consider the simple pendulum, given in Hamiltonian form by the one degree-of-freedom system $dq/dt = p$, $dp/dt = -q$, with Hamiltonian $H = (p^2 + q^2)/2$. Write a program to solve this using Euler's method, given in lectures. Take suitable initial conditions, eg $p = 0$ and $q = 1$ at $t = 0$. Choose a variety of timesteps τ, and confirm that the Hamiltonian grows by a factor $(1 + \tau^2)$ at each timestep. Integrate for a long time and show that given a particular τ, the results become unsatisfactory for sufficiently large time.

Repeat all of the above using Matlab's built-in 4th/5th order Runge-Kutta integrator **ode45**. The first time, use the default error settings; you should find that whilst the results are better than for Euler, they are still eventually unsatisfactory. Investigate the extent to which you can improve this by overriding the default errors with lower settings (see **doc ode45** for how to do this). Note that though you may specify a timestep τ between output times, **ode45** actually varies its internal timestep to satisfy your error demands. In your write-up, specify the error settings you used.

Now try the symplectic 1st order integrator described in lectures; this requires a trivial modification of your Euler code. Run the same cases as before, with a variety of τ values. Calculate and plot the Hamiltonian as a function of time, and compare it with the corresponding plot using Euler's method. Confirm that in the symplectic case there is no secular growth of the Hamiltonian, but that at any fixed time the error is proportional to τ^n where n, the power-law exponent, is to be measured.

Finally in this exercise, program up the 4th order Forest and Ruth symplectic integrator described in the handouts of Yoshida and Thijssen. Repeat your earlier calculations using the new algorithm, and compare with results from the other methods. Again, ascertain the power-law index n of the error at fixed time.

2. Repeat the last exercise for the more interesting case of the nonlinear pendulum, whose Hamiltonian is given by $H = p^2/2 - \cos q$; the corresponding Hamilton's equations are $dq/dt = p$, $dp/dt = -\sin q$. Use Euler's method, **ode45**, the symplectic leapfrog integrator given in lectures, and the 4th order Forest and Ruth integrator. Note that there are particular problems associated with orbits which go through points like $q = \pi$, $p = 0$. These are fixed points which are saddles, and correspond to the case where the pendulum is at the point of cartwheeling. Experiment starting near (but not at!) these points. Give a comparison of your results.

(Symplectic leapfrog integrator:

$$q' = q_n + \frac{1}{2}\tau p_n; \quad p_{n+1} = p_n - \tau \sin q'; \quad q_{n+1} = q' + \frac{1}{2}\tau p_{n+1}. \text{)}$$

3. Now treat the case of the nonlinear double pendulum, which has two degrees of freedom. The Hamiltonian is

$$H = (p_1^2 + p_2^2)/2 - \cos q_1 - \cos q_2 - \epsilon \cos(q_1 - q_2)\,,$$

where ϵ is a coupling parameter. Write down the corresponding Hamilton's equations, and solve them numerically. Check that when $\epsilon = 0$ each (q, p) pair behaves independently and as in the last exercise. Use the same four methods. With $\epsilon \neq 0$, run a variety of cases starting from ten different initial conditions; hand in results for your four most interesting examples. You should find there are parameter regimes that give chaotic behaviour: one example is the case with initial conditions $q_1(0) = 2.5, p_1(0) = 2, q_2(0) = 1.1, p_2(0) = 0$, and $\epsilon = 0.4$. Finally, check how well the Hamiltonian is conserved by your various schemes, particularly for large time. Compare and contrast a chaotic and a non-chaotic case.

4. Symplectic integrators were invented in the early 1980s. In recent years, special versions have been created which attempt to solve the evolution of the solar system over very long timescales. In particular, it has been shown that the motion of Pluto is apparently chaotic, with possible consequences for the long-time stability of the solar system, though it is currently thought that there are no catastrophic instabilities. The classic paper on this subject is due to Wisdom and Holman, and will be handed out. Read this paper and summarise the contents in your own words, restricting your description to three or four pages. (Note that since Wisdom and Holman, others have modified their procedure, particularly to treat better close encounters, where the Wisdom and Holman method loses symplecticity.)